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Monday, February 27, 2012 8:00AM - 11:00AM –

Session A1 GIMS: Focus Session: Novel Instrumentation and measurements for Biomedical Research 203

8:00AM A1.00001 Instrumentation of Molecular Imaging on Site-Specific Targeting Fluorescent Peptide for Early Detection of Breast Cancer¹ PING YU, Department of Physics and Astronomy, University of Missouri, LIXIN MA, Department of Radiology and Biomolecular Imaging Center, University of Missouri — In this work we developed two biomedical imaging techniques for early detection of breast cancer. Both image modalities provide molecular imaging capability to probe site-specific targeting dyes. The first technique, heterodyne CCD fluorescence mediated tomography, is a non-invasive biomedical imaging that uses fluorescent photons from the targeted dye on the tumor cells inside human breast tissue. The technique detects a large volume of tissue (20 cm) with a moderate resolution (1 mm) and provides the high sensitivity. The second technique, dual-band spectral-domain optical coherence tomography, is a high-resolution tissue imaging modality. It uses a low coherence interferometer to detect coherent photons hidden in the incoherent background. Due to the coherence detection, a high resolution (20 microns) is possible. We have finished prototype imaging systems for the development of both image modalities and performed imaging experiments on tumor tissues. The spectroscopic/tomographic images show contrasts of dense tumor tissues and tumor necrotic regions. In order to correlate the findings from our results, a diffusion-weighted magnetic resonance imaging (MRI) of the tumors was performed using a small animal 7-Tesla MRI and demonstrated excellent agreement.

¹This work was supported by NSF grant CBET-0746871 and DOD grant PC081264.

8:12AM A1.00002 Digital Image Speckle Correlation for the Quantification of the Cosmetic Treatment with Botulinum Toxin Type A (BTX-A), DIVYA BHATNAGAR, Department of Materials Science and Engineering, SUNY Stony Brook, NICOLE CONKLING, Stony Brook University Medical Center, MIRIAM RAFAILOVICH, Department of Materials Science and Engineering, SUNY Stony Brook, ALEXANDER DAGUM, Division of Plastic Surgery, Stony Brook University Medical Center — The skin on the face is directly attached to the underlying muscles. Here, we successfully introduce a non-invasive, non-contact technique, Digital Image Speckle Correlation (DISC), to measure the precise magnitude and duration of facial muscle paralysis inflicted by BTX-A. Subjective evaluation by clinicians and patients fail to objectively quantify the direct effect and duration of BTX-A on the facial musculature. By using DISC, we can (a) Directly measure deformation field of the facial skin and determine the locus of facial muscular tension (b) Quantify and monitor muscular paralysis and subsequent re-innervation following injection; (c) Continuously correlate the appearance of wrinkles and muscular tension. Two sequential photographs of slight facial motion (frowning, raising eyebrows) are taken. DISC processes the images to produce a vector map of muscular displacement from which spatially resolved information is obtained regarding facial tension. DISC can track the ability of different muscle groups to contract and can be used to predict the site of injection, quantify muscle paralysis and the rate of recovery following BOTOX injection.

8:24AM A1.00003 Ultra-low field SQUID electron paramagnetic resonance for biomedical applications, P. BHUPATHI, B.H. EOM, Division of Physics, Mathematics and Astronomy, California Institute of Technology, K.I. PENANEN, P.K. DAY, I. HAHN, Jet Propulsion Laboratory, California Institute of Technology — We have constructed a SQUID-magnetometer system operating at 4K, for electron paramagnetic resonance (EPR) detection from room temperature samples in magnetic fields of the order of Earth's field. The magnetometer consists of a home-built gradiometer pick-up coil inductively coupled to the input of a commercially available 2-stage dc SQUID amplifier. Operation at low EPR excitation frequency of a few MHz has advantages of negligible sample heating and finite penetration depth effects in biological systems. The same system can be adapted to detect NMR signals at several kHz range. We describe our detection scheme and discuss the prospects for *in vivo* biomedical EPR imaging.

8:36AM A1.00004 Single cell microfluidics for systems oncology¹, RONG FAN, Department of Biomedical Engineering, Yale University — The singular term “cancer” is never one kind of disease, but deceptively encompasses a large number of heterogeneous disease states, which makes it impossible to completely treat cancer using a generic approach. Rather systems approaches are urgently required to assess cancer heterogeneity, stratify patients and enable the most effective, individualized treatment. The heterogeneity of tumors at the single cell level is reflected by the hierarchical complexity of the tumor microenvironment. To identify all the cellular components, including both tumor and infiltrating immune cells, and to delineate the associated cell-to-cell signaling network that dictates tumor initiation, progression and metastasis, we developed a single cell microfluidics chip that can analyze a panel of proteins that are potentially associated inter-cellular signaling network in tumor microenvironment from hundreds of single cells in parallel. This platform integrates two advanced technologies – microfluidic single cell handling and ultra-high density protein array. This device was first tested for highly multiplexed profiling of secreted proteins including tumor-immune signaling molecules from monocytic leukemia cells. We observed profound cellular heterogeneity with all functional phenotypes quantitatively identified. Correlation analysis further indicated the existence of an intercellular cytokine network in which TNF α -induced secondary signaling cascades further increased functional cellular diversity. It was also exploited to evaluate polyfunctionality of tumor antigen-specific T cells from melanoma patients being treated with adoptive T cell transfer immunotherapy. This platform could be further extended to analyze both solid tumor cells (e.g. human lung carcinoma cells) and infiltrating immune cells (e.g. macrophages) so as to enable systems analysis of the complex tumor microenvironment from small amounts of clinical specimens, e.g. skinny needle biopsies. Thus, it could potentially become a clinical tool for patient stratification based upon the inter-cellular signaling network and designing new anti-cancer therapy by targeting microenvironmental components.

¹We acknowledge the support from the NCI K99/R00 award (4R00 CA136759-02), the Bill & Melinda Gates Foundation GCE Award, the Alzheimer Association NIRG award and the NIH LINC Program Grant (1 U01 CA16425201).

9:12AM A1.00005 High resolution phase-sensitive optical coherence microscopy tracking of magnetic microbeads for cellular mechanics, VASILICA CRECEA, Department of Physics, University of Illinois at Urbana-Champaign, BENEDIKT GRAF, Department of Electrical Engineering, University of Illinois at Urbana-Champaign, QINGSHAN WEI, HYON-MIN SONG, ALEXANDER WEI, Department of Chemistry, Purdue University, STEPHEN BOPPART, Department of Electrical Engineering, University of Illinois at Urbana-Champaign — We present a real-time multi-modal near-infrared imaging technology that tracks externally induced axial motion of magnetic microbeads in mouse macrophages, human breast epithelial cells, and human breast primary ductal carcinoma cells. The imaging technique includes nanometer scale phase-sensitive magnetomotive integrated optical coherence (MM-OCM) and multiphoton (MPM) microscopy. MPM is used to visualize multifunctional microbeads based on their fluorescence, while MM-OCM detects sinusoidal displacements of the magnetic microbeads induced by a magnetic field. This methodology demonstrates imaging of cell dynamics and has the potential for measuring cell biomechanical properties, which are important in assessing cell health.

9:24AM A1.00006 Reagent-free ultrasensitive spectroscopic probes for long term diabetes monitoring¹, N.C. DINGARI, I. BARMAN, J.W. KANG, Laser Biomedical Research Center, G. R. Harrison Spectroscopy Laboratory, MIT, G. HOROWITZ, Division of Clinical Pathology, Beth Israel Deaconess Medical Center, Harvard Medical School, RAMACHANDRA RAO DASARI, Laser Biomedical Research Center, G. R. Harrison Spectroscopy Laboratory, MIT — Long-term glycemic control is essential in developing therapeutics for diabetics. Glycated hemoglobin (HbA1c) and glycated albumin have been increasingly accepted as a functional metric of glycemic control over the past two to three months and three weeks, respectively. In this talk, we present the first demonstration of non-enhanced Raman spectroscopy as a novel analytical method for quantitative detection of HbA1c and glycated albumin. Using the drop coating deposition Raman technique, we observe that the non-enzymatic glycosylation of these proteins results in subtle, but consistent, changes in vibrational features, which with the help of multivariate classification techniques can be used to discriminate the glycated proteins from their unglycated variants with 100%. Additionally, the developed multivariate calibration models show a high degree of prediction accuracy even at substantially lower concentrations than those typically encountered in clinical practice. The excellent accuracy and reproducibility achieved in this proof-of-concept study opens substantive avenues for basic investigations of glycated proteins as well as in high-throughput glycemic marker sensing in multi-component mixtures and potentially even in serum and whole blood samples.

¹The authors wish to thank the NIH National Center for Research Resources for their grant P41-RR02594, at the MIT Laser Biomedical Research Center.

9:36AM A1.00007 The measurand problem in infrared breath alcohol testing, TED VOSK, Of Counsel Cowan, Kirk, Gaston — Measurements are made to determine the value of a quantity known as a measurand. The measurand is not always the quantity subject to measurement, however. Often, a distinct quantity will be measured and related to the measurand through a measurement function. When the identities of the measurand and the quantity actually measured are not well defined or distinguished, it can lead to the misinterpretation of results. This is referred to as the measurand problem. The measurand problem can present significant difficulties when the law and not science determines the measurand. This arises when the law requires that a particular quantity be measured. Legal definitions are seldom as rigorous or complete as those utilized in science. Thus, legally defined measurands often fall prey to the measurand problem. An example is the measurement of breath alcohol concentration by infrared spectroscopy. All 50 states authorize such tests but the measurand differs by jurisdiction. This leads to misinterpretation of results in both the forensic and legal communities due to the measurand problem with the consequence that the innocent are convicted and guilty set free. Correct interpretation of breath test results requires that the measurand be properly understood and accounted for. I set forth the varying measurands defined by law, the impact these differing measurands have on the interpretation of breath test results and how the measurand problem can be avoided in the measurement of breath alcohol concentration.

9:48AM A1.00008 Nanoscale neuroelectronic interface based on open-ended nanocoax arrays, JEFFREY R. NAUGHTON, BINOD RIZAL, MICHAEL J. BURNS, JEE YEOM, SHANNON HEYSE, MICHELLE ARCHIBALD, STEPHEN SHEPARD, GREGORY MCMAHON, THOMAS C. CHILES, MICHAEL J. NAUGHTON, Boston College — We describe the development of a nanoscale neuroelectronic array with submicron pixelation for recording and stimulation with high spatial resolution. The device is composed of an array of nanoscale coaxial electrodes, either network- or individually-configured. As a neuroelectronic interface, it will employ noninvasive real-time capacitive coupling to the plasma membrane with potential for extracellular recording of intra- and interneuronal synaptic activity, with one target being precision measurement of electrical signals associated with induced and spontaneous synapse firing in pre- and post-synaptic somata. Subarrays or even individual pixels can also be actuated for precisely-localized stimulation. We report initial results from measurements using the rat adrenal pheochromocytoma PC12 cell line, which terminally differentiates in response to nerve growth factor, as well as SH-SY5Y neuroblastoma cells in response to retinoic acid, characterizing the basic performance of the fabricated device.

10:00AM A1.00009 Phosphorus-31 MRI of bones using quadratic echo line-narrowing, MERIDETH FREY, SEAN BARRETT, Yale University Physics Dept., KARL INSOGNA, JOSHUA VANHOUTEN, Yale University, School of Medicine Dept. of Internal Medicine — There is a great need to probe the internal composition of bone on the sub-0.1 mm length scale, both to study normal features and to look for signs of disease. Despite the obvious importance of the mineral fraction to the biomechanical properties of skeletal tissue, few non-destructive techniques are available to evaluate changes in its chemical structure and functional microarchitecture on the interior of bones. MRI would be an excellent candidate, but bone is a particularly challenging tissue to study given the relatively low water density and wider linewidths of its solid components. Recent fundamental research in quantum computing gave rise to a new NMR pulse sequence - the quadratic echo - that can be used to narrow the broad NMR spectrum of solids. This offers a new route to do high spatial resolution, 3D ³¹P MRI of bone that complements conventional MRI and x-ray based techniques to study bone physiology and structure. We have used our pulse sequence to do 3D ³¹P MRI of *ex vivo* bones with a spatial resolution of (sub-450 μ m)³, limited only by the specifications of a conventional 4 Tesla liquid-state MRI system. We will describe our plans to push this technique towards the factor of 1000 increase in spatial resolution imposed by fundamental limits.

10:12AM A1.00010 Phosphorus-31 MRI of cell membranes using quadratic echo line-narrowing, SEAN BARRETT, MERIDETH FREY, Yale University Physics Dept., JOSEPH MADRI, MICHAEL MICHAUD, Yale University, School of Medicine Dept. of Pathology — Soft biological tissues have phosphorus concentrated in the membranes, metabolites, RNA and DNA of cells. This leads to a complicated, multi-peak ³¹P nuclear magnetic resonance spectrum (including a broad membrane peak and narrow metabolite peaks), which precludes high-resolution ³¹P MRI of soft tissues. This long-standing barrier has been overcome by a novel pulse sequence - the quadratic echo - recently discovered in fundamental quantum computation research. Applying time-dependent gradients in synch with a repeating pulse block enables a new route to high spatial resolution, three-dimensional ³¹P MRI of the soft solid components of cells and tissues. This is a functionally different kind of MR image, since conventional ¹H MRI probes the intracellular and extracellular free water, whereas our ³¹P MRI signal is dominated by the cell membrane contribution, which in turn depends on the density of mitochondria. The unique aspects of the signal should provide new insights into cellular and tissue function that complement the information revealed by ¹H MRI. So far, various *ex vivo* soft tissue samples have been imaged with (sub-mm)³ voxels. We will describe plans to enhance the spatial resolution in future work, to open a new window into cells.

10:24AM A1.00011 Accelerating the magnetic resonance imaging of hard and soft solids, ZACHARY SETHNA, MERIDETH FREY, SEAN BARRETT, Yale University Physics Dept. — Recent fundamental research in quantum computing gave rise to a new NMR pulse sequence - the quadratic echo - that can be used to narrow the broad MR spectrum of solids by orders of magnitude. This advance enables high spatial resolution, 3D MRI of hard and soft solids (e.g., the ³¹P MRI of bone and soft tissues, which has recently been demonstrated in our group). While this is great progress, the next challenge to address is the slow imaging time in solids. The *T*₁ time of solids can be orders of magnitude larger than that of a liquid (e.g., for some of our samples the *T*₁ time can be >100 s). Since imaging sequences wait a repetition time (of order *T*₁) between scans, a three-dimensional image (requiring many scans) can take >24 hours. Here we discuss approaches under study that aim to decrease the total imaging time of our MRI of solids technique. One method is to implement a variant on the driven equilibrium approach. Another method is to take less data, namely, sparse MRI (i.e., under-sampling of k-space). This leads to artifacts in standard FFT image construction; more advanced alternatives, such as a difference map algorithm, may be used to produce an image closer to the ideal, which is a promising approach to reduce total imaging time.

10:36AM A1.00012 A Comparison of Raman Spectral Features of Frozen and Deparaffinized Tissues in Neuroblastoma and Ganglioneuroma¹ , SUNEETHA DEVPURA, JAGDISH S. THAKUR, Wayne State University, JANET M. POULIK, Children's Hospital of Michigan, RAJA RABAH, University of Michigan-Ann Arbor, VAMAN M. NAIK, University of Michigan-Dearborn, RATNA NAIK, Wayne State University — We have investigated the cellular regions in neuroblastoma and ganglioneuroma using Raman spectroscopy and compared their spectral characteristics with those of normal adrenal gland. Thin sections from both frozen and deparaffinized tissues, obtained from the same tissue specimen, were studied in conjunction with the pathological examination of the tissues. We found a significant difference in the spectral features of frozen sections of normal adrenal gland, neuroblastoma, and ganglioneuroma when compared to deparaffinized tissues. The quantitative analysis of the Raman data using chemometric methods of principal component analysis and discriminant function analysis obtained from the frozen tissues show a sensitivity and specificity of 100% each. The biochemical identification based on the spectral differences shows that the normal adrenal gland tissues have higher levels of carotenoids, lipids, and cholesterol compared to the neuroblastoma and ganglioneuroma frozen tissues. However, deparaffinized tissues show complete removal of these biochemicals in adrenal tissues. This study demonstrates that Raman spectroscopy combined with chemometric methods can successfully distinguish neuroblastoma and ganglioneuroma at cellular level.

¹We would like to acknowledge the support from the Richard J. Barber Foundation for Interdisciplinary Research

10:48AM A1.00013 Expanding Cancer Detection Using Molecular Imprinting for a Novel Point-of-Care Diagnostic Device , YINGJIE YU, MIRIAM RAFAILOVICH, YANTIAN WANG, State University of New York- Stony Brook, ALINA RANJBARAN, Garden City High School, TOM WANG, The Wheatley School, DAVID NAM, Monta Vista High School — We propose the use of a potentiometric biosensor that incorporates the efficient and specific molecular imprinting (MI) method with a self-assembled monolayer (SAM). We first tested the biosensor using carcinoembryonic antigen, CEA, a biomarker associated with pancreatic cancer. No change in detection efficiency was observed when detection was performed in the presence of 100% serum albumin, indicating that the sensor is able to discriminate for the template analyte even in concentrated solution of similar substances. Computer simulations of the protein structure were performed in order to estimate the changes in morphology and determine the sensitivity of the biosensor to conformational changes in the proteins. We found that even small changes in PH can generate rotation of the surface functional groups, without significant change in the morphology. Yet, the results show that only when the detection and imprinting conditions are similar, robust signals occurs. Hence we concluded that both morphology and surface chemistry play a role in the recognition.

Monday, February 27, 2012 8:00AM - 11:00AM —
Session A2 GQI FEd: Invited Session: Teaching Quantum Information Science at Liberal Arts College 204AB

8:00AM A2.00001 Doing quantum theory at a liberal arts college , BENJAMIN SCHUMACHER, Kenyon College — An academic career at a liberal arts college poses some challenges for a researcher in quantum information and quantum foundations, most notably the lack of local collaborators and graduate students. Are there also complementary advantages and opportunities?

8:36AM A2.00002 Quantum Information in Non-physics Departments at Liberal Arts Colleges , MICHAEL WESTMORELAND, Denison University — Quantum information and quantum computing have changed our thinking about the basic concepts of quantum physics. These fields have also introduced exciting new applications of quantum mechanics such as quantum cryptography and non-interactive measurement. It is standard to teach such topics only to advanced physics majors who have completed coursework in quantum mechanics. Recent encounters with teaching quantum cryptography to non-majors and a bout of textbook-writing suggest strategies for teaching this interesting material to those without the standard quantum mechanics background. This talk will share some of those strategies.

9:12AM A2.00003 Theoretical Research Fostered by an Undergraduate Environment , WILLIAM WOOTTERS, Williams College — An undergraduate setting entails certain challenges for a faculty member doing research in theoretical physics, but it also offers particular opportunities. While it is possible to succeed in any area of theoretical research at an undergraduate institution, the experience of teaching at the undergraduate level and doing research with undergraduate students naturally leads one to think about problems that, though possibly very interesting, do not require a high level of technical expertise. Such problems tend to be “close to the trunk of the tree of physics,” as a colleague has suggested, meaning that they may be closer to the central ideas of physics than many highly specialized problems. In this talk I give examples of research projects in quantum information and quantum foundations that have been stimulated in part by undergraduate-level teaching and carried out with undergraduate collaborators.

9:48AM A2.00004 Is Theoretical Physics Locus-dependent? Quantum Information at Liberal Arts Colleges , HERBERT BERNSTEIN, Hampshire College — No abstract available.

10:24AM A2.00005 Fundamental Physics with Table-Top Optics , ENRIQUE GALVEZ, Colgate University — Experimental physics research at an undergraduate institution poses the challenge of requiring the production of publishable results while also being a suitable setting for mentoring undergraduates in research. It is tempting for young faculty to copy/adapt “big-machine” university research, but that is a tough enterprise that is hard to sustain. An option that suits the undergraduate setting better is a small, table-top, apparatus devoted to projects with promising potential. In optics I found such a setting, and a successful transition from big-machine to table-top setups. Optics is a fertile ground for student projects that does not involve heavy maintenance, can achieve substantial depth, and enables student independence. It also allows the creation of projects that match the abilities of the not-so-high achievers. At the conference I will present examples of recent projects involving the study of classical light beams that carry optical vortices and non-classical beams that encode qubits. This work has been funded by Research Corporation, NSF and Air Force.

Monday, February 27, 2012 8:00AM - 11:00AM —
Session A3 DCMP: Invited Session: Superconducting Fluctuations in Cuprates 205AB

8:00AM A3.00001 Decrease of pairing strength with underdoping in cuprate superconductors

, JOHAN CHANG, EPFL, Lausanne, Switzerland — The transition temperature T_c of cuprate superconductors decreases at low hole doping p , but it is still unclear whether the pairing strength decreases or increases. Different interpretations of the pseudogap lead to opposite conclusions. Different estimates of the upper critical field H_{c2} are in sharp contradiction. In this talk, we resolve the latter contradiction by showing that superconducting fluctuations in the underdoped cuprate Eu-LSCO, measured via the Nernst effect, obey the theory of Gaussian fluctuations, as in conventional superconductors [1, 2]. The extracted critical field H_{c2} is small, and it dips at $p = 0.11$, showing that pairing strength is weak where stripe order is strong. In the archetypal cuprate superconductor YBCO, H_{c2} extracted from other measurements [3] has the same doping dependence, also with a minimum at $p = 0.11$, again where stripe order is present [4, 5]. We conclude that competing states such as stripe order weaken the pairing strength and this, rather than phase fluctuations, is the predominant cause for the low T_c of underdoped cuprates. Work done in collaboration with N. Doiron-Leyraud, E. Hassinger, J.-Ph. Reid, O. Cyr-Choinière, F. Laliberté, R. Daou, S. Pyon, T. Takayama, H. Takagi, and Louis Taillefer.

- [1] M. N. Serbyn *et al.*, Phys. Rev. Lett. **102**, 067001 (2009).
- [2] K. Michaeli and A. M. Finkel'stein, Europhys. Lett. **86**, 27007 (2009).
- [3] Y. Ando and K. Segawa, Phys. Rev. Lett. **88**, 167005 (2002).
- [4] F. Laliberté *et al.*, Nature Comm. **2**, 432 (2011).
- [5] T. Wu *et al.*, Nature **477**, 191 (2011).

8:36AM A3.00002 Pseudogap phase and superconducting fluctuation regime of the cuprate superconductors¹

, NEVEN BARIŠIĆ, School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA — The pseudogap phenomenon in the cuprates is one of the most investigated topics in the field of correlated materials. A related question is the extent to which superconducting fluctuation persist between the pseudogap temperature (T^*) and superconducting transition temperature (T_c). We have addressed this question by combining several experimental probes: planar dc-resistivity [1], microwave conductivity [2,3], and torque magnetometry [4]. dc-resistivity measurements in the simple tetragonal model compound $\text{HgBa}_2\text{CuO}_{4+\delta}$ [5], which features the highest T_c (97 K) among all single-layer cuprates, reveal four characteristic temperatures: T^* , coincident with the onset of novel $\mathbf{q}=0$ magnetic order revealed by neutron diffraction [6]; a second, lower pseudogap temperature T^{**} associated with a further rearrangement of the states at the Fermi level; T' , which marks the onset of superconducting fluctuations; and finally T_c . Notably, T' lies only 10-20 K above T_c and closely tracks the superconducting dome with doping. The superconducting fluctuation regime is further investigated by microwave conductivity and torque magnetometry, and these results confirm the latter conclusion. The results for $\text{HgBa}_2\text{CuO}_{4+\delta}$ are complemented by a comprehensive investigation of other cuprates ($\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$, $\text{Bi}_2\text{Sr}_{2-z}\text{La}_z\text{CuO}_{6+\delta}$), which leads to new insights into the phase diagram of cuprate superconductors.

- [1] N. Barišić *et al.*, preprint.
- [2] M.S. Grbić *et al.*, Phys. Rev. B **80**, 094511 (2009).
- [3] M.S. Grbić *et al.*, Phys. Rev. B **83**, 144508 (2011).
- [4] G. Yu *et al.*, preprint.
- [5] N. Barišić *et al.*, Phys. Rev. B **78**, 054518 (2008).
- [6] Y. Li *et al.*, Nature **455**, 372 (2008).

¹This work was done in collaboration with G. Yu, D. Xia, Y. Li, X. Zhao, M. S. Grbić, M. Požek, A. Dulčić, and M. Greven. It was supported by the NSF and by DOE BES.

9:12AM A3.00003 Fluctuations of Superconductivity in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$: A Terahertz Conductivity Study¹

, LUCAS BILBRO, The Institute for Quantum Matter, Department of Physics and Astronomy, Johns Hopkins University — In the underdoped pseudogap regime of the high-temperature superconductors, one expects that due to low superfluid densities and short correlation lengths, superconducting fluctuations will be significant for transport and thermodynamic properties. However, there has been disagreement about how high in temperature they may persist, their role in the phenomenology of the pseudogap regime, and their significance for understanding high-temperature superconductivity. We use THz time-domain spectroscopy (TTDS) to probe the temporal fluctuations of superconductivity above the critical temperature (T_c) in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) thin films over a doping range that spans almost the entire superconducting dome. Signatures of the fluctuations persist in the conductivity in a narrow temperature range above T_c . Our measurements show that superconducting correlations do not make an appreciable contribution to the charge transport anomalies of the pseudogap in LSCO at temperatures well above T_c .² I will compare our results for an underdoped ($x=0.095$) sample with measurements of diamagnetism in a similarly doped crystal of $\text{La}_{1.905}\text{Sr}_{0.095}\text{CuO}_4$. I will show, through a vortex-plasma model, that if the fluctuation diamagnetism originates solely in vortices, then these vortices must exhibit an anomalously large vortex diffusion constant, more than two orders of magnitude larger than the Bardeen-Stephen estimate.³ This points to either the extremely unusual properties of vortices in the underdoped d-wave Cuprates or a contribution to the diamagnetic response that is not superconducting in origin. Finally, I will introduce preliminary results of THz conductivity measurements of critically underdoped LSCO films, where superconductivity is fully suppressed.

¹Work supported by The Institute of Quantum Matter under DOE grant DE-FG02-08ER46544, the Gordon and Betty Moore Foundation, and the US DOE under Project No. MA-509-MACA.

²L.S. Bilbro *et al.*, Nature Physics **7**, 298 (2011).

³L.S. Bilbro *et al.*, Phys. Rev. B **84**, 100511 (2011).

9:48AM A3.00004 Distinct Ranges of Superconducting Fluctuations and Pseudogap in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$

, FLORENCE RULLIER-ALBENQUE, Service de Physique de l'Etat Condense, IRAMIS, CEA Saclay, France — The contribution of superconducting fluctuations (SCF) to the ab-plane conductivity has been determined accurately in a series of $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ single crystals using high magnetic fields to restore the normal state behavior [1]. This allows us to determine within the same set of transport measurements both the field $H'_c(T)$ and the temperature T'_c above which the SCFs are fully suppressed, and the pseudogap temperature T^* . A careful investigation near optimal doping shows that T^* becomes smaller than T'_c , which unambiguously evidences that the pseudogap cannot be assigned to preformed pairs [2]. In the nearly optimally doped samples, the SCF contribution to conductivity can be accounted for by Gaussian Aslamazov-Larkin fluctuations in the Ginzburg-Landau approach [3]. A phase fluctuation contribution might be invoked in the most underdoped sample in a T range which increases when controlled disorder is introduced by electron irradiation. The analysis of the fluctuation magnetoconductance allows us to determine the critical fields $H_{c2}(0)$ which are found to be very similar to $H'_c(0)$ and to increase with hole doping. These two depairing fields which are directly connected to the magnitude of the superconducting gap therefore follow the evolution of T_c , which is at odds with the sharp decrease of the pseudogap with increasing hole doping.

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- [2] F. Rullier-Albenque, H. Alloul, G. Rikken, Phys. Rev. B **84**, 014522 (2011).

10:24AM A3.00005 Fluctuoscropy of Superconductors¹ , ANDREY VARLAMOV, Institute of Superconductivity and Innovative Materials SPIN- CNR — The study of superconducting fluctuations (SF) is a subject of fundamental and practical importance. Since the moment of discovery SF became a noticeable part of research in the field of superconductivity (SC) and a variety of fluctuation effects have been detected. The interest to SF in SC was regenerated by the discovery of HTS, where, due to extremely short coherence length and low effective dimensionality of the electron system, SF manifest themselves in a wide range of temperatures. The characteristic feature of SF is their strong dependence on temperature and magnetic field. This allows to separate SFs from other contributions and to use them as a tool for characterization of SC systems (“fluctuoscropy”) for example to extract the values of T_c , $H_{c2}(T)$ and phase-breaking time from experimental data. We present the complete results for fluctuation magneto-conductivity (FMC) and Nernst signal (FNS) of impure 2D superconductor in the whole phase diagram above the transition line $H_{c2}(T)$, including the domain of quantum fluctuations. Along some line $H_0(T)$, in agreement with experimental findings, FMC becomes zero and beyond it remains small and negative. The corresponding surface in coordinates (T, H) becomes in particular non-trivial at low temperatures and close to $H_{c2}(0)$, where it is trough-shaped. The observation of large FNS in HTS and conventional SC above $T_c(H)$, has attracted much attention recently. The idea to attribute it to the entropy transport by analogy to vortices was proposed. On the other hand this giant effect, close to $T_c(0)$, was explained in terms of SF. Our general results allow to successfully fit the available experimental data in a wide range of magnetic fields and temperatures, to extract the value of the “ghost” field and other parameters of SC. We offer also a qualitative consideration, which gives a natural explanation for the giant value of FNS attributing it to a strong dependence of the fluctuation Cooper pair (FCP) chemical potential on temperature. Close to zero temperature, when the magnetic field approaches $H_{c2}(0)$, a peculiar dynamic state consisting of clusters of coherently rotating FCP forms. We estimate the characteristic size and lifetime of such clusters and present the scenario of fluctuation nucleation of Abrikosov’s lattice.

¹Work supported by the U.S. DOE, Office of Science, under Contract No. DE-AC02-06CH11357. Support of MIUR under project PRIN 2008 and the European Community FP7-IRSES programs “ROBOCON” and “SIMTECH” (contract N 236947) is acknowledged.

Monday, February 27, 2012 8:00AM - 11:00AM – Session A4 DAMOP: Focus Session: Hybrid Systems and Quantum Information Science in Atomic, Molecular, and Optical Physics 205C

8:00AM A4.00001 A Light-Matter Interface with NV Centers , BRENDAN SHIELDS, NATHALIE DE LEON, Harvard University Department of Physics, BIRGIT HAUSMANN, Harvard University School of Engineering and Applied Sciences, YIWEN CHU, Harvard University Department of Physics, MICHAEL BUREK, Harvard University School of Engineering and Applied Sciences, PATRICK MALETINSKY, Institute of Quantum Electronics, ETH Zurich, QIMIN QUAN, Harvard University School of Engineering and Applied Sciences, ALEXANDER ZIBROV, Harvard University Department of Physics, HONGKUN PARK, Harvard University Department of Chemistry, MARKO LONCAR, Harvard University School of Engineering and Applied Sciences, MIKHAIL LUKIN, Harvard University Department of Physics — NV centers in diamond offer much promise as solid state qubits for scalable quantum communication and information processing. However, for bulk diamond systems the low collection efficiency and large phonon sideband emission represent substantial limitations for applications in quantum information science. In this talk we will describe the realization of nanoscale photonic cavities containing NV centers with desired optical properties. The experimental realization of spontaneous emission control and strong coupling regime of cavity QED will be discussed.

8:12AM A4.00002 Probing the motion of a mechanical resonator via coherent coupling to a single spin qubit¹ , SHIMON KOLKOWITZ, QUIRIN UNTERREITHMEIER, Department of Physics, Harvard University, ANIA BLESZYNSKI JAYICH, Department of Physics, UC Santa Barbara, STEVEN BENNETT, Department of Physics, Harvard University, PETER RABL, Austrian Academy of Science, Innsbruck, Austria, J.G.E. HARRIS, Departments of Physics and Applied Physics, Yale University, MIKHAIL LUKIN, Department of Physics, Harvard University — Mechanical systems can be influenced by a wide variety of extremely small forces, ranging from gravitational to optical, electrical, and magnetic. When mechanical resonators are scaled down to nanometer-scale dimensions, these forces can be harnessed to enable coupling to individual quantum systems. In this talk we will present results showing that the coherent evolution of a single electronic spin associated with a Nitrogen Vacancy (NV) center in diamond can be coupled to the motion of a magnetized mechanical resonator. Specifically we use coherent manipulation of the spin to sense the driven and Brownian motion of the resonator under ambient conditions at a picometer length scale. We will discuss potential applications of this technique including the detection of the zero-point fluctuations of a mechanical resonator, the realization of strong spin-phonon coupling at a single quantum level, and the implementation of quantum spin transducers.

¹S.K. acknowledges support by the Department of Defense (DoD) through the National Defense Science and Engineering Graduate Fellowship (NDSEG) Program.

8:24AM A4.00003 A nanoscale quantum interface for single atoms , TOBIAS TIECKE, Harvard University, Department of Physics and Research Laboratory of Electronics, MIT, JEFF THOMPSON, Harvard University, Department of Physics, JOHANNES FEIST, ITAMP, Harvard-Smithsonian center for Astrophysics, CHUN YU, Harvard University, Department of Chemistry, ALEXEY AKIMOV, Harvard University, Department of Physics, DARRICK CHANG, Caltech, ALEXANDER ZIBROV, Harvard University, Department of Physics, VLADAN VULETIC, Center for Ultracold Atoms, Department of Physics, MIT, HONGKUN PARK, Harvard University, Department of Chemistry, MIKHAIL LUKIN, Harvard University, Department of Physics — Neutral atoms are ideal quantum systems: they have long ground-state coherence times and strong optical cycling transitions that enable state detection and preparation. Building quantum networks of atoms interacting through photons is challenging, however, as many schemes for atom-photon interaction are inefficient or hard to scale. We propose a scheme to trap neutral atoms near silver nanowires, which are tightly confining waveguides for surface plasmons. The nanowire tip is used to generate a near-field optical trapping potential, and to enhance and efficiently collect spontaneous emission from the atom. We present experimental results on using the atom to sense the optical field at submicron distances from the wire and our current efforts towards loading the nanotrap.

8:36AM A4.00004 Estimating and characterizing electromechanical coupling of superfluid helium to a microwave resonator , YANG GE, BING LI, University of Chicago, ANDREAS FRAGNER, ROB SCHOELEKOPF, Yale University, DAVID SCHUSTER, University of Chicago — Electrons on helium is a unique two-dimensional electron gas system formed at the interface of a quantum liquid (superfluid helium) and vacuum. The motional state of single-electron quantum dots defined on such systems has been proposed as a good candidate for hybrid quantum computing and as a gateway to measuring the electron spin [1,2]. Incoherent fluctuations of the thickness or density of the helium film are potential sources of motional dephasing, hence require further experimental characterization. In addition, if these ripplons or phonons could be coherently coupled to an electromagnetic cavity one could realize a quantum electro-mechanical system. Here, I will present estimates and preliminary experimental characterization of the electromechanical couplings as well as progress with electrons on helium.

[1] S. Lyon, Phys. Rev. A. 74, 5 (2006)

[2] D.I. Schuster, et al. Phys. Rev. Lett. 105, 040503 (2010)

8:48AM A4.00005 Tunable High Q Superconducting Microwave Resonator for Hybrid System with ^{87}Rb atoms¹, ZAEILL KIM, K.D. VOIGT, JONGMIN LEE, J.E. HOFFMAN, J.A. GROVER, S. RAVETS, JQI/UMD, V. ZARETSKEY, UMD, B.S. PALMER, LPS, M. HAFEZI, J.M. TAYLOR, JQI/NIST/UMD, J.R. ANDERSON, A.J. DRAGT, C.J. LOBB, L.A. OROZCO, S.L. ROLSTON, F.C. WELLSTOOD, JQI/UMD — We have developed a frequency tuning system for a “lumped-element” thin-film superconducting Al microwave resonator [1] on sapphire intended for coupling to hyperfine ground states of cold trapped ^{87}Rb atoms, which are separated by about $f_{Rb} = 6.83$ GHz. At $T=12$ mK and on resonance at 6.81 GHz, the loaded quality factor was 120,000. By moving a carefully machined Al pin towards the inductor of the resonator using a piezo stage, we were able to tune the resonance frequency over a range of 35 MHz and within a few kHz of f_{Rb} . While measuring the power dependent response of the resonator at each tuned frequency, we observed anomalous decreases in the quality factor at several frequencies. These drops were more pronounced at lower power. We discuss our results, which suggest these resonances are attributable to discrete two-level systems.

[1] Z. Kim *et al.*, AIP ADVANCES 1, 042107 (2011).

¹Work supported by NSF through the Physics Frontier Center at the Joint Quantum Institute, Dept. of Physics, Univ. of Maryland.

9:00AM A4.00006 Coupling quantum microwave circuits to quantum optics via cavity electro-optic modulators¹, MANKEI TSANG, National University of Singapore — Experimental circuit quantum electrodynamics has made great strides in recent years, but it remains an open question how the quantum information stored in the microwave circuits can be transferred for long distances. Just as in classical information, the most promising solution is to convert the microwave fields to optical frequencies, where ultra-low-loss photonic devices such as optical fibers can be used. Here I propose the use of cavity electro-optic modulators for coherent coupling between microwave and optical fields. The electro-optic effect is the change in optical refractive index in certain materials, such as lithium niobate, under an applied voltage. Leveraging the fact that cavity electro-optics has the same physics as cavity optomechanics, a cavity electro-optic modulator can realize various joint quantum operations on the microwave and optical fields, including coherent frequency conversion, laser cooling of microwave resonance, hybrid entanglement, hybrid parametric amplification and oscillation, and optical quantum-nondemolition measurements of microwave quadrature and energy.

¹This material is based on work supported by the Singapore National Research Foundation under NRF Grant No. NRF-NRFF2011-07.

9:12AM A4.00007 Hybrid Quantum Systems with Circuit Quantum Electrodynamics¹, DAVID SCHUSTER, University of Chicago — Quantum Information Processing presents daunting challenges, with competing requirements of fast manipulation, long storage, and long distance transport of fragile quantum states. In aggregate, many of the challenges quantum computation have been met with nanosecond manipulations (quantum circuits), coherence times measured in seconds (atomic ions/nuclear spins), and entanglement transported over kilometers (linear optics), yet thus far no system has achieved all of the necessary components simultaneously. One promising direction is to leverage the best aspects of each system in a hybrid system, much as is done in a conventional computer, where transistors provide fast processing, magnetic memory provides massive long term storage, and information is transmitted via microwaves or fiber optics. A review of the constituent quantum systems, and the types of couplings between them will be presented. The coupling of a superconducting cavity/qubit system to electrons floating on helium will be discussed as an example of how to construct a hybrid system. Recent results on trapping and detection of electrons on helium using a superconducting cavity will be presented.

¹Andreas Fragner, Yang Ge, Bing Li, Rob Schoelkopf

9:48AM A4.00008 Nonlinear optics quantum computing with circuit QED¹, PRABIN ADHIKARI, MOHAMMAD HAFEZI, Joint Quantum Institute at UMD, JACOB TAYLOR, Joint Quantum Institute at UMD and NIST — One approach to quantum information processing is to use photons as quantum bits and rely on linear optical elements for most operations. However, some optical non-linearity is necessary to enable universal quantum computing. We consider a circuit-QED approach to linear optics quantum computing in the microwave regime, including a deterministic two-photon phase gate. Our model is a hybrid quantum system comprising an LC resonator coupled to a flux or phase superconducting qubit, which will be used to implement a non-linear two photon phase shift operation. Using this model, we show how fast, low-noise two-qubit gates between photons are possible, and discuss limitations of these ideas based on current technology.

¹This research supported by the Physics Frontier Center at the JQI.

10:00AM A4.00009 Towards Hybrid Quantum Information Processing with Electrons on Helium, ANDREAS FRAGNER, Department of Applied Physics, Yale University, DAVID SCHUSTER, Department of Physics, University of Chicago, MARK DYKMAN, Department of Physics, Michigan State University, STEPHEN LYON, Department of Electrical Engineering, Princeton University, LUIGI FRUNZIO, Department of Applied Physics, Yale University, ROBERT SCHOELKOPF, Department of Physics and Applied Physics, Yale University — Electrons above the surface of superfluid helium form a two-dimensional electron gas in which single-electron quantum dots can be defined using electrostatic gates submerged under the helium film. The quantized motion and spin state of such a trapped electron on helium can be coupled to a high finesse superconducting cavity in a hybrid circuit QED architecture [1]. The cavity is used for nondestructive readout and as a quantum bus mediating interactions between distant electrons or an electron and a superconducting qubit. Coupling between motional states and individual photons in the cavity is estimated at a Rabi frequency of $g/2\pi \sim 20$ MHz with coherence times exceeding 20 μs for charge and 1 s for spin [1, 2]. Here I will discuss recent experiments in which we successfully trap and detect a two-dimensional electron gas on helium in a dc-biased superconducting cavity. Experimental progress towards the single-electron regime will also be presented.

[1] D.I. Schuster, A.Fragner, M.I. Dykman, S. Lyon and R.J. Schoelkopf, Phys. Rev. Lett. 105, 040503 (2010)

[2] S. A. Lyon, Phys. Rev. A 74, 052338 (2006)

10:12AM A4.00010 An ab-initio microscopic theory of anomalous heating in planar ion traps¹, H.R. SADEGHPOUR, ITAMP, Harvard-Smithsonian Center for Astrophysics, A. SAFAVI-NAINI, ITAMP/Dept of Physics MIT, P. RABL, IQOQI, Innsbruck, P.F. WECK, Advanced Systems Analysis, Sandia — Anomalous heating of trapped ions limits the scalability of the planar trap architecture for quantum computation. Measurements of the electric field noise present in ion traps indicate that the noise-induced heating scales as the inverse fourth power of the distance from the trap electrodes to the ion and its spectral density scales with the inverse of frequency [1]. These measurements also suggest that some thermally activated random process is at work. In this work, we present an ab-initio theory of this noise due to oscillating dipoles on the trap electrode surface [2]. The dipoles are formed when atoms are adsorbed on the trap surface, whose interaction with the surface is described with density functional theory (DFT). We present calculations for the spectral noise density and its distance, frequency and temperature dependencies. We consider both independent and correlated dipoles.

[1] Q. A. Turchette *et al.*, Phys. Rev. A. 61, 63418 (2000).

[2] A. Safavi-Naini, P. Rabl, P. F. Weck, H. R. Sadeghpour, Phys. Rev. A. 84, 023412 (2011).

¹NSF

10:24AM A4.00011 Quantum logic for molecular quantum information processing, J. MUR-PETIT, J. PEREZ-RIOS, J. CAMPOS-MARTINEZ, M.I. HERNANDEZ, Instituto de Fisica Fundamental, IFF-CSIC, Spain, S. WILLITSCH, Department of Chemistry, University of Basel, Switzerland, J.J. GARCIA-RIPOLL, Instituto de Fisica Fundamental, IFF-CSIC, Spain — Very recently, molecular ions have been trapped and cooled to the mK regime in well defined internal states [1] opening a new window for precision spectroscopy of molecular species and quantum information with cold molecular ions. A first requirement for both applications is the ability to control and measure the state of molecular ions. I will present our proposal [2] of a fast, non-destructive and temperature independent spectroscopy method suitable to study electronic, vibrational, rotational and Zeeman transitions in complex ions that implements quantum logic schemes [3] between an atomic ion and the molecular ion of interest, using optical forces on the atom, and optical forces or magnetic field gradients on the molecule. This method sets a starting point for a hybrid quantum computation scheme with molecular and atomic ions, covering the measurement and entangling steps. Finally I will discuss the remarkable decoherence properties of two Zeeman states of the $^{16}\text{O}_2^+$ molecular ion that make it a promising system for QIPC purposes [4].

[1] X. Tong *et al.*, Phys. Rev. Lett. **105**, 143001 (2010).

[2] J. Mur-Petit *et al.*, arXiv:1106.3320

[3] P. O. Schmidt *et al.*, Science **309**, 749 (2005).

[4] J. Mur-Petit *et al.*, in preparation.

10:36AM A4.00012 Possibility of “magic” trapping of three-level system for Rydberg blockade implementation¹, MUIR J. MORRISON, ANDREI DEREVIANKO, University of Nevada, Reno — The Rydberg blockade mechanism has shown noteworthy promise for scalable quantum computation with neutral atoms. Both qubit states and gate-mediating Rydberg state belong to the same optically-trapped atom. The trapping fields, while being essential, induce detrimental decoherence. Here we theoretically demonstrate that this Stark-induced decoherence may be completely removed using powerful concepts of “magic” optical traps. We analyze “magic” trapping of a prototype three-level system: a Rydberg state along with two qubit states, which are hyperfine states attached to a $J = 1/2$ ground state. Our numerical results show that the group IIIB metals such as Al are suitable candidates. Such trapping may or may not be possible for the alkalis, as “magic” conditions depend sensitively on the the trap-Rydberg interaction. Calculations of these effects are ongoing, and the results will be presented.

¹This project was supported in part by the NSF and UNR Honors Undergraduate Research Award.

10:48AM A4.00013 Cooling in the single-photon regime of optomechanics, ANDREAS NUNNENKAMP, Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland, KJETIL BORKJE, STEVEN GIRVIN, Departments of Physics and Applied Physics, Yale University, New Haven, Connecticut 06520, USA — Optomechanics experiments are rapidly approaching the regime where the radiation pressure of a single photon displaces the mechanical oscillator by more than its zero-point uncertainty. We show that in this limit the power spectrum has multiple sidebands and that the cavity response has several resonances in the resolved-sideband limit [Phys. Rev. Lett. **107**, 063602 (2011)]. We then discuss how red-sideband cooling is modified in this nonlinear regime. Using Fermi's Golden rule we calculate the transition rates induced by the optical drive. In the resolved-sideband limit we find multiple cooling resonances for strong single-photon coupling. They lead to non-thermal steady states and are accompanied by multiple mechanical sidebands in the optical output spectrum. Our study provides the tools to detect and take advantage of this novel regime of optomechanics.

Monday, February 27, 2012 8:00AM - 11:00AM –

Session A5 DCMP: Surfaces: Structure, Transitions and Morphological Evolution 206A

8:00AM A5.00001 The Relaxation of Vicinal (001) with ZigZag [110] Steps¹, MICAH HAWKINS, Department of Physics, University of Maryland, College Park, AJMI BH HAMOUDA, Faculte des Sciences de Monastir, Monastir, Tunisia, DIEGO LUIS GONZÁLEZ-CABRERA, THEODORE L. EINSTEIN, Department of Physics, University of Maryland, College Park — This talk presents a kinetic Monte Carlo study of the relaxation dynamics of [110] steps on a vicinal (001) simple cubic surface. This system is interesting because [110] steps have different elementary excitation energetics and favor step diffusion more than close-packed [100] steps. In this talk we show how this leads to relaxation dynamics showing greater fluctuations on a shorter time scale for [110] steps as well as 2-bond breaking processes being rate determining in contrast to 3-bond breaking processes for [100] steps. The existence of a steady state is shown via the convergence of terrace width distributions at times much longer than the relaxation time. In this time regime excellent fits to the modified generalized Wigner distribution (as well as to the Berry-Robnik model when steps can overlap) were obtained. Also, step-position correlation function data show diffusion-limited increase for small distances along the step as well as greater average step displacement for zigzag steps compared to straight steps for somewhat longer distances along the step. Work supported by NSF-MRSEC Grant DMR 05-20471 as well as a DOE-CMCSN Grant.

¹NSF-MRSEC

8:12AM A5.00002 Embedded Atom Method Potential for Ni-Cu Alloys and Its Applications for Ni, Cu growth on Cu(111)¹, BERK ONAT, Informatics Institute, Istanbul Technical University, Istanbul, Turkey, SONDAN DURUKANOGLU, Nanotechnology Research and Application Center, Faculty of Engineering and Natural Sciences, Sabanci University, Istanbul, Turkey — We developed a semi-empirical, many-body type model potential to investigate static and dynamic properties of Ni-Cu alloys. The formalism is based on the embedded atom method with improved optimization techniques. The Ni-Cu alloy potential was determined by fitting to data on lattice parameters, cohesive energies for L1₀, L1₁, L1₂, and L1₃ phases, together with vacancy formation energies, bulk modulus and elastic properties for L1₂, L1₃ phases. Our preliminary calculations for energy barriers for the diffusing Ni and Cu atoms on Cu(111) based on the nudged elastic band method are found to be consistent with the available experimental and other theoretical results. Our ultimate goal is to describe the varying characteristics in growing islands of pure Cu, Ni atoms and mixed Ni-Cu combinations on Cu(111) [S. Pons *et al.*, Surf. Sci., **511**, 449, (2002)].

¹This work was supported by TUBITAK under Grant No. 109T105. Computations were carried out through UYBHM at Istanbul Technical University, under Grant No. 20132007.

8:24AM A5.00003 Computational diffusion model of reconstructed regions in Ag/Si epitaxial growth, JOSEPH DRISCOLL, KELLY ROOS, Bradley University, D. WALL, M. HORN-VON HOEGEN, F.-J. MEYER ZU HERINGDORF, Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen, 47057 Duisburg, Germany — The thermal decay of Ag islands, grown epitaxially in a Stranski-Krastanov mode on Si(001) and Si(111) surfaces, has been studied experimentally with photoemission electron microscopy (PEEM). In a range of elevated temperatures the islands decay mainly by dissociation of Ag atoms from island edges, rather than by direct desorption into the gas phase. On the surrounding surface, the Ag atoms are subject to thermally-activated diffusion and desorption. The Ag surface concentration decreases with distance from the island edges. Where the local concentration is above a critical value, coverage-dependent reconstructed overlayers form surrounding the islands. The spread of the overlayers, relative to the position of the decaying island, depends on competition between diffusion and desorption. Previous quasi-static models [1] have shown that the observed reconstructed regions are related to the atomistic parameters describing surface diffusion, and have been applied to extract diffusion coefficients from the experimental data. Here we present results from a dynamic diffusion model that captures many of the qualitative and quantitative time- and temperature-dependent phenomena observed in the experiments.

[1] K.R. Roos et. al. PRL 100, 016103 (2008); D. Wall et. al. NJP 12 (2010) 103019

8:36AM A5.00004 Plasma-assisted molecular beam epitaxy growth of ZnSnN_2 , NATHANIEL FELDBERG, JAMES ALDOUS, YUAN YAO, IMTIAZ TANVEER, BENJAMIN KEEN, University at Buffalo, WOJCIECH LINHART, TIM VEAL, University of Warwick, YOUNG-WOOK SONG, ROGER REEVES, University of Canterbury, STEVE DURBIN, University at Buffalo, UNIVERSITY AT BUFFALO TEAM, UNIVERSITY OF WARWICK COLLABORATION, UNIVERSITY OF CANTERBURY COLLABORATION — The Zn-IV-nitrides are a promising series of “earth abundant element” semiconductors with a predicted band gap range of 0.6 eV to 5.4 eV, which, like the (Al,Ga,In)N family, spans the entire visible solar spectrum. Considering this alternative family has a number of advantages, including the avoidance of indium, the price of which has varied almost an order of magnitude over the past decade, and surface electron accumulation which is present in the In-rich alloys. Not all members of this family have yet been synthesized, in particular ZnSnN_2 , the most important member for PV with its predicted band gap of approximately 2 eV. We have successfully grown a series of these films using plasma-assisted molecular beam epitaxy using elemental Zn and Sn sources. In this report, we discuss the relationship between process parameters and microstructure, as well as stoichiometry as determined by Rutherford backscattering spectrometry. Additionally, we provide preliminary estimates for its bandgap energy based on photoluminescence and optical absorption.

8:48AM A5.00005 Transition between two patterns on an Au-deposited Si(111) surface¹, F.K. MEN, A.L. CHIN, C.P. CHANG, Department of Physics, National Chung Cheng University, Chia-Yi 621, Taiwan, — Two distinct patterns have been observed by depositing sub-monolayer Au onto a Si(111)-(7×7) surface with a small miscut angle. Upon depositing Au at 600 °C, we find that a stripe of (5×2) reconstruction forms at the upper step edge in every terrace. For 700 °C deposition, one entire terrace out of several terraces transforms into the (5×2) reconstruction while the other terraces are totally unaffected by the Au deposition. The relative population between the (5×2) and the (7×7) terrace is governed by the amount of deposited Au. After annealing at a temperature above 700 °C the striped (5×2) pattern transforms into the (5×2)-terrace pattern. The similarity between this coarsening of (5×2) reconstruction and the Ostwald ripening of clusters is striking and will be discussed. One application using the (5×2) pattern as a template to grow nanostructure in designated regions will be demonstrated.

¹Work supported by NSC of the Republic of China.

9:00AM A5.00006 Unusual Island Formations of Iridium on Ge(111) Studied by STM¹, MARSHALL VAN ZIJLL, CORY MULLETT, BRET STENGER, EMILIE HUFFMAN, DYLAN LOVINGER, WILLIAM MANN, SHIRLEY CHIANG, UC Davis — We have used scanning tunneling microscopy (STM) to characterize the growth of iridium onto Ge(111). Iridium was deposited onto the Ge(111) c(2×8) surface at different coverages less than 1ML, and the samples were annealed to temperatures between 550K and 750K. A new form of growth was observed, consisting of pathways connecting larger iridium islands. As the annealing temperature increased, the iridium growth first formed unusual shapes with finger-like protrusions. Next, these shapes broke apart into smaller islands, which ultimately formed into larger islands at higher temperatures. High resolution images have been obtained, which allow insight into the atomic arrangements.

¹Funding from NSF CHE-0719504 and NSF PHY-1004848

9:12AM A5.00007 Thickness-dependent Adatom-Adatom Binding Energy on Pb(111): The Effect of Quantum Size Effect on Critical Nucleus¹, MIAO LIU, FENG LIU, University of Utah — We perform first-principles calculations to investigate adatom-adatom binding energies on Pb(111) as a function of film thickness. An odd-even thickness-dependent oscillation is found in the adatom-adatom binding energies, in analogy to the similar behavior in adatom surface binding energies and diffusion barriers found previously. We will discuss these results in relation to the thickness-dependent island nucleation density and compactness, as observed in recent experiments.

¹The work was supported by NSF-DMR 0909212

9:24AM A5.00008 De-wetting of thin films: Analytic theory of cluster coarsening dynamics, ADI CONSTANTINESCU, Asia Pacific Center for Theoretical Physics, Pohang, South Korea, LEONARDO GOLUBOVIC, West Virginia University, ARTEM LEVANDOVSKY, University of California Riverside — Long range de-wetting forces acting across thin films, such as the fundamental van der Waals interactions, may drive the formation of large clusters (tall multi-layer islands) and pits, observed in thin films of soft materials (polymers), as well as in thin films of liquid and solid metals. These long range de-wetting interactions introduce a distinct long lasting early-time scaling behavior characterized by a slow growth of the cluster height/lateral size aspect ratio (i.e., a time-dependent Young angle), and by effective coarsening exponents that depend on cluster size. In this study, we develop an analytic theory capable to calculate these effective size-dependent coarsening exponents characterizing the cluster growth in the early-time cross-over regime. Such a pronounced cross-over behavior has been indeed seen in experiments; however its physical origin has remained elusive to this date. Our results attribute these observed phenomena to ubiquitous long range de-wetting interactions acting across thin films.

9:36AM A5.00009 Surface morphological stabilization of crystalline solids under the simultaneous action of electric, thermal, and mechanical fields, DWAI PAYAN DASGUPTA, GEORGIOS SFYRIS, RAUF GUNGOR, DIMITRIOS MAROUDAS, Department of Chemical Engineering, University of Massachusetts Amherst — We report a detailed analysis of the morphological stability of planar surfaces of electrically and thermally conducting stressed crystalline elastic solids under the simultaneous action of an electric field, an imposed temperature gradient, and uniaxial tension. Our analysis is based on linear stability theory and self-consistent dynamical numerical simulation according to a fully nonlinear model that accounts for curvature- and stress-driven surface diffusion, surface electromigration and thermomigration, as well as surface diffusional anisotropy. Our self-consistent dynamical simulations combine a front tracking method for monitoring surface morphological evolution with Galerkin boundary-integral computations of the displacement and temperature fields and the electrostatic potential. We determine the surface morphological stability domain boundaries and the critical values of the applied electric-field strength and temperature gradient required to stabilize the planar surface morphology. We explore the synergistic or competing effects on the surface morphological response of the simultaneously applied thermal and electric fields, aiming at optimization of the electric-field strength and temperature gradient requirements for planar surface stabilization.

9:48AM A5.00010 Electromigration-driven morphological evolution of monolayer-thick epitaxial islands on substrates, DIMITRIOS MAROUDAS, DWAIPAYAN DASGUPTA, GEORGIOS SFYRIS, Department of Chemical Engineering, University of Massachusetts Amherst — Electromigration-driven dynamics, with and without the simultaneous action of elastic strain, can lead to pattern formation of surface morphological features that may have significant impact on nanofabrication. An important example is epitaxial islands on substrates; for heteroepitaxial islands, misfit strain is induced due to lattice mismatch with the substrate. We develop a fully nonlinear model for the driven morphological evolution of monolayer-thick coherently strained islands on crystalline elastic substrates with diffusional mass transport limited to the island circumference. We carry out self-consistent dynamical simulations of such island dynamics, combining front tracking methods with solutions to the corresponding electrostatic and elastostatic boundary-value problems. We develop a universal scaling theory that explains the simulation results for the dependence of the island migration speed on the island size, electric field, and epitaxial system parameters for isolated, morphologically stable islands. We investigate systematically thermal, elastic, and size effects on the migration and morphological evolution of heteroepitaxial islands. We also find and characterize a variety of stable asymptotic states in the driven dynamical response of such heteroepitaxial islands.

10:00AM A5.00011 Electromigration-driven surface morphological stabilization of coherently strained thin films on elastically deformable substrates, GEORGIOS SFYRIS, RAUF GUNGOR, DIMITRIOS MAROUDAS, Department of Chemical Engineering, University of Massachusetts Amherst — We study the surface morphological stability of a coherently strained thin film grown epitaxially on a substrate and subjected to an external electric field; both infinitely thick and finite-thickness elastic substrates are examined. Due to its lattice mismatch with the substrate material, the film may undergo a Stranski-Krastanow (SK) instability, resulting in formation of islands on the film surface. To examine the morphological stability of the epitaxial film's planar surface state, we conduct a linear stability analysis based on a three-dimensional model of driven surface morphological evolution. We also consider the use of thin compliant substrates, which partly accommodate elastically the lattice-mismatch strain. We find that, regardless of the substrate type, the simultaneous action of a properly applied and sufficiently strong electric field is necessary to stabilize the planar morphology; in such cases, surface electromigration can inhibit SK-type instabilities and control the onset of island formation on the film surface. Our analysis shows that the critical electric-field strength required to stabilize the planar morphology of a thin film on a compliant substrate can be reduced by up to two orders of magnitude compared to that for a conventional thick substrate.

10:12AM A5.00012 Quantum Monte Carlo Study of Surface Energy, CHENG-RONG HSING, CHING-MING WEI, IAMS, Academia Sinica, Taipei 10617, Taiwan — The accuracy of Density Functional Theory (DFT) is based on the exchange-correlation approximation used and needs to be checked by highly accurate quantum many-body approaches. We have performed calculations of the surface energies using the state-of-the-art diffusion quantum Monte Carlo (QMC) method to examine the accuracy of LDA and GGA (PBE) functionals in the study of surface energy. The systems studied include NaCl(100), MgO(100), CaO(100), TiO₂(110), Si(100)-(2x2), C(100)-(2x2), and Ge(100)-(2x2) surfaces. Our results indicate that (i) the surface energy by DMC is always larger than the surface energy by LDA; and (ii) the surface energy by LDA is always larger than the surface energy by GGA. For the surface energies of NaCl(100) and MgO(100), the DMC results reproduce the experimental measured values accurately. To conclude, when compared the surface energies obtained by DFT and DMC, the results predicted by DFT using either LDA or GGA functional are underestimated.

10:24AM A5.00013 Reconstructions of the GaN(10 $\bar{1}\bar{1}$) surfaces: Density functional theory calculations¹, JUNG-MIN HYUN, Sookmyung Women's University, YONG-SUNG KIM, Korea Research Institute of Standards and Science, HANCHUL KIM, Sookmyung Women's University — GaN has been extensively studied for its potential applicability in optoelectronics as well as in spintronics. The functional performance in such applications depends on the surface characteristics of thin films. Thin films of GaN are typically grown along the polar [0001] direction, but their light-emission efficiency is reduced due to the electron-hole separation. A strategy to remedy such an undesired effect is to grow films along nonpolar or semipolar directions. In this presentation, we will address the reconstructions of the Ga-terminated semipolar (10 $\bar{1}\bar{1}$) surface. We performed the density functional theory calculations using the generalized gradient approximation, the projector augmented wave potentials, and the repeated slabs. From the calculated energetics of various reconstructions, we found that there exist a few structural motifs of GaN(10 $\bar{1}\bar{1}$). They are short Ga chains and Ga vacancies. For instance, a 4 × 2 reconstruction with a Ga tetramer and surface Ga vacancies is stable in the N-rich condition, which is significantly different from the previous results [Akiyama *et al.*, Jpn. J. Appl. Phys. 48, 100201 (2009)]. Our results would provide a comprehensive understanding on the Ga-terminated semipolar surfaces.

¹This work was supported by Nano R&D Program through the National Research Foundation of Korea (NRF) (No. 2009-0082490) and by the Strategic Supercomputing Support Program from KISTI (No. KSC-2008-S02-0010).

10:36AM A5.00014 Cross-sectional scanning tunneling microscopy at GaN (10-10), HOLGER EISELE, LENA IVANOVA, Technische Universität Berlin, SVETLANA BORISOVA, Forschungszentrum Juelich GmbH, MARIO DAEHNE, Technische Universität Berlin, PHILIPP EBERT, Forschungszentrum Juelich GmbH — Group-III nitrides are the materials of choice for optoelectronic devices in the green to ultraviolet wavelength range. Recently, the question arose, whether the growth of GaN based devices could be improved by switching from polar surfaces to the non-polar ones. For non-polar GaN surfaces only little is known about the exact energetic positions of surface states, and thus their possible influence on the Fermi level. Furthermore, GaN still suffers from high dislocation densities, far above that of zincblende type III-V semiconductor crystals, which are detrimental for optoelectronic applications of GaN. Therefore we investigated the GaN(10-10) cleavage surface by cross-sectional scanning tunneling microscopy and spectroscopy. We were able to identify the energetic positions of the intrinsic surface states and the Fermi level. We found that both, the filled N-derived and empty Ga-derived dangling bond states are outside the fundamental band gap, the latter one being 0.1–0.2 eV above the conduction band minimum. The observed band gap is 3.4±0.2 eV, in agreement with the nominal value from the bulk. The observed Fermi level pinning of about 1.0 eV below the conduction band edge is attributed to a high defect density at the surface, but not to intrinsic surface states.

10:48AM A5.00015 Geometrical and Electronic structures of Planar and Buckled Silicene on Ag(111), CHUN-LIANG LIN, Department of Advanced Materials Science, The University of Tokyo, RYUICHI ARAFUNE, International Center for Materials Nanoarchitectonics, National Institute for Materials Science, NORIYUKI TSUKAHARA, Department of Advanced Materials Science, The University of Tokyo, KAZUAKI KAWAHARA, Department of Applied Chemistry, The University of Tokyo, NORIAKI TAKAGI, MAKI KAWAI, Department of Advanced Materials Science, The University of Tokyo — Silicene grown on the Ag(111) surface was investigated by scanning tunneling microscopy / spectroscopy (STM / STS). Two atomic arrangements of honeycomb lattice, planar and buckled, were found. The planar silicene is consisted of Si atoms in the same height while the buckled one shows slightly twisted structure in the vertical direction. Compared to the planar silicene, the lateral distance between two neighboring atoms in the buckled silicene is reduced with about 7%. Assuming that there is no change in the length of Si-Si bond, the angle between the Si-Si bond and the axis normal to the surface is 110 degrees, which is close to the bond angle of 109 degrees in the sp³ hybridization. This might suggest that the Si-Si bonding in the buckled silicene is formed mainly by sp³ hybridization rather than sp². However, our STS observations certainly showed a Dirac cone feature at the Fermi level for both types of silicene. Thus, we conclude that the electronic configuration of buckled silicene partially remains in sp² hybridization and the charge carriers still behave as the massless Dirac fermions.

Monday, February 27, 2012 8:00AM - 10:24AM –

Session A6 DMP: Focus Session: van der Waals Bonding in Advanced Materials - Physisorption and Self Assembly on Metals 206B

8:00AM A6.00001 Application of vdW-DF Methods to Hydrogen Adsorptions and an Organic Ferroelectric¹, KYUHO LEE, Rutgers University — In recent years, several schemes have been proposed to include van der Waals (vdW) interactions into the framework of density functional theory (DFT). These offer the potential to extend the scope and usefulness of DFT, allowing applications to an entire new class of sparse materials. For finite systems, we validated our non-empirical van der Waals density functionals (vdW-DFs) with respect to very accurate quantum chemical calculations of the potential energy curves (PECs) for small molecular duplexes [1]. For extended systems, however, typical tests focus on comparisons with a few accessible observations, such as binding energy and bond length [1]. In this talk, we present a third approach in which full PECs from accurate experiments are used for the assessment of vdW methods for extended systems [2]. We calculate the PECs of the H₂ molecule and light atoms on the (100), (110), and (111) surfaces of Cu. The gas-surface-scattering experiments provide the rich data bank that covers results for the whole shape of the physisorption potentials. We also present an application of vdW-DF2 to an organic ferroelectric, phenazine-chloranilic acid [3]. In spite of extensive experimental efforts to characterize this rare organic material, the origin of the long-range order is unclear and even the ground state structure is not completely determined yet. We study its structure, energetics, ferroelectric properties, structural instability, and the proton-transfer process in it in comparison with PBE results and experiments wherever possible.

[1] K. Lee, E. Murray, L. Kong, B. I. Lundqvist, and D. C. Langreth, *Phys. Rev. B* **82**, 081101 (2010).

[2] K. Lee, A. K. Kelkkanen, K. Berland, S. Andersson, D. C. Langreth, E. Schröder, B. I. Lundqvist, and P. Hyldgaard, *Phys. Rev. B* **84**, 193408 (2011).

[3] K. Lee, B. Kolb, T. Thonhauser, D. C. Langreth, and D. Vanderbilt, *in preparation*.

¹This work was supported by National Science Foundation Grant No. DMR-0801343.

8:36AM A6.00002 Structure and Energetics of Benzene Adsorbed on Transition-Metal Surfaces: Density-Functional Theory with Screened van der Waals Interactions, WEI LIU, VICTOR G. RUIZ-LÓPEZ, GUO-XU ZHANG, XINGUO REN, MATTHIAS SCHEFFLER, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG, Berlin, Germany — The adsorption of benzene on metal surfaces is an important benchmark system for more complex hybrid inorganic/organic interfaces. Here, the recently developed DFT+vdW^{surf} method (density-functional theory including screened van der Waals (vdW) interactions) [1] is used to study the structure and energetics of benzene on transition-metal surfaces (Cu, Ag, Au, Pd, Pt, Rh, and Ir). Benzene adsorbs in a planar configuration at coinage metal surfaces, with almost zero distortion and a flat potential-energy surface. In contrast, benzene is strongly bound to the (111) surface of Pd, Pt, Rh, and Ir, and located at the bridge-30° site. The vdW interactions significantly enhance the binding energy by more than 0.75 eV for all metals. The screening of the vdW energy plays a critical role in coinage metals, shortening the equilibrium distance by 0.2 Å, and lowering the binding energy by 0.25 eV. The validity of our results is confirmed by comparison with calculations using the random-phase approximation including renormalized single excitations (EX+cRPA+rSE scheme [2]), and the experimental data from temperature-programmed desorption and calorimetry measurements. [1] V. G. Ruiz-López et al., submitted. [2] X. Ren et al., *Phys. Rev. Lett.* **106**, 153003 (2011).

8:48AM A6.00003 Physisorption of three amine terminated molecules (TMBDA, BDA, TF-BDA) on the Au(111) Surface: The Role of van der Waals Interaction¹, MARAL AMINPOUR, DUY LE, TALAT S. RAHMAN, Department of Physics, University of Central Florida — Recently, the electronic properties and alignment of tetramethyl-1,4-benzenediamine (TMBDA), 1,4-benzenediamine (BDA) and tetrafluoro-1,4-benzenediamine (TFBDA) molecules were studied experimentally. Discrepancies were found for both the binding energy and the molecule tilt angle with respect to the surface, when results were compared with density functional theory calculations [1]. We have included the effect of vdW interactions both between the molecules and the Au(111) surface and find binding energies which are in very good agreement with experiments. We also find that at low coverages each of these molecules would adsorb almost parallel to the surface. N-Au bond lengths and charge redistribution on adsorption of the molecules are also analyzed. Our calculations are based on DFT using vdW-DF exchange correlation functionals. For BDA (since we are aware of experimental data), we show that for higher coverage, inclusion of intermolecular van der Waals interaction leads to tilting of the molecules with respect to the surface and formation of line structures. Our results demonstrate the central role played by intermolecular interaction in pattern formation on this surface.

[1] M. Dell'Angela et al, *Nano Lett.* **2010**, **10**, 2470; M. Kamenetska et al, *J. Phys. Chem. C*, **2011**, **115**, 12625

¹The work is supported by DOE under Grant No. DE-FG02-07ER15842

9:00AM A6.00004 Effect of physisorbed molecules and an external external fields on the metallic Shockley surface state of Cu(111): A density functional theory study¹, KRISTIAN BERLAND, Chalmers University of Technology, T.L. EINSTEIN, University of Maryland, PER HYLDGAARD, Chalmers University of Technology — To manipulate the Cu(111) partially-filled Shockley surface state, we study its response to an external field² E and physisorbed PAHs and quinone molecules. We use density-functional theory calculations with periodic-boundary conditions. The van der Waals density functional version vdW-DF2 accounts for the molecular adsorption. The issue that the Kohn-Sham wave functions couple to both sides of the Cu slab is handled with a decoupling scheme based on a rotation in Hilbert space. A convergence study reveals that to obtain a proper Shockley surface state, 6 Cu layers is sufficient, while 15 is optimal. We use 6 layers for the response to the molecules and 15 to external field. We find that the surface state displays isotropic dispersion (up to order k^6), free-electron like until the Fermi wave vector but with a significant quartic component beyond. The shift in band minimum and effective mass depend linearly on E , with a smaller fractional change in the latter. Charge transfer occurs beyond the outermost copper atoms, and most of the screening is due to bulk electrons. We find that the molecular physisorption increases the band minimum, with the effect the of a quinone being much stronger than the corresponding PAH.

¹Supported by (KB and PH) Swedish Vetenskapsrådet VR 621-2008-4346 and (TLE) NSF CHE 07-50334 and UMD MRSEC DMR 05-20471.

²KB, TLE, PH; arXiv 1109:6706

9:12AM A6.00005 Computational Study of Supramolecular Self-Assembly Using CH/ π Bonds

, C. HAN, CHIPS, NCSU, Q. LI, S. HORTON, M. FUENTES-CABRERA, B. SUMPTER, CNMS, ORNL, W. LU, J. BERNHOLC, CHIPS, NCSU, P. MAKSY-MOVYCH, M. PAN, CNMS, ORNL — Self assembly is an important research area in supramolecular engineering. We show that CH/ π bonds can be exploited as a vehicle to assemble clusters of well-defined sizes on metal surfaces. Specifically, we theoretically explain the observations of largely uniform distribution of phenylacetylene magic clusters, each consisting of six molecules, on Au(111) surfaces. Using density functional theory with a van der Waals functional, we discuss the reasons for the preference of the hexamer structure, the key effect of CH/ π bonding on the self-assembly, and the critical role of the metal surface. Our calculated STM images and electronic properties are in good agreement with experiment. The cooperative, multi-center CH/ π interactions offer an attractive tunability via chemical functionalization, and thus may provide a new avenue towards rationally designing a desired supramolecular shape and size.

9:24AM A6.00006 Noble Gases on Metal Surfaces: New Insights on Adsorption Site Preference

, DE-LI CHEN, WISSAM AL-SAIDI, KARL JOHNSON, University of Pittsburgh — Experiments have previously found that noble gases (Kr, Xe) adsorb on low-coordination atop sites on several different metal surfaces, rather than on high-coordination hollow sites. This unexpected preference for low-coordination sites has been previously ascribed to reduced Pauli repulsion mostly due to exchange energy at the atop site, based on density functional theory calculations within the local density approximation (LDA). In contrast, our calculations using non-local van der Waals (vdW-DF) density functional show that site preference is due to a delicate balance between the electrostatics which favor the hollow site and kinetic energy which favors the atop site; exchange-correlation energies has a very little role. Moreover, we find, using LDA, GGA, and vdW-DF functionals, that the hollow site is a saddle point of index 1 or 2 on the 2-dimensional potential energy surface, while the atop site is the only true minimum. Therefore, the reason that hollow site occupation is not observed is that it is a transition state and so has a very short life-time. Our results show that the inclusion of non-local vdW interactions is crucial for obtaining results in quantitative agreement with experiments for adsorption energies, equilibrium distances, and vibrational energies.

9:36AM A6.00007 Adsorption of polyvinylpyrrolidone on Ag surfaces: Insight into the workings of a structure-directing agent¹

, WISSAM AL-SAIDI, University of Pittsburgh, HAIJUN FENG, KRISTEN FICHTHORN, The Pennsylvania State University — We use density-functional theory to resolve the role of polyvinylpyrrolidone (PVP) as a structure-directing agent in the shape-selective synthesis of Ag nanostructures. We identify several different binding states for PVP segments on Ag(100) and Ag(111) and find an energetic preference for Ag(100), which arises from a surface-sensitive balance between direct binding and van der Waals attraction. At the chain level, correlated segment binding leads to a strong preference for PVP bind to Ag(100). Our study underscores differences between small-molecule and polymeric structure-directing agents.

¹This work was funded by the Department of Energy, Office of Basic Energy Sciences, Materials Science Division, grant number DE-FG02-07ER46414

9:48AM A6.00008 Adsorption of halogenated molecule on stepped metallic surfaces: the role of van der Waals interactions

, RENGIN PEKOZ, KAREN JOHNSTON, DAVIDE DONADIO, Max Planck Institute for Polymer Research — The deposition of halogenated aromatic molecules on metallic surfaces is the first step for the bottom-up fabrication of atomically precise graphene nanoribbons [1]. Interest in the binding properties in this type of systems and in general in organic/inorganic interfaces has stimulated the inclusion of van der Waals (vdw) interactions within density functional theory (DFT). Using a fully non-local Van der Waals density functional (vdW-DF) [2,3] we have studied the adsorption of dichlorobenzene on stepped Au(332) and Pt(332) surfaces and on flat (111) surfaces. For several different adsorption sites, the energies, and equilibrium geometries have been computed, and electron density analysis has been performed using both conventional generalized gradient approximation (GGA) and vdW-DF. The two approaches yield qualitatively different results, highlighting the importance of non-local dispersions in this class of systems. The non-trivial role of steps edges on adsorption energies and geometries is also elucidated. [1] J. Cai *et al.*, Nature 466, 470 (2010). [2] M. Dion *et al.*, Phys. Rev. Lett. 92, 246401 (2004). [3] A. Gulans *et al.* Phys. Rev. B 79, 201105 (2009).

10:00AM A6.00009 The Nature of Binding in the Phenalenyl Dimer and its Derivatives

, BRIAN KOLB, TIMO THONHAUSER, Wake Forest University, MIKLOS KERTESZ, Georgetown University — The biradical phenalenyl π -dimer and its derivatives have attracted interest recently because of their potentially useful electrical, optical, and magnetic properties. These properties can be tuned by adjusting the binding characteristics between the monomers within the dimer. Typically, this is done by substituting electron withdrawing or donating groups onto the α or β -site carbons. An understanding of this binding lies at the heart of useful application of these materials. In this work, the binding characteristics of phenalenyl dimers were investigated using density functional theory. In particular, the vdW-DF functional was used to explore the role of van der Waals interactions in the binding within this system. A comparison of the binding curves with those of the closed shell derivatives wherein the central carbons have been replaced by either nitrogen or boron sheds light into the nature of the interactions between the monomers.

10:12AM A6.00010 Binding nature of adenine and C60 on graphene: a van der Waals density functional analysis¹

, PER HYLDGAARD, KRISTIAN BERLAND, Chalmers University of Technology, VALENTINO COOPER, Oak Ridge National Laboratory, ANDERS BERGVALL, SERGEY KUBATKIN, TOMAS LÖFWANDER, ELSEBETH SCHRÖDER, Chalmers University of Technology — Based on van der Waals density functional theory (using vdW-DF1 and vdW-DF2), we study and analyze the adsorption of adenine² and C60³ on graphene. Understanding molecular binding on graphene helps development of functionals because the infinite graphene shifts the balance between short-range and long-range contributions to binding as compared dimers or molecular crystals. The potential of graphene as contacts in single-molecule electronics also motivates the study of the interaction between aromatic molecules and graphene; the binding separation affects the magnitude of hopping parameters. We present results on binding energy and separation, vibrational states, overlays, and charge transfer. We find that the hexagonal ring in C60 binds closer to the graphene sheet than what a flat molecule such as adenine does. The role played by the difference in geometry between the flat (adenine) and spherical (C60) shape is discussed.

¹Support from Vetenskapsrådet

²K. Berland *et al.*; J. Phys.: Condens. Matter 23 135001 (2001)

³A. Bergvall *et al.*; Phys. Rev. B 84, 155451 (2011)

Monday, February 27, 2012 8:00AM - 11:00AM –

Session A7 DMP DCOMP: Focus Session: Computational Design of Materials - Structure Prediction 207

8:00AM A7.00001 Crystal structure prediction: a novel approach based on minima hopping, MAXIMILIAN AMSLER, STEFAN GOEDECKER, University of Basel — With increasing computational resources the prediction of crystal structures from first principle calculations has become feasible, but still remains a demanding task. A reliable method to perform an efficient, systematic search for the ground state structure based solely on the system's composition is essential. Motivated by the promising results of the minima hopping method obtained on isolated systems, we have generalized the algorithm for crystal structure prediction. Optimized moves in the configurational space spanned by both atomic coordinates and simulation cell variables are performed to escape from local enthalpy minima, and revisiting known minima is avoided, thus allowing a fast exploration of the enthalpy surface. The predictive power of the novel method has been shown in several applications, of which the following will be presented. Superconducting phases in hydrogen rich materials were investigated, leading to the discovery of novel ground state structures. For the longstanding question of the crystal structure of cold compressed graphite a new candidate phase could be identified to perfectly match experimental results. And at last, new low energy structures for materials with possible applications in hydrogen storage are presented.

8:12AM A7.00002 Adaptive Genetic Algorithm method for Crystal Structure Prediction and Materials Discovery¹, CAI-ZHUANG WANG, MIN JI, SHUNQING WU, Ames Laboratory, Iowa State U, Ames, Iowa 50011, KOICHIRO UMEMOTO, U of Minnesota and Ames Laboratory, Iowa State U, RENATA WENTZCOVITCH, Univ of Minnesota, KAI-MING HO, Ames Laboratory, Iowa State U, Ames, Iowa 50011, AMES TEAM², MINNESOTA TEAM³ — We developed a fast and efficient method for crystal structure prediction and materials discovery. The method is based on the cut-and-paste genetic algorithm (GA) scheme introduced by Deaven and Ho [1]. In the evaluation of energies of target structures, first-principles calculations are accurate but time-consuming. Our method performs GA searches uses auxiliary model potentials to screen the energy of candidate structures, selecting only a few for more extensive first principles evaluation. Parameters of the auxiliary potentials are adaptively adjusted to reproduce the first-principles results during the course of the GA search. Our method combines the speed of empirical potential searches with the accuracy of first principles calculations. We will present results on applications to various systems including metallic alloys and ultrahigh pressure SiO₂, H₂O and Mg-Si-O systems.

[1] D. M. Deaven, K. M. Ho, Phys. Rev. Lett. 75, 288 (1995).

¹USDOE BES

²Min Ji, Shunqing Wu, Koichiro Umemoto, Cai-Zhuang Wang, Kai-Ming Ho

³Koichiro Umemoto, Renata Wentzcovitch

8:24AM A7.00003 Periodic structure optimization via local heat pulse-quench cycles employing the GULP code, ARNULF MÖBIUS, Institute for Theoretical Solid State Physics, IFW, Dresden, Germany, J. CHRISTIAN SCHÖN, Max Planck Institute for Solid State Research, Stuttgart, Germany — We present an optimization algorithm for problems with many continuous degrees of freedom and a huge number of local minima. It is based on the thermal cycling approach, originally developed for combinatorial optimization tasks [1]. The main idea is to cyclically disturb a few randomly chosen degrees of freedom of the current best local minimum and to quench this state by a highly efficient local search code. As the optimization proceeds, the amplitude of the disturbance slowly decreases. This approach is applied to a lattice structure prediction problem. We use the general utility lattice program (GULP) by J.D. Gale and co-workers [2] for local search. As test, the hypothetical periodic Mg₁₀Al₄Ge₂Si₈O₃₆ compound is studied, where both the cell parameters and the atom positions are free to vary. The results demonstrate that the proposed procedure is robust and far more efficient than the previous approaches to this problem by means of multi-start local search, simulated annealing, and evolutionary algorithms in Ref. 3.

[1] A. Möbius et al., Phys. Rev. Lett. 79 (1997) 4297.

[2] J.D. Gale and A.L. Rohl, Mol. Simul. 29 (2003) 291.

[3] A.R. Oganov et al., in "Modern Methods of Crystal Structure Prediction," ed. A.R. Oganov, (Wiley, 2011), p. 223.

8:36AM A7.00004 Mapping the Materials Genome through Combinatorial Informatics, KRISHNA RAJAN, Iowa State University — The recently announced White House Materials Genome Initiative provides an exciting challenge to the materials science community. To meet that challenge one needs to address a critical question, namely *what* is the materials genome? Some guide on how to the answer this question can be gained by recognizing that a "gene" is a carrier of information. In the biological sciences, discovering how to manipulate these genes has generated exciting discoveries in fundamental molecular biology as well as significant advances in biotechnology. Scaling that up to molecular, cellular length scales and beyond, has spawned from genomics, fields such as proteomics, metabolomics and essentially systems biology. The "omics" approach requires that one needs to discover and track these "carriers of information" and then correlate that information to predict behavior. A similar challenge lies in materials science, where there is a diverse array of modalities of materials "discovery" ranging from new materials chemistries and molecular arrangements with novel properties, to the development and design of new micro- and mesoscale structures. Hence to meaningfully adapt the spirit of "genomics" style research in materials science, we need to first identify and map the "genes" across different materials science applications. On the experimental side, combinatorial experiments have opened a new approach to generate data in a high throughput manner, but without a clear way to link that to models, the full value of that data is not realized. Hence along with experimental and computational materials science, we need to add a "third leg" to our toolkit to make the "Materials Genome" a reality, the science of Materials Informatics. In this presentation we provide an overview of how information science coupled to materials science can in fact achieve the goal of mapping the "Materials Genome".

9:12AM A7.00005 Diamondlike carbo-boride C5B compound? Testing crystal structures and stability with Global Space Group Optimization (GSGO)¹, ARKADIY MIKHAYLUSHKIN, National Renewable Energy Laboratory, USA, XIUWEN ZHANG, Colorado School of Mines, Golden, USA, ALEX ZUNGER, University of Colorado, Boulder, USA — Diamond-like C5B has been alleged to be a new exciting material discovered at high pressures and temperatures. Using density-functional based evolutionary Global Space Group Optimization (GSGO) we established the likely structures of BC3 and BC5 phases and the known B4C compound. Examining the ground state line between solid Carbon and solid Boron we find only B4C is a ground state structure. C5B and C3B are high energy structure at high pressure. The reaction between BC3 and solid carbon producing C5B is found to have a positive reaction enthalpy that depends only weakly on pressure. In contrast to the previous reports, we argue that at 0 T the BC5 is less stable than BC3 in access of carbon. However, a small positive enthalpy of the reaction BC5 → BC3 + 2C cannot rule out formation of the BC5 from the BC3 precursor material as thermally stabilized due to vibrational entropy or/and disorder effects.

¹This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Energy Frontier Research Centers.

9:24AM A7.00006 Hands-free thermodynamic alloy modeling of ~700 binary alloys using a Bayesian approach: Part I, GUS HART, LANCE J. NELSON, Brigham Young University, STEFANO CURTAROLO, Duke University, C. SHANE REESE, Brigham Young University — Bayesian approaches have become useful in recent years as increasing computing power has made them practical. Bayes rule itself is nothing more than a simple statement of conditional probability but can be used to make strong inferences. We discuss the general idea behind Bayes rule and how to use it to build physical models. Using a database of about 150,000 first principle calculations, we are building models for ~700 binary alloys.

9:36AM A7.00007 Hands-free thermodynamic alloy modeling of ~700 binary alloys using a Bayesian approach: Part II, LANCE J. NELSON, Brigham Young University, STEFANO CURTAROLO, Duke University, C. SHANE REESE, GUS L.W. HART, Brigham Young University — In recent years, Bayesian statistics has become more popular as a scientific tool. This is mainly due to advances in computing power, which make the Bayesian formalism tractable. Baye's rule, which is a simple statement of conditional probability, is the foundation for Bayesian statistics. When used in conjunction with sampling algorithms, such as Metropolis-Hastings and Gibbs, Baye's rule provides a powerful framework for characterizing important parameters and for making inference. We demonstrate how the Bayesian framework can be applied to alloy modeling, providing the solution to several typical problem areas in this field. Together with our large database of first-principles data this Bayesian framework helps us quickly and accurately characterize hundreds of binary alloys.

9:48AM A7.00008 Sorting stable from unstable hypothetical compounds and determining the electronic structure of interesting candidates : The case of Half-Heusler Filled Tetrahedral ABX structures¹, XIUWEN ZHANG, Colorado School of Mines, Golden, CO 80401, LIPING YU, ANDRIY ZAKUTAYEV, DAVID GINLEY, National Renewable Energy Lab., Golden, CO 80401, ALEX ZUNGER, University of Colorado, Boulder, CO 80305 — Electronic structure theory has recently been used to propose hypothetical compounds, seeking new useful functional materials. In some cases, such hypothetical compounds in presumed crystal structures may be significantly higher in energy than (i) their lowest-energy structures or, than (ii) a combination of their constituents. We use the first-principles thermodynamics to sort (i) the lowest-energy structure and (ii) the thermodynamic stability with respect to disproportionation of the 488 unreported ABX octet compounds. We find that as many as 235 of the 488 are unstable with respect to decomposition, whereas other 235 of the unreported compounds are predicted to be thermodynamically stable. (18 materials are too close to call). The electronic structures of these predicted stable compounds are evaluated based on GW approximation for electron's self-energy. To support the theoretical predictions of new materials, thin film samples of AgYGe were synthesized using combinatorial Pulsed Laser Deposition. AgYSi-type ground state crystal structure and Y-rich composition stability range of AgYGe agree well with theory.

¹This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Energy Frontier Research Centers and REMRSEC at Colorado School of Mines.

10:00AM A7.00009 Band-structure predictions for A2BX4 discovery compounds¹, STEPHAN LANY, V. STEVANOVIC, National Renewable Energy Lab., Golden, CO, A. ZUNGER, University of Colorado at Boulder, CO — The inverse design of materials requires to predict the existence and the properties of previously unknown materials. We have performed a computational search for thermodynamically stable materials within the family of A2BX4 compounds (A, B = main group and 3d cations; X = O, S, Se, Te) resulting in the theoretical discovery of about 100 previously unreported compounds. The challenge for the prediction of band-structures and optical spectra is to obtain accurate results for a wide range of materials within a single computational scheme, so that unknown materials can be predicted with confidence. Whereas the main group chalcogenides are rather accurately predicted by many-body GW calculations, large deviations from experiment are observed for many 3d oxides. In particular, we find that the 3d orbitals consistently occur at too high energies, independent on whether they are occupied (e.g., Cu2O) or unoccupied (e.g., TiO2). While the exact nature of these issues are under investigation, we pursue here a pragmatic approach, using attractive on-site potentials with a single parameter for each 3d element, which leads to good agreement with experiment for binary and ternary 3d oxides. We use this approach to predict the band-structures of the discovery compounds.

¹Supported by the US Department of Energy, Office of Basic Energy Sciences, as part of an Energy Frontier Research Center.

10:12AM A7.00010 New Crystal Structures Identified for PtO and PtO₂ using Density Functional Theory Calculations¹, JUAREZ L.F. DA SILVA, RICARDO K. NOMIYAMA, University of Sao Paulo, MAURICIO J. PIOTROWSKI, Federal University of Santa Maria — Platinum plays an important role in catalysis and electrochemistry, and it has been known that the direct interaction of oxygen with Pt surfaces can lead to the formation of platinum oxides (PtO_x), which can affects the reactivity. To contribute to the atomistic understanding of the atomic structure of PtO_x, we report a density functional theory study of the atomic structure of bulk PtO_x ($1 \leq x \leq 2$). From our calculations, we identified a lowest energy structure (GeS-type, space group *Pnma*) for PtO, which is 0.181 eV lower in energy than the structure suggested by Moore and Pauling (PtS-type). Furthermore, two atomic structures were identified for PtO₂, which are almost degenerate in energy with the lowest energy structure reported so far for PtO₂ (CaCl₂-type). Based on our results and analysis, we suggest that Pt and O atoms tends to form octahedron motifs in PtO_x even at lower O composition by the formation of Pt–Pt bonds.

¹We thank FAPESP (Sao Paulo Science Foundation) for support.

10:24AM A7.00011 Simulation of structural and electronic properties of amorphous tungsten oxycarbides, KALIAPPAN MUTHUKUMAR, HARALD O. JESCHKE, ROSER VALENTI, Institut fuer Theoretische Physik, Goethe-Universitaet Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — Electron beam induced deposition with tungsten hexacarbonyl W(CO)₆ as precursors leads to granular deposits with varying compositions of tungsten, carbon and oxygen. Depending on the deposition conditions, the deposits are insulating or metallic. We employ an evolutionary algorithm to predict the crystal structures starting from a series of chemical compositions that were determined experimentally. We show that this method leads to better structures than structural relaxation based on guessed initial structures. We approximate the expected amorphous structures by reasonably large unit cells that can accommodate local structural environments that resemble the true amorphous structure. Our predicted structures show an insulator to metal transition close to the experimental composition at which this transition is actually observed. Our predicted structures also allow comparison to experimental electron diffraction patterns.

10:36AM A7.00012 Predicting Two-Dimensional Boron-Carbon Compounds by the Global Optimization Method, XINYU LUO, JIHUI YANG, XINGAO GONG, HONGJUN XIANG, Fudan University, HANYU LIU, Jilin University, YANCHAO WANG, Jilin Univ, YANMING MA, Jilin University, CCMG, FUDAN UNIVERSITY TEAM, JILIN UNIVERSITY COLLABORATION — We adopt a global optimization method to predict two-dimensional (2D) nanostructures through the particle-swarm optimization (PSO) algorithm. By performing PSO simulations, we predict new stable structures of 2D boron-carbon (B-C) compounds for a wide range of boron concentrations. Our calculations show that: (1) All 2D B-C compounds are metallic except for BC₃ which is a magic case where the isolation of carbon six-membered ring by boron atoms results in a semi-conducting behavior. (2) For C-rich B-C compounds, the most stable 2D structures can be viewed as boron doped graphene structures, where boron atoms typically form 1D zigzag chains except for BC₃ in which boron atoms are uniformly distributed. (3) The most stable 2D structure of BC has alternative carbon and boron ribbons with strong in-between B-C bonds, which possesses a high thermal stability above 2000 K.

10:48AM A7.00013 Quantum confined Schottky barriers: Tuning the Schottky-Mott and Bardeen Limits, JAMES CHELIKOWSKY, TZU-LIANG CHAN, University of Texas at Austin, KAI-MING HO, Iowa State University and Ames Laboratory, CAI-ZHUANG WANG, Ames Laboratory, SHENGBAI ZHANG, Rensselaer Polytechnic Institute — Even though metal-semiconductor junctions are an essential component in electronic devices, an atomistic understanding of the electronic structure of such junctions has remained elusive. Hundreds, if not thousands, of atoms may be required to model such interfaces, owing to lattice mismatches at the interface. The absence of a detailed understanding of the interface structure has inhibited the application of electronic structure calculations to examine the evolution of Fermi level pinning. Here we capitalize on recent computational breakthroughs and apply them to a prototypical system: a Pb(111) film on a Si(111) substrate. We consider up to 1,500 atoms in our first principle calculations based on real space pseudopotentials, and explicitly model the atomistic details of the metal-semiconductor interface. We propose a pinning mechanism for the Fermi level that depends critically on the role of quantum confinement in the overlying metallic film. By changing the thickness of the overlying film, the pinning mechanism can be tuned from the abrupt interface description of Schottky and Mott to the metal induced gap state description of Bardeen.

Monday, February 27, 2012 8:00AM - 10:48AM — Session A8 DMP GMAG: Focus Session: Frustrated Magnetism - Triangular Lattice 208

8:00AM A8.00001 Spin Correlations in the quasi-triangular magnet, $\text{Cu}_2(\text{OH})_3\text{NO}_3$, JASON S. GARDNER, Indiana University, GEORG EHLERS, SNS, Oak Ridge National Laboratory, FLETCHER WERNER, S.A. SOLIN, Washington U in St. Louis — We have investigated the structural and magnetic properties of the spin $S = 1/2$ antiferromagnetic quasi-triangular lattice materials: $\text{Cu}_{2(1-x)}\text{Zn}_{2x}(\text{OH})_3\text{NO}_3$ ($0 < x < 0.65$) using a.c. susceptibility, heat capacity [1,2] and neutron scattering. After a brief introduction to the bulk properties of this family of materials, we will discuss recent inelastic neutron scattering results from the pure and doped materials. The temperature dependence of the quasielastic scattering reveals an abundance of slow spin dynamics at elevated temperatures. This scattering collapses as the system is cooled through its ordering temperature (11 K) and a Q-independent mode is observed at finite energy. These results will be compared to those seen in other triangular systems with a Kagome motif.

- [1] J. Wu, J.S. Wildeboer, F. Werner, A. Seidel, Z. Nussinov, and S.A. Solin, Europhysics Letters, **93**, 67001 (2011).
- [2] J. Wu, A. K. Gangopadhyay, P. Kanjanaboos and S. A. Solin, J. Phys.: Condens. Matter **22**, 334211 – 334222 (2010).

8:12AM A8.00002 Optical spectroscopy of the Triangular Lattice Antiferromagnets CuCrO_2 and $\alpha\text{-CaCr}_2\text{O}_4$, MICHAEL SCHMIDT, ZHE WANG, F. MAYR, Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany, S. TOTH, B. LAKE, A.T.M.N. ISLAM, Helmholtz-Zentrum Berlin fuer Materialien und Energie, D-14109 Berlin, Germany, V. TSURKAN, A. LOIDL, J. DEISENHOFER, Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — We will compare and discuss our results obtained by optical spectroscopy on CuCrO_2 and $\alpha\text{-CaCr}_2\text{O}_4$. While CuCrO_2 is famous for its multiferroicity [1], in $\alpha\text{-CaCr}_2\text{O}_4$ a polarization can only be observed under the application of electric or magnetic field, despite having a closely related structure [2]. At near infrared and visible light frequencies we observe Cr^{3+} crystal field absorptions and below T_N excitons and exciton-magnon-transitions appear. The width of these exciton-magnon transitions is analyzed with respect to the existence of Z_2 vortices as proposed by Kojima et al. [3].

- [1] S. Seki et al., Phys. Rev. Lett. 101, 067240 (2008)
- [2] K. Singh et al., Phys. Rev. B 84, 064129 (2011)
- [3] N. Kojima et al., J. Phys. Soc. Jpn. 62, 4137 (1993)

8:24AM A8.00003 Quantum Spin Fluctuations for an Incommensurate Spiral, RANDY FISHMAN, Oak Ridge National Laboratory, Oak Ridge, TN 37831 USA — Quantum spin fluctuations are investigated for the incommensurate spiral state of a geometrically-frustrated triangular-lattice antiferromagnet. With increasing anisotropy, the average spin amplitude becomes larger but the spiral becomes more distorted. Quantum fluctuations enhance both the wavevector of the distorted spiral and the critical anisotropy above which it undergoes a first-order transition into a collinear state. An experimental technique is proposed to isolate the effects of quantum fluctuations from the classical distortion of the spiral. Results of this work are used to estimate the change in spin amplitude and ellipticity in the multiferroic state of CuFeO_2 . Research sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy under contract with UT-Battelle, LLC.

8:36AM A8.00004 Phase Diagram of the Spatially Anisotropic Heisenberg Model on a Triangular Lattice, SEDIGH GHAMARI, CATHERINE KALLIN, Dept. of Physics and Astronomy, McMaster University, SUNG-SIK LEE, Dept. of Physics and Astronomy, McMaster University and Perimeter Institute for Theoretical Physics, ERIK SORENSEN, Dept. of Physics and Astronomy, McMaster University — The spatially anisotropic spin-1/2 Heisenberg model on a triangular lattice is examined using a renormalization group (RG) analysis in the limit of weak interchain coupling ($J'/J \ll 1$ or large anisotropy). In agreement with a previous similar study, a collinear antiferromagnetic (CAF) state is found for large anisotropies. Retaining a marginal term that was not previously included, elucidates the strong competition between spiral and CAF order and suggests a direct transition at a fairly large anisotropy to incommensurate spiral order with a significantly renormalized wave vector that smoothly connects to the commensurate spiral state at the isotropic point. The significant renormalization of the ordering vector of this incommensurate spiral phase is argued to explain why many numerical studies found spin liquid behavior close to the isotropic point, (i.e. $J'/J \sim 0.85$). The agreement between the predictions of our RG analysis for the correlation function of the staggered magnetization on next-nearest-neighbor chains with DMRG results for small anisotropies further supports this picture. Finally, the effect on the phase diagram of Dzyaloshinskii-Moriya interactions, relevant to Cs_2CuCl_4 , will be discussed.

8:48AM A8.00005 Variational Monte Carlo study of quantum spin=1 liquid phases in the extended triangular-lattice Heisenberg model, SAMUEL BIERI, MAKSYM SERBYN, TODADRI SENTHIL, PATRICK LEE, Massachusetts Institute of Technology — Recent experiments in the compound $\text{Ba}_3\text{NiSb}_2\text{O}_9$ [PRL 107, 197204] indicated that quantum-spin liquid phases in a spin $S=1$ anti-ferromagnet may exist. Motivated by these experiments, we construct quantum spin=1 liquid states with three flavors of fermionic spinons. We use variational Monte Carlo calculations to investigate the phase diagram of a triangular-lattice quantum Heisenberg model with single-ion anisotropy, bi-quadratic, and ring-exchange terms. We compare the energies of the spin-liquid states with conventional magnetically ordered states. We find that in some parameter ranges, an exotic gapless $U(1)$ spin liquid is stabilized. In other parameter ranges, a BCS pairing instability with unconventional symmetry gaps out some of the spinons. We discuss our findings in relation with present and future experiments.

9:00AM A8.00006 Magnetic Structure and Spin Waves in $\text{Co}_2(\text{OD})_3\text{Cl}$, SACHITH DISSANAYAKE, S. JI, Department of Physics, University of Virginia, C. CHAN, T.K. NG, Department of Physics, Hong Kong University of Science and Technology, J. LEE, Department of Physics, University of Virginia, Y. QIU, NIST Center for Neutron Research, K.C. RULE, B. LAKE, Helmholtz Zentrum Berlin, M. GREEN, NIST Center for Neutron Research, X.G. ZHENG, Department of Physics, Saga University, S.-H. LEE, Department of Physics, University of Virginia — We have examined the magnetic structure of $\text{Co}_2(\text{OD})_3\text{Cl}$ with magnetic Co^{2+} ($3d^7$; $s=3/2$) ions using neutron powder diffraction data. Magnetic structure that yields the best refinement factor is an “umbrella”-type antiferromagnetic structure with ab-components of magnetic moments in the kagome plane forming a $q=0$ 120° structure and the moments are canted out of the plane by $\sim 40^\circ$. The magnetic moments in the triangular plane are aligned ferromagnetically along the c-axis. We have performed linear spin wave calculations considering the nearest neighbor interactions J within the kagome plane and J_F between the kagome and the triangular plane. The effects of J_F/J and the canting angle to the spin wave dispersion was studied thoroughly, to find out an effective spin hamiltonian that explains our inelastic neutron scattering data with two prominent excitation modes centered at 3 meV and 19 meV. Single ion-type anisotropy was also included in the spin hamiltonian to study its effect to the spin wave excitation.

9:12AM A8.00007 Partially disordered state and spin-lattice coupling in an $S=3/2$ triangular lattice antiferromagnet Ag_2CrO_2 , M. MATSUDA, Quantum Condensed Matter Division, Oak Ridge National Laboratory, H. YOSHIDA, M. ISOBE, National Institute for Materials Science (NIMS), Tsukuba, Japan, C. DE LA CRUZ, Quantum Condensed Matter Division, Oak Ridge National Laboratory, R.S. FISHMAN, Materials Science and Technology Division, Oak Ridge National Laboratory — Ag_2CrO_2 consists of triangular lattice planes of CrO_2 , which are well separated by the metallic Ag_2 layers. [1] This compound is an $S=3/2$ frustrated triangular lattice antiferromagnet without orbital degree of freedom. We performed neutron diffraction experiments on a powder sample of Ag_2CrO_2 on a neutron powder diffractometer HB-2A and a triple-axis neutron spectrometer HB-1, installed at HFIR in Oak Ridge National Laboratory. With decreasing temperature, a short-range 4-sublattice spin state develops. However, a long-range partially disordered state with 5 sublattices abruptly appears at $T_N=24$ K, accompanied by a structural distortion, and persists at least down to 2 K. The spin-lattice coupling stabilizes the anomalous state, which is expected to appear only in limited ranges of further-neighbor interactions and temperature. It was found that the spin-lattice coupling is a common feature in triangular lattice antiferromagnets with multiple-sublattice spin states, since the triangular lattice is elastic.

[1] H. Yoshida *et al.*, to appear in J. Phys. Soc. Jpn.

9:24AM A8.00008 Quantum Critical Magnetization Behaviors of the Kagome- and Triangular-Lattice Antiferromagnets, TORU SAKAI, JAEA, Spring-8, HIROKI NAKANO, University of Hyogo — Magnetization process of the $S=1/2$ isotropic Heisenberg antiferromagnets on the kagome and triangular lattices are studied. Data from numerical-diagonalization method up to 39-spin systems, are reexamined from the viewpoint of the derivative of the magnetization with respect to the magnetic field. We find that the behavior of the derivative around the $1/3$ height of the magnetization saturation is quite different from the cases of typical magnetization plateaus for the kagome-lattice antiferromagnet. This new phenomenon is called the “magnetization ramp” [1]. We also compare it with the $1/3$ magnetization plateau of the triangular antiferromagnet. The critical exponent analysis indicates a clear difference between the magnetization plateau and ramp [2]. In addition using the numerical diagonalization up to 42-spin systems we suggest that the kagome-lattice antiferromagnet has a gapless singlet-triplet excitation in the thermodynamic limit [3].

[1] H. Nakano and T. Sakai: J. Phys. Soc. Jpn. 79 (2010) 053707.

[2] T. Sakai and H. Nakano: Phys. Rev. B 83 (2011) 100405(R).

[3] H. Nakano and T. Sakai: J. Phys. Soc. Jpn. 80 (2011) 053704.

9:36AM A8.00009 Phase Diagram of Spin-1/2 Triangular Antiferromagnet in a Magnetic Field, RU CHEN, HYEJIN JU, Department of Physics, University of California, Santa Barbara, CA-93106-9530, HONGCHEN JIANG, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA-93106-9530, OLEG STARYKH, Department of Physics, University of Utah, Salt Lake City, Utah 84112, LEON BALENTS, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA-93106-9530 — We investigate the spin-1/2 quantum Heisenberg antiferromagnet on both two-dimensional triangular lattice and N-leg triangular ladder. The model describes isotropic Heisenberg chains (exchange constant J) coupled antiferromagnetically through interchain diagonal bonds (exchange constant J'). We study different regions using various controlled theoretical methods. Primarily we focus on the region slightly below saturation field. We show that the cone-coplanar state transition is absent, while commensurate-incommensurate transition emerges right below the saturation field for two-dimensional triangular lattice. We also determine the ground states in the limit $J' \ll J$, using one-dimensional bosonization, renormalization group methods and current algebra. Finally, we compare our theoretical result with DMRG result for N-leg ladder.

9:48AM A8.00010 Spin Correlations and Excitations in the Quasi-2D Triangular Bilayer Spin Glass LuCoGaO_4 , K. FRITSCH, McMaster University, Hamilton, G.E. GRANROTH, A.T. SAVICI, Neutron Scattering Sciences Division, ORNL, Oak Ridge, H.M.L. NOAD, McMaster University, Hamilton, H.A. DABKOWSKA, B.D. GAULIN, Brookhouse Institute for Materials Research, Hamilton — LuCoGaO_4 is a layered magnetic-bilayer material wherein Co^{2+} magnetic moments and nonmagnetic Ga^{3+} ions are randomly distributed on planar triangular bilayers. This makes it an ideal case to study the interplay between geometric frustration, site disorder and low dimensionality and its influence on the magnetic ground of the system. This novel material has been grown for the first time in single crystal form at McMaster University. We have performed magnetization measurements, revealing a previously identified spin glass transition near $T_f \sim 19$ K, and a Curie Weiss temperature of $T_{cw} \sim 96$ K, consistent with antiferromagnetic interactions[1]. We discuss time-of-flight neutron scattering measurements using SEQUOIA at SNS which elucidate the evolution of the static and dynamic spin correlations in LuCoGaO_4 over a range of temperatures from $T \ll T_f$ to $T > T_{cw}$. We observe quasielastic scattering at $(1/3, 1/3, L)$ positions in reciprocal space and rods of scattering along the c^* -direction, consistent with short range antiferromagnetic correlations within decoupled bilayers, and which confirm the 2-dimensional character of this system. Inelastic scattering measurements show a gapped ~ 12 meV spin excitation which softens and broadens in energy, filling in the gap on a temperature scale of $\sim T_{cw}/2$. [1] Cava et al., J. Solid State Chem. 140, 337 (1998).

10:00AM A8.00011 Emergence and lifting of frustration for dipolar molecules, SEBASTIAN HUBER, EHUD ALTMAN, The Weizmann Institute of Science, EUGENE DEMLER, Harvard University — Ising spins on a triangular lattice are like a “harmonic oscillator” of geometric frustration. We address the general question of how this frustration is lifted in a system of dipolar molecules confined to $2+\epsilon$ dimensions. When the confinement to two dimensions is strong, the dipoles arrange in a triangular lattice. Upon reduction of the confinement, the dipoles undergo a transition out of the two dimensional plane, leading to an Ising degree of freedom. Spin-lattice coupling gives rise to an effective model in terms of quantum dimers. We discuss the resulting phases and the implications to current experiments with hetero-nuclear molecules.

10:12AM A8.00012 Spin dynamics in Kagomé-staircase multiferroic $\text{Ni}_3\text{V}_2\text{O}_8$, ANDREY PODLESNYAK, G. EHLERS, M. FRONTZEK, Quantum Condensed Matter Division, NScD, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, R.S. FISHMAN, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, O. ZAHARKO, Laboratory for Neutron Scattering, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland, M. KENZELMANN, Laboratory for Developments and Methods, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland, S. BARILO, Institute of Solid State and Semiconductor Physics, Minsk 220072, Belarus — The coupling of magnetic and ferroelectric order has recently been drawing a lot of interest in condensed matter science given the fundamental interest and potential applications. $\text{Ni}_3\text{V}_2\text{O}_8$ (NVO) is a $S = 1$ magnet with Ni^{2+} ions arranged in a weakly coupled buckled Kagomé-staircase planes. Its complex magnetic phase diagram exhibits four different zero field incommensurate and commensurate magnetic phases below 10 K, with only one developing ferroelectric order. We present here a detailed study of low temperature magnetic dynamics in this geometrically frustrated spin system. Using single crystal inelastic neutron scattering technique we map the magnetic excitation spectra across all the magnetic phase transitions. We found that the spin-waves, well formed in the base temperature nonferroelectric phase at $T < 3$ K, are considerably damped when the system enters the low-temperature incommensurate phase with ferroelectric order ($3.9 < T < 6.3$ K). Finally, we discuss models that describe the coupling between magnetic and ferroelectric properties in the incommensurate magnets.

10:24AM A8.00013 Temperature-dependent Raman studies of the magnetodielectric vanadates: $\text{Ni}_3\text{V}_2\text{O}_8$, $\text{Co}_3\text{V}_2\text{O}_8$, and $\text{K}_2\text{V}_3\text{O}_8$ ¹, M. KIM, Y. GIM, S.L. COOPER, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois, Urbana, Illinois, 61801, USA, R.J. CAVA, Department of Chemistry, Princeton University, Princeton, New Jersey 08544 — The kagome staircase compounds, $\text{Ni}_3\text{V}_2\text{O}_8$ and $\text{Co}_3\text{V}_2\text{O}_8$, are known to exhibit dielectric anomalies at the magnetic transitions; and inhomogeneously mixed-valent $\text{K}_2\text{V}_3\text{O}_8$ has been shown to have a strong dependence of the dielectric constant on applied magnetic field. However, while strong spin-lattice coupling is generally associated with the complex phases and phenomena in these materials, there has been little microscopic information about this coupling. In this talk, we present temperature-dependent Raman scattering studies of $\text{Ni}_3\text{V}_2\text{O}_8$, $\text{Co}_3\text{V}_2\text{O}_8$, and $\text{K}_2\text{V}_3\text{O}_8$ that allow us to investigate the microscopic connection between the strong spin-lattice coupling and the magnetodielectric effects in these materials.

¹Work supported by the National Science Foundation under Grant NSF DMR 08-56321.

10:36AM A8.00014 Competing Interactions in the $S=3/2$ Kagome Staircase $\text{Co}_3\text{V}_2\text{O}_8$: Evolution of the Commensurate and Incommensurate Phases in a Magnetic Field, JOEL HELTON, YING CHEN, JEFFREY LYNN, National Institute of Standards and Technology, GEORGII BYCHKOV, SERGEI BARILO, Belarus Academy of Sciences, NYRISSA ROGADO, ROBERT CAVA, Princeton University — Single crystal neutron diffraction studies have been performed on the $S = 3/2$ kagome staircase compound $\text{Co}_3\text{V}_2\text{O}_8$ with a magnetic field applied along the magnetization easy-axis ($\vec{H} \parallel \vec{a}$). Previous zero-field measurements reported incommensurate, transversely polarized spin density wave (SDW) phases [with a temperature dependent propagation vector of $\vec{k} = (0 \delta 0)$] interspersed with multiple commensurate lock-in transitions at temperatures above the ferromagnetic ground state. For small applied fields along $\vec{a}$, $\mu_0 H \approx 0.05$ T, the commensurate lock-in phases are destabilized in favor of the incommensurate SDW, while slightly larger applied fields restore the commensurate lock-in phase with $\delta = 1/2$ and yield a new commensurate phase with $\delta = 2/5$. For measurements in an applied field, higher-order scattering is observed that corresponds to the second-harmonic.

Monday, February 27, 2012 8:00AM - 11:00AM –

Session A9 GMAG DMP: Focus Session: Magnetic Oxide Thin Films And Heterostructures - Cobaltite And Ferrite Thin Films 209

8:00AM A9.00001 Ferromagnetic insulating state in tensile-strained LaCoO_3 thin films¹, HAN HSU, University of Minnesota, PETER BLAHA, TU Vienna, RENATA WENTZCOVITCH, University of Minnesota — With local density approximation + Hubbard U (LDA+ U) calculations, we show that the ferromagnetic (FM) insulating state observed in tensile-strained LaCoO_3 epitaxial thin films is most likely a mixture of low-spin (LS) and high-spin (HS) Co, namely, a HS/LS mixture state. Compared with other FM states, including the intermediate-spin (IS) state (*metallic* within LDA+ U), which consists of IS Co only, and the insulating IS/LS mixture state, the HS/LS state is the most favorable one. The FM order in HS/LS state is stabilized via the superexchange interactions between adjacent LS and HS Co. We also show that Co spin state can be identified by measuring the electric field gradient (EFG) at Co nucleus via nuclear magnetic resonance (NMR) spectroscopy.

¹This work was primarily supported by the MRSEC Program of NSF grants DMR-0212302 and DMR-0819885, and partially by EAR-081272 and EAR-1047629. P.B. was supported by the Austrian Science Fund (SFB F41, “ViCoM”). Calculations were performed at the MSI.

8:12AM A9.00002 Aberration-corrected STEM-EELS studies of epitaxial $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_3$ thin films, MARIA VARELA, Oak Ridge National Laboratory, JAUME GAZQUEZ, NEVEN BISKUP, Universidad Complutense, Spain, STEPHEN PENNYCOOK, Oak Ridge National Laboratory, MARIA TORIJA, MANISH SHARMA, SHAMEEK BOSE, CHRIS LEIGHTON, University of Minnesota — Cobaltite thin films provide a unique opportunity to study magneto-electronic phase separation, which can be strong in this reduced dimensionality environment. Here we present an investigation of epitaxial $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_3$ thin films on SrTiO_3 and LaAlO_3 substrates by scanning transmission electron microscopy and electron energy loss spectroscopy. The different degrees of strain and also different orientations of the substrates (such as (001) vs. (110)) induce major changes of the crystal structure and the depth profile of the chemical composition, observed both in the La/Sr and O sub-lattices. These effects can lead to lower effective doping level at the interface, favoring interfacial magneto-electronic phase separation. Research Council Starting Investigator Award (JS, NB) and the U.S. Dept. of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Div. (MV, SJP). Work at UMN supported by NSF and DOE (scattering).

8:24AM A9.00003 Atomic-Scale Imaging and Control of Interface Magnetic States in Vacancy Ordered Cobaltite Thin Films¹, ALBINA BORISEVICH, YOUNG-MIN KIM, MICHAEL BIEGALSKI, Oak Ridge National Laboratory, JUN HE, Vanderbilt University, HANS CHRISTEN, Oak Ridge National Laboratory, SOKRATES PANTELIDES, Vanderbilt University, STEPHEN PENNYCOOK, Oak Ridge National Laboratory — Magnetic properties of complex oxide thin films are strongly affected by strain, chemical composition, and octahedral tilt of the substrate. Here, we study lanthanum/strontium cobaltite ($\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_{3-x}$, LSCO) thin films via quantitative aberration-corrected scanning transmission electron microscopy and Electron Energy Loss Spectroscopy (EELS) to explore the coupling between magnetic properties, ionic behavior, and oxygen octahedral tilts. LSCO films were grown by PLD in identical conditions on two different substrates, LSAT (cubic) and NGO (orthorhombic). These substrates have nearly identical lattice parameters, but different octahedral tilts. The film on NGO appears to be $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_{2.5}$, while the film on LSAT is less oxygen deficient. Comparison of measured lattice parameters with the first-principles calculations allows us to determine oxygen content in the film. In $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_{2.5}$ /NGO films, EELS reveals different valence states of Co at the interface depending on termination, resulting in different magnetic states. Therefore changes in octahedral tilts can induce changes in oxygen stoichiometry and interface magnetic states of the vacancy ordered structures.

¹This research is sponsored by the MSE Division (YMK, JH, SJP, AYB) and SUF Division (MDB, HMC), Office of BES of the U.S. DOE.

8:36AM A9.00004 Stress and magnetism in LaCoO₃ films¹, ALEX DEMKOV, The University of Texas at Austin — Cobaltates exhibit a wide variety of exciting electronic properties resulting from strong electron correlations; these include superconductivity, giant magnetoresistance, metal-insulator transition, and strong thermoelectric effects. This makes them an excellent platform to study correlated electron physics, as well as being useful for various applications in electronics and sensors. In the ground state in the bulk, the prototypical complex cobalt oxide LaCoO₃ is in a spin-compensated low-spin state (t_{2g}^6), which results in the ground state being nonmagnetic. In a recent experiment, Fuchs *et al.* (*Phys. Rev. B* **75**, 144402 (2007)) have demonstrated that a ferromagnetic ground state could be stabilized by epitaxial tensile strain resulting in a Curie temperature (T_C) of ~ 90 K when LaCoO₃ (LCO) is grown on SrTiO₃ (STO) using pulsed laser deposition. In this talk I will discuss our recent successful attempt to integrate a LCO/STO heterostructure with Si (001) using molecular beam epitaxy. We have grown strained, epitaxial LaCoO₃ on (100)-oriented silicon using a single crystal STO buffer (Appl. Phys. Lett. **98**, 053104 (2011)). SQUID magnetization measurements confirm that the ground state of the strained LaCoO₃ is ferromagnetic with a T_C of 85 K. Our first-principles calculations of strained LaCoO₃ using the LSDA+ U method show that beyond biaxial tensile strain of 2.5% local magnetic moments, originating from the high spin state of Co³⁺, emerge in a low spin Co³⁺ matrix. Ferromagnetism found in tensile-strained LaCoO₃ is tightly coupled to the material's orbital and structural response to applied strain. Theoretical calculations show how LaCoO₃ accommodates tensile strain *via* spin state disproportionation, resulting in an unusual sublattice structure.

¹This work is supported by the National Science Foundation under grant DMR-0548182

9:12AM A9.00005 Ordering of defects induced by epitaxy in LaCoO₃ films¹, VIRAT MEHTA, University of California-Berkeley, NEVEN BISKUP, Universidad Complutense, Madrid 2840, Spain, FRANKLIN WONG, University of California-Berkeley, ELKE ARENHOLZ, Lawrence Berkeley National Laboratory-Advanced Light Source Division, MARIA VARELA, Oak Ridge National Laboratory, YURI SUZUKI, University of California-Berkeley — In the bulk, LaCoO₃ (LCO) undergoes a spin state transition from a diamagnet to a paramagnet with increasing temperature. Recent studies of epitaxial LCO thin films have resulted in the stabilization of a higher spin state and ferromagnetic ordering at low temperatures. Here, we explore the effects of epitaxy on the electronic structure of LCO films with X-ray absorption spectroscopy (XAS) and scanning transmission electron microscopy (STEM). We find differences in XAS spectra in coherently strained thinner films compared to the thicker partially relaxed films which may be due to differences in Co valence and bonding. STEM and electron energy loss spectroscopy of thinner LCO films reveal ordered defect planes that appear to be associated with a change in the O and Co bonding environments. In films on LaAlO₃ strained in compression periodic planes occur parallel to the substrate-film interface, while films on SrTiO₃ strained in tension have perpendicular defect planes. Correlation with magnetic data suggests that defect rich regions may exhibit greater ferromagnetism.

¹Research was sponsored by the ERC Starting Investigator Award Program (NB) and the U.S. DOE, Office of Basic Energy Sciences (MV, VM, YS)

9:24AM A9.00006 Spin state disproportionation and ferromagnetism in strained LaCoO₃: Ab-initio study, SEO HOSUNG, ALEXANDER DEMKOV, Department of Physics, The University of Texas at Austin — Strain engineering of artificial oxide heterostructures opens up routes for the creation of novel electronic phases that do not exist in the bulk. To fully exploit the functionalities of the oxide, understanding its electronic and structural response to epitaxial strain is crucial. One example is the recent demonstration of biaxial tensile strain stabilizing an insulating ferromagnetic ground state in normally non-magnetic LaCoO₃. However, theoretical understanding is incomplete. In this talk, using the LSDA+ U method we discuss the origin of strain induced transition to insulating ferromagnetic ground state in LaCoO₃. We show that beyond biaxial tensile strain of 2.5% local magnetic moments, originating from high spin state of Co³⁺, emerge in low spin Co³⁺ matrix. We further show that these local moments are ferromagnetically coupled via superexchange interaction. In contrast, we find that compressive strain by itself is not able to stabilize a magnetic state, that agrees with recent experiment. Ferromagnetism found in tensile-strained LaCoO₃ is tightly coupled to the material's orbital and structural response to applied strain. We discuss how LaCoO₃ accommodates tensile strain *via* spin state disproportionation, resulting in an unusual sublattice structure.

9:36AM A9.00007 Percolation-Type Ferromagnetic Order in Epitaxial Strained LaCoO₃ Thin Films, GEORGE STERBINSKY, National Institute of Standards and Technology, PHILIP RYAN, JONG-WOO KIM, EVGUENIA KARAPETROVA, Advanced Photon Source, Argonne National Laboratory, J. MA, JING SHI, Department of Physics, University of California, Riverside, JOSEPH WOICK, National Institute of Standards and Technology — Support for percolation-type ferromagnetic order in LaCoO₃ thin films is provided by x-ray diffraction and Co K -edge x-ray absorption fine structure (XAFS) spectroscopy. X-ray diffraction shows considerable changes in structure with respect to bulk LaCoO₃, and extended XAFS (EXAFS) demonstrates a large Jahn-Teller like distortion of the oxygen octahedra in highly strained films. Structural distortions of the oxygen octahedra are strongly coupled to the hybridization between orbitals of Co and O atoms, as shown by x-ray absorption near edge spectroscopy (XANES). Our results indicate that increased Co-O hybridization, and therefore increased magnetic exchange energy, does not cause ferromagnetism to occur in LaCoO₃ thin films. Instead, we suggest that the strain-induced distortions of the oxygen octahedra increase the population of e_g electrons and concurrently depopulate t_{2g} electrons beyond a stabilization threshold for ferromagnetic order.

9:48AM A9.00008 Imaging Local Magnetic Domain Rearrangement in Strained LaCoO₃ Thin Films Using Magnetic Force Microscopy¹, MORGANN BERG, NELIZA LEON, AGHAM POSADAS, ALFRED LEE, University of Texas at Austin, JEEHOON KIM, Los Alamos National Laboratory, ALEX DE LOZANNE, ALEX DEMKOV, University of Texas at Austin — Previous studies we have conducted on thin films of lanthanum cobaltate (LCO) under tensile strain have revealed a tendency toward local magnetic domain rearrangement into streak-like configurations near the ferromagnetic to paramagnetic phase transition. Moreover, the persistence of these streak-like characteristics to lower temperatures after field-cooling appears to be linked to the strength of the applied magnetic field in which these films are field-cooled. This tendency has not yet been verified for thin films of LCO under compressive strain which could indicate whether this magnetic domain rearrangement is intrinsic to thin film samples of LCO or is merely an effect of tensile strain. Using magnetic force microscopy, we investigate the microscale magnetic properties of a thin film of LCO under compressive strain, prepared by molecular beam epitaxy and deposited on a lanthanum aluminate substrate. We observe these properties across a wide temperature range and compare our results to global magnetic characteristics of this film as measured by a SQUID magnetometer.

¹I'd like to acknowledge the IGERT (DGE-0549417) and NSF (DMR-0923231) grants which supported this work and contributions from collaborators which made this research possible.

10:00AM A9.00009 Origin of ferromagnetic ordering in LaCoO₃ epitaxial thin films¹, WOO SEOK CHOI, Oak Ridge National Laboratory, J.-H. KWON, Seoul National University, HYUNGJEEN JEEN, Oak Ridge National Laboratory, VLADIMIR HINKOV, University of British Columbia, M. KIM, Seoul National University, HO NYUNG LEE, Oak Ridge National Laboratory — LaCoO₃ (LCO) film has received attention due to its unexpected ferromagnetic (FM) ordering, which is distinctly different from the bulk counterpart. Although the exact origin has not been understood, previous studies have suggested that the epitaxial strain should play an important role. In this work, we show that the FM ordering could be related to a locally-ordered microstructure. We used PLD to deposit epitaxial LCO thin films on various substrates in order to impose different degree of strain. XRD and XAS studies showed that the films are of high quality, without any secondary phases or changes in the Co valence. In addition, all the films were coherently-strained. From the STEM investigation, however, we noticed that some of the films had an unexpected stripe-like superstructure along the <100> direction. While the microstructure resembles that of oxygen-vacancy or charge ordering, typically found in doped transition metal oxides, we could rule out such possibilities and interpret it as a nanoscale twin boundary. The strain induced structural change seems to originate the FM ordering.

¹The work was supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

10:12AM A9.00010 Magnetic properties of LuFeO₃ thin films¹, XIAOSHAN XU², Oak Ridge National Lab, WENBIN WANG, University of Tennessee, ZHENG GAI, Oak Ridge National Lab, XUEMEI CHENG, Bryn Mawr College, LEYI ZHU, DAVID KEAVNEY, Argonne National Laboratory, PAUL SNIJDER, THOMAS WARD, Oak Ridge National Lab, JIAN SHEN, University of Tennessee — In order to extract their intrinsic magnetic properties, we have grown LuFeO₃ thin films epitaxially on Al₂O₃ (0001), a substrate with minimum magnetic impurities, using pulsed laser deposition. The magnetization measurements reveal strong anisotropy between in-plane and out-of-plane, not only in terms of coercivity and remanence, but also obvious in the zero field cool and field cool splitting. Further experiment using X-ray magnetic linear dichroism suggest magnetic ordering higher than 290 K and a spin reorientation at lower temperature. Over all, the films appear weak-ferromagnetic.

¹Research supported by US DOE, Office of Basic Energy Science, Materials Science and Engineering Division.

²Research performed as a Eugene P. Wigner Fellow and staff member at the Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U.S. Department of Energy under Contract DE-AC05-00OR22725.

10:24AM A9.00011 Fabrication and properties of LuFeO₃ thin film¹, WENBIN WANG, University of Tennessee & Oak Ridge National Lab, XIAOSHAN XU, ZHENG GAI, NINA BALKE, MIAOFANG CHI, THOMAS Z. WARD, PAUL C. SNIJDER, Oak Ridge National Lab, JIAN SHEN, University of Tennessee & Fudan University, UNIVERSITY OF TENNESSEE TEAM, OAK RIDGE NATIONAL LAB TEAM, FUDAN UNIVERSITY COLLABORATION — We have succeeded in growing the hexagonal LuFeO₃ single crystalline thin films on Al₂O₃(0001) substrates using Pulsed Laser Deposition (PLD). The structures, epitaxial relation between film and substrate, ferroelectric and magnetic properties of the samples were characterized by RHEED, LEED, XRD, AFM, TEM, PFM and SQUID magnetometry. The structure of our hexagonal LuFeO₃ films is consistent with that of YMnO₃, and the samples exhibit a piezoelectric effect at room temperature. RHEED data are consistent with a structural change from a polar P6₃cm (185) to non-polar P6₃/mmc (194) at 1050 K. SQUID measurements reveal strong magnetic order in the thin film. All the data suggests a coexistence of ferroelectricity and magnetic order in hexagonal LuFeO₃ films.

¹Research sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy.

10:36AM A9.00012 Enhancement of the Magnetic Moment in Ultrathin Fe-doped CoFe₂O₄¹, JARRETT MOYER, CARLOS VAZ, DIVINE KUMAR, Department of Applied Physics and CRISP, Yale University, DARIO ARENA, National Synchrotron Light Source, Brookhaven National Laboratory, VICTOR HENRICH, Department of Applied Physics and CRISP, Yale University — The magnetic properties of magnetic oxides can be drastically altered through a reduction in film thickness. It has previously been demonstrated that the magnetic moments of CoFe₂O₄ and NiFe₂O₄ are enhanced for ultrathin films; however, the physical mechanisms for this enhancement are still unknown. To determine the physical cause of this increased magnetic moment and to examine the effect of Fe doping, thin films of Co_{1-x}Fe_{2+x}O₄ (0 ≤ x ≤ 0.8) are grown epitaxially on MgO (001) substrates by MBE at thicknesses ranging from 3 – 20 nm. SQUID magnetometry measures the bulk magnetic properties of the samples and confirms that there is an increase in the magnetic moment for all stoichiometries as the film thickness is reduced. XAS, XMLD and XMCD measurements examine the cation-specific magnetic moments and spin directions to explain the physical mechanisms that lead to an enhanced magnetic moment in ultrathin Fe-doped CoFe₂O₄ films.

¹This research is primarily supported by NSF Grant MRSEC DMR-0520495

10:48AM A9.00013 Electronic states and magnetic structure at the Co₃O₄ (110) surface: a first principles study, JIA CHEN, ANNABELLA SELLONI, Princeton University — Tricobalt tetraoxide (Co₃O₄) is an important catalyst and Co₃O₄(110) is a frequently exposed surface in Co₃O₄ nanomaterials. We employed Density-functional theory with on-site Coulomb repulsion U term to study the atomic structures, energetics, magnetic and electronic properties of the two possible terminations, A and B, of this surface. These calculations predict A as the stable termination in a wide range of oxygen chemical potentials, consistent with recent experimental observations. The Co³⁺ ions do not have a magnetic moment in the bulk, but become magnetic at the surface, which leads to surface magnetic orderings different from the one in the bulk. Surface electronic states are present in the lower half of the bulk band gap and cause partial metallization of both surface terminations. These states are responsible for the charge compensation mechanism stabilizing both polar terminations. Furthermore, our calculations predict that the critical thickness for polarity compensation is 4 layers.

Monday, February 27, 2012 8:00AM - 11:00AM –
Session A10 DCOMP: Invited Session: Computational Assessment of a Sustainable Energy Future: The Earth-abundant Materials Approach 210A

8:00AM A10.00001 Computational Design of Solar Energy Harvesting Materials Made of Earth-Abundant Elements¹, YIYANG SUN, Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute — Very large-scale deployment of photovoltaic (PV) technology based on both the first and second generation solar cells poses serious questions on the materials supply as they rely on either high-purity and high-quality silicon crystals or rare elements such as indium and tellurium. “Ancient” PV materials made of earth-abundant elements, such as oxides and sulfides of copper and iron, have attracted resurgent interests. There is also intensive research devoted to the search for “modern” earth-abundant PV materials, with a recent promising example being $\text{Cu}_2\text{ZnSnSe}_4$. Computational approaches play a key role in this endeavor by guiding the screening and optimization of the materials toward high device performance. In this paper, I will focus on two aspects of computational design of earth-abundant PV materials. First, I will discuss the methods for accurately predicting band gaps of semiconductor materials. The emphasis will be on the performance of hybrid functional method on different classes of materials. Based on these understandings, I will discuss how to tune the band gap of a material to match the solar spectrum. For example, one could reduce the band gap of anatase to 1.5 eV by the chemical codoping approach. Second, I will discuss the methods for accurate computation of defect properties, which is important as the defectiveness is intrinsic to the low-cost synthesized materials. I will introduce a method for calculation of defect formation energies by minimizing the error due to the “band-gap problem” of the density functional theory. I will also discuss approaches to mitigating the effects of defects, e.g., by passivation.

¹The author acknowledges the support by NSF under Award No. DMR-1104994 and DOE under Award No. DE-SC0002623.

8:36AM A10.00002 Computational approaches to finding earth-abundant thermoelectric materials¹, VIDVUDS OZOLINS², Dept of Materials Science and Engineering, University of California, Los Angeles — Good thermoelectric materials should possess a combination of seemingly incompatible properties, such as high electronic mobility and low lattice thermal conductivity. Therefore, search for crystalline materials with glass-like thermal conductivity has been an active field of research. Several cubic I-V-VI₂ semiconductors, the paradigm for which is AgSbTe_2 , have been shown to exhibit minimal values of lattice thermal conductivity at ambient temperatures when the phonon mean free path equals the interatomic distance. These modes are due to the existence of highly polarizable lone s^2 electron pairs on the group V cations. Electrostatic repulsion between the lone s^2 pairs and the valence charge on group VI anions tends to favor locally distorted bonding configurations and may lead to unstable phonons. We present the results of first-principles density functional theory (DFT) calculations of phonon dispersion and electron-phonon interactions in cubic I-V-VI₂ semiconductors, where the group I elements are Cu, Ag, Au or alkali metals, the group V elements are P, As, or Bi, and the group VI elements are S, Se, or Te. Compounds that have only marginally stable phonons have extremely large Grüneisen parameters that result in a thermal conductivity limited by Umklapp processes to values at the amorphous limit above 200 K. Following the *ab initio* calculation, we synthesized AgSbTe_2 , AgSbSe_2 , AgBiTe_2 , NaSbTe_2 , NaSbSe_2 , and NaBiTe_2 and report their thermal conductivity and specific heat: in all cases, the experiments confirm the theory.

¹This work was supported as part of the “Revolutionary Materials for Solid State Energy Conversion,” an Energy Frontier Research Center funded by the U.S. Dept of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001054.

²In collaboration with Michele Nielsen and Joseph Heremans, Department of Physics, Ohio State University

9:12AM A10.00003 Solar energy into fuels - the importance of interface catalysis¹, FRANK ABILD-PEDERSEN, SUNCAT Center for Interface Science and Catalysis Photon Science, SLAC National Accelerator Laboratory — Finding sustainable energy solutions for the future will rely heavily on the energy influx from the sun. One convenient way of storing solar energy is by transforming that energy into a chemical form - like a fuel. The efficiency of such a transformation will require catalysts that are optimized for specific reactions, and we will need to find new catalysts for a number of processes, if we are to successfully synthesize fuels from sunlight. A fundamental insight into the way the catalysts work at the molecular level is an essential ingredient if one wants to speed up the discovery process. In this presentation I will discuss some of the challenges in catalyst discovery. In particular, I will focus on the conversion of syngas to methanol, an important sub-reaction in the biomass to fuels process.

¹U.S. Dept. of Energy, Office of Basic Energy Sciences

9:48AM A10.00004 Key electronic processes in organic solar cells: a theoretical perspective, VEACESLAV COROPCEANU, Center for Organic Photonics and Electronics and School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332-0400, USA — In this contribution, we discuss state-of-the-art quantum-chemical approaches used to derive the microscopic parameters and model the key electronic processes in organic solar cells. We illustrate the application of recently developed computational methods by computing the electronic couplings and the rates of exciton dissociation and charge recombination in several model donor-acceptor complexes. The contributions of both intra-molecular and inter-molecular vibrations to the electron-vibrational interaction will be discussed in detail. The impact on the charge-transport characteristics of the interplay between electron-vibration coupling and electronic coupling is investigated in the framework of band, disorder, and semi-classical models.

10:24AM A10.00005 Harvesting the energy from the sun: insights from ab initio materials modeling, GIULIA GALLI, University of California, Davis — Can quantum and atomistic simulations make valuable contributions to the search of materials for sustainable energy sources? We will address this question by discussing some specific examples where quantum simulations have been used to predict optical properties of nanostructured semiconductors and of complex oxides in contact with water. We will also discuss issues related to the comparisons with increasingly complex experiment.

Monday, February 27, 2012 8:00AM - 11:00AM — Session A11 DCMP: Graphene: Transport in Devices and Structures 210B

8:00AM A11.00001 Transport in Graphene: Ballistic, Anomalous, or Diffusive?, MARIO BORUNDA, HOLGER HENNIG, ERIC HELLER, Harvard University — The discovery of graphene, consisting of a layer of carbon atoms arranged in a honeycomb lattice, represents a conceptually new class of materials that are only one atom layer thick. Recent experiments achieved extremely high mobilities in suspended graphene leading to ballistic transport. In this talk, we study implications of diffusive and ballistic transport in graphene devices and ask what could be possible signatures of “anomalous” (or superdiffusive) transport. Experimental setups to differentiate between these stochastic processes are discussed.

8:12AM A11.00002 Transport in high-mobility mesoscale graphitic devices¹, ANDREI GARCIA, FRANCOIS AMET, Applied Physics Department, Stanford University, JAMES WILLIAMS, DAVID GOLDBABER-GORDON, Physics Department, Stanford University — Recent advances in graphene fabrication have allowed for high-mobility structures to be created. We report on the fabrication and measurement of mesoscale devices of graphene on boron-nitride. We present the details by which graphene is transferred on to boron-nitride substrates, where we observed enhanced mobility over similar devices fabricated on silicon dioxide substrates. Transport measurements at low temperature are described with focus given to reconfigurable, mesoscale devices in graphene.

¹This work is supported by FENA, an FCRP center based at UCLA, and the Center for Probing the Nanoscale at Stanford University, an NSF NSEC.

8:24AM A11.00003 Gate defined quantum confinement in suspended bilayer graphene, MONICA ALLEN, Harvard University, JENS MARTIN, University of Exeter, AMIR YACOBY, Harvard University — Devices that confine electrons in graphene have sparked substantial interest due to applications ranging from spin-based quantum computation to valley filters. However, the absence of an intrinsic bandgap in graphene has limited such devices to on-chip nanopatterned structures to date. Here we present high quality quantum dots in suspended bilayer graphene with tunnel barriers defined by external electric fields that break layer inversion symmetry, thereby eliminating both edge and substrate disorder. We demonstrate clean electron confinement in two regimes: at zero magnetic field B using the single particle energy gap induced by a perpendicular electric field and at $B > 0$ using the quantum Hall ferromagnet $\nu=0$ gap. Our devices exhibit clean quantum transport behavior at magnetic fields ranging from zero to seven Tesla, including a highly resistive $\nu=0$ quantum Hall state and over forty consecutive Coulomb blockade oscillations with symmetric source-drain coupling. The data indicate that the dots are defined by local top gating and are not disorder formed. Geometric control over oscillation periodicity is confirmed by electrostatic simulations based on lithographic gate geometry.

8:36AM A11.00004 Quantum Transport in Double-gated Trilayer Graphene *pnp* Junctions, YONGJIN LEE, JAIRO VELASCO JR., LEI JING, WENZHONG BAO, DAVID TRAN, MARC BOCKRATH, CHUN NING (JEANIE) LAU, Department of Physics and Astronomy, University of California, Riverside — Using trilayer graphene *pnp* junctions with suspended top gates, we perform transport measurements. At a magnetic field $B=0$, by an applied perpendicular electric field, the conductance is increased that it is suggestive of a semi-metallic band overlap. At $B=8T$ we observe quantum Hall conductance with fractional values, which can be explained equilibration of edge state between differentially-doped regions, and the presence of an insulating state at filling factor $\nu=0$.

8:48AM A11.00005 Superconducting proximity effect in graphene: Injecting Cooper pairs in quantum Hall edge states, KATSUYOSHI KOMATSU, CHUAN LI, SANDRINE AUTIER-LAURENT, ALIK KASUMOV, HELENE BOUCHIAT, SOPHIE GUERON, Laboratoire de Physique des Solides, Université Paris Sud, 91405 Orsay, France — A superconductor-graphene(SG) hybrid system, such as an SGS junction or an SG interface, provides an ideal platform to investigate the relativistic nature of Dirac fermions combined with superconductivity. Instead of the retro-reflection of carriers in an ordinary superconductor-normal metal interface, an SG interface is theoretically predicted to show the specular reflection of quasiparticle carriers. We show that a supercurrent flows through a SGS junction with Nb electrodes even through a very long graphene distance of $1.2\mu m$, more than 3 times the length previously reported. This supercurrent disappears in the vicinity of the Dirac point, indicating a strong sensitivity of the transmission of Andreev pairs to the formation of charge puddles with size greater than the superconducting coherence length. We also present data on similar size graphene samples with superconducting electrodes with a high critical field (more than 7 Tesla) for which the properties of the normal state are dominated by quantum Hall physics. Whereas the behavior of the supercurrent is similar to the Nb/Graphene/Nb system in zero field, new features are observed in the high field quantum Hall regime.

9:00AM A11.00006 Gate-Tunable Superconducting-Insulating Transition in Tin-Decorated Graphene, VINCENT BOUCHIAT, ZHENG HAN, ADRIEN ALLAIN, Neel Institute, CNRS-Grenoble — We report the measurement of electrostatically tuned superconducting-insulating transition in macroscopic, CVD-Grown samples of graphene which decorated with tin nanoparticles. The self assembled network of Tin islands generates superconducting correlations locally in the Graphene by means of proximity effect. Correlations eventually leads to percolation of a supercurrent. This system exhibits features related to granular superconductivity, a giant magnetoresistance peak, as well as an intermediate metallic behavior. We emphasize outstanding dynamics of the transition, which exhibit a change in resistance of more than 7 orders of magnitude within 40V of gate voltage, thus realizing a real electrostatically driven superconducting-insulating transition. The intense positive magnetoresistance observed for fields below the critical field of Tin nanoparticles is a signature of the localization of Cooper pairs. This hybrid superconductor provides a model system to better understand the physics of inhomogeneous superconductivity, as crossing the transition by adjusting the carrier density is conceptually simpler than using a magnetic field. It also allows to cross the transition continuously and under constant disorder.

9:12AM A11.00007 Transport through Andreev Bound States in a Graphene-base Quantum Dot¹, YANJING LI, NADYA MASON, University of Illinois at Urbana-Champaign — We perform tunneling spectroscopy on a graphene-quantum dot (QD)-superconductor junction, a system in which sharp, gate-tunable Andreev bound states (ABS) in the spectra have been observed [1]. Here we extend previous results, particularly regarding the origins of the QD. In particular, we discuss how a discontinuous layer of AlO_x between the superconductor and the graphene plays a role in the formation of the QD. We also discuss additional spectroscopic features that may be due to multiple QDs and energy levels. Finally, we show that a robust superconducting tunneling junction can be created in a lead-graphene structure, without the explicit deposition of a tunneling barrier.

[1] Dirks, T., Nature Physics 7, 386–390 (2011)

¹Supported by NSF 491119-244006-191100 and DOE-DMS DE-FG02- 07ER46453 through the Frederick Seitz Materials Research Laboratory.

9:24AM A11.00008 Direct Measurement of the Fermi Energy in Graphene Using a Double Layer Structure¹, SEYOUNG KIM, INSUN JO, DAVID DILLEN, DOMINGO FERRER, BABAK FALLAHZAD, ZHEN YAO, SANJAY BANERJEE, EMANUEL TUTUC, The University of Texas at Austin — The Fermi energy is a fundamental property of an electron system. Here we introduce a direct measurement technique of the relative Fermi energy as a function of carrier density, using transport measurement in a double layer structure where one of the layers is graphene. The principle of this method is that the Fermi energy in the target material is equal to the applied inter-layer bias required to bring the graphene layer to charge neutrality point. Using a double layer graphene structure, we illustrate the technique by measuring the Fermi energy in one of the graphene layers. By mapping the top graphene layer zero density line as a function of bottom and inter-layer bias, we measure the Fermi energy as a function of carrier density at zero and in high magnetic fields. We extract the Fermi velocity, Landau level spacing and Landau level broadening.

¹We thank C. P. Morath and M. P. Lilly for discussions. This work was supported by NRI, ONR, and Intel. Part of this work was performed at the National High Magnetic Field Laboratory, which is supported by NSF (DMR-0654118), the State of Florida, and DOE.

9:36AM A11.00009 Magnetic field dependence of the carrier's effective mass and the g-factor in graphene¹, ANDRII IUROV, Hunter College and Graduate Center, City University of New York, GODFREY GUMBS, OLEKSIY ROSLYAK, Hunter College, City University of New York, DANHONG HUANG, USAF Research Lab (AFRL/RVSS) — It has been established that the intrinsic Zeeman energy is one half of the cyclotron energy for “bare” electrons in graphene. Consequently, there could be Landau-level mixing between the energy bands. We investigate how the band mixing is affected by the Coulomb interaction. Pairing of the electrons and holes in the presence of a circularly polarized light is also considered for several filling factors. We calculate the quasiparticle effective mass and effective g -factor for dressed electrons and holes in monolayer graphene. As an intermediate step of these calculations, we obtain the dielectric function for the case of electron dressed states and investigate how the magnetoplasmons modes are affected by the electron-photon interaction.

¹This research was supported by contract # FA 9453-11-01-0263 of AFRL. DH would like to thank the Air Force Office of Scientific Research (AFOSR) for its support.

9:48AM A11.00010 Magnetic-field tunable electron-phonon coupling in graphite, LI-CHUN TUNG, Dept. of Phys. and Astrophys., University of North Dakota, W. YU, School of Physics, Georgia Institute of Technology, P. CADDEN-ZIMANSKY, Department of Physics, Columbia University, M. KINDERMANN, School of Physics, Georgia Institute of Technology, D. SMIRNOV, National High Magnetic Field Laboratory, Z. JIANG, School of Physics, Georgia Institute of Technology — Electron-phonon coupling (EPC) plays a pivotal role in condensed matter physics, governing intriguing phenomena such as superconductivity, ballistic transport, and excited-state dynamics. In graphitic systems, EPC is found to be strongly related to the quasiparticle excitations, electronic states and optical properties. Thus, the EPC may be manipulated via external parameters, such as electric field or magnetic field, and provide alternative access to adjust the characteristics of carbon-based devices. Here, we explore the EPC in graphite via magnetophonon resonance using cyclotron resonance (CR) spectroscopy. A marked avoided-level-crossing splitting of the CR and a Fano resonance-like behavior are observed, when the CR energies intersect the specific phonon energies via tuning the magnitude of the magnetic field. We attribute these results to the resonance between the CR excitations and the large momentum zone-edge, and the long-wavelength zone-center phonons, respectively. This work suggests that rich interacting physics exists in graphitic materials, which may have profound implications in future optoelectronics.

10:00AM A11.00011 High frequency high magnetic field response of graphene monolayers, IVANA PETKOVIC, Laboratoire National de Métrologie et d'Essais, Trappes, France, FRANCIS WILLIAMS, FABIEN PORTIER, PATRICE ROCHE, KEYAN BENNACEUR, CHRISTIAN GLATTLI, Commissariat à l'Energie Atomique, Saclay, France — We study the electronic magnetotransport in graphene at rf frequencies (5-50GHz). Our aim is to investigate the dynamics of charge carriers in the quantum Hall regime. The graphene sample is placed in a break made in a coplanar waveguide and the transmitted power is measured. In order to isolate the response of the sample from the direct transmission between the input and output waveguides, the graphene electron density distribution is modulated with a side gate and the resulting modulation in the transmitted power detected via a standard lock-in technique. The fixed frequency graphene response as a function of magnetic field reveals two different components. One is symmetric in B and dominates under large side gate voltage, and the other shows reproducible fluctuations revealed only at low gate voltage modulation amplitude. The first part is thought to be related to the bulk conductivity and the fluctuations to the carrier dynamics close to the edge. The amplitude of the fluctuations depends on the trajectory of the carriers, since the parity with respect to magnetic field reversal is not conserved. We thus demonstrate the chiral nature of the transport. We assume that the fluctuations of impedance originate in the scattering from localized states close to the sample edge.

10:12AM A11.00012 Impurity-limited carrier transport in graphene nanoribbons¹, C.W. SMITH, MASAHIRO ISHIGAMI, Department of Physics and Nanoscience Technology Center, University of Central Florida, Orlando, FL 32816 — We have measured the transport property of graphene nanoribbons as a function of impurity density in ultra high vacuum. Specifically, the impact of Coulomb and van der Waals impurities on the transport and source-drain gap of nanoribbons is investigated. Our results have direct consequences on fundamental science using graphene constrictions and graphene-based devices.

¹This work is based upon research supported by the National Science Foundation under Grant No. 0955625.

10:24AM A11.00013 Electrical Transport Study of Suspended Graphene Nanoribbons, MING-WEI LIN, KULWINDER DHINDSA, LEZHANG LIU, QING LAN, Department of Physics and Astronomy, Wayne State University, MARK MING-CHENG CHENG, Wayne State University, LUIS AGAPITO, NICHOLAS KIOUSSIS, California State University, ZHIXIAN ZHOU, Department of Physics and Astronomy, Wayne State University — Suspended graphene nanoribbon field effect transistors from unzipped multiwall carbon nanotubes have been fabricated. Electrical transport measurements show that current-annealing effectively removes the adsorbed impurities on the suspended graphene nanoribbons. Further increasing the annealing current creates a narrow constriction in the ribbons with non-negligible disorder, leading to the formation of a large band-gap and subsequent high on/off ratio. On the other hand, uniform suspended graphene nanoribbons with ultra-low-disorder reveal a high mobility exceeding 3000 cm² V⁻¹ s⁻¹ and an intrinsic band gap. The width and length dependence of the electrical transport properties of ultra-low-disorder graphene nanoribbons with nearly atomically smooth edges will also be discussed.

10:36AM A11.00014 Quantum Transport in Graphene Nanoribbon Networks, ANDRÉS RAFAEL BOTELLO-MÉNDEZ, Institute of Condensed Matter and Nanosciences(IMCN), Université Catholique de Louvain (UCL), Belgium, EDUARDO CRUZ-SILVA, Oak Ridge National Laboratory (ORNL), USA, JOSÉ MANUEL ROMO-HERRERA, Departamento de Química Física, Universidad de Vigo, Spain, FLORENTINO LÓPEZ-URÍAS, IPICYT, Mexico, MAURICIO TERRONES, Materials Research Institute, The Pennsylvania State University, USA, BOBBY G. SUMPTER, ORNL, USA, HUMBERTO TERRONES, JEAN-CHRISTOPHE CHARLIER, IMCN, UCL, Belgium, VINCENT MEUNIER, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, USA — Focusing on systems that can be realized experimentally, both in-plane conductance of inter-connected graphene nanoribbons and tunneling conductance in out-of-plane nanoribbon intersections are investigated. The quantum transport properties of such networks are computed using first-principles calculations based on the density functional theory formalism. The electronic transport through in-plane nanoribbon cross-points is found to be significantly affected by scattering at the intersections with the exception of all zigzag nanoribbon terminals arranged at a 60 degree angle. This result demonstrates the possibility of designing graphene nanoribbon networks capable of guiding electron along desired and predetermined paths. In addition, the electron transport properties of out-of-plane nanoribbons cross-points with realistic size are described within a simple tight-binding approach. The stacking angle is predicted to play a key role on the electronic transmission through nanoribbon networks.

10:48AM A11.00015 Current Quantization in Corrugated Graphene Nanoribbons, UPALI APARAJITA, OLEKSIY ROSLYAK, GODFREY GUMBS, Physics & Astronomy Department, Hunter College, CUNY, DANHONG HUANG, USAF Research lab, Kirtland AFB, NM — Corrugated graphene provides such a phenomenon as curvature induced $p-n$ junction band gap opening and decoherence. We report yet another effect of current quantization in graphene nanoribbons via energy minigaps induced by the corrugation. Effects of edge roughness and long range charged scatterers on the quantization are investigated. Comparison is drawn with acoustically induced minigaps in carbon nanotubes [Talyanskii et al., PRL 87,276082(2001)].

Monday, February 27, 2012 8:00AM - 11:00AM —

Session A12 DCMP: Graphene: Electronic Structure and Interactions - Adsorbates, Doping and Defects 210C

8:00AM A12.00001 Transport study of electrochemically decorated and intercalated graphene, DMITRI K. EFETOV, KIN FAI MAK, YINSHENG GUO, TONY F. HEINZ, LOUIS BRUS, PHILIP KIM, Columbia University in the City of New York — Due to the surface-only properties of graphene, the decoration and/or intercalation of single, bi- and multi-layer graphene with foreign atoms can severely modify its electronic interactions, similar to those observed in its 3D counterpart the graphite intercalation compounds. Supported by a highly increased density of state due to a strong charge transfer above 10¹⁴ cm⁻² into the graphene π -bands, certain adatoms are expected to induce strong electronic interactions to the graphenes own Dirac fermions, where theoretical predictions reach from the Kondo-effect and magnetism to as far as superconductivity in graphene. In this study we will present evidence of specific adsorption and intercalation of diverse atomic species by electrochemical means. We will present a detailed transport study, including resistivity-, Hall- and magneto-resistivity measurements of single-, bi- and multi-layer graphene devices which were subjected to electrochemical doping by a variety of electrolytes and ionic species such as Li⁺, ClO₄⁻, Cs⁺, Ca²⁺, etc.

8:12AM A12.00002 Electronic detection of phase transition of adsorbed water on graphene, SHUDONG XIAO, MICHAEL FUHRER, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742-4111 — Graphene is sensitive to overlayers on its surface through charge transfer and also through changes in dielectric constant, which can alter the scattering by static disorder in graphene. We performed transport measurement on graphene devices *in situ* in ultra-high vacuum at low temperature. Water vapor is introduced to the chamber and is adsorbed on graphene at low temperature. After deposition of a few monolayers of water, the resistivity of graphene at fixed gate voltages is measured as the temperature is raised from 40K to room temperature. Sharp features in the temperature-dependent resistivity mark reproducible, irreversible (upon re-cooling) changes in the sample which we interpret as phase transitions in the adsorbed water overlayer, likely corresponding to dewetting and desorption. This work has been supported by the University of Maryland NSF-MRSEC under Grant No. DMR 05-20471 with supplemental funding from NRI.

8:24AM A12.00003 *GW* study of the effect of various defects on the band gap of fluorographene, YOUNG-MOO BYUN, JORGE SOFO, VINCENT CRESPI, Penn State University — Recently synthesized fluorographene, fully fluorinated graphene in a chair configuration, is a wide band-gap (E_g) semiconductor with an experimental optical band gap of ~ 3 eV. However, first-principles calculations have shown that pristine fluorographene should have E_g of 5.4 to 7.5 eV. To explain this discrepancy, we have studied the effect of F vacancies, a Stone-Wales (SW) defect, C single vacancies and C double vacancies on E_g of fluorographene using density functional theory and the *GW* approximation. F vacancies and a SW defect are not likely to affect E_g of fluorographene, whereas a C single vacancy with a doubly fluorinated C atom, a C double vacancy, and a C double vacancy with two doubly fluorinated C atoms lead to a *GW* band gap of ~ 4 eV, which is consistent with the optically measured E_g , and they are energetically more favorable than other C vacancies at a wide range of chemical potential of F (μ_F).

8:36AM A12.00004 Controlled electrochemical functionalization of epitaxial graphene¹, CALVIN CHAN, THOMAS BEECHEM, TAISUKE OHTA, DAVID WHEELER, Sandia National Laboratories, KEITH STEVENSON, University of Texas, Austin — Chemical functionalization is a promising means of modifying graphene for applications ranging from nanoelectronics to transparent electrodes. Various schemes have been demonstrated, but control over functionalization density with well-specified molecules is still a challenge. We report on the controlled electrochemical functionalization of epitaxial graphene with trifluoromethylphenylene (CF₃Ph), where the functionalization density was controlled by the electron injection rate. CF₃Ph peaks were observed in x-ray photoemission spectroscopy, along with binding energy shifts consistent with bonding between CF₃Ph and graphene. A maximum functionalization density of one molecule per six graphene carbons was inferred from the peak intensities. Spectroscopic Raman mapping revealed increasing graphene D:G peak intensity ratios that scaled with increasing functionalization-induced localized defects. While a minimal shift in the π orbital structure and the emergence of CF₃Ph related features were observed in ultraviolet photoemission spectroscopy, a work function increase by 0.5 eV in CF₃Ph-graphene suggests a shift of the electron distribution towards the CF₃ moieties on the surface. This work has positive implications for transparent electrode applications.

¹This work was supported by the Early Career LDRD program at SNL, and the DOE EFRC in Charge Separation and Transfer (DE-SC0001091). SNL is operated by Sandia Corp., a Lockheed Martin Co., for the US DOE-NNSA (DE-AC04-94AL85000).

8:48AM A12.00005 Adsorption of NH₂ on Graphene in the Presence of Primary Defects, CHAD JUNKERMEIER, NRC Post-Doctoral Associate, U.S. Naval Research Laboratory, STEFAN BADESCU, U.S. Air Force Research Laboratory, THOMAS REINECKE, U.S. Naval Research Laboratory — The primary amine, NH₂, is of interest as a linker between graphene and organic molecules in novel biotechnologies using graphene platforms. We are using *ab initio* electronic structure calculations to study NH₂ adsorption on graphene. We find that the adsorption energy on pristine graphene is on the order of 0.778 eV, a relatively weak bond. We are interested in situations in which the bonding of NH₂ is stronger and are studying systems in which NH₂ adsorbs near defects. We find the adsorption energy of a NH₂ molecule near a second NH₂ molecule is as high as 1.037 eV and that the adsorption near a substitutional N atom is 1.063 eV. We find that there is a RKKY-like interaction between the adsorbate molecules in the case of two NH₂. We will also give results for NH₂ adsorption near other defects.

9:00AM A12.00006 Influence of subsurface hydrogen on the properties of single layer graphene grown on Ru(0001)¹, BOGDAN DIACONESCU, Los Alamos National Laboratory, FRANK HAGELBERG, East Tennessee State University, MAXWELL GRADY, KARSTEN POHL, University of New Hampshire — Graphene has aroused tremendous interest due to its remarkable electronic and mechanical properties. The lack of a band-gap, however, causes a serious challenge for implementing graphene as a material for electrical switches and therefore creative ways of inducing this band-gap are needed. We will present a STM/LEED/DFT study of the single layer graphene on Ru(0001) system in the presence of hydrogen. Structural studies show arrays of Moire superlattices with sizes ranging from 0.9 to 3.0 nm in the presence of hydrogen on the compact surface of ruthenium. First principle calculations help explain the appearance of these arrays of graphene reconstructions driven by the H presence at the Ru(0001) interface, and furthermore, predict the appearance of a bandgap with values correlated with the Moire superstructure sizes in the presence of hydrogen.

¹This work was supported by the Nanoscale Science and Engineering Center for High-rate Nanomanufacturing (NSF NSEC-425826) and NSF DMR-1006863.

9:12AM A12.00007 Graphene symmetry-breaking with molecular adsorbates: modeling and experiment¹, M.A. GROCE, M.K. HAWKINS, Y.L. WANG, W.G. CULLEN, T.L. EINSTEIN, U. of Maryland — Graphene's structure and electronic properties provide a framework for understanding molecule-substrate interactions and developing techniques for band gap engineering. Controlled deposition of molecular adsorbates can create superlattices which break the degeneracy of graphene's two-atom unit cell, opening a band gap. We simulate scanning tunneling microscopy and spectroscopy measurements for a variety of organic molecule/graphene systems, including pyridine, trimesic acid, and isonicotinic acid, based on density functional theory calculations using VASP. We also compare our simulations to ultra-high vacuum STM and STS results.

¹Supported by U. of Maryland NSF-MRSEC under Grant No. DMR 05-20471.

9:24AM A12.00008 Overcoming Doping Difficulty in Graphene via Substrate¹, SU-HUAI WEI, BING HUANG, HONGJUN XIANG, National Renewable Energy Laboratory — Controlling the type and density of charge carriers by doping is the key step for developing graphene electronics. However, direct doping of graphene is rather challenge. Using first-principles method we find that doping could be strongly enhanced in epitaxial graphene grown on silicon carbide substrate. Compared to free-standing graphene, the formation energies of the dopants can decrease by as much as 8 eV. The type and density of the charge carriers of epitaxial graphene layer can be effectively manipulated by suitable dopants and surface passivation. More importantly, contrasting to the direct doping of graphene, the charge carriers in epitaxial graphene layer are weakly scattered by dopants due to the spatial separation between dopants and conducting channel.

¹Work is supported by DOE/BES and NREL LDRD Program

9:36AM A12.00009 Calculations of double-sided coverage of transition metals on graphene, TIMOTHY HECHT, BRET HESS, Brigham Young University — We study the properties of transition metal atoms adsorbed in high coverage on graphene using first principles density functional theory. While there have been many studies on single-sided coverage of adatoms on graphene, we focus on coverage of both sides of graphene. We have observed systems with significantly stronger binding with double-sided coverage than systems with only single-sided coverage. We discuss the effect of double-sided coverage on the electronic structure of these systems.

9:48AM A12.00010 Excited Carriers Relaxation and Hydrogen Dissociation on Hydrogenated Graphene: A Theory, JUNHYEOK BANG, Y.Y. SUN, D. WEST, S.B. ZHANG, Department of Physics, RPI, Troy, New York 12180, USA, S. MENG, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, Z.G. WANG, F. GAO, PNNL, Richland, Washington 99352, USA — Using *ab initio* molecular dynamics coupled with time-dependent density functional theory (TDDFT), we show that the energy transfer of photo-excited carriers into atomic kinetic energy on hydrogenated graphene depends sensitively on the surface H coverage. Here, the energy transfer rate plays a crucial role in the determination of the H dissociation dynamics from graphene. In the low density “isolated” hydrogen atom limit, the energy transfer is significantly suppressed 80 fs after the excitation. Thus, it is difficult to dissociate hydrogen due to the faster energy dissipation from H into carbon backbone, despite that initially the H kinetic energy had increased to around 1.5 eV and the C-H bondlength had stretched to 2.4 Å. In sharp contrast, at the high-density graphene limit, an efficient energy transfer channel is established when the C-H bondlength exceeds 1.4 Å. A fraction of the H readily dissociates within 15 fs. This is because ionized H forms a charged layer that expels, and as such accelerates the H ions with higher initial thermal velocities flying away. Our study thus reveals the importance of performing TDDFT calculations for excited carrier dynamics as from the widely adopted ground-state or constrained DFT dynamics one would expect the C-H bonds in graphene to be significantly stronger, due to full surface passivation, than that of isolated H.

10:00AM A12.00011 Theory of hydrogen induced giant spin-orbit coupling in graphene¹, MARTIN GMITRA, DENIS KOCHAN, JAROSLAV FABIAN, University of Regensburg — Adatoms seem for now the most perspective way of increasing and controlling spin-orbit coupling in graphene. Hydrogen in particular is a role representative, as it gives both lattice deformation and covalent bonding, both contributing towards sigma-pi hybridization needed for the increase of the spin-orbit coupling around K. To establish the relevant physics of the H induced spin-orbit coupling in graphene, we have performed systematic calculations of hydrogenated graphene. We found that the magnitude of the coupling is of the order of meVs, exactly what is needed to explain the experimental data on spin relaxation. Doing both first-principal calculations and tight-binding modeling we calculate the spin-orbit splittings and introduce an effective hopping model that can be used in realistic investigations.

¹The work is supported by the DFG SFB 689.

10:12AM A12.00012 Understanding electron-phonon interactions in doped graphene: the case of Li-intercalated graphite, ANDREW WALTERS, MPI for Solid State Research, Germany, MARK DEAN, Brookhaven National Lab, USA, CHRISTOPHER HOWARD, MARK ELLERBY, JONATHAN PAYNE, University College London, UK, MICHAEL KRISCH, ALEXEI BOSAK, European Synchrotron Radiation Facility, France, GIANNI PROFETA, University of L'Aquila, Italy, MATTEO CALANDRA, FRANCESCO MAURI, University Paris 6, France — The recent explosion of research on doped graphene systems together with the discovery of superconductivity in CaC₆ has reignited the interest in graphite intercalation compounds (GICs). While it is generally agreed that the superconductivity observed in GICs is BCS-like, there is still much controversy over which electrons and which phonons are primarily involved in the electron-phonon (e-ph) coupling leading to superconductivity. Moreover, thanks to the close similarity between the electronic structure of GICs and doped graphene, the study of e-ph interactions in GICs provides a unique approach to help elucidate the complex e-ph interactions in doped graphitic systems. We present inelastic x-ray scattering measurements of the high energy (~ 200 meV) graphitic phonons in LiC₆ across the Brillouin zone. The LiC₆ phonons are much softer than in pure graphite, as the electron doping destabilizes the C-C bonds. We observe large phonon broadening for all phonons at the graphite Brillouin zone center, suggestive of unusual e-ph interaction phenomena. We discuss our results in the light of the e-ph coupling reported from angle-resolved photoemission spectroscopy and in relation to strong non-adiabatic effects observed using Raman scattering.

10:24AM A12.00013 p-n codoping induced improvement of adsorption, magnetism, and electronic structure in 3d transition metal adatoms on graphene¹, SHIFEI QI, Shanxi Normal Univ. and Univ. of Science & Technology of China, ZHENYU ZHANG, Univ. of Science & Technology of China and Harvard Univ., XIAOHONG XU, Shanxi Normal Univ. — Generating ferromagnetism and preserving its unique properties in graphene are crucial to the development of graphene-based spintronics. Using first-principles calculations, we investigate the effects of p-n codoping method on absorption, magnetic properties, and of electronic structures 3d transition metal adatoms (TMs, i.e., Fe, Co, and Ni) on graphene. It is found that p-n codoping can strengthen the adsorption of TMs on graphene, and enhance the magnetic moments of Fe and Co adatoms on graphene. It can also cause Ni to transition from nonmagnetic to magnetic states. Furthermore, magnetic coupling between two p-n pairs is also explored. Electronic structure analysis indicates that p-type dopant turns graphene into an electron-deficient system, and compensates for the shift in Fermi level caused by adsorption of TMs. Therefore, p-n codoping can bring about increases in the magnetic moment and adsorption of TM-adsorbed graphene systems while preserving the unique properties of graphene.

¹Supported by NNSF of China, USNSF, and DMSE/BES of USDOE.

10:36AM A12.00014 Directed Assembly of Molecules on Graphene/Ru(0001)¹, L.Z. ZHANG, H.G. ZHANG, J.T. SUN, Y. PAN, Q. LIU, J.H. MAO, H.T. ZHOU, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, T. LOW, IBM Thomas J. Watson Research Center, New York 10598, USA, H.M. GUO, S.X. DU, H.-J. GAO, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES TEAM, IBM THOMAS J. WATSON RESEARCH CENTER COLLABORATION — Recently, the graphene monolayers have been seen to adopt a superstructure - moiré pattern - on Ru(0001). By using low temperature scanning tunneling spectroscopy, we identified the laterally localized electronic states on this system. The individual states are separated by 3 nm and comprise regions of about 90 carbon atoms. This constitutes a highly regular quantum dot-array with molecular precision. It is evidenced by quantum well resonances with energies that relate to the corrugation of the graphene layer. By using scanning tunneling microscopy/spectroscopy, we demonstrate the selective adsorption and formation of ordered molecular arrays of FePc and pentacene molecules on the graphene/Ru(0001) templates. With in-depth investigations of the molecular adsorption and assembly processes we reveal the existence lateral electric dipoles in the epitaxial graphene monolayers and the capability of the dipoles in directing and driving the molecular adsorption and assembly. When increasing the molecular coverage, we observed the formation of regular Kagome lattices that duplicate the lattice of the moiré pattern of monolayer graphene.

¹Supported by MOST (2009CB929103, 2011CB932700) of China

10:48AM A12.00015 Study on the Adsorption of Small Gas Molecules on graphene by the Density Functional Theory Calculations, YIMING MI, Graduate Department, Shanghai University of Engineering Science, 333 Longteng Rd., Shanghai 201620, PR CHINA, XINXIN ZHAO, School of Fundamental Studies, Shanghai University of Engineering Science, 333 Longteng Rd., Shanghai 201620, PR CHINA, SHUICHI IWATA, Graduate School of Frontier Sciences, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8654, JAPAN — The absorption of different small gas molecules on graphene is investigated based on the pseudopotential method within the density functional theory formalism. The preferred adsorption site (among the top, bridge, and hollow positions) and orientations of these molecules on the graphene surface are analyzed and the related adsorption energies are calculated. The charge transfer between the adsorbed molecules and the graphene is discussed as well.

Monday, February 27, 2012 8:00AM - 10:48AM –
Session A13 DMP GMAG: Focus Session: Magnetic Nanostructures-Patterned Nanostructures and Nanowires 211

8:00AM A13.00001 High Frequency Excitation of Nanometer-Scale, Strongly Coupled FM / NM / FM Disks¹, JAVIER PULECIO, PETER WARNICKE, SHAWN POLLARD, DARIO ARENA, YIMEI ZHU, Brookhaven National Laboratory — There is great interest in the manipulation of magnetic domains in nanostructures from both a fundamental and applications perspective. In particular, the use of resonant frequency excitations permits a power reduction of the driving forces necessary to induce detectable motion in magnetic vortex structures. Here we present an experimental and numerical study of patterned tri-layered disk stacks which are composed of 25nm Permalloy|1nm Copper|15nm Permalloy, excited at resonance, ranging from 250-500nm in radii. In-situ Lorentz microscopy was used to acquire time averaged real space images of the vortices' gyrotropic motion and micromagnetic simulations were implemented to further understand the coupled dynamics between the ferromagnetic layers across the thin non-magnetic spacer layer. We discuss the effects of interlayer coupling on the vortex trajectories and resonant frequencies for the individual ferromagnetic layers.

¹Work supported by Department of Energy, Office of Basic Energy Science, under contract No. DE-AC02-98CH10886

8:12AM A13.00002 Controlling the formation process of vortex states in magnetic nanodots with asymmetric geometry¹, MI-YOUNG IM, PETER FISCHER, CXRO/LBNL, ANDREAS VOGEL, GUIDO MEIER, IAP/U Hamburg — Magnetic vortex structures in nanoscale elements are currently highly attractive, since they offer exciting topological spin configurations to study on a fundamental level nanoscale spin behavior and they show great potential for applications in data storage and memory technologies. One of the primary questions is to tailor the nucleation process of vortex structures, which would open the opportunity for the control of magnetic/spin phenomena in magnetic vortices such as the resonant motion of a magnetic vortex core, etc. We have investigated the stochastic character of the formation process of vortex states in permalloy (Ni₈₀Fe₂₀) nanodots with different geometries by direct imaging of vortex structures with high resolution magnetic transmission soft X-ray microscopy (MTXM). We observe that the formation process of vortex state sensitively depends on the geometry of nanodots. Based on our experimental result, we will discuss the possibility to control the generation process of magnetic vortex states by directed modifications of the geometry of nanodots.

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¹Supported by DOE/BES No. DE-AC02-05CH11231, DFG/SFB 66 and GK 1286.

8:24AM A13.00003 Quantum depinning of the magnetic vortex core in micron-size permalloy disks, RICARDO ZARZUELA, SAÜL VÉLEZ, JOAN MANEL HERNANDEZ, JAVIER TEJADA, Departament de Física Fonamental, Universitat de Barcelona, VALENTYN NOVOSAD, Materials Sciences Division, Argonne National Laboratory, GRUP DE MAGNETISME TEAM, MATERIALS SCIENCES DIVISION TEAM — The vortex state being characterised by an in-plane closed flux domain structure and an out-of-plane magnetization at its centre (known as the vortex core) is one of the magnetic equilibria of thin soft ferromagnetic micron-size dots. The vortex core is a mesoscopic object and so it is a suitable candidate to observe quantum tunneling of its magnetic moment between classically stable magnetic configurations. For the first time, we report experimental evidence of quantum dynamics of the vortex core of micron-size Permalloy (Fe₁₉Ni₈₁) disks induced by the application of an in-plane magnetic field. It is attributed to the quantum tunneling of the vortex core through pinning barriers, which are associated to structural defects in the dots, towards its equilibrium position. The crossover temperature from the thermal to the quantum regime is obtained within the framework given by the Caldeira-Leggett theory. Comparison between experiments and theory points to tunneling of the vortex core by steps of the order of 0.3 nm and gives estimates to the parameters characterising the pinning barriers.

8:36AM A13.00004 Energy barriers for vortex nucleation and annihilation in sub-100 nm magnetic dots¹, ANDREW T. KING, IGOR V. ROSHCHIN, Texas A&M University — Understanding energy barriers involved in nucleating and annihilating magnetic vortices in nanodots is important for magnetic memories and nano-oscillators. We used a "rigid-vortex approximation" and micromagnetic approach to calculate the total magnetic energy of a nanodot for various magnetic configurations. This was done for 20 nm-thick iron nanodots with different diameters (30, 40, 65, and 80 nm) as a function of applied magnetic field. By analyzing the energy landscape for different magnetic configurations, we calculated the energy barrier for switching from the vortex to the single-domain state (vortex annihilation) and the converse (vortex nucleation). The applied fields required to overcome these two barriers are compared to those obtained from the simulations directly and to the experimental values.² The role of the thermal fluctuations in the temperature dependence of these critical fields will be discussed by comparison of the energy barriers with the thermal energy, kT.

¹Work is supported by Texas A&M University, TAMU-CONACYT Collaborative Research Program.

²R. K. Dumas, et al., *Appl. Phys. Lett.* **91**, 202501 (2007).

8:48AM A13.00005 A Novel Non-lift-off Block Copolymer Nanolithography Technique for Etch-damage Susceptible Magnetic Materials, A. BARUTH, A. SHANKAR, K. WALSTER, M.D. RODWOGIN, M.J. ERICKSON, M.A. HILLMYER, C. LEIGHTON, University of Minnesota - Twin Cities — Nanolithographic techniques based on self-assembled block copolymer templates offer exceptional potential for fabrication of large-area nanostructure arrays from a wide variety of functional materials. Despite significant progress with control of the template ordering and development of pattern transfer schemes, significant issues exist with common techniques such as lift-off and etching. Here, we demonstrate successful execution of a nanolithographic process based on climate-controlled solvent annealing of easily degradable cylinder-forming poly(styrene-*b*-lactide) block copolymer films that avoids both lift-off, and some of the most challenging aspects of etching. In particular, our overfill/planarize/etch-back scheme leads to retention of robust ferromagnetism even in 24 nm diameter dots of a material ($\text{Ni}_{80}\text{Fe}_{20}$) that is both magnetically soft and susceptible to etch damage. The result is a large-area array of 24 ± 1.6 nm diameter magnetic nanodots with exceptional hexagonally-close-packed long range order that retain their crystallinity and $\sim 70\%$ of the bulk magnetization. Extensive diffraction, microscopy, magnetometry, and electrical measurements provide detailed characterization of the pattern formation and fidelity. Funded by NSF MRSEC.

9:00AM A13.00006 Quenching of the initial ac Susceptibility in Single Domain Ni Nanobars, ZHENG GAI, XIAOGUANG ZHANG, IVAN I. KRAVCHENKO, SCOTT T. RETTERER, J. WENDELKEN, Oak Ridge National Laboratory — The ac susceptibility measurement probes the dynamic properties of a magnetic material, which is believed to consist of magnetization rotation and domain wall motion contributions. Here we report the observation of a complete quenching of the initial ac susceptibility for a single domain Ni nanobar array, when the ac field is aligned with the long axis of the bars. The vanishing of the susceptibility in one direction is a unique nanoscale phenomena, allowing an unambiguous determination of the magnetic state of the nanostructure and a clean separation of different contributions to its dynamic properties. For example, an unambiguous determination of the temperature dependent surface anisotropy energy is obtained when the field is applied perpendicular to the long axis. This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Office of Basic Energy Sciences, U.S. Department of Energy.

9:12AM A13.00007 Microwave assisted magnetization reversal in cylindrical antidot arrays with in-plane and perpendicular anisotropy, MEHMET YUMAK, KERIM TURE, GULEN AKTAS, Bogazici University Department of Physics, VICTOR VEGA, VICTOR PRIDA, Dpto. Física, Universidad de Oviedo, Calvo Sotelo, CARLOS GARCIA, Bogazici University Department of Physics — Porous anodic alumina is a particularly attractive self-ordered system used as template to fabricate nanostructures. The anodic film contains a self-ordered hexagonal array of parallel pores with tunable pore size and interpore distance, and whose pore locations can be templated. Deposition of magnetic films onto porous alumina leads to the formation of porous magnetic films, whose properties differ significantly from those of unpatterned films. The study of antidot arrays has both technological and fundamental importance. Although porous alumina films are typically synthesized in a planar geometry, in this work we deposited NiFe and Ti/CoCrPt magnetic films with in-plane and out-of-plane anisotropy onto cylindrical-geometry porous anodic alumina substrates to achieve cylindrical antidot arrays. The effect of both, the magnitude of the AC current and the circular magnetic field on the magnetization reversal has been studied for in-plane and perpendicular anisotropies. The level of reduction in the switching field was found to be dependent on the power, the frequency of the microwave pulses and the circular applied magnetic field. Such a reduction is associated with the competition between pumping and damping processes.

9:24AM A13.00008 DC and High-frequency Magnetic Properties of Patterned Ferromagnetic Nanostructures¹, HUAJIE KE, YITZI CALM, MARK TUOMINEN, Department of Physics, Center for Hierarchical Manufacturing, University of Massachusetts Amherst — Magnetic mesoscopic and nanostructures have promising applications such as high-density data storage, magnetic field sensors, and microwave devices. Patterned magnetic structures are especially interesting because their constitutive material, sizes and geometry are easily adjustable in fabrication. This work aims to study dc and radio frequency magnetic properties of Co and permalloy patterned structures and the effect of magnetic coupling. We use electron-beam lithography and complementary techniques to ferromagnetic nanostructures with various separations to control the strength of magnetic interaction. SQUID and complementary MFM characterization are performed to observe the dc magnetic properties. AC susceptibility is used to investigate the low frequency response. Microstrip transmission lines are then incorporated to measure the scattering parameters between 300kHz and 6GHz. The equivalent RLCG circuit elements can be extracted to obtain the effective magnetic permeability for different ferromagnetic structures.

¹This research is supported by NSF grants CMMI-1025020 and DMR-0907201.

9:36AM A13.00009 Precise control of vortex chirality and polarity in “Pac-Man”-like magnetic nanodots by in-plane magnetic field¹, VLADIMIR CAMEL, JAROSLAV TÓBIK, Institute of Electrical Engineering, Slovak Academy of Sciences, Slovakia, GORAN KARAPETROV, Department of Physics, Drexel University and Institute of Electrical Engineering, Slovak Academy of Sciences — Here we explore size-dependent magnetic states of sub-100 nm Permalloy nanomagnets of specific geometry. The geometry is suitable for independent setting and readout of vortex polarity and chirality by applying *in-plane magnetic fields* only. Micromagnetic calculations show that in “Pac-Man”-like magnetic nanodots the relaxation channels to specific chirality and polarity states from uniform magnetization state are deterministic and are not influenced by the presence of moderate out-of-plane fields. The particular geometry opens straight channel for magnetization relaxation towards stable closure-domain vortex state with specific chirality and polarity. We explore a wide geometrical phase space in search for stable and predictable remanent vortex configurations. We find that in these nanomagnets the write process is simple and the signal is easily readable.

¹This publication is the result of the following project implementations: Development of the Centre of Excellence for New Technologies in Electrical Engineering - 2nd, ITMS code 26240120019, supported by the R & D Operational Program funded by ERDF.

9:48AM A13.00010 Direct imaging of complex domain walls and chirality sensors in magnetic nanostripes, S.R. BOWDEN, J. UNGURIS, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD 20899, Y. JANG¹, M. MASCARO, C.A. ROSS, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge MA 02139 — Domain walls (DWs) in patterned ferromagnetic nanostripes are increasingly being considered for non-volatile and radiation hard data storage and logic applications. We use scanning electron microscopy with polarization analysis (SEMPA) to image the formation of complex domain walls in nanostripes and local patterned structures used for sensing DW chirality. The DWs studied have a transverse orientation, where the in-plane spin direction of a 180° DW is perpendicular to the nanostripe axis. We demonstrate a technique where two 180° DWs of alternating chirality may interact to form a stable DW with 360° rotation as opposed to DW annihilation. Higher order DWs with $n\pi$ rotation are demonstrated, where n is an integer number of interacting 180° DWs. The detection of moving 180° DWs via external fields is studied by placing patterned magnetic triangular elements above and below the nanostripe in-plane. As the DW propagates across the wire, the stray field interacts and switches the magnetization of the triangles. The chirality of the DW may be sensed by designing the triangles to respond to the inherent asymmetry of the DW's stray field.

¹Present Address: Samsung Advanced Institute of Technology, Gyeonggi-Do 446-712, Republic of Korea

10:00AM A13.00011 A high-spin atomic 1-D system with a spin-induced CDW instability¹, NADER ZAKI, CHRIS MARIANETTI, Columbia University, PETER JOHNSON, Brookhaven National Lab, RICHARD OSGOOD, Columbia University — We report on low-temperature STM measurements of a Co atomic-wire system that has been realized by the technique of self-assembly on a vicinal Cu(111) substrate [1,2]. We show that for this bimetallic case, the Co-wire system undergoes a CDW instability leading to a 1-D high-spin system. This type of instability does not appear to have been previously reported for a bi-metallic system, particularly for a chain of Co atoms. Using ab initio theoretical calculations, it is deduced that the CDW instability is spin-induced by way of symmetry breaking in the spin population. This result presents a fundamental electronic-structure mechanism for CDW instability that is distinct from previously reported metal-semiconducting systems [3], in that spin clearly plays an essential role in lowering the energy of the system. Furthermore, the calculations indicate that the high-spin correlated state of the constituent Co atoms is a necessary consequence of this CDW instability. Finally, the ferromagnetic nature of this realized system raises questions with regard to substrate spin mediation, such as the possible role of Kondo and RKKY interaction. [1] N. Zaki et al, Phys. Rev. B 80, 155419 (2009) [2] N. Zaki et al, Phys. Rev. B 83, 205420 (2011) [3] P. C. Snijders and H. H. Weitering, Rev. Mod. Phys. 82, 307 (2010)

¹Department of Energy Contract No. DE-FG 02-04-ER-46157

10:12AM A13.00012 Spin resonance in Luttinger liquid with spin-orbit interaction, OLEG TRETIKOV, K.S. TIKHONOV, V.L. POKROVSKY, Texas A&M University — The spin-orbit interaction leads to a narrow spin resonance at low temperatures, even in the absence of an external magnetic field [1]. We study the effect of electron-electron correlations on the resonance. These correlations are strong in quantum wires and cannot be neglected. We show that the electron correlations change the shape and width of the resonance and produce an additional weak resonance at the plasmon frequency.

[1] Ar. Abanov, V. L. Pokrovsky, W. M. Saslow, and P. Zhou, arXiv:1008.1225.

10:24AM A13.00013 Telegraph Noise in LSMO Nanowires¹, NICHOLAS BRONN, XIAOQIAN CHEN, University of Illinois at Urbana-Champaign, Department of Physics, Materials Research Laboratory, JASON HOFFMAN, ANAND BHATTACHARYA, Argonne National Laboratory, Center for Nanoscale Materials, PETER ABBAMONTE, NADYA MASON, University of Illinois at Urbana-Champaign, Department of Physics, Materials Research Laboratory — Hole-doped manganites with the perovskite structure exhibit a variety of superlative properties because of close competition among ferromagnetic metallic, paramagnetic insulating, as well as various charge, spin, and orbitally ordered phases. We have recently observed random telegraph noise (RTN) in low-temperature conductance measurements of epitaxially-grown $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ nanowires patterned by electron-beam lithography and ion milling to widths of $\sim 80\text{nm}$. The RTN is apparent at temperatures less than 30K. It is thought that the RTN is the result of domain fluctuations, which are more clearly observable in such narrow wires.

¹This research was supported by the DOE-DMS under grant DE-FG02-07ER46453 through the Frederick Seitz Materials Research Laboratory at the University of Illinois at Urbana-Champaign.

10:36AM A13.00014 Direct Imaging of Non-Adiabatic Spin Torque Effects on Vortex Core Orbits, SHAWN POLLARD, LEI HUANG, Department of Condensed Matter Physics, Brookhaven National Laboratory, NY 11973, KRISTEN BUCHANAN, Department of Physics, Colorado State University, Fort Collins, CO 80523, DARIO ARENA, National Synchrotron Source, Brookhaven National Laboratory, NY 11973, YIMEI ZHU, Department of Condensed Matter Physics, Brookhaven National Laboratory, NY 11973 — Recently high frequency, current induced vortex motion has received a great deal of interest from a spintronic perspective, as it suggests a possible low power, high speed writing process. However, understanding the processes that govern this motion, specifically the relative contributions of adiabatic and non-adiabatic spin torque effects, has been difficult due to experimental constraints. We developed a novel TEM sample stage in which we apply high frequency currents in-situ to excite resonant motion in Permalloy disc structures ($2000 \times 2000 \times 50\text{nm}$) with high spatial resolution ($< 5\text{nm}$ for dynamic measurements). We have imaged the time-averaged vortex trajectory through resonance. We find that the orbital amplitudes are drastically different for clockwise and counterclockwise chiralities, indicating the presence of both Oersted fields and non-adiabatic spin torque effects, and that the orbital size scales linearly with current density varied between $(7.1-10.0) \times 10^{10} \text{ A/m}^2$. These results allow us to extract a value for the non-adiabatic spin torque with unprecedented precision. Additionally, we report on off-resonance effects, such as tilting and variations in the ellipticity of the orbit as it is swept through resonance, with first of their kind experimental observations.

Monday, February 27, 2012 8:00AM - 11:00AM –
Session A14 GMAG DMP FIAP: Focus Session: Spins in Semiconductors - Magnetic Semiconductors I 212

8:00AM A14.00001 Oxygen Annealing Studies of $\text{SnO}_2\text{:Co}$ Thin Films Deposited by RF Sputtering¹, GRATIELA STOIAN, Florida State University, P.A. STAMPE, R.J. KENNEDY, Florida A&M University, Y. XIN, National High Magnetic Field Laboratory, Tallahassee, S. VON MOLNAR, Florida State University — We report on post-deposition oxygen annealing studies of $\text{SnO}_2\text{:Co}$ thin films to examine the origin of the room temperature ferromagnetism (RTFM) observed in such materials. Materials are deposited on r-cut sapphire substrates by RF sputtering from a doped target with 5 at.% Co nominal concentration. Magnetization measurements reveal that as-grown samples in Ar atmosphere are non-magnetic at RT. However, by annealing them in low O_2 pressure (10^{-4} - 2×10^{-4} Torr), the saturation moment increases to $\sim 0.78 \mu_B/\text{Co}$ at RT, somewhat lower than the expected value for Co^{2+} ions. This verifies that the Co ions are incorporated in the matrix. X-ray diffraction data show a decrease in crystallinity for the most magnetic samples annealed in O_2 at 2×10^{-4} Torr. To confirm this, further structural and temperature-dependent magnetic measurements for various annealing protocols are underway to determine the nature of magnetism in $\text{SnO}_2\text{:Co}$ sputtered thin films.

¹Work supported by NSF DMR-0605734.

8:12AM A14.00002 Embedded Ferromagnetic GdN Nano-Islands in GaN by Molecular Beam Epitaxy¹, T.F. KENT, J. YANG, L. YANG, M.J. MILLS, R.C. MYERS, Department of Materials Science and Engineering, The Ohio State University, Columbus, OH — Nano-islands of GdN are embedded into a GaN matrix by plasma-assisted molecular beam epitaxy. X-ray diffractometry shows that the cubic rocksalt islands are (111) oriented to the c-axis of the hexagonal wurtzite GaN matrix. Cross-sectional scanning transmission electron microscopy allows for the study of island formation, which occurs after 1.2 monolayers of GdN coverage, forming discrete particles, which the GaN matrix grows epitaxially around. Magnetometry reveals two ferromagnetic phases, one due to the GdN particles with Curie temperature of 70K and an anomalous phase with ferromagnetism persistent to room temperature. This room temperature ferromagnetic phase is strongly anisotropic, with out of plane magnetization nearly 300% larger than in-plane at fields less than 1T. Optical characterization reveals that GdN, when strained to GaN, is a semiconductor with direct and indirect bandgaps at 1.2eV and 0.75eV, respectively.

¹Funding provided by the Center for Emergent Materials under NSF Award Number DMR-0820414 and the Institute for Materials Research at OSU under the Interdisciplinary Materials Research Grants (IMRG) program at OSU.

8:24AM A14.00003 Synthesis and Characterization of Co-doped ZnO Dilute Magnetic Semiconducting Nanorods¹, N. DAS, S. KHANRA, S. BHAMIDIPATI, K. MANIVANNAN, P. KAHOL, K. GHOSH, Missouri State University, DEPARTMENT OF PHYSICS ASTRONOMY AND MATERIALS SCIENCE TEAM — Transition-metal doped ZnO dilute magnetic semiconducting nanomaterials are considered as ideal systems for carrying out research in the field of spintronics as they can successfully combine magnetism and electronics in a single substance. ZnO is a wurtzite-type wide-bandgap semiconductor of the II-VI semiconductor group with band gap energy of 3.37 eV. Hydrothermal synthesis of undoped ZnO and Co-doped ZnO nanorods is carried out using aqueous solutions of $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, $\text{Co}(\text{C}_2\text{H}_3\text{OO})_2 \cdot 4\text{H}_2\text{O}$, and using NH_4OH as hydrolytic catalyst. Nanomaterials of different sizes and shapes were synthesized by varying the process parameters such as molarity (0.15M, 0.3M, 0.5M) and pH (8-11) of the precursors, growth temperature (130°C), and annealing time during the hydrothermal Process. Structural, morphological, optical and magnetic properties are studied using various techniques such as XRD, SEM, UV-vis spectroscopy, and SQUID magnetometer. XRD and SEM studies reveal nanorods with hexagonal wurtzite structure with length in the range of 200 to 500 nm, and cross section in the range of 30 to 60 nm. Detailed structural, optical, and magnetic properties will be discussed in this presentation.

¹This work is supported by National Science Foundation (Award Number DMR-0907037).

8:36AM A14.00004 Defect-Induced High- T_C Ferromagnetism and Spinodal Nanodecomposition in MgO, MASAYOSHI SEIKE, Grad. School of Eng. Sci., Osaka Univ. and Cent. Research Labs., Sysmex Corp., TETSUYA FUKUSHIMA, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA, Grad. School of Eng. Sci., Osaka Univ. — Based on a first-principles study of the magnetic properties of MgO with Mg vacancies [1,2], we calculated the electronic structures and exchange coupling constants for Monte Carlo Simulation (MCS) of the Curie temperature (T_C). We also performed MCS of the spinodal nanodecomposition based on the calculated chemical pair interactions between the vacancies. In this study, it was found that hole-doping by Mg vacancies leads to a ferromagnetic ground state, invoking long-range magnetic interaction, and that T_C can reach room temperature at sufficient vacancy concentrations of 15 at.% under a homogeneously distributed condition. However, it was also found that the chemical pair interactions between vacancies are significantly attractive and that the system can form super-paramagnetic clusters of vacancies with strong ferromagnetic coupling in the clusters. These results suggest that, by the spinodal nanodecomposition, the T_C or blocking temperature (T_B) can be enhanced and reach room temperature at smaller vacancy concentrations compared with those estimated for room-temperature ferromagnetism under the homogeneous distribution condition.

[1] M. Seike, et al. Jpn. J. Appl. Phys. 50, 090204 (2011).

[2] K. Sato, et al. Rev. Mod. Phys. 82, 1633 (2010).

8:48AM A14.00005 Gd in GaN: the role of magnetic vacancy clusters¹, ALEXANDER THIESS, PETER H. DEDERICH, STEFAN BLÜGEL, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany, WALTER R.L. LAMBRECHT, Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106-7079, USA — Five years after the experimental discovery of colossal magnetic moments and ferromagnetic ordering above room temperature in gadolinium doped gallium nitride the identification of its microscopic origin is still not accomplished. Here, we are proposing a new model explaining the origin: the clustering of magnetic gallium vacancies. First, we show that such clustered gallium vacancies indeed can preferentially occur by utilizing a simplified growth model, for which we provide the input by large-scale first-principles Green function calculations. The same calculations reveal that the dangling bond nitrogen states around gallium vacancies become significantly spin-polarized. Moreover, we are able to extract a rich set of information on the magnetic exchange interactions between those spin-polarized atoms. These exchange interactions are the basis for our study on the thermal behavior of magnetic vacancy clusters by means of Monte-Carlo simulations. We present the resulting magnetic properties of our simulations and highlight important similarities to the experiment that all point at gallium vacancy clusters as the origin of the experimentally observed magnetic properties in GaN:Gd.

¹Financial support from the DAAD is gratefully acknowledged.

9:00AM A14.00006 Photoluminescence studies of various magnetic phases in (Zn,Mn)Te/ZnSe QDs¹, JOSEPH MURPHY, LARS SCHWEIDENBACK, BIPLOB BARMAN, RAFAL OSZWALDOWSKI, ALEXANDER CARTWRIGHT, BRUCE MC-COMBE, ATHOS PETROU, IGOR ZUTIC, SUNY at Buffalo, Buffalo, NY, IAN SELLERS, University of Oklahoma, Norman, OK, WEN CHUNG CHOU, WU-CHING FAN, National Chiao Tung University, Hsinchu, Taiwan — We have carried out a magneto-PL study of a single layer of (Zn,Mn)Te/ZnSe quantum dots. The CW PL from a previously studied 5 layer sample exhibits high circular polarization but very small Zeeman splitting. Time-resolved PL exhibited a temperature independent temporal red shift, associated with the magnetic polaron formation. These data have been interpreted as due to the presence of an antiferromagnetic phase for the Mn ions. In the present study, the CW magneto-PL spectra exhibit high circular polarization, but significantly larger Zeeman splittings. Furthermore the Zeeman splitting depends strongly on temperature and vanishes at 50 K. These results indicate the presence of a different magnetic phase for the Mn ions in the single layer QD sample. Time-resolved PL experiments suggest the formation of magnetic polarons in this sample.

¹Work at SUNY is supported by DOE-BES, ONR, AFOSR-DCT, NSF, and CAREER

9:12AM A14.00007 Controlling Curie Temperature of (GaMn)As Through Location of the Fermi Level Within the Impurity Band¹, MARGARET DOBROWOLSKA, University of Notre Dame — This talk will address the unresolved issue of ferromagnetism in the ferromagnetic semiconductor GaMnAs, a material whose understanding is of central importance to semiconductor-based spintronics. The above unresolved issue concerns the question of whether the ferromagnetic order in GaMnAs is mediated by valence band holes or by holes residing in the impurity band. The results to be presented are based on the investigation of a wide range of GaMnAs samples using a comprehensive set of experiments that include magnetization, electrical transport and magneto-optics, along with studies of microscopic composition by channeling Rutherford back-scattering and particle-induced x-ray emission. These experiments show unambiguously that the holes underlying ferromagnetic order in GaMnAs reside in the impurity band; and that it is not only the concentration of Mn and of holes, but also the specific location of the Fermi level in the impurity band that establishes the Curie temperature of this material. Specifically, we show that having the Fermi level near the middle of the impurity band, where the states are most extended, is more important for raising T_c than increases in the effective Mn or hole concentrations. Since the location of the Fermi level can be controlled by a variety of means both during and after growth, this new understanding automatically provides practical guidelines for increasing the critical temperature.

¹Collaborators: K. Tivakornsasithorn, X. Liu, J.K. Furdyna, M. Berciu, K.M. Yu and W. Walukiewicz

9:48AM A14.00008 Interstitial Cu Codoping Method for High Curie Temperature (Ga,Mn)As, HITOSHI FUJII, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA, Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University, Japan, LARS BERGQVIST, Retired Department of Materials Science and Engineering, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden, PETER H. DEDERICH, Peter Gruenberg Institut, Forschungszentrum Juelich, D-52425 Juelich, Germany — Based on first principles calculations, we propose a solubility control method of magnetic impurities in dilute magnetic semiconductors (DMSs). We show that donor atoms, such as Cu, introduced at the interstitial sites in GaAs enhance the solubility of Mn. As a result, Mn can be doped to more than 20 percent in GaAs in the thermal equilibrium condition [1]. Due to the carrier-induced nature of the ferromagnetism in DMSs, the ferromagnetism is suppressed because of the compensation of hole from Mn acceptors by the codoped interstitial Li or Cu. In order to recover the ferromagnetism, we propose low temperature annealing after crystal growth to remove only the interstitials. Our NEB (Nudged Elastic Band method) calculation results show that the effective migration barrier of Cu in GaMnAs is about 0.2eV. This value is small compared with the migration barrier of Li in GaMnAs (about 0.5eV). Even if Li, it is possible to diffuse Li in (Ga_{0.7}Mn_{0.3})As at 0.12 micron in 24 hours [2]. In case of Cu, therefore, we can expect further annealing distance than Li case because of the low migration barrier.

[1] H. Fujii, et al.: Appl. Phys. Express 4 (2011) 043003.

[2] L. Bergqvist, K. Sato: Phys. Rev. B 83, 165201 (2011)

10:00AM A14.00009 Tight binding study of single ion magnetic anisotropy of Mn²⁺ in Ga(Mn)As¹, HEMACHANDER SUBRAMANIAN, JONG HAN, University at Buffalo, State University of New York — Bulk uni-axial magnetic anisotropy of Ga(Mn)As observed in experiments has not been well understood as much as cubic magnetic anisotropy in the same material. We propose that the uni-axial anisotropy arises due to the coupling of local lattice distortions around Mn²⁺ impurity ion to its spin state through spin-orbit coupling of holes bound to the impurity ion. We model the coupling using nearest-neighbor tight-binding and many-body perturbation theory. The model includes intra-atomic Coulomb interaction inside Mn²⁺ ion, spin-orbit interaction of holes at the Γ point, $p-d$ hopping interaction between Mn²⁺ ion d orbitals and As ion p orbitals, and strain due to local lattice distortions. We observe breaking of tetrahedral symmetry around the Mn²⁺ ion when the system is paramagnetic. We explore the effect of this broken symmetry in stabilizing certain magnetization directions through spin-orbit coupling in the ferromagnetic regime.

¹NSF DMR-0907150

10:12AM A14.00010 Infrared to visible magneto-optical effects in (Ga,Mn)As, N. TESAROVA, C.T. ELLIS, G. ACBAS, A. MUKHERJEE, K. VYBORNÝ, J. CERNE, Physics Dept., University at Buffalo, SUNY, J. SUBRT, T. OSTATNICKY, P. NEMEC, Faculty of Mathematics and Physics, Charles University in Prague, Czech Rep., V. NOVAK, Institute of Physics ASCR, v.v.i., Prague, Czech Rep., J. SINOVA, Dept. of Physics, Texas A&M Univ., College Station, TX — (Ga,Mn)As is perceived as a model material for future low-power spintronics devices due to its carrier mediated ferromagnetic properties. Despite the extensive theoretical and experimental studies, the energy band structure and the mechanism of ferromagnetic order (of Mn spins) still remains a matter of controversy [Ohya, Nature Physics 2011; Jungwirth, PRL 2010]. In our study, we employ magneto-optical Faraday and Kerr measurements to probe the character of the states near the Fermi energy, which is expected to be responsible for Mn-ordering. We also study the spectral dependence of magnetic linear dichroism that is mainly sensitive to the states mediating the Mn-Mn interaction [Kimel, PRL 2005]. The measurements are performed from the infrared to visible range (100 – 2600 meV) on high quality samples with different Mn concentration (1.5 – 14 %) with Curie temperatures up to 190 K. The results are compared with the predictions of $k \cdot p$ theory with antiferromagnetic $p-d$ exchange. We acknowledge the financial support provided by NSF-DMR1006078 and Faculty of Mathematics and Physics, Charles University in Prague.

10:24AM A14.00011 Spin-Transfer-Torque Driven Domain Wall Motion in (Ga,Mn)(As,P), E.K. VEHSTEDT, Dept of Physics & Astronomy, Texas A&M Univ; Inst of Physics, ASCR vvi, L.P. ZARBO, Inst of Physics, ASCR vvi, K. VYBORNÝ, Dept of Physics, SUNY Buffalo; Inst of Physics, ASCR vvi, E. DE RANIERI, Hitatch-Cambridge Laboratory, Uni of Cambridge, H.G. KATZGRABER, Dept of Physics & Astronomy, Texas A&M Univ; ETH Zurich, J. WUNDERLICH, Hitatch-Cambridge Laboratory, Uni of Cambridge; Inst of Physics, ASCR vvi, T. JUNGWIRTH, Inst of Physics, ASCR vvi; School of Physics & Astronomy, Uni of Nottingham, J. SINOVA, Dept of Physics & Astronomy, Texas A&M Univ; Inst of Physics, ASCR vvi — Precise control of domain wall (DW) motion in magnetic materials is a prerequisite for the realization of novel non-volatile and down-scalable logic/memory devices which promise to overcome the limitations of current technologies. While magnetic fields are the obvious choice for DW manipulation, in spin-orbit (SO) coupled materials, electric fields provide an additional means of control via current-induced spin torque. We extend the existing theoretical framework used to describe magnetization dynamics in uniform ferromagnets (FM) to dilute FM semiconductors. Analogous to the study of homogeneous systems, we compute the current-induced internal fields (CIF) corresponding to the spin torques and perform a quantitative analysis of the effect of CIFs on DW motion by solving the phenomenological Landau-Lifshitz-Gilbert equations. Microscopic calculations based on an accurate description of the SO coupling effects are used to estimate the observed anisotropies. Our theoretical efforts are complemented by experimental studies in the SO coupled FM (Ga,Mn)(As,P).

10:36AM A14.00012 Magnetic properties of Ga_{1-x}Mn_xAs/Ge heterojunctions, JONATHAN LEINER, XINYU LIU, JACEK FURDYNA, MARGARET DOBROWOLSKA, University of Notre Dame — It has been shown that the incorporation of Mn in substitutional and interstitial positions of GaAs is linked to the Fermi level of GaMnAs during the growth [1]. Additionally, experiments with samples that are doped with either Be or Si reveal the role of the Fermi level in determining T_c [2]. To further investigate this effect, we deposited Ge in varying thicknesses on top of GaMnAs layers. Germanium is very nearly lattice matched to GaMnAs, and the valence band offset of the two materials (~0.54 eV) places the top of the valence band as well as the Mn acceptor level of GaMnAs significantly below the top of the valence band of Ge. Thus, when Ge is grown on GaMnAs, the incorporation of Mn has already been fixed during its growth, but the holes are drained off into Ge. SQUID measurements on these samples show that the T_c of the GaMnAs drops very rapidly when layers of Ge are deposited over it, the decrease in T_c scaling roughly with the thickness of the Ge layers. This behavior is consistent with the expected “draining away” of holes from the GaMnAs layer into the Ge. Results of our efforts to fine-tune the amount of holes removed from GaMnAs by Ge will be presented.

[1] Wojtowicz et al., Physica E 25, 171 (2004).

[2] Cho et al., JAP 103, 07D132 (2008); APL 93, 262505 (2008).

10:48AM A14.00013 Spin-dependent Transport in GaAs/MnAs Core/shell Nanowires, JING LIANG, JIAN WANG, A. PAUL, B.J. COOLEY, D.W. RENCH, N.S. DELLAS, S.E. MOHNEY, R. ENGEL-HERBERT, N. SAMARTH, Center for Nanoscale Science and Materials Research Institute, Penn State University, University Park PA 16802 — Hybrid GaAs/MnAs core/shell nanowires synthesized by molecular beam epitaxy [APL 97, 072505 (2010)] are of potential interest for proof-of-concept room temperature nanospintronics applications. Magnetic order in these nanostructures is directly influenced by a unique competition between the magnetocrystalline and shape anisotropies in MnAs. We report four probe measurements of the temperature dependence of the resistivity and the anisotropic magnetoresistance (AMR) in single nanowires over a temperature range 1 K - 300 K and in magnetic fields ranging up to 80 kOe, applied both parallel and perpendicular to the nanowire axis. We used the measured AMR in conjunction with micromagnetic simulations to reveal the detailed magnetization reversal process in the MnAs nanoshell. The micromagnetic simulations also provide insights into interesting structures for spin engineering at the nanoscale. Supported by NSF-MRSEC and ONR.

Monday, February 27, 2012 8:00AM - 11:00AM — **Session A15 DMP FIAP GMAG: Focus Session: Spins in Metals - Thermal Effects on Magnons and Spin Currents** 213

8:00AM A15.00001 Theory of phonon-driven spin Seebeck effect, HIROTO ADACHI, Japan Atomic Energy Agency, JUN-ICHIRO OHE, Toho University, SABURO TAKAHASHI, Tohoku University, SADAMICHI MAEKAWA, Japan Atomic Energy Agency — Spin Seebeck effect refers to a thermal spin injection occurring over millimeter scales from a ferromagnet into an attached nonmagnetic metal [Uchida et al., Nature 455, 778 (2008)]. We discuss the importance of the phonon-drag process in the spin Seebeck effect. Our theory of phonon-drag spin Seebeck effect [Adachi et al., Appl. Phys. Lett. 97, 252506 (2010)] explains simultaneously the local nature of the spin Seebeck effect [Jaworski et al., Nature Materials 9, 898 (2010); Uchida et al., Nature Materials 10, 737 (2011)] and the signal enhancement at low temperatures [Jaworski et al., Phys. Rev. Lett. 106, 186601 (2011)]. We also discuss the difference between our approach and that developed in Xiao et al., Phys. Rev. B 81, 214418 (2010).

8:12AM A15.00002 Spin Seebeck Effect Measurements on Ferromagnetic Thin Films Using Micromachined Thermal Isolation Platforms, AZURE D. AVERY, DAIN BASSETT, University of Denver, MATT R. PUFALL, NIST, Boulder, CO, BARRY L. ZINK, University of Denver — The newly discovered thermoelectric effect, called the spin Seebeck effect (SSE), refers to a spin imbalance generated by a thermal gradient. This spin imbalance, capable of driving a pure spin current into a contact, is detected by measuring the conversion of the spin current into a transverse voltage (V_T) via the inverse spin Hall effect. A robust theoretical treatment of the SSE has so far eluded the community at large, and more experimental data are needed to understand the underlying physics. In this talk we present V_T measurements associated with the SSE and AMR measurements for Ni, Fe, and Ni-Fe alloy thin films, along with Au as a control, made using our micromachined thermal isolation platforms. The sensitive thermal transport measurements we make using these platforms offer several advantages including concurrent measurements at hot and cold ends of the sample, equal heating of the sample ends to isolate traditional thermoelectric effects, and a large reversible thermal gradient. Additionally, the substrate thickness results in a virtually 2-D thermal platform that dramatically reduces the likelihood of thermal gradients perpendicular to the sample.

8:24AM A15.00003 Search For Spin Seebeck effect in in situ grown thin films¹, PRIYANGA JAY-ATHILAKA, DUSTIN BELYEA, HILLARY KIRBY, CASEY W. MILLER, Department of Physics, University of South Florida, SPINLAB TEAM — The Spin Seebeck Effect (SSE) is a phenomenon in which the application of a temperature gradient across a ferromagnet causes a measurable electric potential difference transverse to the gradient when a normal metal is grown onto the ferromagnet. The spin current diffusing into the normal metal is transduced to a voltage via the Inverse Spin Hall Effect. Measuring the SSE accurately is challenging due to presence of other effects, possibly including regular Seebeck effect and anomalous thermo-magnetic phenomena. Here we report on our efforts to measure the SSE in thin films of NiFe and Co, using Au and Ta as the electrodes. All samples were grown on Si/SiO_x substrates by magnetron sputtering through contact masks. The mask exchange was done in situ in a chamber where the base pressure was 2.0x10⁻⁷ Torr in order to limit contamination of the interfaces. The samples were measured using a rig with a reversible temperature gradient of 15K/cm and the resultant voltage was measured at the hot and cold ends of the sample using nanovoltmeters. The voltage signal we observe is strongly correlated with the magnetic hysteresis loops measured by Magneto-Optical Kerr Effect magnetometer.

¹Supported by NSF

8:36AM A15.00004 Intrinsic spin-dependent thermal transport¹, C.L. CHIEN, Department of Physics and Astronomy, The Johns Hopkins University — Spin caloritronic effect, such as spin Seebeck effect, has attracted a great deal of attention recently. In most cases such studies have been made on patterned ferromagnetic thin films on substrates. The mechanism of spin Seebeck effect has evolved from intrinsic difference in the spin chemical potentials to magnon-phonon interaction through the substrate. We use patterned ferromagnetic thin film to demonstrate the profound effect of a substrate on the spin-dependent thermal transport. With different sample patterns and on varying the direction of temperature gradient, both longitudinal and transverse thermal voltages exhibit asymmetric instead of symmetric spin dependence. This unexpected behavior is due to an out-of-plane temperature gradient imposed by the thermal conduction through the substrate and the mixture of the anomalous Nernst effects. Only with substrate-free samples have we determined the intrinsic spin-dependent thermal transport with characteristics and field sensitivity similar to those of anisotropic magnetoresistance effect.

¹In collaboration with S. Y. Huang (JHU), W. G. Wang (JHU), S. F. Lee (IoP, Academia Sinica in Taiwan), and J. Kwo (NTHU and NTU in Taiwan). This work has been supported by the US NSF grant DMR 05-20491 and the Taiwan NSC grant 99-2911-I-007-510.

9:12AM A15.00005 Thermoelectric coating based on the spin Seebeck effect, AKIHIRO KIRIHARA, NEC Corporation, KEN-ICHI UCHIDA, YOSUKE KAJIWARA, Tohoku University, MASAHICO ISHIDA, YASUNOBU NAKAMURA, TAKASHI MANAKO, SHIGERU KOHMOTO, NEC Corporation, EIJI SAITOH, Tohoku University, SHINICHI YOROZU, NEC Corporation — Thermoelectric (TE) technologies have been drawing great interest, since they can directly generate electricity from thermal energy that is available in various places. However, their complicated module structure, which is based on a number of thermocouples, still makes it difficult to fabricate large-area TE devices at low cost. In this work, we show a novel concept based on the spin Seebeck effect (SSE) called TE coating, which is characterized by a simple film structure, convenient scaling capability, and easy fabrication. We fabricated a TE-coating film with a bismuth-substituted yttrium iron garnet (Bi:YIG) by a highly productive spin-coating-based process on a nonmagnetic substrate, and demonstrated the SSE-induced TE conversion. The TE-coating layer amounts to only 0.01 % of the total sample thickness, suggesting that such an ultrathin magnetic film can work as a useful thermal-energy collector. This new concept may enable us to implement low-cost and large-area TE functions on various objects, opening opportunities for innovative energy harvesting applications.

9:24AM A15.00006 Linear response theory for magnon transport in ferromagnetic insulators, SHUICHI MURAKAMI, RYO MATSUMOTO, Tokyo Institute of Technology — We study transverse response of magnons in ferromagnetic insulators within linear response theory. In analogy with the corresponding theory for electrons [1], magnon transverse response is described, including the Hall effect, Nernst effect, and thermal Hall effect. As is also the case for electrons [1], the response functions for magnons consist of the Kubo-formula term, and the term corresponding to the orbital angular momentum. We can rewrite the response functions in terms of the Berry curvature in momentum space [2]. We apply this theory to the (quantum-mechanical) magnons and to the classical magnetostatic waves. For the magnetostatic waves, the eigenmodes are given by a generalized eigenvalue problem, giving rise to the special form of the Berry curvature [2]. We explain various properties of this Berry curvature for the generalized eigenvalue problem, and discuss its implications for the physical properties of magnetostatic modes. [1] L. Smrcka and P. Streda, J. Phys. C, 10, 2153 (1977); H. Oji, P. Streda, Phys. Rev. B 31, 7291 (1985); [2] R. Matsumoto and S. Murakami, Phys. Rev. Lett. 106, 197202 (2011); Phys. Rev. B 84, 184406 (2011).

9:36AM A15.00007 Thermally-assisted magnetization reversal in nanomagnets with spin-transfer torque: a GPU approach, DANIELE PINNA, ANDREW KENT, ADITI MITRA, DANIEL STEIN, New York University — Spin transfer magnetization reversal has a direct impact on magnetic information storage technologies. The probability that a nanomagnet switches under an applied magnetic field is expected to follow a simple thermally activated LLG model¹. However, a direct current applied to a nanomagnet produces a spin-transfer torque that drives the magnetization out of equilibrium². Such dynamics have been studied in limits where both the low and high current regimes allow analytical treatment³. Nonetheless, the inability to study numerically the long time behavior has hampered with theoretical verification and comparison to current experimental data⁴. In this talk, we present results obtained by employing modern GPU computational techniques to massively parallelize the Langevin equations of the model. We test the numerics by considering a simplified uniaxial case. The full current spectrum is reviewed, verified and compared to the present literature. We then proceed to break the symmetries in the problem and explore the general macrospin model.

¹M. L. Néel, Ann. Geophys. 5, 99 (1949); W. F. Brown, Phys. Rev. B 130, 1677 (1963).

²J. C. Slonczewski, JMMM. 159, L1 (1996)

³J. Sun, Phys. Rev. B 62 1 (2000)

⁴D. Bedau et al. Appl. Phys. Lett. 97, 262502 (2010)

9:48AM A15.00008 Can heat flow induced spin currents move a magnetic domain wall?, AAKASH PUSHUP, TIMOTHY PHUNG, LUC THOMAS, KONSTANTINOS ALEXANDROU, XIN JIANG, SEE-HUN YANG, BRIAN HUGHES, CHARLES RETTNER, STUART PARKIN, IBM Almaden Research Center — It has been established in the past few years that heat flow within a ferromagnet can induce a spin current and an associated voltage. This Spin Seebeck effect, initially reported in ferromagnetic metals, has also been observed in magnetic semiconductors as well as magnetic insulators. An open question has been whether heat flow induced spin currents can also move magnetic domain walls in 'racetrack' magnetic nanowires. In order to answer this question, we investigate the interaction of a magnetic domain wall with spin currents induced by sharp temperature gradients in magnetic nanowire spin valves. We use optical as well as electrical techniques to create sharp temperature gradients on the order of 1-10 K/nm on nanosecond timescales. We will describe our experimental setup and present data that show the various roles that temperature plays on the saturation magnetization of the material as well as on the induced spin currents that influence magnetic domain wall motion.

10:00AM A15.00009 Observation of spin-wave cooling effect in magnets, TOSHU AN, KEN-ICHI UCHIDA, KAZUYA HARI, YOSUKE KAJIWARA, KAZUYA YAMAGICHI, M.B. JUNGFLISCH, The Institute for Materials Research, Tohoku University, A.V. CHUMAK, V.I. VASYUCHKA, BURKARD HILLEBRANDS, Technische Universität Kaiserslautern, Germany, EIJI SAITOH, The Institute for Materials Research, Tohoku University — We focused on utilizing a surface spin wave (Damon-Eshbach mode); traveling on top and bottom surfaces in a non reciprocal manner, as a good carrier of heat. As a sample, Yttrium iron garnet (YIG) was chosen because the spin waves excited in the YIG is known to have a long coherence length propagating distances even a few millimeters. By exciting the surface spin wave of only one side, heat transportation was successfully observed by measuring sample temperature with an infrared thermocamera. More interestingly, the temperature where the spin wave is initially excited shows cooling effect to drop its temperature just after the excitation of the surface spin wave. Here we call this effect as microwave cooling effect which is introducing a new cooling principle.

10:12AM A15.00010 Thermodynamics of magnetic systems from first principles, MARKUS EISENBACH, Oak Ridge National Laboratory, GREGORY BROWN, Florida State University, AURELIAN RUSANU, University of Tennessee, DON M. NICHOLSON, Oak Ridge National Laboratory — Density functional calculations have proven to be a useful tool in the study of ground state properties of many materials. The investigation of finite temperature magnetism on the other hand has to rely usually on the usage of empirical models that allow the large number of evaluations of the system's Hamiltonian that are required to obtain the phase space sampling needed to obtain the free energy, specific heat, magnetization, susceptibility, and other quantities as function of temperature. We have demonstrated a solution to this problem that harnesses the computational power of today's large massively parallel computers by combining a classical Monte-Carlo calculations with our first principles multiple scattering electronic structure code (LSMS) for constrained magnetic states. Here we will present recent advances in our method that improve the convergence as well as applications to 3d element based ferromagnets. This research was performed at Oak Ridge National Lab and sponsored in parts by the Center for Nanophase Material Sciences, Scientific User Facilities Division, the Center for Defect Physics, an Energy Frontier Research Center funded by the US DOE Office of Basic Energy Sciences and the Division of Materials Science and Engineering, Office of Basic Energy Science of

10:24AM A15.00011 Effect of Temperature and Spin Torque on the Stoner-Wohlfarth Astroid of a Nanomagnet, YU-JIN CHEN, University of California, Irvine, JORDAN KATINE, Hitachi Global Storage Technologies, JUERGEN LANGER, Singulus Technologies, MARK LEWIS, University of California, Los Angeles, GRAHAM ROWLANDS, JIAN ZHU, University of California, Irvine, PEDRAM KHALILI AMIRI, KANG WANG, University of California, Los Angeles, ILYA KRIVOROTOV, University of California, Irvine — We report measurements of the Stoner-Wohlfarth switching astroid curves of the free layer nanomagnet in CoFeB/MgO/CoFeB/Ru/CoFe/PtMn elliptical nanoscale magnetic tunnel junctions made as a function of applied voltage and temperature. Measurements of the astroid area as a function of temperature allow us to determine the magnetic anisotropy energy barrier of the free layer and thereby quantify its thermal stability - an important performance parameter of spin torque nonvolatile magnetic memory. Measurements of the astroid as a function of voltage (V) applied to the junction at the bath temperature of 4 K reveal significant voltage-induced deformations of the astroid curve. We observe a decrease of the hard-axis length of the astroid, which arises from ohmic heating of the junction. Comparison of the hard-axis astroid length measured at $T = 4$ K and $-V \rightarrow 0$ to the hard-axis astroid length measured at $T \rightarrow 4$ K and $V = 0$ allows us to quantify ohmic heating of nanoscale tunnel junctions by the applied voltage. The applied voltage reduces the easy-axis length of the astroid as well, but the reduction is asymmetric for positive and negative easy-axis directions. This easy-axis asymmetry reverses upon the applied voltage sign reversal and thus it can be attributed to spin transfer torque.

10:36AM A15.00012 Magnetization dynamics at elevated temperatures¹, LEI XU, SHUFENG ZHANG, The University of Arizona — The conventional Landau-Lifshitz (LL) equation is the basis for simulation of magnetic structure and dynamics as long as the temperature is not too close to Curie temperature. In order to model the magnetization dynamics at elevated temperatures, one needs to extend the LL equation by including a finite longitudinal relaxation. Here within the self-consistent mean-field treatment of ferromagnetism, we propose an effective equation which is capable of addressing magnetization dynamics for a wide range of temperatures. At low temperatures, the equation reduces to the Landau-Lifshitz equation, namely, the transverse relaxation governs the dynamics. At high temperatures, it reduces to paramagnetic Bloch equation. Near the Curie temperature, the longitudinal relaxations play a more important role on the magnetization reversal. We present numerical calculations to simulate a heat-assisted-magnetic-recording process when the temperature is heated and cooled through the Curie temperature.

¹This work is supported by the U.S.DOE (DE-FG02-06ER46307).

10:48AM A15.00013 Temperature dependence of magnetic losses in GMR and TMR devices¹, KEVIN HAUGHEY, RYAN STEARRETT, ARIF OZBAY, EDMUND NOWAK, University of Delaware — Thermally induced magnetization fluctuations in the free and reference magnetic layers of giant and tunneling magnetoresistance (GMR and TMR) spin valves (SV) devices typically give rise to a low-frequency 1/f power spectral density that has been related to local dissipative processes [1]. Understanding the origin of these magnetic losses is essential for increasing the magnetic field sensitivity of GMR and TMR sensors. The low-frequency magnetic losses can be parameterized through a loss angle, $\varepsilon(T, H)$. $\varepsilon(T)$ for the reference layer in our GMR SV is non-monotonic: first decreasing with increasing T, then exhibiting a minimum near 50K and what may be the onset of a plateau or peak near 300K. The peak and minimum shift to lower temperatures when the applied field is oriented perpendicular to the exchange pinning direction. Data for TMR devices show similar trends. The measurements will be described in the context of a model involving thermally activated kinetics and a field-dependent distribution of activation energies for the nanoscale magnetic fluctuators.

[1] Z. Diao et al., PRB **84**, 094412 (2011)

¹DOE under award DE-FG02-07ER46374

Monday, February 27, 2012 8:00AM - 11:00AM – Session A16 DCMP: Liquid and Solid Helium 251

8:00AM A16.00001 Solid helium in rigid torsional oscillators¹, D.Y. KIM, M.H.W. CHAN, Department of Physics, The Pennsylvania State University, University Park, PA 16802, USA — In torsional oscillator experiments on solid helium, separating out the effect of shear modulus stiffening is important to measure true non-classical rotational inertia (NCRI). An increase in the shear modulus of solid helium stiffens the oscillator and causes the resonant period to drop thus mimicking NCRI. This effect can be multiplied in a torsional oscillator that is not completely rigid. We have carried out measurements in torsional oscillators specially designed to minimize the shear modulus effect. These oscillators are different from conventional ones in two aspects. Annulus sample spaces are located in the outermost part from rotational axes and all other parts consist of rigid metal. In this design, the resonant period change by loading solid helium is maximized and the effect of shear modulus change is minimized. We found a NCRI fraction on the order of 3×10^{-5} in these torsional oscillators.

¹Support for this experiment was provided by NSF Grants No. DMR 1103159.

8:12AM A16.00002 Thermal Conductivity of Solid ⁴He in Vycor¹, ZHIGANG CHENG, SAMHITA BANAVAR, STEFAN T. OMELCHENKO, MOSES H.W. CHAN, The Pennsylvania State University — In addition to non-classical rotational inertia (NCRI) observed in torsional oscillator (TO), we have carried out thermal conductivity measurement of solid ⁴He embedded in porous Vycor glass to search for possible anomaly related to the onset of NCRI. Because of the high thermal conductivity of bulk solid ⁴He, it is difficult to resolve any small 'extra' thermal conductivity signal due to the onset of supersolidity. However, when it is confined in porous Vycor, the thermal conductivity of solid ⁴He is significantly reduced. This makes it easier to single out possible anomaly. Preliminary measurements show a rounded peak in the thermal conductivity near 0.1 K.

¹This work is supported by NSF Grants No. DMR 1103159

8:24AM A16.00003 NMR studies of very dilute concentrations of ³He in solid ⁴He, SUNG SU KIM, C. HUAN, L. YIN, J. XIA, Department of Physics and National High Magnetic Field Laboratory, University of Florida, D. CANDELA, Department of Physics, University of Massachusetts, N. S. SULLIVAN, Department of Physics and National High Magnetic Field Laboratory, University of Florida — We compare the results of recent measurements of the nuclear spin-lattice relaxation time (T_1) and nuclear spin-spin relaxation time (T_2) for very dilute concentrations of ³He ($16 \leq x_3 \leq 2000$ ppm) in solid ⁴He with results from previous studies in the temperature range where the relaxation is attributed to the quantum tunneling of ³He atoms in the ⁴He lattice. The comparison shows that the results cannot be explained in terms of a unique correlation time and the effects of ⁴He lattice are important.

8:36AM A16.00004 Observation of superfluid components in solid ^4He ¹, HANS LAUTER, SNS-ORNL, ECKHARD KROTSCHKE, University at Buffalo SUNY Buffalo, EFIM KATS, Institut Laue Langevin France, ALEXANDER PUCHKOV, IPPE Obninsk Russia, VALERIA LAUTER, SNS-ORNL, VESA APAJA, University of Jyväskylä Finland, IVAN KALININ, IPPE Obninsk Russia, MAREK KOZA, Institut Laue Langevin France — Neutron scattering demonstrated that localized superfluid components exist at high pressure within solid helium in aerogel [1]. Two sharp phonon-roton spectra are clearly distinguishable from modes in bulk superfluid helium. These roton excitations exhibit different roton gap parameters than the roton observed in the bulk fluid at freezing pressure. One of the roton modes disappears after annealing. Comparison with theoretical calculations suggests that the model that reproduces the observed data best is that of superfluid double layers within the solid and at the helium-substrate interface. The elastic scattering evidenced in addition to the hcp phase also the bcc-phase. both consisting of a small crystallites as a consequence of the confinement. The structural aspect of coexisting hcp and bcc phases in the aerogel matrix seems to be important for the creation of the localized superfluid components.

[1] H. Lauter, E. Krotschke, E. Kats, A. V. Puchkov, V. V. Lauter, V. Apaja, I. Kalinin, M. Koza, PRL submitted

¹Support by RFBR grant 09-02-97501, AmadeeProject FR 06/2008, Finish Academy Project 7115066 and FWFOroject P21264

8:48AM A16.00005 Evidence for a BCC to HCP Phase Transition for Solid Helium in Porous Vycor Glass at 100 bar and 800 mK¹, LAURENCE LURIO, SAMBUNATH BERA, JONATHAN MALONEY, Department of Physics Northern Illinois University, NORBERT MULDER, Department of Physics, University of Delaware, ZHIGANG CHENG, MOSES CHAN, Department of Physics, Pennsylvania State University, CLEMENT BURNS, Department of Physics, Western Michigan University, ZHAN ZHANG, Argonne National Laboratory — In 2004, Kim and Chan² found evidence that solid helium grown in porous vycor glass exhibited changes in rotational inertia at millikelvin temperatures similar to that observed for superfluids. The nature of this putative supersolid phase is a question of current debate. Subsequent experiments have shown that supersolid behavior depends strongly on crystal quality. For the case of solid helium in vycor, little is known about the crystal quality, or even the crystal phase. In the present work we have performed transmission x-ray diffraction experiments on solid helium in porous vycor glass, over a range of pressures from 1 bar to 162 bar. At pressures up through 96 bar a single peak is observed in the diffraction pattern. At 114 bar and above this peak is observed to split into three peaks. We tentatively identify the low pressure phase as BCC and the high pressure phase as coexistence between BCC and HCP. We interpret the absence of higher order peaks as due to a combination of zero-point motion and defects.

¹This work was supported by NSF grant DMR-0804725.

²Kim, E. and Chan, M. H. W., Nature 427, 225 (2004).

9:00AM A16.00006 Simultaneous observation of 10 MHz ultra sound in solid ^4He contained in torsional oscillator¹, BETTINA HEIN, University of Wuerzburg, JOHN GOODKIND, UCSD, HARRY KOJIMA, Rutgers University — Kim and Chan[1] were motivated in part by an anomalous ultra sound propagation observed by Ho et al.[2] in solid ^4He near 200 mK to carry out torsional oscillator(TO) experiments which led to the discovery of supersolid phenomena. We constructed a 270 Hz TO oscillator which incorporated quartz transducers for simultaneously observing 10 MHz longitudinal ultra sound and torsional oscillation of solid ^4He samples. We are searching for correlation between behaviors in ultra sound propagation and TO response. The length and density of dislocations extracted from ultra sound and the frequency shifts of TO measured in some half a dozen solid ^4He samples have not shown clear correlation.

[1] E. Kim and M. Chan, Nature 427, 225(2004).

[2] P. Ho, I. Bindloss and J. Goodkind, JLTP 109, 409(1997).

¹Research supported in part by NSF.

9:12AM A16.00007 More on the shear modulus of solid helium¹, NORBERT MULDER², University of Delaware — In experiments on solid ^4He one finds a striking similarity between the response of torsional oscillators and the shear modulus. It has been suggested that in fact the observed increase in the torsional oscillator frequency at low temperature is just a reflection of the stiffening of the solid helium, and thus that of the oscillator as a whole. In some cases this may indeed be the case, but a recent experiment by Keiya Shirahama and Eunseong Kim's groups in which a measurement of the shear modulus was incorporated in a torsional oscillator cell seemed to indicate that the response of the solid to shear is decoupled from that of the oscillator. However, one may object that a) the shear was not applied at a frequency different from that of the oscillator, and that b) the direction of the applied shear was orthogonal to the stress imposed by the motion of the oscillator. In a series of experiments using two stacks of piezoelectric transducers that can be excited, and are able to detect, in orthogonal shear directions, we show that shearing the solid at one frequency affects the shear modulus at different frequencies, and similarly, that shearing in one direction affects the modulus as measured at the orthogonal direction. We conclude that quite generally shear and torsional oscillator responses are decoupled. And while they may both reflect the same underlying physics, it is unlikely that one causes the other.

¹supported by the NSF through DMR-0804725

²Department of Physics and Astronomy, Newark, DE 19716

9:24AM A16.00008 Simultaneous Measurement of Non-Classical Rotational Inertia and Shear Modulus of Solid ^4He , WONSUK CHOI, JAEHO SHIN, Center for Supersolid & Quantum Matter Research and Department of Physics, KAIST, Daejeon 305-701, R. O. K., HYOUNG CHAN KIM, National Fusion Research Institute(NFRI), Daejeon 305-333, R. O. K., KEIYA SHIRAHAMA, Department of Physics, Keio University, Yokohama, Japan, EUNSEONG KIM, Center for Supersolid & Quantum Matter Research and Department of Physics, KAIST, Daejeon 305-701, R. O. K. — A failure to rotate or oscillate is the essential nature of low temperature superfluid helium, and more technically known as non-classical rotational inertia (NCRI). It is counter-intuitive, but NCRI is also found in solid helium-4 below ~200 mK [1,2]. Recently, shear modulus showed unusual increase with striking resemblance to those of NCRI [3]. Extended measurements show the NCRI occurs only in a stiffened Bose solid, but it is not understood how they are related. Here we report the first simultaneous measurement of shear modulus and NCRI in solid helium to elucidate the fundamental connection between them. Both emerge at remarkably similar temperatures, whereas no quantitative agreement between the increase of the shear modulus and the magnitude of NCRI is found. The increase of shear modulus seems to be the necessary condition for the onset of NCRI.

[1] E. Kim and M. H. W. Chan Nature 427, 225-227 (2004)

[2] E. Kim and M. H. W. Chan Science 305, 1942 (2004)

[3] J. Day and J. Beamish Nature 450, 853-856 (2007)

9:36AM A16.00009 Interplay of Aerogel Anisotropy and Superfluid ^3He Textures, JIA LI, J. POLLANEN, C.A. COLLETT, W.J. GANNON, W.P. HALPERIN, Department of Physics and Astronomy, Northwestern University, Evanston, IL 60208, USA — The effect of aerogel anisotropy on the ^3He superfluid order parameter and the relative stability of A and B -phases has been investigated. We have performed pulsed NMR on ^3He in high porosity aerogel samples that have different types of anisotropy, characterized with an optical, cross-polarization technique. One aerogel sample has 14.3% growth-induced axial stretching. Its superfluid phase diagram is occupied by the A -phase. Linewidth analysis gives the distribution of the orbital angular momentum, $\vec{l}$. The orientation of $\vec{l}$ is consistent with an easy plane distribution that is perpendicular to the strain axis. A second aerogel sample is axially compressed mechanically by 22.5%. The major part of the zero magnetic field phase diagram is occupied by the B -phase. Additionally, our results show that aerogel anisotropy introduced by compressing and stretching have different orienting effects on the ^3He superfluid order parameters. This work was supported by the National Science Foundation, DMR-1103625.

9:48AM A16.00010 Experiments with ^3He in 10% uniaxially compressed aerogel: the superfluid phase diagram, NIKOLAY ZHELEV, ROBERT BENNETT, ERIC SMITH, Cornell University, JOHANNES POLLANEN, WILLIAM HALPERIN, Northwestern University, JEEVAK PARPIA, Cornell University — Entraining ^3He in aerogel provides a way to introduce disorder in the otherwise ideal quantum fluid. Motivated by the recent prediction that uniaxially compressed aerogel can stabilize the anisotropic A phase over the isotropic B phase, we use a torsional oscillator technique to measure the superfluid phase diagram of ^3He entrained in 10% axially compressed, 98% porous aerogel. We observe that a broad region of the temperature-pressure phase diagram is occupied by the metastable A phase. The reappearance of the A phase on warming from the B phase, before superfluidity is extinguished at T_c , is in contrast to its absence in uncompressed aerogel. We also find that the anticipated alignment of the angular momentum vector by compression is not observed.

10:00AM A16.00011 Application of MEMS Devices to the Study of Liquid ^3He ¹, MIGUEL GONZALEZ, PAN ZHENG, ERIK GARCELL, Department of Physics, University of Florida, Gainesville, FL 32611, USA, HO BUN CHAN, Department of Physics, The Hong Kong University of Science and Technology, Hong Kong, China, YOONSEOK LEE, Department of Physics, University of Florida, Gainesville, FL 32611, USA — We report measurements on the mechanical properties of a micro-electro-mechanical (MEMS) resonator submerged in liquid ^3He at millikelvin temperatures and at pressures 3, 21 and 29 bar. The device consists of a pair of parallel plates with a well-defined gap of $0.75\text{ }\mu\text{m}$. The sub-micron gap size and geometry of the device gives access to physics in the high Knudsen regime and allows the investigation of surface scattering effects in thin films of quantum fluids. Details of design, fabrication, and operation will be presented along with a study of the damping characteristics of the submerged resonator through a wide range of temperatures spanning from classical fluid to degenerate Fermi liquid. The device shows potential for the use in low temperature experiments and to investigate novel phenomena in quantum fluids at the micro/nano scale such as superfluid ^3He films.

¹Supported by NSF through DMR- 0803516 (YL)

10:12AM A16.00012 Partial depinning of dislocation in ^4He from ^3He impurities induced by thermal roughening¹, DARYA ALEINIKAVA, ANATOLY KUKLOV, College of Staten Island, CUNY — The mechanism of the roughening induced partial depinning of gliding dislocations from ^3He impurities is proposed [1] as an alternative to the standard “boiling off” scenario [2]. We give a strong argument that ^3He remains bound to dislocations even at large temperatures due to very long equilibration times. This conjecture is based on two observations: First, the experimental data [2] for shear modulus temperature dependence obtained at very different ^3He concentrations (1 ppb and 300 ppb) can be, practically, collapsed on each other by a simple rescaling of temperature; Second, both moduli can be fit by the Monte-Carlo simulations data within the assumption that the impurities remain confined to the spatial region occupied by dislocation. Conversely, impurities evaporation violates strongly the data collapse and is absolutely inconsistent with the simulations. We propose that such long equilibration time is due to the very narrow band of ^3He impuritons [3].

[1] D.Aleinikava, A.B.Kuklov. arXiv:1110.5884v1;

[2] J. Day and J. Beamish, Nature **450**, 853 (2007); J. Day, O. Syshchenko, and J. Beamish, Phys. Rev. B **79**, 214524 (2009);

[3] A.F. Andreev, Sov. Phys. Usp. **19**, 137 (1976)

¹This work is supported by NSF, Grant PHY 1005527

10:24AM A16.00013 Microscopic Dynamics of Liquid Helium Confined in 1D Nanopores, TIMOTHY PRISK, PAUL SOKOL, NARAYAN DAS, Indiana University, SOULEYMANE DIALLO, Oak Ridge National Laboratory, NOBUO WADA, Nagoya University, SHINJI INAGAKI, Toyota Central R and D Laboratories — Recently, Toda et al. performed torsional oscillator and heat capacity measurements on liquid He^4 confined within FSM-16. This porous silica glass has 1D pores with a very narrow diameter of $d = 2.8\text{ nm}$. This system is an example of a 1D quantum fluid in the sense that the thermal wavelength λ is longer than the pore diameter d . Because neutron time-of-flight (ToF) spectroscopy probes elementary excitations, it can be used to study the microscopic dynamics underlying the thermodynamic properties of this 1D quantum liquid. Using the Cold Neutron Chopper Spectrometer (CNCS) at the Spallation Neutron Source (SNS), we performed the first direct measurements of the elementary excitation spectrum of liquid He^4 confined in FSM-16. Measurements were performed at full pore at temperatures $T = 33, 80, 800$, and 1500 mK with an elastic energy resolution of approximately $80\text{ }\mu\text{eV}$. We will discuss the temperature T dependence of the static structure factor $S(Q)$, the energies $\hbar\omega$ and line widths Γ of the phonon-roton spectrum, and the evidence for 2D layer modes in this system. This research was supported by NIST and employed facilities sponsored by the Scientific User Facilities Division of the US Department of Energy.

10:36AM A16.00014 Path-Integral Monte Carlo Simulations of the Ideal Strength of HCP Helium ⁴, MAURICE DE KONING, EDGAR JOSUÉ LANDINEZ BORDA, Universidade Estadual de Campinas — Using path-integral Monte Carlo simulations we assess the ideal strength of solid He-4 in its HCP phase. This fundamental material parameter is defined as the stress necessary to produce irreversible deformation in a defect-free crystal. For this purpose we impose slowly increasing homogeneous deformations to defect-free He-4 crystals and measure the corresponding internal stress state. In this manner, we determine the ideal shear strength in the basal plane as a function of the shear orientation, as well as the tensile and compressive strength perpendicular to this plane. Our results establish upper bounds to the strength of real HCP He-4 crystals.

10:48AM A16.00015 Fitting of m^*/m with Divergence Curve for He_3 Fluid Monolayer using Hole-driven Mott Transition, HYUN-TAK KIM, MIT Creative Research Center in ETRI — The electron-electron interaction for strongly correlated systems plays an important role in formation of an energy gap in solid. The breakdown of the energy gap is called the Mott metal-insulator transition (MIT) which is different from the Peierls MIT induced by breakdown of electron-phonon interaction generated by change of a periodic lattice. It has been known that the correlated systems are inhomogeneous. In particular, He_3 fluid monolayer [1] and $\text{La}_{1-x}\text{Sr}_x\text{TiO}_3$ [2] are representative strongly correlated systems. Their doping dependence of the effective mass of carrier in metal, m^*/m , indicating the magnitude of correlation (Coulomb interaction) between electrons has a divergence behavior. However, the fitting remains unfitted to be explained by a Mott-transition theory with divergence. In the case of He_3 regarded as the Fermi system with one positive charge (2 electrons + 3 protons), the interaction between He_3 atoms is regarded as the correlation in strongly correlated system. In this presentation, we introduce a Hole-driven MIT with a divergence near the Mott transition [3] and fit the m^*/m curve in He_3 [1] and $\text{La}_{1-x}\text{Sr}_x\text{TiO}_3$ systems with the Hole-driven MIT with $m^*/m=1/(1-\rho^4)$ where ρ is band filling. Moreover, it is shown that the physical meaning of the effective mass with the divergence is percolation in which m^*/m increases with increasing doping concentration, and that the magnitude of m^*/m is constant.

[1] Phys. Rev. Lett. 90, 115301 (2003).

[2] Phys. Rev. Lett. 70, 2126 (1993).

[3] Physica C 341-348, 259 (2000); Physica C 460-462, 1076 (2007).

Monday, February 27, 2012 8:00AM - 11:00AM —
Session A17 DMP GERA FIAP: Focus Session: Thermoelectrics - Nanostructured and Oxide TE 252A

8:00AM A17.00001 Thermoelectric properties of filling-controlled zinc-antimonides with layer structure, T. SUZUKI, M.S. BAHRAMY, CMRG and CERG, RIKEN ASI, Japan, R. ARITA, Dept. of Appl. Phys., Univ. of Tokyo, CMRG and CERG, RIKEN ASI, Japan, Y. TAGUCHI, CMRG and CERG, RIKEN ASI, Japan, Y. TOKURA, Dept. of Appl. Phys., Univ. of Tokyo, CMRG and CERG, RIKEN ASI, ERATO MF, JST, Japan — Thermoelectric properties have been investigated for polycrystalline samples of layer-structured $R_{1-x}A_x\text{ZnSbO}$ ($R=\text{La, Ce}$; $A=\text{Ca, Sr}$) as two-dimensional analogues of a conventional thermoelectric semiconductor ZnSb [1]. By substituting A^{2+} for R^{3+} in the charge-reservoir layers, carrier concentration can be successfully controlled without lowering the carrier mobility. The hole doped materials showed low thermal conductivity and moderately high thermopower, whose temperature- and doping-dependence were well explained by theoretical calculation. The values of dimensionless figure of merit ZT were found to increase without showing any sign of saturation up to 390 K, and even higher values can be expected along the conducting ZnSb layers for a single crystal. These results indicate the potential of the hole-doped $R\text{ZnSbO}$ as a good thermoelectric material. This work was in part supported by FIRST program on "Quantum Science on Strong Correlation" from JSPS.

[1] T. Suzuki, M. S. Bahramy, R. Arita, Y. Taguchi, and Y. Tokura, Phys. Rev. B 83, 035204 (2011)

8:12AM A17.00002 Enhancing thermoelectric properties of FeSb_2 by altering stoichiometry and nanostructure, MANI POKHAREL, HUAIZHAU ZHAO, KEVIN LUKAS, ZHIFENG REN, CYRIL OPEIL, Boston College, BC TEAM — FeSb_2 is a strongly correlated semiconductor that has been shown to have an extraordinarily large Seebeck coefficient in single crystal samples. Bienten *et al.* report a Seebeck Coefficient of -45000 $\mu\text{V/K}$ at 10K. The peak value of the dimensionless figure of merit (ZT_{max}) for single crystal samples is calculated to be approximately 0.005 at 10 K and is constrained by its relatively high thermal conductivity. In our previous studies, we find that nanocomposites (NC) tend to decrease thermal conductivity substantially by introducing phonon mismatches between crystal grains. Given that the Seebeck coefficient on the FeSb_2 system is quite sensitive to carrier concentration, we focus on the effects of stoichiometric changes that heighten thermoelectric properties of FeSb_x where $x=2.04, 2.00, 1.96, 1.92$. By tuning the stoichiometry and using the nanocomposite method, the peak value of ZT_{max} was found to be 0.0123 at 43K. Carrier concentration and Hall-mobility measurements will also be discussed.

8:24AM A17.00003 Local Structure of Thermoelectric Clathrates¹, SCOTT MEDLING, FRANK BRIDGES, University of California, Santa Cruz, TOSHIRO TAKABATAKE, Hiroshima University — We present local structure results from extended X-ray absorption fine structure (EXAFS) analysis of two new kinds of clathrates: type I clathrates with a light 'rattler' atom and type VIII clathrates. The rattler atom is extremely important for the thermoelectric properties as it is what strongly scatters phonons and lowers the thermal conductivity without affecting the electrical conductivity. In most thermoelectric clathrates, the rattler atom is a heavy atom, typically Ba or Eu, and such type I clathrates have been discussed extensively in the literature; a smaller rattler atom such as K results in more free space inside the cage. Type VIII clathrates have the same chemical formula as type I clathrates, but have a different, more distorted, cage structure resulting in differing electronic properties. Recent studies indicate a thermoelectric figure of merit at least as high as 1.2 at 400 K is attainable. For both kinds of clathrates, we collect and analyze temperature-dependent data over the range 10-300 K and compare the results with our models.

¹NSF Grant DMR-1005568

8:36AM A17.00004 Nanostructured Thermoelectrics and the New Paradigm¹, MERCOURI KANATZIDIS, Northwestern University — A comprehensive and stable energy strategy would require proportionate attention to all three legs of the "energy stool"; supply (sources), demand (efficiency) and storage/transport (delivery). Thermoelectric materials, that convert waste thermal energy into useful electrical energy, have an important role to play in any and all these three legs. The efficacy and efficiency of thermoelectrics is reflected in the figure of merit ZT , which is directly proportional to the power factor (comprising electrical conductivity and Seebeck coefficient) and inversely proportional to thermal conductivity (comprising carrier and lattice contributions). The recent emergence of nanostructured thermoelectrics has ushered in a new era for bulk thermoelectrics, which show considerable promise to enhance the "contra-indicating" parameters of high electrical conductivity and low thermal conductivity. This is achieved by introducing nanostructures in bulk thermoelectric host materials to significantly reduce lattice thermal conductivity via effective scattering of heat carrying phonon through hierarchical architecture of nanostructured thermoelectrics. The presentation will cover recent developments, current research in our EFRC and future prospects for high performance bulk materials. Systems based on lead chalcogenides (e.g., PbTe , PbSe , PbS) present key science challenges with promising properties and are given particular emphasis. We have achieved excellent control of synthesis and crystal growth of such materials resulting in record enhancements in the figure of merit. These enhancements derive from very large reductions in lattice thermal conductivity possible with nanostructuring. We have experimentally realized concurrent synergistic effect of phonon blocking and charge transmission via the endotaxial placement of nanocrystals in thermoelectric material host. In particular, we have shown that the enhanced performance is due to nanostructuring of thermoelectric host matrix, with a compelling influence of hierarchy of length-scales associated with these systems. The presentation will outline possible future strategies for enhancing the thermoelectric figure of merit of bulk thermoelectric materials.

¹This work is supported as part of the Revolutionary Materials for Solid State Energy Conversion, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001054

9:12AM A17.00005 Assessing the thermoelectric properties of sintered compounds via high-throughput *ab initio* calculations, SHIDONG WANG, Department of Mechanical Engineering and Materials Science, Duke University, ZHAO WANG, LITEN, CEA-Grenoble, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France, WAHYU SETYAWAN, Department of Mechanical Engineering and Materials Science, Duke University, NATALIO MINGO, LITEN, CEA-Grenoble, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France, STEFANO CURTAROLO, Department of Mechanical Engineering and Materials Science and Department of Physics, Duke University — In order to identify promising thermoelectric materials, we study several thousand compounds from the ICSD database. In particular, we consider nano-grained sintered power thermoelectric compounds with the high-throughput *ab initio* AFLOW framework (<http://afwlib.org> and <http://materials.duke.edu/aflow.html>). By regression analysis, we find that the power factor is positively correlated to electronic band gap, carrier effective mass, and the number of atoms per unit cell. This work illustrates the important role that experimental and theoretical databases can play in the development of novel materials.

9:24AM A17.00006 Enhancement of the figure-of-merit in strongly correlated multilayers¹, VELJKO ZLATIĆ, Institute of Physics, Zagreb, JIM FREERICKS, Physics Department, Georgetown University, Washington, D.C. — A theory of charge and heat transport in inhomogeneous multilayers (ML) with correlated electrons is presented. We consider the device which consists of several strongly correlated metallic planes (channel) sandwiched between two semi-infinite Mott insulators (barriers). A driving field is applied parallel to the ML planes and the gate voltage perpendicular to the ML planes. The device is described by the Falicov-Kimball model and transport coefficients are calculated by the linear response theory using the DMFT. The device is tuned by i) increasing the correlation strength so as to enhance the slope of the local density of states in the channel-planes at the chemical potential and ii) changing the gate voltage so as to shift the position of the chemical potential with respect to the band-edge. Both effects have a large impact on the thermoelectric properties and are used to optimize the figure-of-merit, ZT, of the device. The effect of the number of planes is discussed as well. The results for the electrical conductivity, the Seebeck coefficient, the power factor, the Lorenz number and ZT are presented. Optimal tuning gives $ZT \gg 1$.

¹Supported by the NSF grant No. DMR-1006605

9:36AM A17.00007 Thermoelectric and Structural Properties of the Chemically Doped $\text{Ca}_3\text{Co}_4\text{O}_9$ System, JIANMING BAI, Oak Ridge National Laboratory, TAO WU, TREVOR A. TYSON, HAIYAN CHEN, New Jersey Institute of Technology — The Cu and Y doped thermoelectric oxide system $[\text{Ca}_2\text{CoO}_3][\text{CoO}_2]_{1.61}$, also referred to as $\text{Ca}_3\text{Co}_4\text{O}_9$, was prepared by solid state reaction followed by annealing under oxygen. The temperature dependent thermoelectric properties, including resistivity (ρ), Seebeck coefficient (S) and thermal conductivity (κ), were measured on Cu doped $[\text{Ca}_2\text{Co}_{1-x}\text{Cu}_x\text{O}_3][\text{CoO}_2]_{1.61}$ and Y doped $[\text{Ca}_{2-x}\text{Y}_x\text{CoO}_3][\text{CoO}_2]_{1.61}$. In order to understand the origin of the changes in ZT with doping, local (XAS) and long range (XRD) structural measurements as a function of doping were conducted. Identification of the locations of the doping sites and the impact on ZT will be discussed. This work is supported by DOE Grant DE-FG02-07ER46402. The Physical Properties Measurements System was acquired under NSF MRI Grant DMR-0923032 (ARRA award).

9:48AM A17.00008 The effects of increased Co-ion spin states on the Seebeck coefficient in thermoelectric $\text{Ca}_3\text{Co}_4\text{O}_9$ ¹, ROBERT KLIE, TADAS PAULAUŠKAS, QIAO QIAO, ALEJANDRO REBOLA, SERDAR OGUT, University of Illinois at Chicago, DIPANJAN MAZUMDAR, ARUN GUPTA, Center of Materials for Information Technology, University of Alabama, STANISLAW KOLESNIK, Northern Illinois University, JUAN-CARLOS IDROBO, Materials Science and Technology Division, Oak Ridge National Laboratory — Thermoelectric oxides have attracted increasing attention due to their high thermal power and temperature stability. In particular, $\text{Ca}_3\text{Co}_4\text{O}_9$ (CCO), a misfit layered structure consisting of single layer hole-doped CoO_2 sandwiched between insulating Ca_2CoO_3 rocksalt layers, exhibits a high Seebeck coefficient at 1,000 K. It was previously suggested that the Seebeck-coefficient can be further improved by stabilizing an increased Co-ion spin state in the CoO_2 layers. Here we report a significant increase in the room-temperature in-plane Seebeck coefficient of 40 nm thick CCO films grown by pulsed laser deposition on SrTiO_3 substrates. We combine aberration-corrected Z-contrast imaging, atomic-column resolved electron energy-loss spectroscopy, and density-functional calculations to show that the increase is caused by CoO_2 stacking faults with Co^{4+} -ions in a higher spin state compared to that of bulk CCO. The higher Seebeck coefficient makes the CCO system suitable for many high-temperature waste-heat-recovery applications. The role of dopants, such as Bi and Ti will also be explored.

¹This work was supported by the National Science Foundation [DMR-0846748 (RFK), DMR-0938330 (J-CI)].

10:00AM A17.00009 Anisotropic thermopower and magnetothermopower in a misfit-layered calcium cobaltite¹, HUAHONG GUO, TENG YANG, ZHIDONG ZHANG, Institute of Metal Research, Chinese Academy of Sciences — An unusual anisotropy of thermopower and magnetothermopower has been observed in the powerful thermoelectric $\text{Ca}_3\text{Co}_4\text{O}_{9+\delta}$ single crystal. The in-plane thermopower is about twice as big as the out-of-plane thermopower. Combining *ab initio* band structure calculation with semi-classical model analysis, we understand this anisotropy with band structure effects and especially with anisotropic Fermi surface. We find that a strong anisotropy in the topology of Fermi surface leads to the anisotropy of (magneto)thermopower. This study may also shed light on anisotropic properties of other layered cobalt oxides.

¹We thank the NSFC under Grant 11004201 and the Ke TingSui fellowship of IMR-CAS for the financial support

10:12AM A17.00010 The Origin of Enhanced High Temperature Electron Transport in Thermoelectric $\text{Ca}_3\text{Co}_4\text{O}_9$, TAO WU, TREVOR A. TYSON, HAIYAN CHEN, New Jersey Institute of Technology, JIANMING BAI, Oak Ridge National Laboratory, CHERNO JAYE, National Institute of Standards and Technology — Temperature dependent measurements of resistivity, crystal structure and heat capacity reveal significant hysteresis occurring near 400 K in $\text{Ca}_3\text{Co}_4\text{O}_9$. The largest changes in structure occur in the CoO_2 layer associated with electron transport: manifested mainly by b_2 axis changes. Application of magnetic fields up to 8 T reduces the area of the resistivity hysteresis loop with saturation at ~ 4 T. Reduced resistivity associated with this first order phase transition from metallic to semiconducting behavior enhances the thermoelectric properties at high temperatures and points to the metal-insulator transition as a mechanism for improved ZT in high temperature thermoelectric oxide. This work is supported by DOE Grant DE-FG02-07ER46402. The Physical Properties Measurements System was acquired under NSF MRI Grant DMR-0923032 (ARRA award).

10:24AM A17.00011 Electrical and Thermal Transport Properties of $\text{Bi}_2\text{Sr}_2\text{Co}_2\text{O}_{9-\delta}$ Single Crystals and Thin Films, ZHENYU DIAO, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, H.N. LEE, M. CHISHOLM, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, RONGYING JIN, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803 — Layered $\text{Bi}_2\text{Sr}_2\text{Co}_2\text{O}_{9-\delta}$ possesses rich physical properties, promising for thermoelectric applications. We have successfully synthesized $\text{Bi}_2\text{Sr}_2\text{Co}_2\text{O}_{9-\delta}$ in both single crystal and epitaxial thin film forms by applying various oxygen pressures. We found that their electrical and thermal transport properties are sensitive to the oxygen content, suggesting that the oxidation state of Co plays an important role in thermoelectric properties. Comparison of power factor between single crystals and thin films will be presented.

10:36AM A17.00012 Transport Properties of La- doped SrTiO₃ Ceramics Prepared Using Spark Plasma Sintering¹, ARASH MEHDIZADEH DEHKORDI, Department of Materials Science and Engineering, Clemson University, Clemson, South Carolina, SRIPARNA BHATTACHARYA, TERRY M. TRITT, Department of Physics and Astronomy, Clemson University, Clemson, South Carolina, HUSAM N. ALSHAREEF, Materials Science and Engineering, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia — In this work, thermoelectric transport properties of La-doped SrTiO₃ ceramics prepared using conventional solid state reaction and spark plasma sintering have been investigated. Room temperature power factor of single crystal strontium titanate (SrTiO₃), comparable to that of Bi₂Te₃, has brought new attention to this perovskite-type transition metal-oxide as a potential n-type thermoelectric for high temperature applications. Electronic properties of this model complex oxide, SrTiO₃ (ABO₃), can be tuned in a wide range through different doping mechanisms. In addition to A site (La-doped) or B site (Nb-doped) substitutional doping, introducing oxygen vacancies plays an important role in electrical and thermal properties of these structures. Having multiple doping mechanisms makes the transport properties of these perovskites more dependent on preparation parameters. The effect of these synthesis parameters and consolidation conditions on the transport properties of these materials has been studied.

¹The authors wish to acknowledge financial support from the KAUST-Clemson Faculty Initiated Collaboration (FIC) fund.

10:48AM A17.00013 Transition-metal-based perovskite oxides for enhanced thermopower, STANISLAW KOLESNIK, BOGDAN DABROWSKI, Department of Physics, Northern Illinois University, DeKalb, IL and Materials Science Division, Argonne National Laboratory, Argonne, IL, KRZYSZTOF WOJCIECHOWSKI, Faculty of Materials Science and Ceramics, AGH-UST, Cracow, Poland, KONRAD SWIERCZEK, Faculty of Energy and Fuels, AGH-UST, Cracow, Poland — Due to the enhancement of thermopower by spin and orbital degrees of freedom, transition-metal-based perovskite oxides are good candidates for stable and nontoxic materials with a large thermoelectric figure of merit ZT. We have investigated the most promising Mn-, Co- and Ti-based perovskite oxides. Electron doping of SrMnO₃ materials on either Mn or Sr sites induces a rapid decrease in both electrical resistivity and thermopower with the doping level due to the introduction of itinerant charge carriers. The thermopower of electron-doped SrTiO₃ materials satisfy the basic Heikes description, however, no additional enhancement is observed. The hole-doped RCoO₃ perovskites exhibit limited solubility of alkaline earth's for small rare earth ion sizes. The dependence of thermopower on charge doping and temperature appears to follow the extended Heikes formulation only at low doping and below 300 K, which indicates that Co³⁺ and Co⁴⁺ exist in several spin states beyond that range. Among all investigated compounds the largest ZT~0.3 values were observed for 3-8% Nb-substituted SrTiO₃ materials at about 700 K. Supported by the U.S. DOE-BES DE-AC02-06CH11357.

Monday, February 27, 2012 8:00AM - 11:00AM – Session A18 DCMP: Dynamics in II-VI Nanocrystals 252B

8:00AM A18.00001 Blinking and spectral diffusion of CdSe/ZnS nanoparticles, AXEL LORKE, DANIEL BRAAM, ANDREAS MÖLLEKEN, MATTHIAS OFFER, GÜNTHER PRINZ, MARTIN GELLER, Fakultät für Physik und CeNIDE, Universität Duisburg-Essen, 47048 Duisburg — Even though the tunable optical properties of colloidal nanoparticles have been studied extensively, their luminescent behaviour is still not fully understood. The random emission intermittency and the power-law of on- and off-times as well as shifts in the emission wavelength still lack a comprehensive understanding [1]. We investigate the excitonic structure of CdSe/ZnS core/shell nanoparticles using a micro-photoluminescence (PL) setup with confocal as well as imaging optics. The nanoparticles are dispersed in toluene with 1% PMMA and deposited by spin-coating on different substrates (bare Si/SiO₂ as well as Si/SiO₂ covered with different rough metallic layers). Depending on the substrate, we observe emission intermittency or nearly blinking-free emission with spectral jumps of 25 meV in the emission energy. Both can be assigned to excitonic transitions affected by additional charge inside or outside the nanoparticle [2]. Furthermore, we observe a phonon replica of 25 meV and smaller (<10 meV) energetic shifts of the emission lines, which are likely caused random charge variations in the environment of the nanoparticle.

[1] P. Frantsuzov et al., *Nature* 4, 519 (2008).

[2] A. Efros, *Nature Mat.* 7, 612 (2008)

8:12AM A18.00002 Photoluminescence blinking and carrier dynamics in giant nanocrystals with different electron confinement, SID SAMPAT, University of Texas at Dallas, YIJUN GUO, JAVIER VELA, Iowa State University, ANTON MALKO, University of Texas at Dallas — Quantum dots have shown great promise as high quantum yield photon sources for applications in bioimaging, LEDs, lasers, etc. However, their photoluminescence (PL) intermittency (blinking) often complicates practical implementations. Recently, a new breed of giant nanocrystal quantum dots (gNQDs) with a large number of shell monolayers (ML) has been developed that show strongly suppressed blinking¹ and existence of multiexcitons.^{2,3} So far, their PL emission has been limited to around 630nm. In this work, we broadened this approach and extended gNQD emission to shorter wavelength in the visible spectrum. We investigated photostable CdSe/CdS gNQDs with small (480nm emission) core and compared them to large (625nm emission) core non-blinking gNQDs with similar shell thickness (14-17 ML). The small core dots show increased blinking behavior and shorter PL decay times in comparison to large core dots. The observed difference in blinking behavior is suggestive of different carrier confinement regimes leading to enhanced electron trapping at the dot's surface as well as modifications to non-radiative Auger recombination rates.

¹Y. Chen et al., *JACS* 130, 5026 (2008)

²Y.S. Park et al., *Phys. Rev. Lett.* 106, 187401 (2011)

³A. V. Malko et al., *Nano Lett.*, accepted (2011)

8:24AM A18.00003 Lifetime Blinking in Non Blinking Quantum Dots¹, VICTOR KLIMOV, YAGNASENI GHOSH, ANDREA STEINBRUECK, JENNIFER HOLLINGSWORTH, HAN HTOON, CHRISTOPHE GALLAND, Los Alamos National Laboratory — Photoluminescence (PL) blinking is a common property of nanoscale light emitters. Nanocrystal quantum dots have often been used as model systems in studies of this intriguing phenomenon. Here, we use recently developed thick-shell CdSe/CdS NQDs to demonstrate a new regime of blinking where discrete fluctuations in the PL lifetime ("lifetime blinking") occur without appreciable changes in the PL intensity. Single-dot measurements under controlled electrochemical charge injection [1] yield the PL lifetimes of neutral and charged excitons. We show that the observed "lifetime blinking" are due to random charging/discharging of the nanocrystal [2]. Indeed, the injection of electrons does not appreciably modify the PL quantum yield, which explains the coexistence of a nonblinking intensity with a "blinking" lifetime. At higher excitation power, charged excitons dominate the PL emission. We build a quantitative model showing that nanocrystal charging is caused by Auger-assisted ejection of a hole, producing negatively charged species. Importantly, Auger recombination that involves excitation of an electron is suppressed while hole-based processes remain efficient.

[1] Galland et al., *Nature* 479, 203-207 (2011)

[2] Galland et al., Submitted (2011)

¹Funding: Center for Advanced Solar Photophysics, an Energy Frontier Research Center funded by the US Department of Energy (DOE, BES), NIH-NIGMS grant 1R01GM084702-01.

8:36AM A18.00004 Two types of luminescence blinking revealed by spectroelectrochemistry of single quantum dots¹, CHRISTOPHE GALLAND, YAGNASENI GHOSH, ANDREA STEINBRUECK, MILAN SYKORA, JENNIFER HOLLINGSWORTH, VICTOR KLIMOV, HAN HTOON, Los Alamos National Laboratory — The phenomenon of fluorescence intermittency (blinking between ON/OFF states) has been observed for both naturally occurring fluorophores and artificial nanostructures. This study aims to resolve the long-standing controversy surrounding the origin of photoluminescence blinking in core/shell nanocrystal quantum dots. Researchers usually evoke the Auger, or A-type, mechanism in which photo-ionization of the dot leads to the OFF state, but recent observations have raised doubts about this explanation. Here we report time-resolved photoluminescence studies of individual nanocrystal quantum dots performed while electrochemically controlling the degree of their charging [1]. We find that a second mechanism (called B-type) is the dominant cause for blinking. During B-type blinking, a photo-excited, “hot” electron is trapped in a surface state before being released to the core; the luminescence is quenched without any Auger process. By controlling the applied potential and the shell thickness, we can control the frequency and type of blinking, or suppress it completely.

[1] Galland *et al.*, *Nature* **479**, 203-207 (2011).

¹C.G. and V.I.K. acknowledge support of the Center for Advanced Solar Photophysics, an Energy Frontier Research Center funded by the US Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences (BES).

8:48AM A18.00005 Ultrafast Cathodoluminescence Studies of Colloidal Nanocrystals, LAZARO PADILHA, WAN KI BAE, VICTOR KLIMOV, JEFFREY PIETRYGA, Los Alamos National Laboratory, RICHARD SCHALLER, Argonne National Laboratory, Northwestern University — Despite possessing numerous desirable properties, including excellent photostability, high stopping-power, and fast, efficient fluorescence, semiconductor nanocrystal quantum dots are only mediocre gamma-ray scintillator materials. Efforts to improve performance are forestalled by a lack of understanding of how those materials respond to high energy radiation, which in turn comes from a lack of appropriate ultrafast tools for examining the relaxation of gamma-excited quantum dots. To this end, we have developed a 20keV as a surrogate for spontaneous gamma irradiation. We apply this technique to study the time-resolved response of thin films of CdSe/ZnS core/shell quantum dots. Energetic excitation produces a variety of excited states that can be separately resolved by consideration of their established energies and relaxation dynamics. We analyze the relative branching ratios of single excitonic, multi-excitonic and charged excitonic states to derive surprising conclusions regarding the physics of highly-excited quantum dots, as well as the probable source of poor gamma-scintillating performance.

9:00AM A18.00006 Dynamic fluctuations in ultrasmall nanocrystals induce white light emission, TIMOTHY J. PENNYCOOK, JAMES R. MCBRIDE, SANDRA J. ROSENTHAL, Vanderbilt University, STEPHEN J. PENNYCOOK, Oak Ridge National Laboratory, SOKRATES T. PANTELIDES, Vanderbilt University — Nanocrystals typically emit monochromatically at their size-dependent energy gaps. Recently, it was found that by pushing the size of a nanocrystal to its lower limits, absorption occurs at increasingly larger energies, but the expected blue to ultraviolet emission does not occur. Instead, ultrasmall nanocrystals begin to emit a broader spectrum. For instance, ultrasmall CdSe nanocrystals emit white light [1]. We have investigated small to ultrasmall CdSe nanocrystals using a combination of state-of-the-art scanning transmission electron microscopy and finite-temperature quantum molecular dynamics simulations. Our findings indicate that following excitation, partial thermalization sets the ultrasmall nanocrystals into a fluxional state, with a continuously varying energy gap, which results in white light emission when averaged over time. Furthermore, although the larger monochromatic emitting nanocrystals we have observed possess stable crystal cores, their surfaces are fluxional. Dynamic fluxionality should be taken into consideration when optimizing nanocrystals for applications. This work is supported by DOE grant DE-FG02-09ER46554 and Basic Energy Sciences Materials Sciences and Engineering Division.

[1] Bowers II, M.J. *et al.* *J. Am. Chem. Soc.* **127**, 15378 (2005).

9:12AM A18.00007 Dynamics of charge separation and multicarrier recombination in CdS/CdTe heterodimer nanocrystals, SEIJI TAGUCHI, Institute for Chemical Research, Kyoto University, MASAKI SARUYAMA, University of Tsukuba, TOSHIHARU TERANISHI, YOSHIHIKO KANEMITSU, Institute for Chemical Research, Kyoto University — Heterostructured semiconductor nanocrystals provide new ways to manipulate electronic wave functions and carrier recombination pathways. Recently, we developed a novel anion exchange reaction and synthesized anisotropically phase-segregated CdS/CdTe heterodimers with staggered band-edge alignment [1]. Here we report the ultrafast carrier dynamics in the heterodimers measured by transient absorption spectroscopy. While pump laser energy was tuned to create excitons only in the CdTe phase, we observed the bleaching of the CdS excitonic transition. The bleaching of CdS exciton states should be induced by electron injection from the CdTe phase to the CdS phase. Very rapid electron transfer time was evaluated to be about 400 fs. Moreover we found that temporal evolutions of CdS excitonic bleaching are almost independent of excitation intensity over a wide range, implying the suppression of Auger recombination. Our results indicate that charge separation efficiency of the heterodimers is enhanced due to their centrosymmetry-broken structures, and the designed nanocrystals are useful for next generation solar cells. [1] Saruyama *et al.*, *J. Am. Chem. Soc.* **133**, 17598 (2011).

9:24AM A18.00008 Transient Photoluminescence in Ligand-Exchanged Quantum Dot Assemblies¹, MICHAEL E. TURK, PATRICK M. VORA, AARON T. FAFARMAN, BENJAMIN T. DIROLL, CHRISTOPHER B. MURRAY, CHERIE R. KAGAN, JAMES M. KIKKAWA, University of Pennsylvania — Improving electronic contact between nanocrystals (NCs) within self-assembled NC solids is a long standing goal, and recent work on ligand exchange using ammonium thiocyanate has demonstrated marked improvements in the charge mobility of NC films over longer, more insulating ligands [1]. Here, we use transient photoluminescence (PL) to study changes in radiative lifetime caused by ligand exchange. Our work begins by examining differences in lifetime and radiative efficiency between liquid dispersions and solid films of CdSe semiconductor NCs, and moves on to study additional changes in both types of samples correlated with ligand substitution. We use a combination of time-correlated single photon counting and non-linear optical Kerr gating to study PL on nanosecond and sub-picosecond time frames, respectively. We discuss the relationship between nanosecond and picosecond dynamics, and examine temperature dependence from 300 to 5 Kelvin. Initial data indicate a decrease in PL lifetime with ligand exchange, which we discuss in the context of increased transport mobilities and decreased interparticle separations, as well as changes in the steady-state optical spectra of these systems. [1] A.T. Fafarman, *et al.*, *J. Am. Chem. Soc.*, **133**, 15753 (2011).

¹Transient PL work supported by the Department of Energy Office of Basic Energy Sciences Award DE-SC0002158, and sample synthesis supported by the NSF Solar Program under Award No. DMS-0935165.

9:36AM A18.00009 Optically Excited Exciton Transfer of Spherical Quantum Dots via Optical Near-Field Interactions, TOGAY AMIRAHMADOV, Bilkent University, PEDRO LUDWIG HERNANDEZ MARTINEZ, HILMI VOLKAN DEMIR, Bilkent University, Nanyang Technological University — We study a system composed of a mixture of different-sized spherical quantum dots (QDs) involving optical near-field (ONF) interactions to induce effective optical excitation transfer. Here energy transfer was explained by resonant energy transfer via the optical near-field interaction between the first excited state of small QDs and the second excited state of large QDs. The energy transfer in a film of different-sized QDs made of CdTe and CdSe were experimentally demonstrated. An analysis between the optical near field transfer rate [1] and Förster type transfer rate was made. The proper understanding of the exciton transfer between these QDs is important for the design and implementation of near-field photonic devices employing them. [1] M. Ohtsu, *et al.*, *Principles of Nanophotonics*, CRC Press (2008).

9:48AM A18.00010 Efficient Exciton Transfer from an Epitaxial Quantum Well to an Energy Gradient Structure Composed of Layer-by-Layer Assembled Colloidal Quantum Dots, SEDAT NIZAMOGLU¹, Bilkent University, PEDRO LUDWIG HERNANDEZ MARTINEZ, Bilkent University, Nanyang Technological University, EVREN MUTLUGUN, Bilkent University, HILMI VOLKAN DEMIR, Bilkent University, Nanyang Technological University — In this work, we study exciton migration from a violet-emitting epitaxial quantum well (QW) to an energy gradient structure that consists of layer-by-layer assembled, green- and red-emitting quantum dot (QD) bilayer. In the experimental study, the energy gradient of these green and red QDs provides an increase of 64.2% in the exciton transfer efficiency with respect to the bilayer of only red-emitting QDs. These results suggest that the energy difference between the QD layers significantly boosts the QW-QD exciton transfer rate compared to the mono-dispersed case. To support this experimental observation, we propose a theoretical model based on optical near field and density matrix to investigate the effects of energy difference between the QD layers. The strong exciton transfer from the epitaxial QWs to the colloidal QDs is essential to the energy efficiency of hybrid optoelectronic devices [1-3].

[1] A. Ruland, et al., Adv. Mater. 23, 4573–4577 (2011).

[2] M. Naruse, et al., Phys. Rev. 82, 125417 (2010).

[3] S. Nizamoglu, et al., Appl. Phys. Lett. 98, 163108 (2011).

¹currently at Wellman Center for Photomedicine, Massachusetts General Hospital & Department of Dermatology, Harvard Medical School, 55 Fruit Street, Boston, Massachusetts 02114, USA

10:00AM A18.00011 Anomalous photo-induced spectral changes in CdSe/ZnS quantum dots¹, GEORGIY SHCHERBATYUK, University of California, Merced, RICHARD INMAN, University of California, San Diego, PATRICK TALBOT, SAYANTANI GHOSH, University of California, Merced — We study photo-induced static and dynamic spectral changes in self-assembled CdSe/ZnS quantum dot (QD) thin films with varying QD concentrations under ambient conditions. Using spatially resolved scanning photoluminescence microscopy in conjunction with spectrally resolved time-correlated photon counting, we measure the variations in spectral intensity, emission wavelength, and recombination lifetimes as functions of photo-exposure time. We find that at low concentrations photo-darkening and photo-oxidation rates slow down with increasing QD density, but in the high concentration limit these rates are strongly enhanced. Our measurements lead us to conclude that the interplay of photo-induced surface trap discharging with preferential photo-oxidation of smaller QDs is further modulated by resonant energy transfer driven by strong inter-dot interactions in highly concentrated samples. Finally, we extend our studies to thin films with two different QD diameters to vary the ratio of donors to acceptors and modify the energy transfer efficiency

¹This work is supported by UC SOLAR

10:12AM A18.00012 ABSTRACT WITHDRAWN —

10:24AM A18.00013 Waveguide Integrated Colloidal Quantum Dot Emitters, MINGMING JIANG, DONGFANG LI, RASHID ZIA, Brown University — High-yield II-VI colloidal quantum dots (QDs) have received considerable attention as quantum emitters for photonic device applications. Given their scalable synthesis and self-assembly, these QDs could serve as the basis for large arrays of single photon sources. Here, we present preliminary results on the integration of CdSe-based QDs into dielectric waveguides. Specifically, we will show how the local optical environment can be used to direct and enhance QD emission into specific spatial and spectral modes. First, we will present fabrication techniques to safely embed QDs into thin film dielectric waveguides. Then, we will present experimental back-focal-plane (BFP) measurements that demonstrate how thin-film interference effects can be used to control the QD angular emission patterns. Experimental BFP data will be discussed and analyzed in terms of theoretical predictions based on the local density of optical states (LDOS), thus demonstrating how interference effects can be used to effectively direct emission from randomly oriented QDs. If time permits, we will also show how the extension of these techniques to individual QD emitters in ridge waveguides.

10:36AM A18.00014 Comparison of carrier multiplication yields in the PbX salts¹, JAYSON STEWART, LAZARO PADILHA, JEFFREY PIETRYGA, Los Alamos National Laboratory, AARON MIDGETT, JOSEPH LUTHER, MATTHEW BEARD, ARTHUR NOZIK, National Renewable Energy Laboratory, VICTOR KLIMOV, Los Alamos National Laboratory — In this talk I will present recent results of a collaborative effort investigating the quantum efficiency of carrier multiplication (CM) of the lead salt nanocrystals: PbS, PbSe and PbTe. These materials are promising candidates for exploring generation-III photovoltaic concepts that rely on carrier multiplication, the process in which a single photon generates more than one electron-hole pair. Despite the many apparent similarities of these materials in their bulk form, we find that these compounds exhibit strikingly different CM yields in their nanocrystalline form. We suggest that the difference in CM yields in these nanomaterials is the consequence of different competing relaxation rates, such as phonon emission. Indeed, we estimate the rate of energy dissipation due to phonon emission mediated by a polar Frohlich-type interaction for these three materials and find excellent qualitative agreement with the data. This approach could prove useful for predicting future materials to investigate for increasingly high CM yields.

¹Center for Advanced Solar Photophysics

10:48AM A18.00015 ABSTRACT WITHDRAWN —

Monday, February 27, 2012 8:00AM - 11:00AM —

Session A19 DCMP: Invited Session: New Correlated Electron Physics Using Scanning Tunneling Microscopy and Other Probes 253AB

8:00AM A19.00001 Local Kondo screening and spatial coherence in YbRh_2Si_2 ¹, STEFFEN WIRTH,

Max-Planck-Institute for Chemical Physics of Solids Dresden — Heavy fermion metals are often characterized by a variety of relevant energy scales and competing interactions which may result in such fascinating phenomena as quantum criticality and unconventional superconductivity. Therefore, these materials have advanced to suitable model systems by means of which electronic interactions can be studied in detail. This will be discussed for the interplay of localized and itinerant electronic states in Kondo lattice systems in which heavy charge carriers are generated. We investigate the generic Kondo lattice system YbRh_2Si_2 , one of the heaviest heavy fermion metals, by utilizing atomically resolved Scanning Tunneling Spectroscopy (STS) [1]. An analysis of the topography allows for a determination of the terminating surface as well as a comparison to results from chemical analysis. Importantly, the crystal field excitations are unambiguously reflected by our STS measurements, clearly relating STS to bulk properties. The hybridization of conduction and $4f$ electrons results in a gap-like feature in the tunneling conductance. In addition, a strongly temperature dependent peak in the tunneling conductance is attributed to a resonance resulting from the Kondo lattice. The experimental data are discussed in relation to results obtained within the non-crossing approximation (NCA) and renormalized band structure calculation. In a brief outlook we discuss further investigations by STS, e.g. with respect to the quantum critical phenomena observed in YbRh_2Si_2 [2], to substitutions-induced changes of the relevant energy scales [3], or on heavy fermion superconductors.

[1] S. Ernst *et al.*, Nature **474** (2011) 362.

[2] S. Friedemann *et al.*, Proc. Natl. Acad. Sci. USA **107** (2010) 14547.

[3] S. Friedemann *et al.*, Nature Phys. **5** (2009) 465.

¹Work partly supported by the German Research Foundation through DFG Forschergruppe 960

8:36AM A19.00002 Correlated Spin Phenomena in Molecular Systems, WILSON HO, University of California,

Irvine — While a great deal of work has been carried out on molecular magnets, the spatial distribution of the spin wave function and the many body interactions between the delocalized molecular spin and its surrounding electrons can now be obtained with atomic scale resolution with the scanning tunneling microscope (STM). The combination of surface science, self-assembly, and STM enables correlated spin phenomena, such as the Kondo state, to be probed in a wide range of well characterized systems from single molecules to a two-dimensional lattice of interacting spins. Nonlocality, Kondo gap, and the Kondo lattice in correlated electron physics are revealed by the atomic-scale spatial resolution and high energy resolution spectroscopy and imaging with the STM from oxygen to porphyrins and phthalocyanine molecules adsorbed on metal and oxide surfaces.

9:12AM A19.00003 Long-range Kondo signature of a single magnetic impurity¹, MARTIN WEN-

DEROTH, 4. Physikalisches Institut, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — Scanning tunneling spectroscopy (STS) has provided an approach to study the Kondo effect - one of the oldest many particle phenomena known in condensed matter physics - in real space. In spite of the high spatial resolution of scanning tunneling spectroscopy, experiments performed on single magnetic atoms on metal surfaces, have shown that the fingerprint of the Kondo effect is only visible if the tip is placed directly above the impurity (e.g. [1]). In the present work we follow a novel route and investigate single isolated Co and Fe impurities not on top but buried below a Cu(100) surface. It has been shown recently [2] that the anisotropy of the copper Fermi surface leads to a strongly directional propagation of quasi particles called electron focusing which gives access to individual bulk impurities in a metal. We have studied the energy-dependent scattering characteristics for single isolated atoms of Ag, Co and Fe buried under a Cu(100) surface using low temperature scanning tunnelling spectroscopy (STS). For the case of a non-magnetic Ag impurity a Friedel oscillation in the local density of states is observed. For both magnetic impurity atoms we observe, in contrast to previous works, a long range Kondo signature which is periodic with the distance to the impurity [3]. The comparison of Co and Fe atoms demonstrates that both impurity species show similar behavior on completely different energy scales, which is determined by the Kondo temperature. We investigate the scattering amplitude as well as the phase. A theoretical interpretation based on a combined approach of band structure and many-body numerical renormalization group calculations is able to describe the rich spatially and spectroscopically resolved experimental data.

[1] M. Ternes *et al.*, Journal of Physics: Condensed Matter **053001** (2009)

[2] A. Weismann *et al.*, Science **323**, 1190 (2009)

[3] H. Prueser *et al.*, Nature Physics **7**, 203 (2011)

¹This work was supported by DFG SFB 602 TP A3.

9:48AM A19.00004 Defects in Heavy-Fermion Materials: Unveiling Strong Correlations in Real Space¹, DIRK MORR, University of Illinois at Chicago — Heavy-fermion materials exhibit a plethora of puzzling phenomena which are believed

to arise from the competition between Kondo screening and antiferromagnetic ordering. The microscopic origin of these phenomena, such as the non-Fermi-liquid properties observed in the quantum critical region, is still a topic of debate. Recent groundbreaking scanning tunneling spectroscopy (STS) experiments [1-4] have shed new light on this debate by providing important insight into the electronic and magnetic structure of heavy fermion materials. In this talk, I review some recent progress made in our theoretical understanding of the differential conductance, dI/dV and the resulting quasi-particle interference (QPI) patterns [5-7], observed in these experiments. In particular, I will demonstrate that defects in heavy-fermion materials provide an unprecedented opportunity to disentangle electronic correlations arising from Kondo screening, and antiferromagnetic correlations between the magnetic moments by inducing perturbations in the electronic and magnetic structure that exhibit characteristically different spatial patterns. The spatial extent of these perturbations grows with the strength of the magnetic interactions, and thus directly reflects the degree of correlations [5]. In addition, I show that non-magnetic defects (Kondo holes) in heavy fermion materials can give rise to the formation of an impurity bound. Our prediction of spatial hybridization oscillations and the formation of an impurity bound state were recently confirmed by STS experiments [4]. Moreover, I will demonstrate that QPI spectroscopy, utilizing spatial oscillations in the LDOS induced by defects, does not only provide important insight into the electronic structure of heavy fermion materials, but also in the entanglement of electronic and magnetic states [6,7]. Finally, the strongly correlated nature of heavy-fermion materials leads to a highly non-linear quantum interference between defects, and the creation of order from disorder. These results provide unique insight into the spatial complexity of heavy fermion materials.

[1] A.R. Schmidt *et al.*, Nature **465**, 570 (2010).

[2] P. Aynajian *et al.*, PNAS **107**, 10383 (2010).

[3] S. Ernst *et al.*, Nature **474**, 362 (2011).

[4] M. Hamidian *et al.*, PNAS **108**, 18233 (2011).

[5] J. Figgins and D.K. Morr, Phys. Rev. Lett. **107**, 066401 (2011).

[6] J. Figgins and D.K. Morr, Phys. Rev. Lett. **104**, 187202 (2010).

[7] T. Yuan, J. Figgins, and D.K. Morr, arXiv:1101.2636.

¹This work was performed in collaboration with J. Figgins and T. Yuan, and was supported by the U.S. Department of Energy under Award No. DE-FG02-05ER46225

10:24AM A19.00005 Tunable Kondo Effect in SrTiO_3 ¹, JAMES WILLIAMS, Stanford University — Correlated, low-dimensional systems offer the possibility of tuning complex physical phenomena. Using strong electric fields applied with an electrolytic gate, we continuously tune through three regimes of transport in SrTiO_3 : an insulator, a metal and a Kondo metal. Two of these regimes – the metallic and Kondo metal state – are investigated as a function of temperature and magnetic field, where clear signatures of each regime are evident and discussed. This diverse system not only displays behavior distinct from conventional two-dimensional electron gases, but also show similarities to the $\text{LaAlO}_3/\text{SrTiO}_3$ interface, elucidating on some of the phenomena observed in this heterostructure of debated origin.

¹Supported by the MURI program 5 of the Army Research Office Grant No. W911-NF-09-1-0398.

Monday, February 27, 2012 8:00AM - 11:00AM – **Session A20 FIAP: Invited Session: Advanced Quantum Materials for Future Information Technology 253C**

8:00AM A20.00001 Graphene-based Electronics and Optoelectronics¹, PHAEDON AVOURIS, IBM, T.J. Watson Research Center, Yorktown Heights, NY 10598 — Graphene has rather unique electrical and properties and there is currently strong interest in taking advantage of these properties for technological applications. In my talk I will review some of the key properties of free graphene, how these properties are affected by environmental interactions and under technologically relevant conditions, and how they can be utilized in electronics and optoelectronics. In electronics, I will focus on high frequency (≥ 300 GHz) graphene transistors and simple IC circuits, as well as related device physics problems, such as the role of electrical contacts, scattering effects, graphene topology, device size scaling, energy dissipation, etc. I will then review the key optical properties of graphene and their use in optoelectronics. Specifically, I will focus on the far-infrared and THz range of the spectrum, on ways of controlling graphene's absorption in this spectral range and provide examples of corresponding applications. I will also discuss photocurrent generation in graphene and its use in ultrafast graphene photodetectors.

¹Work in collaboration with: Y.-M. Lin, D. E. Farmer, Y. Wu, F. Xia, H. Yan, C. Dimitrakopoulos, W. Zhu, M. Freitag, K. Jenkins, A. Valdes-Garcia, T. Low, V. Perebeinos.

8:36AM A20.00002 Visualizing Helical Metals on Topological Insulators¹, ALI YAZDANI, Princeton University — During the last few years, it has become apparent that there can be a distinct type of insulator, which can occur because of the topology of electronic wavefunctions in materials comprised of heavier elements. Strong interaction between the spin and the orbital angular momentum of electrons in these compounds alters the sequence in energy of their electronic states. The key consequence of this topological characteristic (and the way to distinguish a topological insulator from an ordinary one) is the presence of metallic electrons with helical spin texture at their surfaces. I will describe experiments that directly visualize these novel quantum states of matter and demonstrate their unusual properties through spectroscopic mapping with the scanning tunneling microscope (STM). These experiments show that the spin texture of these states protects them against backscattering and localization. These states appear to penetrate through barriers that stop other electronic states. I will also describe more ongoing efforts focused on unraveling the physics of topological surface states and their potential for device-like applications.

References:

P. Roushan et al, *Nature* **460** 1106 (2009).

J. Seo et al, *Nature* **466** 343 (2010).

H. Beidenkopf et al, to appear *Nature Physics* (2011).

¹Work is supported by NSF, NSF-MRSEC, ONR, and DARPA.

9:12AM A20.00003 Quantum information processing with defect spins in diamond and silicon carbide¹, WILLIAM KOEHL², Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 USA — Many proposals for quantum information technologies require quantum systems that can be easily manipulated by an outside observer, while remaining largely unaffected by destructive interactions with the surrounding environment. One system that matches this description is a defect in the crystal lattice of diamond known as the nitrogen-vacancy (NV) center. Electrons trapped at this defect form an atomic scale spin state that can be used as an individually addressable, solid state quantum bit (qubit) even at room temperature. The exceptional quantum properties of the diamond NV have motivated recent efforts to search for similar defects in other semiconductors, as these would expand the technological opportunities available to defect-based quantum systems [1]. We discuss these efforts, which make use of techniques from both computational materials science and experimental quantum physics, focusing on explorations of the 4H polytype of silicon carbide (4H-SiC). In particular, we present recent experimental results that identify several defect spin states in 4H-SiC that function as analogs to the diamond NV. Using optical and microwave techniques similar to those used with diamond NV qubits, the spins of these defects can be optically addressed and coherently controlled in the time domain at temperatures ranging from 20 – 300 K. Additionally, these defects are optically active near telecom wavelengths, inhabit a host material for which there already exist industrial scale crystal growth and advanced microfabrication techniques, and possess desirable spin coherence properties comparable to those of the diamond NV. This makes them promising candidates for various photonic, spintronic, and quantum information applications that merge quantum degrees of freedom with classical electronic and optical technologies [2].

[1] J. R. Weber*, W. F. Koehl*, J. B. Varley*, A. Janotti, B. B. Buckley, C. G. Van de Walle, and D. D. Awschalom, *Proc. Natl Acad. Sci. USA* **107**, 8513 (2010).

[2] W. F. Koehl, B. B. Buckley, F. J. Heremans, G. Calusine, and D. D. Awschalom, *Nature* **479**, 84 (2011); A. Dzurak, *Nature* **479**, 47 (2011).

¹This work is funded by AFOSR and DARPA.

²In collaboration with B. B. Buckley, F. J. Heremans, G. Calusine, and D. D. Awschalom.

9:48AM A20.00004 Quantum Transport in Dirac Materials, PABLO JARILLO-HERRERO, MIT — Over the past few years, the physics of low dimensional electronic systems has been revolutionized by the discovery of materials with very unusual electronic structures. Among these, graphene and topological insulators have taken center stage due to their relativistic-like electron dynamics and their potential applications in nanotechnology. In this talk I will briefly review the properties of graphene and topological insulators and discuss some of our recent quantum electronic transport experiments in these systems.

10:24AM A20.00005 GHz - THz plasmonic circuits using low dimensional electronic systems¹, DONHEE HAM, Harvard University — Nature offers a broad variety of plasma systems consisting of electrons unbound from atoms, e.g.; astrophysical plasmas in intergalactic, interstellar, and stellar media; the Earth's ionosphere; and solid-state plasma, the free electrons in metals and semiconductors, only to name a few. A key feature of many plasma systems is collective motions of electrons; as the electron density profile is perturbed from equilibrium, Coulomb restoring forces (and sometimes quantum pressure in dense plasma) arise to power these collective motions, usually in the form of bulk electron density oscillations or electron density waves. Solid-state plasmas are particularly interesting, as the fabrication technologies available for solid-state materials allow us to alter the boundaries and interfaces of the plasma media in various ways to engineer the collective motion. A notable example is the surface plasmons, which have been a source of many breakthroughs in photonics. I will talk about a set of our recent developments where the plasmons are brought down to the electronics-regime (GHz~THz) and manipulated to produce a range of functionalities, while offering unique advantages to electronics over their purely electromagnetic counterparts. (Co-workers) William Andress (Harvard), Hosang Yoon (Harvard), Kitty Yeung (Harvard), Ling Qin (Harvard), Ken West (Princeton), and Loren Pfeiffer (Princeton).

¹The authors are grateful to the support of this research by the Air Force Office of Scientific Research under contracts no. FA 9550-09-1-0369 and no. FA 9550-08-1-0254.

Monday, February 27, 2012 8:00AM - 11:00AM – Session A21 DCMP: Superconductivity: Josephson, Tunneling and Proximity Effects 254A

8:00AM A21.00001 Equal-spin Andreev reflection from quasiparticle interference effects in high- T_C /half metallic ferromagnet junctions¹, C. VISANI, R. BERNARD, J. BRIATICO, M. BIBES, A. BARTHÉLÉMY, J.E. VILLEGAS, Unité Mixte de Physique CNRS/Thales, J. TORNOS, Z. SEFRIOUI, J. SANTAMARIA, GFMC, Universidad Complutense de Madrid — We report evidence for long-range superconducting correlations in the half-metallic ferromagnet (F) $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$, obtained from conductance measurements along the c-axis in SFS and SF junctions (with S the high- T_C superconductor $\text{YBa}_2\text{Cu}_3\text{O}_7$). Well below the superconducting T_C , we observed oscillations in the differential conductance as a function of the voltage bias, in which we identified two sets of resonances: i) quasiparticle interferences in the S (top) layer (Tomasch resonances) and ii) in the half-metallic F layer (McMillan-Rowell resonances). Both of them imply Andreev-like reflections at the SF interface and the coherent propagation of the resulting phase-conjugated quasiparticles through the entire S and F layers thickness (up to 30 nm for the F layer). Because conventional Andreev reflection and the coherent long-range propagation of the outcoming opposite-spin electron/hole pairs are heavily suppressed in strongly polarized ferromagnets, the observation of the above effect implies the occurrence of equal-spin Andreev reflection at the studied SF interfaces.

¹Work supported by French RTRA “Supraspin”, ANR “SUPERHYBRIDS-II” and EU-FP7 “PIXIE.”

8:12AM A21.00002 Proximity Effect in Mesoscopic Superconductor-Normal-Superconductor Arrays¹, SERENA ELEY, SARANG GOPALAKRISHNAN, University of Illinois Urbana-Champaign, PAUL GOLDBART, Georgia Institute of Technology, NADYA MASON, University of Illinois Urbana-Champaign — Systems of superconducting islands on normal metal films provide a tunable medium with which to study the superconducting proximity effect, phase transitions, and vortex dynamics. Such systems are predicted to exhibit 2D zero-temperature metallic states. Although there has been experimental evidence of such states, they cannot be explained by conventional transport theory. Here, we report transport measurements on triangular arrays of mesoscopic, proximity-coupled Nb islands placed on normal metal Au films. The arrays undergo a two-step transition to a superconducting state; we characterize the superconducting transitions in these systems as a function of island thickness and spacing. The temperature of the first step of the transition linearly decreases with increasing island spacing, and the spacing-dependence of the second step deviates from conventional theories. Moreover, the trends of both steps suggest that the system is approaching zero-temperature metallic states. Through a phenomenological model, we resolve these transitions as a consequence of intra- and inter-island coupling between superconducting phases of individual Nb grains.

¹This research was supported by the DOE-DMS under grant DE-FG02-07ER46453 through the Frederick Seitz Materials Research Laboratory at the University of Illinois at Urbana-Champaign.

8:24AM A21.00003 Coherent Two Photon Production in Superconductor-Semiconductor Heterostructures¹, PAUL BAIREUTHER, Karlsruhe Institute of Technology, Karlsruhe, Germany, ILYA VEKHTER, Louisiana State University, Baton Rouge, LA, USA, JÖRG SCHMALIAN, Karlsruhe Institute of Technology, Karlsruhe, Germany — Connecting a thin (direct band gap) p-n junction to a superconductor allows Cooper pairs to tunnel into the junction. This leads to an enhancement of the luminescence at the junction via Cooper pair based radiative recombination[1,2], an effect that has recently been observed experimentally[3]. Due to the proximity-induced Cooper pairs in the junction, anomalous photon production related to coherent two photon processes becomes allowed. Using a simple model for direct band gap luminescence we study a superconductor-p-n-superconductor heterostructure where the two photon state depends on the relative phase between the two superconductors. We investigate to what extent the production rate of entangled photons is controlled by the phase difference between the attached superconductors.
[1] E. Hanamura, Phys. Stat. Sol. (b) 234, 166 (2002).
[2] Y. Asano, I. Suemune, H. Takayanagi, and E. Hanamura, Phys. Rev. Lett. 103, 187001 (2009).
[3] I. Suemune, T. Akazaki, K. Tanaka, M. Jo, K. Uesugi, M. Endo, H. Kumano, E. Hanamura, H. Takayanagi, M. Yamanishi and H. Kan, Jpn. Journ. of Appl. Phys. 45, 9264 (2006).

¹Supported by the DFG-Center for Functional Nanostructures, Karlsruhe Institute of Technology

8:36AM A21.00004 Field-Dependent Effects in Superconductors Coupled to Semiconducting Heterostructures¹, STEPHANIE LAW, Department of Physics and Materials Research Lab, University of Illinois at Urbana-Champaign, WADE DEGOTTARDI, SMITHA VISHVESHWARA, NADYA MASON, JAMES ECKSTEIN, University of Illinois at Urbana-Champaign — We report transport measurements between superconducting leads separated by a small InAs gap. The NbTi superconducting layer is grown in-situ on top of the InAs to allow good contact. The samples are then fabricated into Hall bars with narrow gaps between the superconducting leads. Differential resistance and IV characteristics are measured in two and four terminal setups at 300mK both on and off quantum Hall plateaus. Multiple Andreev reflection peaks are observed (up to $n=4$ in some cases) and their field dependence measured. As the field increases, the MAR peaks shift to lower voltages and follow a general scaling law which holds across devices with different gap lengths. One device shows a supercurrent at all fields and in this device, MAR peaks corresponding both to the superconducting gap as well as a proximity-induced normal gap are seen. Explanations for the field-dependence of the MAR peaks will be discussed.

¹This material is based upon work supported by the U.S. Department of Energy, Division of Materials Sciences under Award No. DE-FG02 07ER46453, through the Frederick Seitz Materials Research Laboratory at the University of Illinois at Urbana-Champaign

8:48AM A21.00005 Transport Properties Characterized by Magnetic Domain-Wall Motion in Josephson Junction¹, MICHYASU MORI, Japan Atomic Energy Agency, SIN-ICHI HIKINO, WATARU KOSHIBAE, RIKEN, Japan, SADAMICHI MAEKAWA, Japan Atomic Energy Agency — Nano-scale magnetic materials for spintronics devices are extensively studied due to many advantages. Non-volatile memory using a magnetic domain wall (DW) is one example of such devices, and the oscillatory DW is examined toward several applications. Once such devices are realized in a microscopic circuit, one needs to measure the DW motion more precisely. In this talk, we discuss the transport properties characterized by a magnetic domain wall (DW) motion in a ferromagnetic Josephson junction, which is composed of a ferromagnetic wire with DW and two superconducting electrodes. Our previous theory [1] is developed to include the DW motion into the Josephson current. By supposing a simplified DW structure, we find that the current-voltage curve exhibits stepwise structures, when DW oscillates in the ferromagnetic wire. The mechanism behind this result is common to the electric field generated by the vortex motion in the superconductor.

[1] S. Hikino, M. Mori, S. Takahashi, and S. Maekawa, J. Phys. Soc. Jpn, **77**, 053707 (2008).

¹Grants-in-Aid for Scientific Research from MEXT (No. 19204035, No. 21360043, No. 22102501), the “K” computer project of Nanoscience Program, JST-CREST, and FIRST Program.

9:00AM A21.00006 Dramatic suppression of the Josephson effect in floating superconductors, MARIA JOSE MARTINEZ-PEREZ, FABIO TADDEI, FRANCESCO GIAZZOTTO, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, Piazza S. Silvestro 12, I-56127 Pisa, Italy — A number of devices exploiting the Josephson effect consist of floating superconducting islands. A well-known example are SISIS junctions (where S and I stand for superconductor and insulating barrier, respectively) present in many applications such as SQUIDS. The Josephson effect relies on the macroscopic phase describing the wave function of the electrons in the superconducting electrodes. This phase is fixed by the electrochemical potential of the superconductor that is settled experimentally. An intriguing situation arises then when dealing with floating superconducting islands that have no well-defined reference potential. Here we present an experimental characterization of Al/AlO_x/Al/AlO_x/Al junctions. We focus, on the one hand, on genuine SISIS junctions in which the central aluminium island remains floating and, on the other, on virtually grounded samples in which the central aluminium island is referred to a fixed potential through a metallic contact. We observe that, under identical circumstances, floating junctions exhibit a dramatic suppression of their Josephson current compared to their grounded counterparts. Possible reasons such as the overheating of the central island or quasiparticle fluctuations are addressed.

9:12AM A21.00007 Escape and retrapping phenomena in HTS and LTS Josephson Junctions¹, L. LONGOBARDI, Seconda Università degli Studi di Napoli, Dipartimento di Ingegneria dell'Informazione, via Roma 29, 81031 Aversa (Ce) Italy, D. STORNAIUOLO, CNR-SPIN, UOS Napoli, D. MASSAROTTI, L. GALLETTI, Università degli Studi di Napoli, Dipartimento di Scienze Fisiche, F. CARILLO, G. PAPARI, NEST CNR-NANO, Pisa Italy, A. KAWAKAMI, Advanced ICT Research Institute, National Institute of Information and Communications Technology, 588-2 Iwaoka-cho, Nishi-ku, Kobe 651-2492, Japan, G.P. PEPE, A. BARONE, Università degli Studi di Napoli, Dipartimento di Scienze Fisiche, G. ROTOLI, F. TAFURI, Seconda Università degli Studi di Napoli, Dipartimento di Ingegneria dell'Informazione — We investigate escape and retrapping dynamics in Josephson junctions characterized by different levels of dissipation. Measurements are carried out both on high (HTS) and low (LTS) critical temperature superconductor Josephson systems, characterized by different types of barriers, i.e. grain boundary and standard insulating layers. Based on the damping level we observe various regimes ranging from macroscopic quantum tunneling, thermal activation and phase diffusion processes. Experimental data are compared with a numerical model allowing a precise determination of the damping parameter.

¹We acknowledge partial support by STREP-MIDAS and by a Marie Curie International Reintegration Grant number 248933 “hybMQC” within the 7th European Community Framework Programme.

9:24AM A21.00008 Dominant second harmonic in the Josephson current–phase relation: Manifestation of the long-range spin-triplet proximity effect in SFF’S junctions, ZORAN RADOVIC, University of Belgrade, Serbia, LUKA TRIFUNOVIC, University of Basel, Switzerland, MILOŠ KNEZEVIC, University of Cambridge, UK — We present theoretical study of the Josephson effect and pairing correlations in planar SFF’S junctions that consist of conventional superconductors connected through two metallic monodomain ferromagnets. Both singlet and triplet pair amplitudes, the Josephson current-phase relations, and density of states for arbitrary orientation of magnetizations are calculated from the self-consistent solutions of Eilenberger equations in the clean limit and for moderate disorder in ferromagnets. We find that in highly asymmetric SFF’S junctions the long-range spin-triplet proximity effect manifests itself as a dominant second harmonic in the Josephson current-phase relation [1] and gives distinctive tunneling conductance spectra [2]. Unambiguous detection of the long-range spin-triplet proximity effect by tunneling spectroscopy and experimental realization of the Josephson junctions ground state degeneracy (like at 0- π transitions) is accessible for small interface roughness and moderate disorder in ferromagnets at low temperatures.

[1] L. Trifunovic, Z. Popovic and Z. Radovic, Phys. Rev. B **84**, 064511 (2011).

[2] M. Knezevic, L. Trifunovic, and Z. Radovic (to be published).

9:36AM A21.00009 Andreev bound states in proximitized InAs nanowires¹, WILLY CHANG, VLADIMIR MANUCHARYAN, MERRITT MOORE, FERDINAND KUEMMETH, CHARLES MARCUS, Harvard University, THOMAS SAND JESPERSEN, JESPER NYGARD, University of Copenhagen — We present measurements of individual Andreev bound states (ABS) in semiconducting InAs nanowires contacted by a superconductor. The two ends of a U-shaped Al lead are deposited on the nanowire to form low-resistance contacts, between which a normal lead is then deposited to form a high-resistance tunnel contact to the nanowire. A tunneling current through the nanowire is formed by grounding the Al leads and by applying a voltage bias to the tunnel contact. Measurements of the differential conductance of the device as a function of voltage bias, magnetic field, and backgate show resonances that are associated with the density of states in the proximitized nanowire. This sub-gap structure depends periodically on magnetic flux, with a period of $\phi_0 = h/2e$. At voltages and magnetic fields exceeding the gap and the critical field of the Al leads, this structure disappears completely. Further control is achieved via a global backgate, with the tunneling current completely switched off at sufficiently low gate voltages. We interpret this structure as ABS arising from the normal electronic properties of the nanowires.

¹Research funded by Microsoft Corporation Station Q

9:48AM A21.00010 A Superconductor in the Presence of an Exchange Field and Spin-orbit Interaction¹, MARIUS EICH, FBML, MIT, JOHANNES C. LEUTENANTSMEYER, FBML, MIT and I. Phys. Inst., Georg-August-Universitaet Goettingen, PENG WEI, FBML, MIT, MARKUS MUENZENBERG, I. Phys. Inst., Georg-August-Universitaet Goettingen, JAGADEESH S. MOODERA, FBML and Physics Dept., MIT — A superconductor (SC) in contact with a magnetic semiconductor experiences a large internal exchange field (IEF) that acts on the spins [1,2]. The quasi particle density of states (*q-DOS*) in the SC splits by the Zeeman energy, $2\mu H_{EX}$ where μ is the electron magnetic moment and H_{EX} is the IEF [1,2]. Here we combine IEF and spin-orbit (S-O) interaction to investigate the properties of Al by superconductive (SIS) tunneling spectroscopy [1]. Thin film sandwich junction 4EuS/4.5Al/(*d*-Au)/Al₂O₃/8Al (film thickness in nm and *d* from 0 to 0.06nm) was studied: ferromagnetic EuS layer provides the IEF whereas the Au layer creates the S-O scattering in Al. Tunnel conductance measured at 0.4K showed a large Zeeman splitting of *q-DOS* in Al film due to the IEF, even at $H_{appl} = 0$. In zero H the large asymmetry in the conductance peaks and reduction in the Zeeman splitting were observed due to S-O scattering when compared to control junctions (no Au). The sharp features in the SIS tunnel conductance allowed these studies even at the lowest level of S-O scattering.

[1] R. Meservy and P. M. Tedrow, Phys. Rep. 238, 173 (1994).

[2] J. S. Moodera, T. S. Santos and T. Nagahama, J. Phys.: Condens. Matter 19, 165202 (2007)

¹This work is supported by NSF DMR 0504158 and DFG SFB 602.

10:00AM A21.00011 Quantum tunneling of Normal-Superconducting interfaces in a type-I superconductor, SAUL VELEZ, ANTONI GARCIA-SANTIAGO, RICARDO ZARZUELA, JOAN MANEL HERNANDEZ, JAVIER TEJADA, Universitat de Barcelona, Spain, EUGENE CHUDNOVSKY, The City University of New York, New York, USA — The magnetic irreversibility in the intermediate state in various disks of pure type-I superconducting lead (Pb) with structural defects of diverse nature is presented. The results are discussed in terms of the contributions of the shape-dependent geometrical barrier (which is the origin of the so-called topological hysteresis) and the energy barriers associated to stress defects that act as pinning centers on normal-superconductor interfaces (NSI). The effect of the defects is to enhance the capability of the system to trap magnetic flux along the descending branch of the hysteresis cycle driving the system in a set of metastable states that would originate the occurrence of time-dependent phenomena. Magnetic relaxation studies reveal that the dynamics of the intermediate state of a type-I superconductor with defects is ruled by nonthermal processes for low enough temperatures. It is attributed to quantum tunneling of NSI mediated by the formation/flattening of bumps at the defects of the sample. The average value of the tunneling barriers is estimated and the temperature of crossover from the thermal to the quantum regime is obtained from the Caldeira-Leggett theory. Comparison between theory and experiment points to tunneling of interface segments of a size comparable to the coherence length, by steps of the order of 1 nm. Finally, the effect of an applied magnetic field on the quantum dynamics of the system is also explored.

10:12AM A21.00012 Josephson superjunction: an SIS junction with a correlated insulator¹, DAVID STROUD, CHRIS PORTER, Ohio State University, KWANGMOO KIM, Korea Institute of Advanced Study — We consider the properties of an SIS Josephson junction, in which the insulating region is itself a superconductor, but below its superconducting-insulating transition. The junction could, for example, be made of a superconducting film, in which the central region is much thinner than the two regions on either side. To treat quantum fluctuations in both the insulating and the superconducting region, we model the insulator as itself an SIS Josephson array below its S/I transition and the superconductor as an array above that transition. We calculate the coupling energy of the junction as a function of insulator thickness using two methods. The first is a mean-field approach, generalized to allow for spatial variation of the order parameter. The second approach is to use quantum Monte Carlo simulation, which we use to calculate the phase stiffness as a function of insulator thickness. In both cases, the properties of the junction can be tuned by varying the thickness of the insulating region, and the properties of both superconducting and insulating materials.

¹Supported in part by NSF MRSEC, Grant No. DMR 08-20414 and the Ohio Supercomputer Center.

10:24AM A21.00013 Neural dynamics in superconducting networks, KENNETH SEGALL¹, Colgate University, DAN SCHULT², Colgate University, PATRICK CROTTY³, MAX MILLER⁴, Colgate University — We discuss the use of Josephson junction networks as analog models for simulating neuron behaviors. A single unit called a “Josephson Junction neuron” composed of two Josephson junctions [1] displays behavior that shows characteristics of single neurons such as action potentials, thresholds and refractory periods. Synapses can be modeled as passive filters and can be used to connect neurons together. The sign of the bias current to the Josephson neuron can be used to determine if the neuron is excitatory or inhibitory. Due to the intrinsic speed of Josephson junctions and their scaling properties as analog models, a large network of Josephson neurons measured over typical lab times contains dynamics which would essentially be impossible to calculate on a computer. We discuss the operating principle of the Josephson neuron, coupling Josephson neurons together to make large networks, and the Kuramoto-like synchronization of a system of disordered junctions.

[1] “Josephson junction simulation of neurons,” P. Crotty, D. Schult and K. Segall, Physical Review E 82, 011914 (2010).

¹Department of Physics and Astronomy

²Department of Mathematics

³Department of Physics and Astronomy

⁴Department of Physics and Astronomy

10:36AM A21.00014 Half-metallic *d*-wave Josephson junctions, HENRIK ENOKSEN, JACOB LINDER, ASLE SUDBØ, Department of Physics, Norwegian University of Science and Technology, N-7491 Trondheim, Norway — We examine the dc Josephson effect in a ballistic superconductor/half-metal/superconductor junction by means of the Bogoliubov-de Gennes equations. We study the role of spin-active interfaces and compare how different superconductor symmetries affect the Josephson effect. We analyze critical current as a function of junction width, spin-flip strength and direction, and temperature. We show that the temperature-dependence of the supercurrent in the d_{xy} -symmetry case differs qualitatively from the *s*- and $d_{x^2-y^2}$ -symmetries. Finally, we have found a general analytical expression for the Andreev Bound State-energies which shows how we can either induce $0 - \pi$ -transitions, or continuously change the ground state phase of the junction by controlling the magnetic misalignment at the interfaces.

10:48AM A21.00015 A Microfabricated Phonon Spectrometer to Spectrally Resolve Phonon Transport, OBAFEMI OTELAJA, JARED HERTZBERG, RICHARD ROBINSON, Cornell University, Department of Materials Science and Engineering — In this work we show how frequency-dependent phonon transport can be probed with non-equilibrium phonons. We demonstrate a method of generating and detecting non-equilibrium phonons in micron- and nanoscale structures [1]. Our scalable method of fabricating phonon generators and detectors involves formation of Al-AlxOy-Al superconducting tunnel junctions on the sidewalls of a silicon mesa. In the line-of-sight path in these mesas, we generate and detect non-equilibrium, ballistically propagating phonons with a frequency ~ 100 GHz. Phonons are generated through the decay of quasiparticles injected into one superconducting film of the generator. This process excites phonons in a tunable, non-thermal spectral distribution. The phonons radiate into the mesa and are observed by the detector after passing through the mesa. By utilizing electron-beam lithography and plasma etching, we demonstrate the fabrication of high aspect ratio nanostructures along the ballistic path in order to observe surface scattering effects. This work is supported by DOE (DE-SC0001086).

[1] J. B. Hertzberg et al, Rev. Sci. Instrum. 82, 104905 (2011).

Monday, February 27, 2012 8:00AM - 11:00AM –

Session A22 DMP DCOMP: Focus Session: Fe-based Superconductors - Gap Structure 254B

8:00AM A22.00001 Anisotropic Energy-Gaps of Iron-based Superconductivity from Intra-band Quasiparticle Interference in LiFeAs, ANDREAS W. ROST, University of St Andrews / Cornell University, MILAN P. ALLAN, CMPMS Department, Brookhaven National Laboratory, ANDREW P. MACKENZIE, University of St Andrews, YANG XIE, J.C. DAVIS, Cornell University, K. KIHOU, C.-H. LEE, A. IYO, H. EISAKI, Institute of Advanced Industrial Science and Technology, Tsukuba, T.-M. CHUANG, Institute of Physics, Academia Sinica, Nankang, Taipei — Cooper pairing in the iron-based high- T_C superconductors is thought to occur due to the projection of the antiferromagnetic interactions between neighboring iron atoms onto the complex momentum-space electronic structure. A key consequence is that distinct anisotropic energy gaps $\Delta_i(k)$ with specific relative orientations should occur on the different electronic bands i . However, the high-precision spectroscopy required to demonstrate anisotropy of the energy gaps, and to determine the relationship between the $\Delta_i(k)$ on different bands, has not been achieved. Here we introduce intra-band Bogoliubov quasiparticle scattering interference (QPI) to iron-based superconductor studies, focusing specifically on LiFeAs. This approach provides direct spectroscopic confirmation of multiple anisotropic energy gaps on different bands. We identify the QPI signatures of the three hole-like bands assigned by photoemission studies to be γ , α_2 and α_1 . Then, by introducing a new QPI technique, we determine the magnitude and relative orientations of the anisotropic $\Delta_i(k)$. Intra-band Bogoliubov QPI therefore yields the spectroscopic information required to identify the mechanism of superconductivity in iron-based superconductors.

8:12AM A22.00002 Low temperature specific heat of the codoped iron-arsenic superconductor $\text{Ba}_{0.55}\text{K}_{0.45}\text{Fe}_{1.95}\text{Co}_{0.05}\text{As}_2$ ¹, K. GOFRYK, J. LASHLEY, Los Alamos National Laboratory, A. LEITHE-JASPER, W. SCHNELLE, Max-Planck Institute for Chemical Physics of Solids, Dresden, F. RONNING, Los Alamos National Laboratory, M. NICKLAS, Max-Planck Institute for Chemical Physics of Solids, Dresden, F. WEICKERT, Los Alamos National Laboratory, H. ROSNER, Max-Planck Institute for Chemical Physics of Solids, Dresden, J.L. SMITH, Los Alamos National Laboratory — Despite large experimental and theoretical efforts the structure of the superconducting gap and the origin of the pairing mechanism in iron-based superconductors is still unresolved. Measurements of the low temperature specific heat and its magnetic response inside the superconducting state give important information about the symmetry of the gap. Here, we present results of our studies of codoped $\text{Ba}_{0.55}\text{K}_{0.45}\text{Fe}_{1.95}\text{Co}_{0.05}\text{As}_2$ with a T_c of 32.5 K. The high quality of the material is marked by a pronounced peak at T_c as well as by a low residual specific heat $\gamma_0 = 2.4 \text{ mJ/mol K}^2$. We will discuss the implications of the new specific heat results on the symmetry of the order parameter in this system.

¹The work at MPI has been supported by the DFG through SPP 1458

8:24AM A22.00003 Gap structure of the iron-based superconductor KFe_2As_2 via thermal conductivity, A. JUNEAU-FECTEAU, R.T. GORDON, J.-PH. REID, N. DOIRON-LEYRAUD, L. TAILLEFER, University of Sherbrooke, Canada, M.A. TANATAR, R. PROZOROV, Ames Laboratory and Iowa State University, USA, T. SAITO, H. FUKAZAWA, Y. KOHORI, Chiba University and JST-TRIP, Japan, K. KIHOU, C.H. LEE, A. IYO, H. EISAKI, AIST and JST-TRIP, Japan — The thermal conductivity of the iron-based superconductor KFe_2As_2 was measured at temperatures down to 50 mK in magnetic fields up to 15 T, as a way to probe the superconducting gap structure. A large residual linear term in the $T = 0$ limit is observed in zero field, showing that the gap structure contains nodes, consistent with a previous report [J.K. Dong et al., PRL 104, 087005 (2010)]. We discuss the possible interpretations for the nature of these nodes, in light of three different theoretical proposals: accidental line nodes in an extended s -wave state which are either horizontal [K. Suzuki et al., arXiv:1108.0657] or vertical [S. Maiti et al., arXiv:1111.0306], or symmetry-imposed vertical line nodes in a d -wave state [R. Thomale et al., PRL 107, 117001 (2011)].

8:36AM A22.00004 Gap structure of iron-based superconductors via directional thermal conductivity, JEAN-PHILIPPE REID, University of Sherbrooke — Because the structure of the superconducting gap as a function of direction reflects the pairing interaction, it can shed light on the nature of the pairing mechanism. In the iron pnictides, the experimental situation in this respect remains unclear and so far suggests the lack of a universal picture. Here I present a systematic study of the superconducting gap structure through directional thermal conductivity measurements [1] on hole-doped K-Ba122 [2,3], electron-doped Co-Ba122 [4,5], self-doped LiFeAs [6] and the chalcogenide FeTeSe. We observe a general trend for the evolution of the superconducting gap with doping. At optimal doping, the gap structure is nodeless and isotropic (3D). Away from optimal doping, nodes appear on the Fermi surface at the edges of the superconducting dome, as seen for K-Ba122 and Co-Ba122. This strongly suggests that the presence of these nodes is accidental and therefore not imposed by symmetry. It would instead depend on the competition between intra- and inter-band interactions controlled by the evolving band structure and Fermi surface, and by the onset of antiferromagnetic order.

Work done in collaboration with M. A. Tanatar, X. G. Luo, H. Shakeripour, R. Gordon, A. Juneau-Fecteau, N. Doiron-Leyraud, S. René de Cotret, F. Laliberté, E. Hassinger, J. Chang, N. Ni, S. L. Bud'ko, P. C. Canfield, H. Kim, R. Prozorov, B. Shen, H. Luo, Z. Wang, H.-H. Wen, K. Cho, Y. J. Song, Y. S. Kwon, and Louis Taillefer.

[1] H. Shakeripour et al., New Journal of Physics **11**, 055065 (2009).

[2] X. G. Luo et al., Physical Review B **80**, 140503 (2009).

[3] J.-Ph. Reid et al., arXiv:1105.2232.

[4] M. A. Tanatar et al., Physical Review Letters **104**, 067002 (2010).

[5] J.-Ph. Reid et al., Physical Review B **82**, 064501 (2010).

[6] M. A. Tanatar et al., Physical Review B **84**, 054507 (2011).

9:12AM A22.00005 Proximity fingerprint of $s_{\pm}$ superconductivity¹, ALEXEI KOSHELEV, VALENTIN STANEV, Materials Science Division, Argonne National Laboratory — We suggest a straightforward and unambiguous test to identify possible opposite signs of superconducting order parameter in different bands proposed for iron-based superconductors ($s_{\pm}$ -state). We consider proximity effect in a weakly coupled sandwich composed of a $s_{\pm}$ -superconductor and thin layer of s -wave superconductor. In such system the s -wave order parameter is coupled differently with different $s_{\pm}$ -gaps and it typically aligns with one of these gaps. This forces the other $s_{\pm}$ -gap to be anti-aligned with the s -wave gap. In such situation the aligned band induces a peak in the s -wave density of states (DoS), while the anti-aligned band induces a dip. Observation of such contact-induced negative feature in the s -wave DoS would provide a definite proof for $s_{\pm}$ -superconductivity.

¹This work was done within the “Center for Emergent Superconductivity,” an EFRC funded by the U.S. DOE, Office of Science, Office of BES, Award # DE-AC0298CH1088.

9:24AM A22.00006 Doping dependence of the specific heat of single crystal $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ ¹,

CARLOS CHAPARRO, LEI FANG, HELMUT CLAUS, GEORGE CRABTREE, VALENTIN STANEV, WAI-KWONG KWOK, ULRICH WELP, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA, MORTEN ESKILDSEN, Department of Physics, University of Notre Dame, Notre Dame, IN 46556, USA, ANDREAS RYDH, Department of Physics, Stockholm University, SE-10691 Stockholm, Sweden — We present a systematic study of the specific heat transitions on a series of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ single crystals with phosphorous doping ranging from near optimum doped $x = 0.3$ to strongly over doped $x = 0.55$. Our results reveal that $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ follows the scaling $\Delta C/T_c \sim T_c^2$ remarkably well.² The clean-limit nature of this material imposes new restraints on theories aimed at explaining the scaling. We find that the Ginzburg-Landau parameter decreases significantly with doping whereas the superconducting anisotropy is $\Gamma \sim 2.6$, independent of doping.

¹Crystal synthesis was supported by the CES, an EFRC funded by US DOE, Office of Science, Office of Basic Energy Sciences (CC,LF,WKK); materials characterization by DOE, Office of Basic Energy Sciences, (UW,HC, GWC), under contract No. DE-AC02-06CH11357.

²S. L. Bud'ko, N. Ni, P. C. Canfield, Phys. Rev. B **79**, 220516 (2009).

9:36AM A22.00007 Gap Symmetry in KFe_2As_2 ¹, SAURABH MAITI, Dept. of Physics, University of Wisconsin-Madison,

MAXIM KORSHUNOV, L.V. Kirensky Institute of Physics, Siberian Branch of Russian Academy of Sciences, Russia; Siberian Federal University, Russia., ANDREY CHUBUKOV, Dept. of Physics, University of Wisconsin-Madison — We revisit the issue of the gap symmetry in KFe_2As_2 , which is an Fe-pnictide superconductor with only hole pockets. Previous theoretical studies mostly argued for a d -wave gap in KFe_2As_2 since transport and thermodynamic measurements point to the presence of the gap nodes. However, a d -wave gap is inconsistent with recent laser-based angle-resolved photoemission measurements. We propose the scenario for a nodal s -wave superconductivity induced by a non-magnetic intra-band and inter-band interactions between fermions near the two hole pockets at Γ point. The superconducting gap that we find changes sign between the two hole pockets at Γ point and has $\cos 4\theta$ angular dependence and can have accidental nodes on one or several hole pockets. We argue that strong angle dependence is the consequence of near-degeneracy between inter-pocket and intra-pocket interaction on the hole pockets. We also provide a connection between the relative phase of 4θ oscillations and the shapes of the Fermi surface and discuss the implications in the light of photoemission and tunneling experiments.

¹The authors acknowledge: NSF-DMR-0906953, Humboldt foundation, RFBR, Presidium of RAS program N5.7, FCP scientific and Research-and-Educational Personnel of Innovative Russia, and President of Russia(grant MK-1683.2010.2)

9:48AM A22.00008 Disorder induced transition between $s_{\pm}$ and s_{++} states Fe-based superconductors¹, M.M. KORSHUNOV, Kirensky Institute of Physics, Krasnoyarsk 660036, Russia, D.V. EFREMOV, O.V. DOLGOV, Max-Planck-Institut FKF, D-70569 Stuttgart, Germany, A.A. GOLUBOV, Faculty of Science and Technology and MESA+ Institute of Nanotechnology, University of Twente, The Netherlands, P.J. HIRSCHFELD, Department of Physics, University of Florida, Gainesville, Florida 32611, USA — The symmetry and structure of the superconducting gap in recently discovered Fe-based materials is one of the main challenges in this exciting new field (see, e.g. P.J. Hirschfeld, M.M. Korshunov, and I.I. Mazin, Rep. Progr. Phys. 2011). We have reexamined the problem of disorder in 2-band superconductors, and shown within the framework of the T -matrix approximation that the suppression of T_c can be described by a single parameter depending on the intra- and interband impurity scattering rates. T_c is shown to be more robust against nonmagnetic impurities than would be predicted in the trivial extension of Abrikosov-Gor'kov theory. We find disorder-induced transition from the $s_{\pm}$ state to a gapless and then to a fully gapped s_{++} state, controlled by the sign of the average coupling constant.

¹Partial support was provided by DOE DE-FG02-05ER46236 (PJH and MMK), and RFBR 09-02-00127, Presidium of RAS program N5.7, Russian FCP GK P891, President of Russia MK-1683.2010.2 (MMK)

10:00AM A22.00009 Doping - dependent anisotropic superconducting gap in $\text{Na}_{1-\delta}\text{FeAs}$ and $\text{NaFe}_{1-x}\text{Co}_x\text{As}$ pnictides, KYUIL CHO, M.A. TANATAR, N. SPYRISON, H. KIM, R. PROZOROV, The Ames Laboratory, IA, USA, G. TAN, J. YAN, P. DAI, C. ZHANG, Oak Ridge National Laboratory, TN, USA — London penetration depth, λ (T), was measured in single crystals of self electron-doped $\text{Na}_{1-\delta}\text{FeAs}$ and chemically electron-doped $\text{NaFe}_{1-x}\text{Co}_x\text{As}$ superconductors. Doping level δ in self-doped ones was controlled by the deintercalation of Na^+ ions, stimulated by ultrasonic treatment. Use of the two doping techniques allowed us to cover the whole doping phase diagram from underdoped parent NaFeAs to heavily Co-overdoped compositions, with the optimal doping, $T_c \sim 25$ K, achieved for $x = 0.025$. Use of two protocols also allowed us to monitor the effect of disorder, introduced by chemical substitution in Fe sublattice. The low-temperature variation of λ (T), measured as a function of doping, was analyzed using a power-law fit, $\Delta\lambda = A T^n$. The exponent, n , changes from $n \sim 1.85$ at the optimal doping to much lower values in the underdoped, $n \sim 1.1$, and heavily overdoped, $n \sim 1.3$, samples. This doping-evolution of λ (T) cannot be explained by isotropic gap with scattering and suggests that while the superconducting gaps are isotropic at the optimal doping, at least one of them develops strong anisotropy at the dome edges. This scenario appears to be common for many other Fe-based superconductors.

10:12AM A22.00010 Proximity effect of iron-based superconductor in conventional s -wave superconducting thin films, NICK GROLL, THOMAS PROSLIER, ALEX KOSHELEV, VALENTIN STANTEV, DUCK-YOUNG CHUNG, Argonne National Laboratory — The proximity effect has been proposed as a mechanism to unambiguously identify the possible $s_{\pm}$ -state in iron-based superconductors.¹ With a thin s -wave superconductor atop a $s_{\pm}$ -superconductor it is suggested that the s -wave order parameter will couple to the $s_{\pm}$ -gaps differently, inducing a correction to the s -wave density of states that can be probed using electron tunneling spectroscopy. In this talk, we will present recent results of the superconducting proximity effect in s -wave MoGe thin films sputtered on top of bulk superconducting $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ ($T_c=35\text{K}$) pnictide. Electron tunneling spectroscopy measurements were performed for several MoGe film thicknesses using a homemade point contact setup. Finally, results will also be presented for similar measurements using two conventional s -wave superconductors.

¹A. E. Koshelev, V. Stanev, Europhysics Letters, Vol. 96, 27014 (2011)

10:24AM A22.00011 Volovik effect in the $s_{\pm}$ state of $\text{Ba}_{0.67}\text{K}_{0.33}\text{Fe}_2\text{As}_2$ from high field NMR¹, SANGWON OH, ANDREW MOUNCE, WILLIAM HALPERIN, Northwestern University, CHENGLIN ZHANG, PENGCHENG DAI, The University of Tennessee, PHILIP KUHN, ARNEIL REYES, National High Magnetic Field Laboratory — The spatially averaged density of states of an unconventional d -wave superconductor is magnetic field dependent, proportional to $H^{1/2}$, owing to the Doppler shift of quasiparticle excitations in a background of vortex supercurrents. [1, 2] This phenomenon, called the Volovik effect, is absent in an s -wave state; however, it has been predicted [3] to exist for a sign changing $s_{\pm}$ state with a characteristic field dependence, proportional to H . We have observed this behavior in the ^{75}As NMR spin-lattice relaxation rate of a single crystal of $\text{Ba}_{0.67}\text{K}_{0.33}\text{Fe}_2\text{As}_2$ studied over a wide range of fields up to 28 T. Our spatially resolved measurements show that Doppler contributions to the rate increase toward the vortex core, consistent with the superconducting state having unconventional $s_{\pm}$ symmetry.

[1] G. E. Volovik, J. Phys. C. **21**, L221 (1988)

[2] G. E. Volovik, JETP Lett. **58**, L221 (1988)

[3] Y. Bang, Phys. Rev. Lett. **104**, 217001 (2010)

¹This work is supported by DE-FG02-05ER46248, DE-FG02-05ER46202 and the NHMFL by NSF and the State of Florida.

10:36AM A22.00012 Origin of the variety of superconducting gap structure in iron-based superconductors: competition between orbital and spin fluctuations, SEIICHIRO ONARI, TETSURO SAITO, HIROSHI KONTANI, Nagoya University — To understand the pairing mechanism in iron-based superconductors, we study the three-dimensional gap structure based on the orbital fluctuation theory. We focus on the fully-gapped state in (i) heavily electron-doped KFe_2Se_2 [1], nodal gap structure in (ii) isovalent-doped $\text{BaFe}_2(\text{As,P})_2$, and strongly band-dependent gap structure in (iii) hole-doped $(\text{Ba,K})\text{Fe}_2\text{As}_2$. Based on the three-dimensional ten orbital model for (i), we obtain orbital-fluctuation-mediated fully-gapped s_{++} wave state without sign reversal. For (ii), we reproduce the loop-shaped nodal structure on the electron-Fermi surface, due to the competition between orbital and spin fluctuations. For (iii), we obtain a drastic change in the gap structure by hole-doping, reflecting the variation of orbital fluctuations due to the topological change of electron-pockets. These results indicate the significant role of orbital fluctuations in iron-based superconductors. [1] Saito et al., PRB **83**, 140512(R) (2011)

10:48AM A22.00013 Microscopic Mechanism for a Pairing State with Time-Reversal Symmetry Breaking in Iron-Based Superconductors, WERNER HANKE, Theoretical Physics, University of Würzburg, SHOU-CHENG ZHANG, Department of Physics, Stanford University, CHRISTIAN PLATT, Theoretical Physics, University of Würzburg, RONNY THOMALE, Department of Physics, Stanford University — The multipocket Fermi surfaces of iron-based superconductors promote pairing states with both $s_{\pm}$ -wave and dx^2-y^2 -wave symmetry. We argue that the competition between these two order parameters could lead to a time-reversal-symmetry breaking state with $s + id$ -pairing symmetry in the iron-based superconductors, and propose several scenarios in which this phase may be found. To understand the emergence of such a pairing state on a more rigorous footing, we start from a microscopic 5-orbital description representative for the pnictides. Using a combined approach of functional renormalization group and mean-field analysis, we identify the microscopic parameters of the $s + id$ -pairing state. There, we find the most promising region for $s + id$ -pairing in the electron doped regime with an enhanced pnictogen height.

[1] arXiv:1106.5964v1

Monday, February 27, 2012 8:00AM - 11:00AM — Session A23 DCMF: Metals Magnetic 255

8:00AM A23.00001 Bulk electronic structure of FeRh undergoing metamagnetic transition via hard x-ray photoemission, ALEXANDER GRAY, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, DAVID COOKE, Department of Physics, University of California, Berkeley, PETER KRUGER, CNRS Université de Bourgogne, CATHERINE BORDEL, Department of Physics, University of California, Berkeley, ERIC FULLERTON, Center for Magnetic Recording Research, University of California, San Diego, SHIGENORI UEDA, KEISUKE KOBAYASHI, NIMS Beamline Station at SPring-8, FRANCES HELLMAN, Department of Physics, University of California, Berkeley, CHARLES FADLEY, Department of Physics, University of California, Davis — In this study changes in the electronic structure accompanying a temperature-induced metamagnetic transition from anti-ferromagnetic to ferromagnetic order are investigated in strained epitaxial FeRh thin films via valence-band and core-level hard x-ray photoelectron spectroscopy with a photon energy of 6 keV. At such high photon energy, the resulting inelastic mean-free paths of the photoemitted electrons and therefore the average probing depths are on the order of 60 Å, corresponding to about 20 unit cells and ensuring truly bulk-sensitive measurement. Clear differences between the AFM and FM states are observed across the entire valence-band spectrum and these are well reproduced using density functional theory. Changes in the Fe 2p core-levels of Fe are also observed and interpreted using Anderson impurity model calculations. These results suggest that significant electronic structure changes are involved in this AFM-FM transition.

8:12AM A23.00002 Random magnet with competing anisotropies in $\text{Fe}_x\text{Ni}_{1-x}\text{F}_2$ alloys¹, TRENT JOHNSON, FELIO PEREZ, TUDOR STANESCU, DAVID LEDERMAN, West Virginia University — A series of epitaxial (110) $\text{Fe}_x\text{Ni}_{1-x}\text{F}_2$ films were deposited on (110) MgF_2 via molecular beam epitaxy. The Fe concentration x was determined by measuring the lattice parameter along the [110] direction using x-ray diffraction. The film thicknesses and the roughness of each interface were found by fitting of x-ray reflectivity data. The magnetic ordering as a function of x was analyzed by SQUID magnetometry. Enhancement of the Néel temperature in alloys as well as evidence of spontaneous magnetization along the c -axis after field-cooling were observed for samples with $x > 0.1$; for samples with $x < 0.1$ the magnetization was perpendicular to the c -axis. Two phase transitions were observed for alloy samples with $x > 0.1$. The phase diagram of the upper transition was consistent with mean field theory of a system with competing anisotropies. The transition at lower temperatures was unaffected by the application of a magnetic field, whereas the upper temperature transition was broadened by the application of fields as small as 50 Oe. This suggests the presence of a spin-glass phase at lower temperatures, followed by melting of the spin glass prior to the main transition to paramagnetic behavior as the temperature is raised.

¹This work was supported by the National Science Foundation.

8:24AM A23.00003 Structural and electronic origin of large magnetostrictive $Fe_{1-x}Ga_x$ alloys¹

, HUI WANG, Shenyang National Laboratory of Materials Science, Institute of Metal Research and International Centre of Materials Physics, Chinese Academy of Scie, YANNING ZHANG, RUQIAN WU, LIZHI SUN, University of California, Irvine, SONSHENG XU, ZHIDONG ZHANG, Shenyang National Laboratory of Materials Science, Institute of Metal Research and International Centre of Materials Physics, Chinese Academy of Scie — $Fe_{1-x}Ga_x$ binary alloys exhibiting large magnetostriction and excellent ductility have great potentials for various applications. The origin of large magnetostriction has not been thoroughly studied, especially at high Ga concentration ($x > 18.75\%$). We conduct extensive ab initio molecular dynamics simulation of $Fe_{1-x}Ga_x$ alloys to generate atomic structures; and find that the alloys adopt the disordered A2 structure for $x < 18.75\%$ and the A2+D0₃ mixed structures for $18.75\% < x < 23.4\%$, respectively. The formation of D0₃-like structure play a key role for the decrease of magnetostriction beyond $x = 19\%$. Interestingly, the magnetostriction may greatly enhance, up to $\lambda_{001} = 850$ ppm in ternary alloys with incorporation of 3 – 5% Cu and Zn.

¹Work was supported by the ONR (Grant No: ONR N00014-11-1-0444). Calculations were performed on the DOD supercomputers.

8:36AM A23.00004 Thin film deposition of Mn₂Ga under various growth condition , MINGYANG LI, LI

GAO, XIN JIANG, MAHESH SAMANT, BRIAN HUGHES, KEVIN ROCHE, IBM Almaden Research Center, CLAUDIA FELSER, University of Mainz, STUART PARKIN, IBM Almaden Research Center — The tetragonal DO_{22} phase of $Mn_{3-x}Ga$ is a ferromagnetic Heusler with perpendicular magnetic anisotropy. It has high spin polarization, high Curie temperature and low magnetic moment, and thus becomes a good candidate for spin-transfer-torque magnetic random access memory. This work reports the epitaxial growth of tetragonal Mn_2Ga thin films using sputtering method. The effect of various substrates, buffer layers, and substrate temperature on the film roughness is presented and compared. The formation of Mn_2Ga islands are observed at the beginning of growth on most buffer layers by reflection-high-energy-electron-diffraction. The smoothest film with root-mean-square roughness 0.10nm is obtained by using Pt buffer layer. The magnetic properties are also compared.

8:48AM A23.00005 Magneto Caloric Effect in Ni-Mn-Ga alloys: First Principles and Experimental studies , KHORGOLKHUU ODBADRAKH, DON NICHOLSON, Oak Ridge National Laboratory, GREGORY BROWN, Florida State University, AURELIAN RUSANU, ORLANDO RIOS, JASON HODGES, ATHENA SAFA-SEFAT, GERARD LUDTKA, MARKUS EISENBACH, BOYD EVANS, Oak Ridge National Laboratory — Understanding the Magneto-Caloric Effect (MCE) in alloys with real technological potential is important to the development of viable MCE based products. We report results of computational and experimental investigation of a candidate MCE materials Ni-Mn-Ga alloys. The Wang-Landau statistical method is used in tandem with Locally Self-consistent Multiple Scattering (LSMS) method to explore magnetic states of the system. A classical Heisenberg Hamiltonian is parametrized based on these states and used in obtaining the density of magnetic states. The Curie temperature, isothermal entropy change, and adiabatic temperature change are then calculated from the density of states. Experiments to observe the structural and magnetic phase transformations were performed at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL) on alloys of Ni-Mn-Ga and Fe-Ni-Mn-Ga-Cu. Data from the observations are discussed in comparison with the computational studies. This work was sponsored by the Laboratory Directed Research and Development Program (ORNL), by the Mathematical, Information, and Computational Sciences Division; Office of Advanced Scientific Computing Research (US DOE), and by the Materials Sciences and Engineering Division; Office of Basic Energy Sciences (US DOE).

9:00AM A23.00006 First principles determination of the rhombohedral magnetostriction of $Fe_{100-x}Ga_x$ and $Fe_{100-x}Al_x$ ($x < 20$) alloys¹ , RUQIAN WU, YANNING ZHANG, University of California, Irvine — Extensive efforts have been dedicated to investigate the extraordinary magnetostriction of Galfenol ($Fe_{100-x}Ga_x$) and Alfenal ($Fe_{100-x}Al_x$) alloys, which are very promising magnetostrictive materials for various applications such as sensors, transducers and spintronic devices. In contrast to the strong response of the tetragonal magnetostriction (λ_{100}) to the Ga/Al concentration (x), the rhombohedral magnetostriction, λ_{111} , vs. x curves for both FeGa and FeAl alloys show negative and steady values for $0 < x < 15$. Strikingly, the sign of λ_{111} changes at $x = 18$, a concentration that corresponds to the first peak of λ_{100} - x curves. Through highly-accurate full potential linearized augmented plane-wave method (FLAPW), our theoretical results nicely reproduce the main features of experimental λ_{111} - x curves, except the opposite sign of λ_{111} of pure Fe. Detailed analyses on the structural and electronic properties of Galfenol provide deeper understandings of the origins of the sign change, as well as the large magnetostriction anisotropy in these alloys. Possible reasons on the disagreement between the calculated and observed rhombohedral magnetostriction of bcc Fe will also be given.

¹Work was supported by the ONR (Grant No: ONR N00014-11-1-0444). Calculations were performed on the DOD supercomputers.

9:12AM A23.00007 Intrinsic Magnetic Properties of $L1_0$ Derivates¹ , RALPH SKOMSKI, Dept. of Physics & Astronomy and NCMN, University of Nebraska, PRIYANKA MANCHANDA, PANKAJ K. SAHOTA, ARTI KASHYAP, IIT Jaipur, India, BALAMURUGAN BALASUBRAMANIAN, Dept. of Physics & Astronomy and NCMN, University of Nebraska, J.E. SHIELD, Dept. Mechanical Engineering, University of Nebraska, D.J. SELLMYER, Dept. of Physics & Astronomy and NCMN, University of Nebraska — It is investigated how atomic substitutions modify the magnetization, exchange and anisotropy of $L1_0$ -ordered ferromagnets. Emphasis is on properties of interest in permanent magnetism, including the reduction of raw-materials costs by substituting iron-series transition metals for expensive heavy (4d/5d) transition-metal elements. In particular, VASP calculations are used to determine the magnetizations of the Fe-Co-Pt, Mn-Al-C and Fe-Ni-S systems. We perform supercell calculations to determine the moments of Fe and Co in various $L1_0$ derivates with chemical disorder. The local magnetic moments exhibit a subtle dependence on the environment, not only in each Fe-Co layer but also through alternating 4d/5d layers. However, the magnitude of these spatial fluctuations is not very large, and after configurational averaging, the moments exhibit very simple dependencies on the concentrations of the involved atoms. The FeNi system is also interesting because $L1_0$ -ordered FeNi was originally discovered in meteorites (tetrataenite), formed with cooling times in excess of one million years.

¹This research is supported by ARPA-E REACT (RS) , BREM (JES), DOE (DJS), ARPA-E Delaware (BB), and DST (AK).

9:24AM A23.00008 Growth of Mn₂TiSn alloy and its magnetic and structural characterizations¹ , YUNG HUH, Physics Department, South Dakota State University, Brookings, 57007, P. KHAREL, V.R. SHAH, X.Z. LI, N. AL-AQTASH, K. TARAWNEH, E.S. KRAGE, R.F. SABIRIANOV, R. SKOMSKI, D.J. SELLMYER, NCMN, University of Nebraska, Lincoln, NE 68588 — A ternary inter-metallic alloy Mn_2TiSn is one of the candidates predicted to be a Heusler compound with high spin polarization and Curie temperature well above room temperature, which is suitable for spintronic applications. Mn_2TiSn powder samples were prepared by arc melting and annealing under controlled environment to study magnetic and structural properties. Temperature and field dependent magnetization measurements show the sample is ferromagnetically ordered with a Curie temperature above 400 K. The low temperature magnetization at 10 K is about 2.5 emu/g under 100 Oe. The coercivity increases as temperature decreases from 1 kOe at room temperature to 2.4 kOe at 10 K. Theoretical calculation from the high field data shows the anisotropy energy is 4.0×10^5 ergs/cm³ at 300 K but it becomes slightly more than doubled at 10 K. TEM and XRD characterizations reveal that the compound crystallizes in the hexagonal structure (D0₁₉, P6₃/mmc) rather than the theoretically proposed L2₁ cubic structure, which is supported by the first-principle structure calculations where the total energy per unit cell volume is preferred for the hexagonal structure.

¹This research is supported by ARO (W911NF-10-2-0099) (DJS, PK, XZL, VRS), NSF-MRSEC (NSF-DMR-0820521) (YH, EK, RFS, KT, NA and RS) and NCMN (Central Facility support).

9:36AM A23.00009 Unusual temperature dependence of the magnetic anisotropy constant in barium ferrite $\text{BaFe}_{12}\text{O}_{19}$, FAN ZHAO, JUN WANG, WEI WU, Ningbo University, GUO-MENG ZHAO, California State University, Los Angeles — We report magnetic hysteresis loops in a wide temperature range (4-700 K) for silica-coated barium ferrite $\text{BaFe}_{12}\text{O}_{19}$ nanoparticles. The saturation magnetization M_s and the first magnetic anisotropy constant K are determined simultaneously from the magnetic hysteresis loop using the law of approach to saturation. It is remarkable that K is linearly proportional to M_s and varies precisely with temperature as $K(T) = K(0)[1 - (T/T_C)^{1.58}]$ in the whole temperature range below the Curie temperature T_C (740 K). The unusual temperature dependence of the anisotropy constant and its linear relation with the saturation magnetization in $\text{BaFe}_{12}\text{O}_{19}$ are not predicted from the existing theoretical models.

9:48AM A23.00010 First principles study of magnetic properties of Zn-Sn substituted M-type Sr-hexaferrite, SEONG-GON KIM, LAALITHA LIYANAGE, Department of physics and astronomy, Mississippi state university, JEFF HOUZE, None, SUNGHO KIM, Center for advanced vehicular systems, Mississippi state university — Site occupancy and magnetic properties of Zn-Sn substituted M-type Sr-hexaferrite $\text{SrFe}_{12-x}(\text{Zn}_{0.5}\text{Sn}_{0.5})_x\text{O}_{19}$ with $x = 1$ were studied using density functional theory and generalized gradient approximation (GGA). Using the GGA+U method the description of strongly correlated $3d$ electrons of Fe was improved. Our results show that Zn and Sn atoms prefer to occupy $4f_1$ and $4f_2$ sites respectively. Favorable Zn-Sn substituted configurations show an increase in saturation of magnetization (M_s), and a decrease in magnetic anisotropy energy (MAE), over the pure M-type Sr-hexaferrite ($x = 0$). Experimental observations agree with the decrease of MAE and the increase of M_s for Zn-Sn substituted Sr-hexaferrite.

10:00AM A23.00011 The Origin of Secondary Hematite Phase in Non-stoichiometric Co-ferrite Prepared by Ceramic Method¹, DAVID JILES, Electrical and Computer Engineering Department, Iowa State University, Ames, IA 50011, USA, CAJETAN NLEBEDIM, Ames Laboratory, US Department of Energy, Ames, IA 50011, USA, ANTHONY MOSES, Wolfson Centre for Magnetics, School of Engineering, Cardiff University, Cardiff CF24 3AA, UK, MAGNETICS RESEARCH GROUP TEAM, MAGNETICS RESEARCH GROUP TEAM, WOLFSON CENTRE FOR MAGNETICS TEAM — Surprising results have shown the formation of a secondary phase of hematite in co-ferrite. Co-ferrite based materials have been increasingly studied for magnetoelastic and magnetoelectric applications. Enhancement of the properties for such applications can be made by cation substitution, heat treatment or processing. Often, samples whose compositions deviate from stoichiometry or targeted compositions are made. It is not yet known, how far from stoichiometric composition one would go to create other phases; which would also affect the properties. This study shows that, when samples are made by the ceramic method, a secondary hematite phase forms with the spinel Co-ferrite phase. The origin of the hematite phase is related to the processing temperature, sintering environment and deviation from stoichiometric composition. Consequently, deviation from targeted or stoichiometric compositions may explain why properties of co-ferrite reported in literature vary.

¹Research at Ames Lab. was supported by Dept. of Energy-Basic Energy Sciences (Contract No. DE-AC02-07CH11358); research at Cardiff University was supported by UK EPSRC (Grant No. EP/D057094).

10:12AM A23.00012 Magnetic Characterization of heavily proton-irradiated MnAl Hall bars¹, MARC COSTANTINE, NATTAWUT ANUNIWAT, YISHEN CUI, STU WOLF, JIWEI LU, University of Virginia, BRAD WEAVER, Navy Research laboratory — τ -MnAl has L1_0 structure with the perpendicular magnetic anisotropy and it attracts some interests due to the potential application in magnetic recording media and spintronics. We fabricate $\sim 2\mu\text{m}$ wide Hall bar devices from 40 nm MnAl thin film to study the transport properties. Anomalous Hall Effect (AHE) resistance loops of the devices and out-of-plane magnetization loops of unpatterned films mimic one another. This correlation shows that the electrical transport of the material is strongly spin dependent at room temperature. Crystallinity and chemical ordering characterization are performed using X-ray diffraction on unpatterned films. Both patterned and unpatterned films are then exposed to 2 MeV-energy protons for 2 hours at Naval Research Laboratory for displacement damages study. The magnetic and magneto-transport properties were not degraded after the irradiation, which shows promising radiation hardness for future spintronics devices. The heavier, more energetic beam sources and larger dose radiations will be performed and discussed.

¹We acknowledge the financial support from DARPA and DTRA.

10:24AM A23.00013 Structural and magnetic properties of high anisotropy $\text{HfCo}_{7-x}\text{Fe}_x$ alloys¹, BALAMURUGAN BALASUBRAMANIAN, BHASKAR DAS, RALPH SKOMSKI, SHAH VALLOPILLY, JEFFREY SHIELD, DAVID SELLMYER, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE 68588. — An increasing demand of rare-earth elements in recent years intensifies the search for rare-earth free permanent magnetic materials with magnetocrystalline anisotropy $K_1 = 1 \text{ MJ/m}^3$. The present study reports melt-spun HfCo_7 alloys with a high K_1 of 1.3 MJ/m^3 along with an appreciable saturation-magnetic polarization (J_s) of 8.9 kG. A substitution of Fe for Co in $\text{HfCo}_{7-x}\text{Fe}_x$ further improves K_1 and J_s to 1.5 MJ/m^3 and 10.4 kG, respectively. XRD studies of HfCo_7 are in agreement with an orthorhombic structure and also reveal a lattice expansion on substituting Fe for Co. These results show that $\text{HfCo}_{7-x}\text{Fe}_x$ can be a promising candidate for permanent-magnet and other significant applications. In brief, the structural and magnetic properties of $\text{HfCo}_{7-x}\text{Fe}_x$ alloys ($0 \leq x \leq 1$) investigated using XRD, EDX, TEM, and SQUID magnetometer will be presented.

¹This work is supported by DOE (D.J.S.), ARPA-E (B.B., J.E.S.), BREM (B.D., R.S.), and NCMN (S.R.V.)

10:36AM A23.00014 Calciothermic Preparation of Sm-Co From Nanostructured Precursor Oxides¹, BRIAN KELLY, Department of Physics and Astronomy, University of Delaware, GERALD POIRIER, Princeton Institute for the Science and Technology of Materials, Princeton University, KARL UNRUH, Department of Physics and Astronomy, University of Delaware — A calciothermic reduction/diffusion process has been developed for the preparation of Sm-Co alloys with good magnetic properties using nanostructured Co- and SmCo -oxide powders as precursors. The precursor oxides were obtained from an aqueous solution of $\text{Sm}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$, $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, and citric acid which, after the removal of excess water, spontaneously reacts to form a fine mixture of Co_3O_4 and SmCoO_3 nanoparticles. These nanoparticles were then mixed with metallic Ca granules, sealed under inert gas in Nb tubes, and heated to temperatures between 850 and 1000 °C for various lengths of time. The products of the reduction/diffusion reaction were studied by scanning electron microscopy with elemental analysis, vibrating sample magnetometry, and x-ray diffraction. These measurements revealed that (in addition to the oxidation product CaO) the products of the reduction/diffusion process were micron-sized particles of essentially single phase SmCo_5 with a coercivity in excess of 40 kOe and a Curie temperature of about 950 °C.

¹This work was supported by DOE ARPA-E DE-AR0000046.

10:48AM A23.00015 Theoretical search for new permanent magnets with no rare earth atoms, LIQIN KE, VLADIMIR ANTROPOV, Ames Laboratory, MARK VAN SCHILFGAARDE, King's College, London, UK — We use the density functional theory and Quasiparticle Self-Consistent GW approximation to investigate the crystal and electronic structure, magnetic moment, anisotropy, and exchange coupling of Fe_{16}N_2 , $\text{Fe}_{13}\text{Al}_3$, Co_7Hf and $\text{Zr}_2\text{Co}_{11}$. Both methods show similar results for magnetization and electronic structure. The experimentally unknown crystal structures of Co_7Hf and $\text{Zr}_2\text{Co}_{11}$ are obtained using structural optimization. We also discuss possible usage of these materials as permanent magnets.

Monday, February 27, 2012 8:00AM - 11:00AM –

Session A24 FIAP: Materials: Synthesis, Growth and Processing (Bulk and Films) 256

8:00AM A24.00001 Epitaxial Growth of Zinc Oxide on Single Crystalline Gold Plates, KATHRYN GREENBERG, JOHN JOO, MOR BARAM, DAVID CLARKE, EVELYN HU, Harvard University School of Engineering and Applied Sciences — Although metal-oxide interfaces are the critical components of many electronic and optical devices, it is rare to find epitaxial metal-oxide structures. We demonstrate for the first time, a method for the low temperature, epitaxial growth of zinc oxide (ZnO) on single crystalline gold plates. The gold plates, up to 100 μ m in width, are grown from a gold-surfactant complex. Even with the large lattice mismatch between (111) gold and (0001) ZnO, we are able to form epitaxial zinc oxide at 90°C on top of the single crystal gold plates. This epitaxial growth is confirmed using transmission electron microscopy, electron diffraction, and electron backscatterer diffraction. Micro-photoluminescence is also performed to investigate the optical properties of the epitaxial zinc oxide. We remove the grown ZnO membranes from the gold plates using a stamping and etching process. These membranes can potentially be used to fabricate high quality microdisks and photonic crystals. The metal-oxide interfaces that we have fabricated may have the ability to be used in a number of technologically important applications, including as better electrical contacts and for improved light extraction from planar LED structures.

8:12AM A24.00002 Forward Raman scattering in ZnO: observation of phonon polaritons¹, D.A. TENNE, T. ENGMAN, A.K. FARRAR, Department of Physics, Boise State University, Boise, ID 83725, USA — Single crystal wurtzite ZnO samples have been studied by forward Raman scattering. Spectra were measured at 295 and 75 K using 442 and 448 nm laser lines for excitation below the fundamental absorption edge. Measuring spectra in forward geometry at varied scattering angles allowed achieving small and variable magnitudes of phonon wave vector necessary to observe a polariton effect. The observed frequencies of the polaritons formed by A₁ TO phonons will be compared to the calculated dispersion of phonon polaritons in ZnO.

¹Supported in part by NSF Grant DMR-1006136

8:24AM A24.00003 SiGe Nanomembranes: Defect-Free Single-Crystalline Substrates for Growth of Strained Si/SiGe Heterostructures¹, DEBORAH M. PASKIEWICZ, BOY TANTO, DONALD E. SAVAGE, PAUL G. EVANS, MARK A. ERIKSSON, MAX G. LAGALLY, University of Wisconsin-Madison — Silicon-Germanium semiconductor alloys play a pivotal role in the strain engineering of heterostructures for microelectronic devices; however, high quality, single crystalline, defect free films with more than minimal Ge concentration do not exist. The lattice mismatch between Si and bulk SiGe results in biaxial tensile strain in thin Si films and leads to electronic band offsets that allow for the confinement of electrons in the strained Si layer, i.e., a two-dimensional electron gas. Many of the current techniques used to create relaxed SiGe rely on plastic relaxation of the alloy, which impose strain variations and inject crystalline defects into all epitaxial layers grown on top. These defects can significantly degrade the performance of any device in the active layer. We demonstrate the fabrication of SiGe nanomembranes (NM): fully elastically relaxed, smooth, single-crystalline sheets of SiGe alloy. These SiGe NMs can be transferred to new handling substrates, bonded, and used as templates for growth of new defect-free materials. We compare the material quality of strained Si/SiGe heterostructures grown on SiGe NMs with those created on SiGe substrates relaxed via dislocations.

¹Research supported by DOE and NSF.

8:36AM A24.00004 XRD analysis of high purity germanium single crystals grown by Czochralski method, GANG YANG, GUOJIAN WANG, WENCHANG XIANG, MUHAMMAD KHIZAR, YUTONG GUAN, YONGCHEN SUN, DONGMING MEI, CHAOYANG JIANG, BRUCE GRAY, University of South Dakota — Two high purity germanium (HPGe) crystals were grown in argon and hydrogen atmosphere by Czochralski method, respectively. Both XRD 2θ scanning and rocking curve (ω -scanning) were used to investigate the quality of the grown crystals. XRD 2θ scanning results show that an extremely strong (400) peak at 2θ of 66.15° and a very feeble (200) peak at 31.56° were observed in three samples cut from the crystal grown in Ar atmosphere, indicating the crystals with <100> orientation. However, there is an obvious split on (400) peak for three samples, which could be attributed to defects in the crystal. Additionally, according to the reflection and extinction law of germanium crystal with face-centered cubic lattice, the reflection of 200 should be forbidden. The presence of (200) peak at 31.56° could be resulted from XRD multiple-beams scattering. For the crystal grown in hydrogen atmosphere, only very strong and non-split (400) peak at 2θ of 66.15° was observed in all three samples. The ω -scanning results of two crystals at the fixed 2θ of 66.15° show that the crystal grown in hydrogen atmosphere has much more highly symmetric rocking curve with narrower FWHM, which exhibits that the crystal grown in hydrogen atmosphere has very high quality. This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota.

8:48AM A24.00005 Growth and characterization of room temperature antiferromagnetic I-Mn-V semiconductors¹, X. MARTI, Charles University in Prague, T. JUNGWIRTH, P. WADLEY, H. REICHLÖVA, V. NOVAK, Institute of Physics ASCR, O. STELMAKHOVYCH, K. UHLIROVA, Charles University in Prague, P. BERAN, Nuclear Physics Institute ASCR, M. CUKR, Institute of Physics ASCR, F. MACA, Institute of Physics ASCR, Czech Republic, A.B. SHICK, Institute of Physics ASCR, J. MASEK, Institute of Physics ASCR, Czech Republic, P. HORODYSKÁ, P. NEMEC, V. HOLY, Charles University in Prague, J. ZEMEK, P. KUZEL, Institute of Physics ASCR, I. NEMEC, Charles University in Prague, B. GALLAGHER, R. CAMPION, C.T. FOXON, University of Nottingham, J. WUNDERLICH, Hitachi Cambridge Laboratory — The integration of ferromagnetism and semiconductors has been studied extensively, but devices operate well below room temperature. Recent theoretical and experimental works have opened a new route for spintronics based on antiferromagnets. Remarkably, high-temperature antiferromagnetic order is much more compatible with semiconductors than the ferromagnetic order. In our work we focus on the family of I-Mn-V antiferromagnetic semiconductor. We report on our synthesis of bulk and thin-film epilayers of the I-Mn-V compounds and on their basic electrical and magnetic properties. We will discuss the utility of these materials for designing antiferromagnetic semiconductor spintronic devices.

[1] Phys. Rev. B 83, 035321 (2010)

[2] <http://arxiv.org/abs/1102.5373>

¹Project P204/11/P339 (Czech Science Foundation) is acknowledged

9:00AM A24.00006 Nonequilibrium growth of GaInAsSb on GaSb across the immiscibility region by molecular beam epitaxy for midinfrared materials¹ , ASLI YILDIRIM, JOHN PRINEAS, Department of Physics and Astronomy, and Optical Science and Technology Center, University of Iowa, Iowa City, IA, 52242 — GaInAsSb is a potentially important mid-infrared material, because alloys can in theory be grown with cut-off wavelengths from 1.7 to 4.9 μm . That potential has been hampered in the past by the presence of large alloy immiscibility regions. In this work, 2 μm bulk GaInAsSb layers lattice-matched to GaSb substrates were grown across the entire compositional range, including the immiscibility region, by molecular beam epitaxy. Lower than typical growth temperatures (410-450 °C) were used to limit the adatom diffusion length and move growth conditions further from equilibrium. Using a variety of techniques to characterize the optical, structural, and morphological quality of films, no phase separation was observed to occur for any alloy concentration. High resolution X-ray scans showed one narrow peak, and a single bright photoluminescence peak was observed for all samples. Smooth GaInAsSb surfaces were observed for all samples by AFM measurements, and XTEM images also show GaInAsSb layers to be homogeneous and defect free, with no sign of phase separation. EDS studies have been done, and results show low alloy scatter.

¹This work is supported by NSF DMR 100-6956

9:12AM A24.00007 Electronic and Structural Properties of InGaZnO Thin Films , D.S. WILLIAMS, S. SALLIS, L.F.J. PIPER, B.E. WHITE, Binghamton University — We examine the effects of oxygen partial pressure during deposition and the structural changes resulting from a post-deposition anneal on the transport properties of InGaZnO. Amorphous oxygen-deficient samples sputter-deposited from a target with an atomic ratio of 2:2:1:7 at 50 watts DC in a 3 mTorr argon atmosphere have a resistivity of 0.16 ohm-centimeters. Amorphous oxygen-rich samples deposited similarly, except for a 10% oxygen partial pressure, are insulating. For both samples, the as-deposited surfaces show a consistent grain size of approximately 30 nm. A subsequent rapid thermal anneal at 600°C for 10 seconds leads to the coalescing and vertical growth of the grains with a resultant thinning of the background matrix. After anneal, the resistivity of the oxygen-deficient sample is decreased to 0.003 ohm-centimeters and 0.005 ohm-centimeters for the oxygen-rich sample. X-ray diffraction, scanning electron microscopy, atomic force microscopy and x-ray photoelectron spectroscopy data are presented to explain these changes and suggest possible methods of tuning the properties of InGaZnO for future use in thin film transistors, flexible electronics, transparent conductors and thermoelectric materials.

9:24AM A24.00008 Low temperature atomic layer deposition of $\alpha\text{-Fe}_2\text{O}_3$ ¹ , JEFFREY KLUG, THOMAS PROSLIER, Argonne National Laboratory, NICHOLAS BECKER, Argonne National Laboratory and Illinois Institute of Technology, JEFFREY ELAM, MICHAEL PELLIN, Argonne National Laboratory — There is significant interest in the use of $\alpha\text{-Fe}_2\text{O}_3$ (hematite) as a semiconducting thin film in a variety of applications including solar energy conversion, water oxidation, and gas sensing. In many such applications, devices may depend on non-planar geometries where traditional thin film deposition techniques are limited by line-of-sight constraints. Atomic layer deposition (ALD) is a gas-phase synthesis technique utilizing sequential self-saturating surface chemical reactions to produce uniform coatings with atomic scale control on substrates with arbitrary shape. However, ALD processes explored for Fe_2O_3 to date generally suffer from either extremely low growth rates, narrow temperature windows for self-saturating growth, or precursors with limited reactivity. In this respect, we will present a detailed study of a new, previously unexplored process for ALD of $\alpha\text{-Fe}_2\text{O}_3$ at technologically relevant temperatures between 200-300°C. Self-limiting growth at ~ 0.7 Å/cycle was confirmed via situ quartz crystal microbalance. The results of in situ process characterization and ex situ analysis of film structure, morphology, composition, and electrical properties will be presented.

¹This work was supported by the U.S. Department of Energy, Office of Science under contract No. DEAC02-06CH11357 and by the American Recovery and Reinvestment Act (ARRA) through the US Department of Energy, Office of High Energy Physics.

9:36AM A24.00009 Impact of atmosphere on HPGe crystal growth¹ , GUOJIAN WANG, GANG YANG, WENCHANG XIANG, JAYESH GOVANI, MUHAMMAD KHIZAR, YUTONG GUAN, DONGMING MEI, Department of physics, University of South Dakota — The growth of high-purity germanium crystals for radiation detectors is being developed at the University of South Dakota. High-purity germanium crystals were grown in argon and hydrogen atmosphere, individually. The growth parameters were compared and analyzed. The relationship between thermal field and crystal quality was discussed. Based on the thermal properties of argon and hydrogen gases, different thermal fields were designed to grow lower dislocation density of high-purity germanium crystals.

¹This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota.

9:48AM A24.00010 Performance optimization of diffused Li on Ga/In eutectic, In/Sn solder and eutectic Ga/In Ohmic contacts to n-high purity-crystalline (100) Ge , KHIZAR KHAN, YANG GANG, GUOJIAN WANG, WENCHANG XIANG, YUTONG GUAN, DONGMING MEI, Department of Physics, University of South Dakota, Vermillion, SD 57069 — Performance optimization study of novel contacts such as diffused lithium on Ga/In eutectic (75.5/24.5 wt%), In/Sn solder (95.0/5.0 wt%) and Ga/In eutectic (75.5/24.5 wt%) to n-high purity-crystalline <100> Ge (HP-SC-Ge) has been presented. Ultrasonically clean samples taken from same substrate were used to process the contacts followed by their characterization utilizing current-voltage (I-V), Hall-effect and AFM measurements. Extreme care was introduced to minimize the effect of parasitic oxide layers. Contacts such as diffused Li on eutectic Ga/In and In/Sn solder were processed in an inert glove box and characterized at 305 K (RT) and 77 K (LN) respectively. Comparative study revealed that Ga/In eutectics contacts behave throughout linear and stable, showing strong hall-effect to that of its counter parts. This was attributed due to the high adsorption behavior of anions at liquid (Ga-In) contacts and improved wettability. Whereas, for In/Sn solder case, the contacts processing considerations were substantially different, mainly because of its poor solder flow, excessive void formation, and heterogeneous phase distribution responsible for process yield loss. For diffused Li on Ga/In eutectic contacts, the linearity of the obtained Ohmic profiles was not consistent due to the high reactivity of the Li with HP-SC-Ge substrate. This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota.

10:00AM A24.00011 Crystal-growth Underground Breeding Extra-sensitive Detectors¹ , DONGMING MEI, The University of South Dakota, CUBED COLLABORATION — CUBED (Center for Ultra-Low Background Experiments at DUSEL) collaborators from USD, SDSMT, SDSU, Sanford Lab, and Lawrence Berkeley National Laboratory are working on the development of techniques to manufacture crystals with unprecedented purity levels in an underground environment that may be used by experiments proposed for DUSEL. The collaboration continues to make significant progress toward its goal of producing high purity germanium crystals. High quality crystals are being pulled on a weekly basis at the temporary surface growth facility located on the USD campus. The characterization of the grown crystals demonstrates that the impurity levels are nearly in the range of the needed impurity level for detector-grade crystals. Currently, the crystals are being grown in high-purity hydrogen atmosphere. With an increase in purity due to the zone refining, the group expects to grow high-purity crystals by the end of 2011. The one third of the grown crystals will be manufactured to be detectors; the remaining will be fabricated in to wafers that have large applications in electro and optical devices as well as solar panels. This would allow the research to be connected to market and create more than 30 jobs and multi millions revenues in a few years.

¹This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota

10:12AM A24.00012 Lattice matched quaternary alloy, BGaAsBi: growth and characterisation¹, DANIEL BEATON, AARON PTAK, KIRSTIN ALBERI, ANGELO MASCARENHAS, National Renewable Energy Lab — The ternary semiconductor alloy GaAs_{1-x}Bi_x has been the focus of many recent studies due to the large decrease in the fundamental band gap, $\Delta E_g \simeq -85 \text{ meV/\%}$ for small incorporated amounts. However, the large size of the bismuth atom relative to the arsenic it replaces results in significant lattice mismatch to GaAs substrates. We now report on the lattice matched quaternary alloy, B_yGa_{1-y}As_{1-x}Bi_x. Incorporating a smaller atom (boron) along with the larger atom (bismuth) allows for a reduction of the epi-layer strain and lattice matched compositions, [B]:[Bi] $\simeq$ 1. The benefit of the choice of boron is that it does not effect the band structure of the host GaAs; no change in the band gap is observed with increasing boron content. Samples were grown by molecular beam epitaxy under conditions conducive to bismuth incorporation: low growth temperatures and low V:III ratios. Both high-resolution X-ray diffraction (XRD) and secondary ion mass spectroscopy were used to verify material composition and photoluminescence used to measure the band gap, and these results will be presented. The increasing observation of a distribution of shallow, in-gap boron related defects will also be discussed.

¹This work is supported by the DOE, BES and MS&E.

10:24AM A24.00013 Optimization of high purity germanium (HPGe) crystals growth rate through the simulation and modeling of growth system geometry¹, JAYESH GOVANI, DONGMING MEI, GUOJIAN WANG, GANG YANG, Physics Department, University of South Dakota, Vermillion, SD 57069 U.S.A — The growth rate and quality of high-purity germanium (HPGe) single crystals depend largely on the control of the thermal field such as the temperature profile and heat transfer. The control parameters of the thermal field can only be regulated externally through the growth system geometry, hydrogen and argon gas pressure, flow rate, pulling rate, and power and frequency of a RF heater. Since quantitative determination of the control parameters is exceptionally challenging and expensive, computer modeling and simulation of Cz growth processes play an imperative role in the advances of innovative pulling procedures and augmentation of Ge crystal quality. We present a detailed modeling and simulation study of radial and vertical temperature gradient, radial and vertical heat flux, temperature profile, thermo-elastic stresses, and defect density analysis for different crystal positions and diverse growth system geometry. We also virtually studied the consequences of targeted growth rate on temperature gradient and induction heating. A comparative analysis of simulated and available experimental results is also presented. In this effort, we have demonstrated the importance of simulation and modeling as it helps reducing the number of growth experiments significantly for the optimization of crystal quality and targeted growth rate.

¹This work is supported by DOE grant DE-FG02-10ER46709 and the State of South Dakota.

10:36AM A24.00014 Passivation Layer by SiC Thin Film Deposition for High Efficiency Solar Cells, MAHDI HAGHZEDEH, ECE U. Mass Lowell, DANIEL SCHMIDT, Plastics Eng U. Mass Lowell, JOEL THERRIEN, ECE U. Mass Lowell — Deposition of a polymer derived SiC thin film as a novel, chemically and physically stable passivation layer to enhance the efficiency of solar cells by way of reducing surface recombination was studied. Starfire Matrix Polymer number 10 (SMP-10) is used to produce thin films of SiC on ion implanted silicon wafers. To ascertain the best method to deposit, three methods were tested: spin coating, spray coating, and dip coating are used. Various concentrations of SMP-10 diluted in xylene as an appropriate solvent are examined. To test the films, a contactless inductive coupling method is used. The thinner layers of SiC are grown by a lower percentage of SMP-10 (5%), higher spin speed in spin coating (3000 RPM), and lower pulling out speed in dip coating (50 mm/minute). All of the methods yield controllable, repeatable, and uniform thin films. Although eliminating oxygen as an impurity in the passivation layer remains a challenge, the described approach has promise as a simple, low-cost passivation layers for higher efficiency solar cells.

10:48AM A24.00015 Growth of ZnO Nanowire Arrays for Advanced Ultraviolet Detectors, JOHN ZELLER, Magnolia Optical Technologies, Inc., TARIQ MANZUR, Naval Undersea Warfare Center, 1176 Howell Street, Newport, RI 02841, A.F. MEHDI ANWAR, Department of Electrical Engineering, University of Connecticut, Storrs, CT 06269, ASHOK K. SOOD, Magnolia Optical Technologies, Inc., 52-B Cummings Park, Woburn, MA 01801 — Zinc oxide (ZnO) provides a unique wide bandgap biocompatible material system exhibiting both semiconducting and piezoelectric properties. Bulk ZnO has a bandgap of 3.37 eV that corresponds to emissions in the solar blind ultraviolet (UV) spectral band (240-280 nm). We have grown highly ordered vertical arrays of ZnO nanowires using the metal organic chemical vapor deposition (MOCVD) technique on Si, silicon dioxide, c-plane sapphire, and GaN epitaxial substrates. UV detectors based on ZnO nanowires offer the highest UV sensitivity and lowest visible sensitivity for applications such as missile plume detection and threat warning. The development of UV detectors based on vertical nanowire arrays requires an innovative fabrication approach involving precise deposition of metal contacts, where UV sensor performance depends to a large extent on the growth conditions as well as on the substrate used. We will present experimental results on the structural, electrical, and optical properties of ZnO nanowires grown for UV sensing applications.

Monday, February 27, 2012 8:00AM - 11:00AM –
Session A25 DCOMP GSCCM DMP: Focus Session: Simulation of Matter at Extreme Conditions - Energetic Materials 257A

8:00AM A25.00001 Instability of planar detonation front in energetic materials, MIKALAI BUDZEVICH, VASILY ZHAKHOVSKY, AARON LANDERVILLE, University of South Florida, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — Detonation wave propagation in solid energetic materials (EMs), as described by the standard AB model, was studied using a novel moving window molecular dynamics (MW-MD) technique. Parameters of the AB model were modified to investigate the mechanisms of detonation propagation in EMs as a function of the activation barrier for the chemical reaction $AB+B \rightarrow A+BB + 3 \text{ eV}$. For barriers below 0.2 eV, the detonation front structure remained planar regardless of the cross-section of the sample. For higher activation barriers, the one-dimensional planar detonation evolves into a cellular detonation upon increase of one of the transverse dimensions of the sample. The cellular detonation transforms into a stable three-dimensional turbulent-like detonation upon simultaneous increase of both transverse dimensions of the sample. These various instabilities of the planar detonation front in solid EMs observed in our MW-MD simulations mirror the major regimes of gas-phase detonation, thus confirming the universal nature of detonation phenomena.

8:12AM A25.00002 Shock-induced chemical reactions in organic materials and explosives, DANA DATTELBAUM, STEPHEN SHEFFIELD, SHAWN MCGRANE, PETER GOODWIN, Los Alamos National Laboratory, SHOCK AND DETONATION PHYSICS TEAM — Interrogating chemical reactions behind a shock front is immensely difficult and, as a result, the details of shock-induced chemistry remain poorly understood. Previous research has shown that dimerizations, polymerizations, ring-opening and decomposition reactions can occur under shock compression, depending on molecular structure. Questions regarding the thresholds for incipient reaction, the nature of first and subsequent reaction steps, and the influence of shock input conditions on reaction kinetics remain to be answered. Here, we have applied *in-situ* electromagnetic gauging at multiple Lagrangian positions to elucidate the evolution of multiple-wave structures associated with shock-induced reactions of several simple functional groups: carbon-carbon double ($-C=C-$) and triple bonds, and nitriles. The relative order of group reactivity under single shock conditions for these simple molecules is discussed. From measurements of the reactive flow, we have obtained detailed information about the temporal evolution of the waves, and global kinetic rates associated with transformation(s) between partially- and fully-reacted states. Near the reactive thresholds, evolution in particle velocities point to reaction timescales on the order of tens-to-hundreds of nanoseconds. We further compare evidence of reaction from gas gun-driven experiments to recent results using laser-driven shocks. Spectroscopic details will be presented from both types of experiments.

8:24AM A25.00003 Molecular dissociation under extreme conditions¹, IGOR SCHWEIGERT, US Naval Research Laboratory — Molecular dissociation under extreme temperatures and pressures is the first step towards thermal or shock initiated decomposition of energetic materials. Fast dissociation rates are challenging to measure, but amenable to first principles calculations. We combine transition-state theory with molecular dynamics simulations based on density-functional theory to predict the temperature-dependent dissociation rates in the gas and the condensed phase. Current applications focus on gas-, solution-, and liquid-phase thermal dissociation of nitramines. These studies will be discussed in the context of developing mesoscale models of initiation of energetic materials.

¹This work is supported by the Naval Research Laboratory via the Jerome and Isabella Karle Distinguished Scholar Fellowship and by the Office of Naval Research, both directly and through the Naval Research Laboratory.

8:36AM A25.00004 Thermodynamic Properties of energetic materials from density functional theory with van der Waals corrections, AARON LANDERVILLE, University of South Florida, MICHAEL CONROY, Naval Research Laboratory, MIKALAI BUDZEVICH, YOU LIN, University of South Florida, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — The calculation of thermodynamic properties for energetic materials from first-principles offers the promise to provide key parameters for mesoscopic and continuum-level simulations of explosives performance for a wide range of pressures and temperatures. While density functional theory with empirical van der Waals corrections, together with corrections for temperature and zero-point effects, can give excellent agreement between calculated and experimentally determined equations of state, quantities such as heat capacities and coefficients of thermal expansion suffer from inaccuracies in the lower frequencies of the calculated vibration spectrum. Additional approaches are discussed to account for the lowest intermolecular modes to increase the accuracy in prediction of thermal properties.

8:48AM A25.00005 Relating polymorphism and decomposition of RDX under static and dynamic compression¹, ZBIGNIEW DREGER, YOGENDRA GUPTA, Insitute for Shock Physics, Washington State University — Knowledge of the reactive behavior of energetic crystals at static high pressures and high temperatures (HP-HT) is an important step toward understanding the shock wave initiation of these crystals. Vibrational spectroscopy in a diamond anvil cell was used to examine the behavior of RDX crystals at the pressures and temperatures relevant to shock wave initiation. Phase boundaries between three RDX polymorphs (α , γ , and ε) were determined up to 12 GPa and 600 K. Decomposition kinetics for the ε - and γ -phases were examined at various pressures and temperatures, and were found to have positive volumes of activation. CO_2 , N_2O and H_2O were identified as the main decomposition species. Static HP-HT results were used to identify and understand the following processes in shocked RDX: $\alpha - \gamma$ phase transition, identification of the crystal phase at decomposition, and the role of pressure and temperature in accelerating the RDX decomposition under shock compression. This work demonstrated that static HP-HT results provide an important complementary route to elucidate the physical and chemical processes in shocked RDX crystals.

¹Work was supported by DOE/NNSA and ONR/MURI.

9:00AM A25.00006 Atomistic Simulations of Orientation and Shock Velocity Dependences on Pentaerythritol Tetranitrate Detonation, TZU-RAY SHAN, AIDAN THOMPSON, RYAN WIXOM, ANN MATTSSON, Sandia National Laboratories, Albuquerque, NM 87185, SANDIA TEAM — Predicting the behavior of energetic materials requires a detailed description of how chemical reaction, energy and pressure fronts propagate during initial stages of detonation. In this talk, classical molecular dynamics (MD) simulations are used to examine orientation and shock velocity dependences in single crystal pentaerythritol tetranitrate (PETN). This work utilizes an empirical, variable charge reactive force field (ReaxFF) that is implemented in the LAMMPS package with a time-averaged bond-order method for on-the-fly chemical species identification. The accuracy of ReaxFF is validated by comparisons of activation barriers for dissociation of a single PETN molecule along various dissociation channels with higher-fidelity, but more expensive, density functional theory (DFT) calculations. The response of single-crystal PETN to shock compression is simulated using the multi-scale shock technique (MSST) along the insensitive (100) directions, as well as the sensitive (001) and (110) directions, at steady shock velocities ranging from 6-10 km/s. Hugoniot curves, particle velocities of shocked molecules, and evolution of reaction products with time from MD simulations with ReaxFF will be discussed and compared to that from DFT calculations.

9:12AM A25.00007 Atomic-Scale Theoretical Studies of Energy Transfer, Inelastic Deformation, and Void Collapse in Molecular Crystals and Polymers, THOMAS D. SEWELL, Department of Chemistry, University of Missouri-Columbia, Columbia, MO 65211 — Recent atomic-scale theoretical studies of shock waves in polyatomic molecular crystals and polymers will be presented, with an emphasis on the results and interpretation of molecular dynamics simulations for pentaerythritol tetranitrate (PETN), hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), nitromethane, and poly(butadiene) (PBD). The effects of structural and mechanical anisotropy on the material response are of particular interest. Among the topics to be discussed are orientation dependent energy transfer pathways and inelastic deformation mechanisms subsequent to shock wave passage in initially defect-free nitromethane and PETN crystals, shock-induced collapse of variously shaped voids in crystalline RDX, and details of shock wave propagation and energy localization in bulk PBD and at the PBD/RDX interface.

9:48AM A25.00008 Explosive initiation of pentaerythritol tetranitrate (PETN) by laser irradiation, ROMAN TSYSHEVSKIY, ONISE SHARIA, MAIJA KUKLJA, Materials Science and Engineering Department, University of Maryland, College Park, MD — Understanding of explosive decomposition of energetic materials triggered by laser irradiation is of great importance for design of new economical formulations with high performance and tunable sensitivity. Earlier, laser irradiation was only considered as a source of heat. Nowadays, it is realized that optical excitation may set off initiation of rapid chemical reactions and govern further decomposition in energetic materials. However, mechanisms of this phenomenon are yet to be established. We present quantum-chemical calculations of the electronic structure of molecular and crystalline PETN to explore the effect of common impurities on its optical properties. We found that charged or excited PETN molecules exhibit significantly different electronic, optical, and chemical behavior. For example, new decomposition pathways that were not available in the ground state become favorable in the charged state of PETN. Three calculated lowest excitation energies of ionized PETN require 0.6, 0.7 and 1.13 eV, which is considerably lower than those for equilibrium PETN. The activation energy of the rate limiting decomposition stage is within 9-12 kcal/mole, while it is 35 kcal/mole in the ground state. We discuss possible ways that originate charge transfer in PETN and presented results in the context of recent experimental data.

10:00AM A25.00009 Condensation of carbon during high explosive detonation, LAURENCE FRIED, SORIN BASTEA, RAUL GARZA, Lawrence Livermore National Lab — The formation of nano-carbon clusters is believed to be responsible for the non-ideal detonation behavior of carbon-rich explosives, such as triamino-trinitrobenzene (TATB). We have developed a new model of carbon formation during detonation. The model is based on the assumption that carbon cluster growth has features of both activated Arrhenius kinetics and diffusion controlled kinetics. In our model the variation of temperature, density, and viscosity throughout the high explosive reaction zone and expansion is calculated using a thermochemical model linked to a hydrodynamic code. We compare our model to new experimental results on the size scaling of detonations in TATB-based explosives.

10:12AM A25.00010 Surface-induced effect on sensitivity of beta and delta HMX crystals, ONISE SHARIA, MAIJA KUKLJA, Department of Materials Science and Engineering, University of Maryland, College Park — It is accepted that sensitivity of energetic materials depends on many factors, including presence of defects, surfaces, interfaces, or voids. However, details of atomistic mechanisms that govern sensitivity to initiation of detonation and correlations between structure, morphology, and degradation of chemical bonds are far from being understood. In this talk, we present quantum chemical calculations combined with transition state theory to analyze chemical decomposition reactions in beta and delta HMX crystals. We calculate the activation barriers and reaction rates in the ideal crystals and materials containing internal surfaces, vacancies, and voids. We show that N-NO₂ homolysis is the most favorable decomposition reaction in all cases. We discuss whether a large space available in the vicinity of voids facilitates the N-NO₂ break in comparisons to an ideal crystal, and if this effect is enhanced in the delta phase in comparison to beta phase. The conclusions and revealed trends are presented in the context of experimental data.

10:24AM A25.00011 ABSTRACT WITHDRAWN —

10:36AM A25.00012 1,1-Diamino-2,2-Dinitroethylene Under High-Pressure-High-Temperature¹, MATTHEW BISHOP, University of Alabama at Birmingham, NENAD VELISAVLJEVIC, Los Alamos National Laboratory, ZHENXIAN LIU, Carnegie Institution of Washington, MATRIN GALLEY, University of Nevada Las Vegas — 1,1-Diamino-2,2-dinitroethylene (FOX-7) is an insensitive high explosive (IHE) which shows promise for use in low vulnerability ammunitions. With performance comparable to RDX and HMX, there is a growing interest in understanding the behavior under denotation conditions. Through the use of diamond anvil cell (DAC) technology and electrical resistive heating, the vibrational behavior of FOX-7, in both the mid and far-IR, were recorded at multiple isotherms under elevated pressure-temperature (PT). Energy-dispersive x-ray diffraction (XRD) was also employed along with a multi-anvil press for further investigating pressure-temperature phase space. Future planned experiments will focus on using high-resolution angular-dispersive XRD and neutron diffraction techniques to resolve high pressure-temperature structural information and obtain P-V-T data. The experiments on FOX-7 have revealed previously uninvestigated knowledge on the elevated-PT decomposition and phase boundaries allowing for a more developed basis for the behavior of FOX-7 under detonation conditions.

¹Los Alamos National Laboratory (LANL) is operated by Los Alamos National Security (LANS), LLC for the Dept. of Energy and National Nuclear Safety Admin. Support for this research was provide by DOE/NNSA Science Campaign 2 under the HE Science Program.

10:48AM A25.00013 Study on the deflagration-to-detonation transition course of porous energetic material, LAN WEI, PENGCHENG HAO, HEFEI DONG, XIAOMIAN HU, JIANSHI ZHU, Institute of Applied Physics and Computational Mathematics — The deflagration-to-detonation transition (DDT) course of energetic material with different porosity ratio was studied utilizing a one-dimensional two-phase flow code. The equations were numerically solved by space-time conservation element and solution element (CE/SE) method. The distribution of physical quantities such as pressure and temperature were obtained together with their evolution history. The physical rules before detonation were mainly analyzed and the effect of convection on the chemical reaction of energetic material was emphasized on.

Monday, February 27, 2012 8:00AM - 11:00AM —

Session A26 DCOMP DMP: Focus Session: Physics of Energy Storage Materials - Materials, Stability and Transport 257B

8:00AM A26.00001 Nanostructured Materials for Portable and Stationary Energy Storage, YI CUI, Stanford University — Storing energy electrochemically involves electronic and ionic processes and chemical transformation inside and at the interface of materials. The ability to understand and design nanostructures and their interfaces afford the great opportunities for controlling these fundamental processes, which can ultimately lead to high performance energy storage devices. Here I will present several exciting examples on designing nanostructures and their interfaces to realize high performance energy storage devices. One example is on designing nanowires and heterostructured nanowires for ultrahigh capacity storage of lithium ions in silicon anodes and sulfur cathodes. The challenges associated with large volume expansion, electron and ion transport, and solid-electrolyte-interphase (SEI) have been addressed. Another example is to design open framework stucture of nanocrystals, which facility facile insertion of sodium and potassium ions. The high power, high energy efficiency and low-cost aqueous batteries can be enabled for grid scale stationary storage.

8:36AM A26.00002 Enhanced electrochemical performance in LiFePO₄/graphene nanocomposite cathode material for lithium ion batteries, KULWINDER DHINDSA, B. MANDAL, M.W. LIN, M. NAZRI, Wayne State University, P. VAISHNAVA, Kettering University, V. NAIK, University of Michigan-Dearborn, G.A. NAZRI, R. NAIK, Z.X. ZHOU, Wayne State University — We synthesized LiFePO₄/graphene nano-composite employing a sol-gel method, where graphene oxide solution was added to the LiFePO₄ precursors during the synthesis. Electrical measurement reveals that the addition of 10% graphene (by weight) to LiFePO₄ increases its conductivity by 5 orders of magnitude. SEM images of the composite show that the material consists of LiFePO₄ nanoparticles (with a mean particle size ~ 50 nm) homogeneously mixed with graphene sheets; the latter provides a three-dimensional conducting network for Li⁺ ion and electron transport. A large specific capacity of 170 mAh/g was observed at a discharge rate of C/2. To further increase the conductivity and inhibit particle size growth of LiFePO₄ (thus to increase the rate capacity), we coated the nanoparticles with a thin carbon layer by adding 0.25M lauric acid as precursor in addition to graphene oxide during the synthesis. The respective roles of graphene and lauric-acid-induced carbon coating in the specific capacity and charge-discharge rate of the LiFePO₄ cathode material will be discussed.

8:48AM A26.00003 Simultaneous enhancement of electronic and Li⁺ ion conductivity in LiFePO₄¹, JAEKWANG LEE, Oak Ridge National Laboratory and Vanderbilt University, STEPHEN J. PENNYCOOK, Oak Ridge National Laboratory, SOKRATES T. PANTELIDES, Vanderbilt University — The electronic conductivity is generally highly sensitive to the electronic properties of a material while the ionic conductivity is mainly sensitive to the structural properties. Thus, the simultaneous control of both is very challenging. Furthermore, many electrochemical systems for advanced energy technologies require materials in which both ionic and electronic conductivities are optimized. Here we explore the influence of biaxial strain on the electronic and Li⁺ ion conductivities of the battery cathode material LiFePO₄ by performing first-principles calculations. We show that biaxial tensile strain leads to simultaneous increases in electronic and ionic conductivities of LiFePO₄. The results unveil a generic mechanism that should be present in other materials with polaronic transport and provide a promising new approach to enhance the performance of energy-related materials.

¹This research was supported in part by the DoE Basic Energy Sciences.

9:00AM A26.00004 Optimization of the surface stability of the LiMn_2O_4 spinel by employing DFT calculations, ALTAF KARIM, KRISTIN PERSSON, Lawrence Berkeley National Laboratory — One of the most important materials for the lithium batteries electrodes is LiMn_2O_4 . We used GGA+U method to calculate the bulk and surface properties of LiMn_2O_4 . Our calculations show that the both correct AFM and electron localization (GGA+U) are necessary to obtain the semiconducting, Jahn-Teller distorted electronic ground state of LiMn_2O_4 . Further we calculated energies of different surfaces such as (100), (110), and (111) to study their stability. Our calculations show that (111) surface has the lowest energy which makes it more stable than other surfaces and it also confirms the experimental results, whereas (101) and (001) similar energies. Absolute surface energies change with +U value, but the ratios between the energies are very similar. Based on these calculations we constructed the equilibrium (Wulff) shape of LiMn_2O_4 particle, which is similar to the cubo-octahedral shape with predominant {1 1 1} facets as it was found in experiments. Our density of states calculations show that the bulk and (100) are semiconducting, whereas (110) and (111) surfaces exhibit metallic behavior. We also calculated the LiMn_2O_4 bulk and surface potentials as a function of lithium concentration.

9:12AM A26.00005 Atomistic Simulation Studies of Nanostructured TiO_2 ¹, PHUTI NGOEPE, MALILI MATSHABA, University of Limpopo, DEAN SAYLE, Cranfield University — TiO_2 has been confirmed as a safe anode material in lithium ion batteries due to its higher Li-insertion potential, ($\sim 1.5\text{V}$) in comparison with commercialised carbon anode materials. Recently in order to attain high rate capabilities of TiO_2 anode, for application in lithium ion batteries with both high power and high energy density, intensive attention has been paid to various TiO_2 nanostructures, such as nanoparticles, nanowires and mesoporous structures. In the current study, amorphisation recrystallization method is used to produce nano-porous, sheets and bulk structures for TiO_2 which have been extensively studied experimentally. Simulated X-ray diffraction patterns are produced from such structures and compared with the experimental XRDs. The simulated microstructures are analysed and compared with available high resolution transmission experimental results. Lithiation of TiO_2 nanostructures is considered and discussed in the context of current investigations and concentration profiles of different ions are shown in the structures. Semi-empirical models based on DFT tightbinding methods, are introduced for TiO_2 and lithiated its forms.

¹We acknowledge the support of SARCHI under the National Research Foundation.

9:24AM A26.00006 First-principles study of electronic structures and phase transitions of lithiated molybdenum disulphide¹, JUN LI, XIAOBO CHEN, Ningbo Institute of Material Technology and Engineering, Chinese Academy of Sciences, Ningbo 315201 PR China, NINGBO INSTITUTE OF MATERIAL TECHNOLOGY AND ENGINEERING TEAM — By first-principles calculations, electronic structures of MoS_2 , intercalation-induced 2H to 1T phase transition and reversibility are investigated. It is revealed that change of interlayer stacking from 2H to 3R imposes negligible influence on the band structure and stability of MoS_2 . In contrast, the change of intralayer stacking from 2H to 1T changes the character of p-d repulsion, resulting in a semiconductor-to-metal transition. We demonstrate that the Kohn-Sham band energy, rather than the coulomb repulsion energy, plays dominant roles in both the phase stabilization and transition during Li intercalation. It is found that the evolution of 1T phase is crucially determined by chemical hardness, which underlies the cycle irreversibility. Due to the charge-density-wave (CDW) phase, Li extraction is impeded by the enhancement of Li-host binding. It is indicated that the cycle reversibility can be improved by electron-donor doping in MoS_2 , because the resultant pre-reduction of Mo and S eliminates the electron transfer from Li to host.

¹Programs supported by the Ningbo Natural Science Foundation, grant no. 2011A610207, by Department of Science and Technology, Zhejiang Province, grant no. 2011C21031, and by the National Natural Science Foundation of China (NSFC), grant no. 11174301.

9:36AM A26.00007 Simulating Dendritic Formation on the Cathode of Lithium-ion Batteries, NING SUN, DILIP GERSAPPE, Department of Materials Science and Engineering, Stony Brook University — The Lattice-Boltzmann method was used to simulate the process of dendrite formation on the cathode of lithium-ion batteries. "In-Situ" maps of the electrodeposition process under constant charging current conditions were obtained. The results showed preferential dendrites formation on higher curvature spots of the cathode, because of the higher electrical field intensity. Different morphologies were obtained due to different initial roughness of the electrode. A mossy-like electrode can be observed after deposition on a rough electrode with randomly generated initial conditions. A tree-like dendrite can be observed when depositing on a single small dendrite. A smooth surface can be obtained when the initial electrode is ideally smooth. The influence of current density was also studied.

9:48AM A26.00008 Density functional and molecular dynamics studies of solid electrolyte $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$, MICHELLE JOHANNES, KHANG HOANG, NOAM BERNSTEIN, Naval Research Laboratory — Garnet-type structured $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO) is considered as a promising candidate for Li-ion battery solid electrolytes because of its high ionic conductivity and electrochemical and chemical stability. We use first-principles density-functional theory calculations and molecular dynamics simulations to reveal the underlying mechanism that drives a tetragonal to cubic transition at elevated temperatures, and also to explain why the cubic phase can be stabilized with the incorporation of a certain amount of impurities such as Al. We show that the relationship between the observance of a cubic phase and the measurement of a substantially higher ionic conductivity is a secondary effect not directly attributable to the presence of Al in the crystal structure. Suggestions for enhancing the ionic conductivity in LLZO will also be discussed.

10:00AM A26.00009 First principles investigation of the superionic electrolyte $\text{Li}_7\text{P}_3\text{S}_{11}$ ¹, NICHOLAS LEPLY, N.A.W. HOLZWARTH, Wake Forest University — $\text{Li}_7\text{P}_3\text{S}_{11}$ has been shown to be a promising superionic conductor for solid state rechargeable batteries with a room temperature conductivity as high as 10^{-3} S/cm and a thermal activation energy as small as $E_A=0.12\text{ eV}$.² We have performed first principles modeling studies³ on this material in order to explain its stability and Li ion migration properties. Our investigation considers optimized crystal structures, migration involving both vacancy and interstitial mechanisms, as well as related materials. We find optimized crystal structures in reasonable agreement with experiment,⁴ and the lowest calculated activation energy barrier was found to be $E_A=0.15\text{ eV}$ in good agreement with the experimental value.

¹Supported by NSF Grant DMR-0705239.

²F. Mizuno et al., *Solid State Ionics* **177**, 2721 (2006).

³N. A. W. Holzwarth, N. D. Lepley, Y. A. Du, *J. Power Sources* **196**, 6870 (2011).

⁴H. Yamane et al., *Solid State Ionics* **178**, 1162 (2007); Y. Onodera et al., *J. Phys. Soc. Jpn.* **79**, 87 (2010), suppl. A.

10:12AM A26.00010 Solid Electrolyte for Advanced Lithium Batteries, GHOLAM-ABBAS NAZRI, BALAJI P MANDAL, Wayne State University, MARYAM NAZRI, Applied Sciences Inc., VAMAN NAIK, University of Michigan - Dearborn, PREM VASHINAVA, Kettering University, RATNA NAIK, Wayne State University, ENERGY STORAGE AND GENERATION TEAM — Lithium battery is a promising energy storage system due to its high energy density and high rate capability and its application ranges from micro to large scale megawatt batteries. The current technology is using liquid electrolyte that limits its application due to flammable nature of the electrolyte, particularly at high temperatures, and difficulty in fabrication and miniaturization of the device. We report a novel solid electrolyte with high lithium ion conductivity as a replacement for the current liquid electrolyte, particularly for electronic applications. The solid state lithium ion conductor is based on lithium germanium phosphorous sulfide compound. The compound is prepared by solid state reaction at 500 °C. The crystallinity and phase purity of the sample is checked by XRD. We also measured ionic conductivity of the sample using both 4-probe and impedance techniques. High lithium ion conductivity at room temperature is observed. In this study we have investigated the dynamics of ion conduction, XRD, and Raman spectra of the super ion conductor. Electrochemical performance of the solid electrolyte in a lithium cell and its stability against high voltage cathodes and lithium anode will also be presented.

10:24AM A26.00011 First principles computer simulations of $\text{Li}_{10}\text{GeP}_2\text{S}_{12}$ and related lithium superionic conductors¹, N.A.W. HOLZWARTH, Wake Forest University — A recent paper by Kamaya *et al.*² reported a new crystalline superionic conductor having a compact tetrahedral structure and a stoichiometry of $\text{Li}_{10}\text{GeP}_2\text{S}_{12}$. The room temperature conductivity was reported to be 0.01 S/cm, comparable to liquid electrolyte conductivities and five times higher the compositionally related thio-LISICON material $\text{Li}_{3.25}\text{Ge}_{0.25}\text{P}_{0.75}\text{S}_4$ developed earlier.³ This talk will present a progress report on our work to perform first principles computer simulations for these materials focussing on the structural, stability, and Li ion mobility properties of idealized crystalline models. From the perspective of our previous studies of Li ion conductivity in lithium thiophosphate electrolytes,⁴ the effects of introducing Ge can be assessed.

¹Supported by NSF Grants DMR-0705239 and DMR-1105485.

² N. Kamaya *et al.*, *Nature Materials* **10**, 682 (2011).

³R. Kanno *et al.*, *J. Electrochem. Soc.* **148**, A742 (2001).

⁴ N. A. W. Holzwarth *et al.*, *J. Power Sources* **196**, 6870 (2011).

10:36AM A26.00012 Exploring Li^+ Potential Energy Surface in Poly(ethylene oxide)-based Sulfonate Ionomers¹, HUAI-SUEN SHIAU, MICHAEL J. JANIK, RALPH H. COLBY, Pennsylvania State University, University Park — Ion-containing polymers are of interest as single-ion conductors for use as electrolytes in electrochemical devices, including lithium ion batteries. Current ion conductivities of the best ionomers are roughly 100X too small for practical applications and have a small fraction of their Li^+ counterions participating in conduction. We are using ab initio methods to investigate the Li^+ conduction mechanism, and specifically the role of transient positive triple ions ($\text{Li}^+\text{A-Li}^+$) in the conduction process. The positive triple ion has a lower energy separated state that allows for facile transport, if there is a pair within 1.4 nm. We will discuss the competition between cation solvation with ether oxygen atoms and cation-anion interaction. The importance of anion-anion separation in altering Li^+ hopping barriers will be examined, as well as the variation in hopping rates with solvent identity. Ab initio calculations are used to evaluate the relative energy of ion states (contact and separated states), and this analysis is used to explain experimental phenomena of Li^+ mobility in ionomers.

¹NSF

10:48AM A26.00013 Ab initio molecular dynamics simulations of organic electrolytes, electrodes, and lithium ion transport for Li-ion batteries, P.R.C. KENT, P. GANESH, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge 37831, DE-EN JIANG, Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, O. BORODIN, Electrochemical Branch, U.S. Army Research Laboratory, Adelphi MD 20783 — Optimizing the choice of electrolyte in lithium ion batteries and an understanding of the solid-electrolyte interphase (SEI) is required to optimize the balance between high-energy storage, high rate capability, and lifetime. We perform accurate ab initio molecular-dynamics simulations of common cyclic carbonates and LiPF₆ to build solvation models which explain available Neutron and NMR spectroscopies. Our results corroborate why ethylene carbonate is a preferred choice for battery applications over propylene carbonate and how mixtures with dimethyl carbonate improve Li-ion diffusion. We study the role of functionalization of graphite-anode edges on the reducibility of the electrolyte and the ease of Li-ion intercalation at the initial stages of SEI formation. We find that oxygen terminated edges readily act as strong reductive sites, while hydrogen terminated edges are less reactive and allow faster Li diffusion. Orientational ordering of the solvent molecules precedes reduction at the interphase. Inorganic reductive components are seen to readily migrate to the anode edges, leading to increased surface passivation of the anode. We are currently quantifying Li-intercalation barriers across realistic SEI models, and progress along these lines will be presented.

Monday, February 27, 2012 8:00AM - 11:00AM —

Session A27 DCMP: Invited Session: Excitonic and Correlation Effects in Single-Layer Graphene
258AB

8:00AM A27.00001 Dynamic screening and the effective fine structure constant of graphene¹, PETER ABBAMONTE, University of Illinois — Electrons in graphene behave, in the low energy sector, like massless Dirac fermions. The degree to which Coulomb correlations influence these fermions is still subject to debate. In this talk I will describe inelastic x-ray scattering experiments on crystals of graphite, to which we have applied newly developed reconstruction algorithms to image the dynamical screening of charge in (effectively) a freestanding graphene sheet. We found that the polarizability of the Dirac fermions in graphene is amplified by excitonic effects in the particle-hole spectrum, which enhances screening of interactions among low energy quasiparticles. I will argue that interactions should be characterized by an effective, screened fine-structure constant, $\alpha_g^*(\mathbf{k}, \omega)$, which our measurements suggest converges to the value $\alpha_g^* = 0.14 \pm 0.092$ in the small wave vector limit. This value is smaller than the bare $\alpha_g = 2.2$, and suggests that the strength of interactions in graphene is similar to that in band semiconductors like Si or GaAs. I will discuss the implications of this result for other Dirac systems, such as nodal quasiparticles in cuprates and topological insulator surface states.

¹Supported by DOE grant DE-FG02-07ER46453

8:36AM A27.00002 Observation of strong excitonic effects in the optical spectrum of graphene¹, TONY HEINZ, Columbia University —

¹This work was done in collaboration with K. F. Mak and J. Shan (Case Western Reserve University).

9:12AM A27.00003 Electron-electron interaction and excitonic effects in graphene systems¹

STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory — Owing to the unique electronic structure of graphene and enhanced electron-electron and electron-hole interactions in lower dimensions, graphene structures exhibit interesting and novel electronic and optical properties. We discuss in this talk results from recent theoretical studies on several graphene systems. First-principles calculations, based on the GW-Bethe-Salpeter Equation approach, have predicted very strong features in the optical absorption spectra of single-layer graphene and multi-layer graphene, arising from resonant excitons. Many of these features have since been observed experimentally. We also explore the effects of charge carrier doping and of having an external electric field on the absorbance of graphene and bilayer graphene. Graphene nanoribbons are semiconductors that, owing to electron-electron interactions, also exhibit extraordinarily magnetic and excitonic effects. Another intriguing phenomenon is one in the magneto-optical response of graphene, which involves resonant transitions of absorption of a photon together with the simultaneous creation of an intervalley, intra-Landau level exciton and a K-phonon. Finally, first-principles results on the plasmon satellite structures in the spectral function of graphene computed with the GW method and beyond are presented. We discuss the origin of these phenomena and make comparison with experiments.

¹This work was supported by NSF, U.S. Department of Energy, and ONR MURI program.

9:48AM A27.00004 Graphene Update, ANDRE GEIM¹, University of Manchester — I will overview the latest experimental progress

made by our group in Manchester. This will cover several subjects with particular attention being paid to interaction effects that have been observed in graphene and its double layer heterostructures.

¹Other contributing authors: Leonid Ponomarenko, Roman Gorbachev, Kostya Novoselov, Daniel Elias, Liam Britnell, Rashid Jalil, Sasha Mayorov, Paco Guinea, Misha Katsnelson, Volodya Fal'ko and Irina Grigorieva

10:24AM A27.00005 Electron-electron interactions in doped graphene sheets¹, MARCO POLINI, NEST,

Istituto Nanoscienze-CNR — In this talk I will review some of the most important electronic properties of graphene. I will first discuss the appearance of plasmaron satellite bands in both angle-resolved photoemission [1] and STM spectra [2,3], emphasizing the important role of the sublattice pseudospin degree of freedom. I will then illustrate some unusual features, which appear only beyond the widely used Random Phase Approximation, characterizing plasmons and Drude weight of the electron gas in this material [4].

[1] A. Bostwick et al., Science 328, 999 (2010).

[2] V.W. Brar et al., Phys. Rev. Lett. 104, 036805 (2010).

[3] A. Principi, M. Polini, and A.H. MacDonald, to be submitted

[4] S.H. Abedinpour et al., Phys. Rev. B 84, 045429 (2011).

¹I acknowledge financial support from the Italian Ministry of Research through the Program “FIRB - Futuro in Ricerca 2010”, Project Title “PLASMOGRAPH.”

Monday, February 27, 2012 8:00AM - 11:00AM –

Session A28 DMP: Focus Session: Dopants and Defects in Semiconductors - ZnO 258C

8:00AM A28.00001 The trends of oxygen vacancy levels in metal oxides, WANJIAN YIN, SUHUI WEI,

MOWAFAK AL-JASSIM, National Renewable Energy Laboratory, YANFA YAN, Department of Physics, University of Toledo, OH — Most of the d or d^{10} oxides such as ZnO, SnO₂, In₂O₃, and TiO₂ are wide-bandgap n -type semiconductors even though they are not intentionally doped. For quite a long time, it was commonly believed that oxygen vacancies (V_O) in metal oxides are the electron donors because the formation energy of V_O in metal oxides is low and the electrical conductivity of the n -type oxides is closely linked to the formation of V_O . However, recent theoretical and experimental studies have put this point of view in question especially with different calculation methods involved. We present a detailed analysis of the wavefunction characters of oxygen vacancy in conventional metal oxides and unveil the chemical trend of oxygen vacancy transition energy levels with respect to the conduction-band minimum (CBM). We show that in the type- s and type- p metal oxides, where the character of an oxygen vacancy level is similar to that of the CBM, the oxygen vacancy levels are generally deep and become deeper when the cation size decreases. In type- d metal oxides, the oxygen vacancy levels are generally shallow and can sometimes even be above the CBM. Our analysis is confirmed by the calculated trends of oxygen vacancy levels in representative metal oxides using hybrid density functional analysis. It also provides guidelines to search a metal oxide that has shallow V_O donor levels, such as the one found in BiVO₄.

8:12AM A28.00002 Highly Efficient Defect Emission from ZnO and ZnO:S, JAY SIMMONS, Department

of Chemistry, Duke University, Durham, North Carolina 27708, JOHN FOREMAN, U.S. Army Aviation and Missile Research Development and Engineering Center, Redstone Arsenal, AL 35898, JIE LIU, Department of Chemistry, Duke University, Durham, North Carolina 27708, HENRY EVERITT, Department of Physics, Duke University, Durham, North Carolina 27708 — Bulk Zinc Oxide (ZnO) is a wide, direct band gap semiconductor with an energy of 3.4 eV that contains two emission bands: the UV band-edge emission and the green defect emission band. We have shown that the external quantum efficiency of the green band can exceed 50%. To investigate the mechanism of efficient defect emission, vacuum annealed (ZnO:Zn) and sulfur-doped (ZnO:S) ZnO were investigated because of their strong defect emission and suppressed UV band edge emission. Continuous wave low temperature photoluminescence (PL) and PL excitation (PLE) spectra were measured for the two compounds. It was found that bound excitons, not free photo-excited carriers, mediate the defect emission in ZnO:Zn, while the defect emission from ZnO:S seems to originate from a Zn-S complex formed in the crystal lattice. Temperature-dependent PLE spectra for the defect and band edge emission were measured to estimate trapping and activation energies of the bound excitons. XPS and X-Ray diffraction studies were also performed to ascertain the concentration and nature of sulfur doping in the ZnO lattice. The results presented here offer hope that engineering defects in ZnO materials may significantly improve the quantum efficiency for white light phosphor applications.

8:24AM A28.00003 Acceptors in bulk and nanoscale ZnO¹, M.D. MCCLUSKEY, Washington State University —

Zinc oxide (ZnO) is a semiconductor that emits bright UV light, with little wasted heat. This intrinsic feature makes it a promising material for energy-efficient white lighting, nano-lasers, and other optical applications. For devices to be competitive, however, it is necessary to develop reliable p-type doping. Although substitutional nitrogen has been considered as a potential p-type dopant for ZnO, theoretical and experimental work indicates that nitrogen is a deep acceptor and will not lead to p-type conductivity. This talk will highlight recent experiments on ZnO:N at low temperatures. A red/near-IR photoluminescence (PL) band is correlated with the presence of deep nitrogen acceptors. PL excitation (PLE) measurements show an absorption threshold of 2.26 eV, in good agreement with theory. Magnetic resonance experiments provide further evidence for this assignment. The results of these studies seem to rule out group-V elements as shallow acceptors in ZnO, contradicting numerous reports in the literature. If these acceptors do not work as advertised, is there a viable alternative? Optical studies on ZnO nanocrystals show some intriguing leads. At liquid-helium temperatures, a series of sharp IR absorption peaks arise from an unknown acceptor impurity. The data are consistent with a hydrogenic acceptor 0.46 eV above the valence band edge. While this binding energy is still too deep for many practical applications, it represents a significant improvement over the ~ 1.3 eV binding energy for nitrogen acceptors. Nanocrystals present another twist. Due to their high surface-to-volume ratio, surface states are especially important. Specifically, electron-hole recombination at the surface give rises to a red luminescence band. From our PL and IR experiments, we have developed a “unified” model that attempts to explain acceptor and surface states in ZnO nanocrystals. This model could provide a useful framework for designing future nanoscale ZnO devices.

¹Work at WSU supported by DOE and NSF.

9:00AM A28.00004 Origin of the “Red” Luminescence Band in Bulk N-doped ZnO, E.R. GLASER,

N.Y. GARCES, Naval Research Laboratory, M.C. TARUN, M.D. MCCLUSKEY, Washington State U. — Optically detected magnetic resonance (ODMR) at 24 GHz was performed on bulk ZnO crystals doped with nitrogen impurities (of high interest for p-type conductivity) to provide more details on the origin of a recently reported red/near-IR photoluminescence (PL) band.¹ PL at 7K revealed strong bandedge excitonic recombination at 3.364 eV, a broad “green” emission band at 2.45 eV, and a broad “red” PL band near 1.7 eV. Two luminescence-increasing ODMR signals were found on this “red” emission. The first was a sharp feature with g-value of 1.957 and FWHM of 1 mT and is attributed to shallow donors based on electron spin resonance (ESR) of n-type ZnO. The second feature exhibited a g-value near 2 and a broad, asymmetric lineshape with FWHM of ~ 10 mT. A simulation of the spectrum showed that the broad resonance could be fit as the sum of three equally spaced lines with magnetic field splitting value and relative intensities in close agreement to those observed for deep nitrogen acceptors as identified from previous ESR studies. Thus, the ODMR results strongly suggest that the “red” PL is due to radiative recombination involving residual shallow donors and deep nitrogen acceptor centers.

¹M.C. Tarun et al., AIP Advances **1**, 022105 (2011).

9:12AM A28.00005 Elevated Temperature Dependent Transport Properties of As- and P-doped Zinc Oxide, B. CAI, M. L. NAKARMI, Department of Physics, Brooklyn College and Graduate Center of the CUNY, Brooklyn, NY, T. ODER, M. MCMASTER, A. SMITH, N. VELPUKONDA, Department of Physics and Astronomy, Youngstown State University, Youngstown, Ohio —

Achieving highly conductive p-type zinc oxide (ZnO) is desired for the development of ZnO based optoelectronic devices. Understanding electrical properties of ZnO, doped with p-type dopants, is necessary for improving p-type conductivity. We employed temperature dependent Hall effect measurement to study the electrical transport properties of As- and P-doped ZnO epilayers. The samples were grown on sapphire substrates by magnetron sputtering technique. From the Hall effect measurements performed at elevated temperatures ranging from 20 to 750 K, we observed double activation processes in both As- and P-doped ZnO epilayers. We will compare the results of uniform doped and delta-doped samples. Correlation between electrical properties from these Hall effect measurements and optical properties from low temperature photoluminescence measurements will also be discussed.

9:24AM A28.00006 Impurity complexes and conductivity of Ga-doped ZnO¹, DENIS DEMCHENKO,

Virginia Commonwealth University — Using hybrid functional theory compared with experimental measurements, we investigate the influence of gallium impurities and their complexes on electrical properties of ZnO. In contrast to the behavior of isolated Ga impurities and native defects, the calculated formation energies of Ga complexes are consistent with experimental data. We show that for high levels of Ga doping the acceptor behavior of $(\text{Ga}_{\text{Zn}} - \text{V}_{\text{Zn}})$ and $(\text{Ga}_{\text{Zn}} - \text{O}_i)$ complexes explains the conductivity measurements and compensation levels in ZnO. The computed binding energies of these complexes are in agreement with the binding energies obtained from the measurements of the temperature dependence of carrier mobility. The binding energy dependence on the Fermi level, as well as the computed barrier heights for the formation of complexes are also consistent with the latest experiments on annealing of Ga doped ZnO samples. Our results show that the formation of defect complexes is essential for capturing the physics Ga defects in ZnO.

¹This work used computational facilities of the VCU Center for High Performance Computing.

9:36AM A28.00007 Cu-Doping of ZnO by Nuclear Transmutation and Electrical and Optical Characterization of Cu Acceptors¹, FARIDA SELIM, MARIANNE TAURN, JIANFENG JI, DONALD WALL, Washington State University,

LYNN BOATNER, Oak Ridge National Laboratory, MATTHEW MCCLUSKEY, Washington State University, SELIM TEAM², COLLABORATION WITH MCCLUSKEY GROUP COLLABORATION, BOATNER COLLABORATION, WALL COLLABORATION — Cu doping is known to have a large effect on the electrical and optical properties of ZnO, its role is different from other dopants, and a fundamental understanding of this role is lacking. One problem of ZnO doping is arising from the difficulty in controlling dopant locations in conventional doping methods. In this work we doped Zn single crystals with copper acceptors by means of the nuclear transmutation doping (NTD) method, which gives highly uniform dopant distributions and has a much higher probability of controlling the dopant locations in the lattice. The Cu doping was confirmed by the infrared absorption signature of Cu^{2+} at 5780 cm^{-1} . Hall-effect measurements indicated that the Cu acceptor level lies 0.160 eV below the conduction band minimum. With respect to optical properties, an interesting low-temperature thermal stimulated luminescence has been observed in as-grown and doped ZnO single crystals. This low-temperature luminescence can reveal the density of donors and acceptors in ZnO and their location in the band gap.

¹Funding was provided by the National Science Foundation (DMR-1006772) and DMR-1004804) and DOE BES.

²Selim and Jianfeng

9:48AM A28.00008 The G0W0 band gap of ZnO: effects of plasmon-pole models, GABRIEL ANTONIUS,

University of Montreal, MARTIN STANKOVSKI, DAVID WAROQUIERS, ANNA MIGLIO, Université Catholique de Louvain, HEMANT DIXIT, University of Antwerpen, KIROUBANAND SANKARAN, MATTEO GIANTOMASSI, XAVIER GONZE, Université Catholique de Louvain, MICHEL COTE, University of Montreal, GIAN-MARCO RIGNANESE, Université Catholique de Louvain, UNIVERSITY OF MONTREAL TEAM, UNIVERSITE CATHOLIQUE DE LOUVAIN TEAM, UNIVERSITY OF ANTWERPEN TEAM — Carefully converged calculations are performed for the band gap of ZnO within the G0W0 approximation. The results obtained using four different well-established plasmon-pole models are compared with those of explicit calculations without such models (the contour-deformation approach). We evaluate the difference between plasmon-pole models that enforce the f-sum rule and those that are fitted to reproduce the low energy response. In the case of ZnO, plasmon-pole models enforcing the f-sum rule underestimate the low-frequency region of the dielectric function probably because of the presence of semi-core states in these calculations. Our results confirm that the band gap of ZnO is underestimated in the G0W0 approach as compared to experiment.

10:00AM A28.00009 Evidence for surface states in ZnO nanostructures using non-linear optical spectroscopy, BENJOY ANAND, Sri Satya Sai Institute of Higher Learning, MARTIN EGBLEWOGBE, University of Ghana, RAMAKRISHNA PODILA, Department of Physics, Clemson University, REJI PHILIP, Raman Research Institute, APPARAO RAO, Department of Physics, Clemson University — An unexpected presence of ferromagnetic (FM) ordering in nanostructured ZnO has been reported previously. Recently, from our detailed magnetization studies and *ab initio* calculations, we attributed this FM ordering in nanostructured ZnO to the presence of surface states, and a direct correlation between the magnetic properties and crystallinity of ZnO was observed. Such defect induced surface states appear as green/yellow emission in the photoluminescence spectrum of ZnO nanostructures. In this study, through a systematic sample preparation of both pristine and Co-doped ZnO nanostructures, and detailed PL and nonlinear optical measurements, we confirm that the observed FM ordering is due to the presence of surface states.

10:12AM A28.00010 Terahertz properties of Tm (Tm=Cu, Ag) doped ZnO thin films, MI HE, XINGQUAN ZOU, TOM WU, ELBERT CHIA, Nanyang Technological University — Optical properties of $\text{Zn}_{0.95}\text{Tm}_{0.05}\text{O}$ (Tm=Cu, Ag) thin films are studied by terahertz time-domain spectroscopy (THz-TDS) at different temperatures (10K – 300K) in the frequency range extending from 0.22 – 3 THz. The measured complex dielectric response and conductivity are well fitted by a Drude-based model. Comparing with undoped ZnO thin films, the doping effect of Ag and Cu is investigated.

10:24AM A28.00011 The growth of non-polar ZnO and $\text{ZnO}/\text{Mg}_{0.25}\text{Zn}_{0.75}\text{O}$ epi-films by radio-frequency magnetron sputtering, BI-HSIUAN LIN, Department of Photonics and Institute of Electro-Optical Engineering, National Chiao Tung University, Taiwan, WEI-REIN LIU, Division of Scientific Research, National Synchrotron Radiation Research Center, Taiwan, SHAO-TING HSU, Department of Photonics and Institute of Electro-Optical Engineering, NCTU, Taiwan, CHIA-HUNG HSU, Division of Scientific Research, NSRRC, Taiwan, WEN-FENG HSIEH, Department of Photonics and Institute of Electro-Optical Engineering, NCTU, Taiwan, NCTU TEAM, NSRRC TEAM, NCKU TEAM — High quality non-polar ZnO and $\text{ZnO}/\text{Mg}_x\text{Zn}_{1-x}\text{O}$ ($x = 0.15, 0.25$) epi-films have been successfully grown on m-plane and r-plane sapphire by using RF magnetron sputtering. The structural properties, including crystalline quality, strain state, and defect structures, of the ZnO and $\text{ZnO}/\text{Mg}_x\text{Zn}_{1-x}\text{O}$ layers are thoroughly examined by synchrotron x-ray scattering, transmission electron microscopy and atomic force microscopy. We found the surface morphology of the a-plane oriented ZnO epi-films is smoother than that of m-plane oriented one. Moreover, the surface of $\text{Mg}_{0.25}\text{Zn}_{0.75}\text{O}$ epi-layer is significantly better than the ZnO epi-film and exhibits the same orientation dependence. The optical properties of these samples are also investigated by temperature, polarization and power dependent photoluminescence, and polarization dependent Raman spectroscopy. The results reveal the a-plane ZnO epi-film grown on r-sapphire with a $\text{Mg}_{0.25}\text{Zn}_{0.75}\text{O}$ buffer layer is promising for bright UV emission application.

10:36AM A28.00012 Excitonic Energy Shifts in Isotopically Controlled $I - III - VI_2$ Chalcopyrites: CuGaS_2 and AgGaS_2 ¹, J.S. BHOSALE, H. ALAWADHI, I. MIOTKOWSKI, A.K. RAMDAS, Purdue University, R. LAUCK, M. CARDONA, MPI for Solid State Research — CuGaS_2 and AgGaS_2 tetrahedrally co-ordinated chalcopyrites are “genealogically related” to $II - VI$ semiconductors like ZnS. We have investigated the shifts in their excitonic signatures by controlling the isotopic mass of the I , III or VI_2 constituent in the crystals grown by physical vapor deposition. The excitonic signatures are observed in wavelength modulated reflectivity employing a high S/N, LED based technique.² For example it reveals a 3.9 meV shift for the A exciton in $\text{Ag}^{71}\text{GaS}_2$ with respect to that of natural AgGaS_2 ; a smaller increase occurs in ZnS ³. These effects have been related to electron-phonon interaction caused by the zero-point vibrations. Similar effects, but with an opposite sign, have been observed for Cu-isotopes in CuGaS_2 as well as in the Cu-monohalides CuCl, CuBr, and CuI⁴; their origin is receiving considerable attention at present though not yet understood. In this context the excitonic temperature dependence^{5,6} will be discussed.

¹Work is supported by US National Science Foundation (DMR 0705793)

²J. S. Bhosale, Rev. Sci. Instrum. 82, 093103 (2011)

³M. Cardona and M.L.W. Thewalt, Rev. Mod. Phys. 77, 575 (2002)

⁴D.Olguin et al., Solid State Commun. 122, 575 (2002)

⁵Cardona, op. cit

⁶H.Alawadhi et al., Phys. Rev.B 75, 205207 (2007)

10:48AM A28.00013 Hybrid Hartree-Fock density functional study of transition-metal doped ZnO, JESUAN BETANCOURT, ALAN KALITSOV, JULIAN VELEV, University of Puerto Rico — Dilute magnetic semiconductors (DMS) obtained by doping semiconductors with transition metals (TM) hold much promise for spintronics. Transition metal doped ZnO (ZnO:TM) has been investigated for a possible room-temperature DMS. Density functional theory gives incorrect prediction for the band gap of ZnO which leads to diverging interpretations for the magnetic behavior of ZnO:TM [1,2]. Here we report Heyd-Scuseria-Ernzerhof (HSE) hybrid functional study of the electronic structure of ZnO:TM (TM=Cu, Ni, Co, Fe, Mn). The hybrid functional corrects for both the bandgap problem on the host and the lack of correlation in the impurity, without the use of *ad-hoc* intra-atomic potentials. Our results show although the HSE opens the band gap of the host, the Hubbard splitting of the impurity levels makes the empty impurity levels reside in the host conduction band. This leaves open the possibility for spin polarized carriers. We discuss the validity of the results and explore their implications for the magnetic behavior of ZnO:TM. [1] H. Raebiger, S. Lany, and A. Zunger, Physical Review B 79, 165202 (2009). [2] P. Gopal and N. A. Spaldin, Phys. Rev. B 74, 094418 (2006).

Monday, February 27, 2012 8:00AM - 11:00AM –
Session A29 GQI: Focus Session: Quantum Optics with Superconducting Circuits: Hybrid Systems and Other Quantum Optics 259A

8:00AM A29.00001 Atomic physics and quantum optics using superconducting circuits: from the Dynamical Casimir effect to Majorana fermions¹, FRANCO NORI, RIKEN and the University of Michigan — This talk will present an overview of some of our recent results on atomic physics and quantum optics using superconducting circuits. Particular emphasis will be given to photons interacting with qubits, interferometry, the Dynamical Casimir effect, and also studying Majorana fermions using superconducting circuits.

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8:36AM A29.00002 Wigner Tomography of Classical and Non-Classical States in a Superconducting Anharmonic Oscillator, NADAV KATZ, ROI RESH, OFER FOGEL, Hebrew University, RADOSLAW BIALZCAK, JOHN MARTINIS, UCSB, YONI SHALIBO, Hebrew University — The Wigner quasi-probability distribution is a powerful tool for characterizing a quantum state and understanding the state dynamics in oscillators. Until now, there have been numerous measurements of this function in harmonic oscillators, and in particular in superconducting devices. However no similar measurement on anharmonic systems has been reported. We utilize the wide-range energy tunability in the multi-level Josephson phase qubit, biased in the small anharmonicity regime, to directly measure the Wigner function of various states. We measure non-classical superpositions of Fock-type states, as well as coherent-like states in this anharmonic system. This method provides an alternative to standard state tomography techniques which usually involve a long calibration process and have limited scalability for multi-level states.

8:48AM A29.00003 Geometric Phases, Noise and Non-adiabatic Effects in Multi-level Superconducting Systems, S. BERGER, M. PECHAL, A.A. ABDUMALIKOV, L. STEFFEN, A. FEDOROV, A. WALLRAFF, S. FILIPP, ETH Zurich — Geometric phases depend neither on time nor on energy, but only on the trajectory of the quantum system in state space. In previous studies [1], we have observed them in a Cooper pair box qubit, a system with large anharmonicity. We now make use of a superconducting transmon-type qubit with low anharmonicity to study geometric phases in a multi-level system. We measure the contribution of the second excited state to the geometric phase and find very good agreement with theory treating higher levels perturbatively. Furthermore, we quantify non-adiabatic corrections by decreasing the manipulation time in order to optimize our geometric gate. Geometric phases have also been shown to be resilient against adiabatic field fluctuations [2]. Here, we analyze the effect of artificially added noise on the geometric phase for different system trajectories.

[1] P. J. Leek *et al.*, *Science* **318**, 1889 (2007)

[2] S. Filipp *et al.*, *Phys. Rev. Lett.* **102**, 030404 (2009)

9:00AM A29.00004 Observing the geometric phase of a superconducting harmonic oscillator, M. PECHAL, S. BERGER, A.A. ABDUMALIKOV, J.M. FINK, J.A. MLYNEK, L. STEFFEN, A. WALLRAFF, S. FILIPP, ETH Zurich — Steering a quantum harmonic oscillator state along cyclic trajectories leads to a path-dependent geometric phase [1]. However, the linearity of the system precludes its observation without a non-linear quantum probe. We therefore make use of a superconducting qubit serving as an interferometer to measure the adiabatic geometric phase of a harmonic oscillator realized as an on-chip resonant circuit [2]. We study the geometric phase for a variety of trajectories and show that, in agreement with theory, it is proportional to the area enclosed by the trajectory in the space of coherent states. At the transition to the non-adiabatic regime, oscillatory dephasing effects caused by residual qubit-resonator entanglement are observed and analyzed. We also discuss the possibility of using the harmonic oscillator geometric phase to implement two-qubit phase gates.

[1] S. Chaturvedi, M. S. Sriram, V. Srinivasan, J. Phys. A: Math. Gen. **20**, L1071 (1987).

[2] M. Pechal *et al.*, arXiv:1109.1157v1 [quant-ph].

9:12AM A29.00005 All-resonant control of superconducting resonator qudits¹, FREDERICK STRAUCH, Williams College — Quantum information processing with using superpositions of Fock states in superconducting resonators holds great promise for multi-level (i.e. qudit) quantum logic. Previous theoretical work has shown that a combination of dispersive and resonant interactions allow for general qudit logic operations. Here I introduce an all-resonant approach to control resonator qudits. This scheme allows for faster logic operations and will be compared to previous methods for Fock state generation and entangled state synthesis.

¹Supported by NSF PHY-1005571

9:24AM A29.00006 Readout of Spin Systems with Superconducting Circuits¹, NATANIA ANTLE, KATER MURCH, R. VIJAY, STEVEN WEBER, ELI LEVENSON-FALK, I. SIDDIQI, UC Berkeley, QNL — We present progress in coupling superconducting circuitry, in particular linear resonators and dispersive magnetometers, to an ensemble of spins. Species with a zero-field splitting (ZFS), such as bismuth doped silicon or NV centers in diamond, are particularly attractive as the absence of a strong magnetic bias field facilitates compatibility with superconducting devices. We present studies of the spin linewidth, and progress towards the observation of collective strong coupling. Furthermore, we will present data on the operation of a highly sensitive nanobridge SQUID magnetometer with a flux sensitivity of $26 \text{ n}\Phi_0/\sqrt{\text{Hz}}$ and tens of MHz of signal bandwidth. We also discuss the resilience of our superconducting measurement circuitry to in-plane magnetic fields, which can be used to tune the spin splitting.

¹This research is supported by the NSF E3S center and the AFOSR.

9:36AM A29.00007 Hybrid quantum circuit with a superconducting qubit coupled to a spin ensemble¹, YUIMARU KUBO, CECILE GREZES, ANDREAS DEWES, DENIS VION, CEA-Saclay, JUNICHI ISOYA, University of Tsukuba, VINCENT JACQUES, ANAIS DREAU, JEAN-FRANCOIS ROCH, ENS de Cachan, IGOR DINIZ, ALEXIA AUFFEVE, CNRS-Grenoble, DANIEL ESTEVE, PATRICE BERTET, CEA-Saclay — We report the experimental realization of a hybrid quantum circuit combining a superconducting qubit and an ensemble of electronic spins. The qubit, of the transmon type, is coherently coupled to the spin ensemble consisting of nitrogen-vacancy (NV) centers in a diamond crystal via a frequency-tunable superconducting resonator acting as a quantum bus [1,2]. Using this circuit, we prepare arbitrary superpositions of the qubit states that we store into collective excitations of the spin ensemble and retrieve back later on into the qubit [3]. These results constitute a first proof of concept of spin-ensemble based quantum memory for superconducting qubits.

[1] Y. Kubo *et al.*, Phys. Rev. Lett. **105**, 140502 (2010).

[2] Y. Kubo *et al.*, arXiv: 1109.3960.

[3] Y. Kubo *et al.*, arXiv: 1110.2978.

¹We acknowledge support from European projects MIDAS and SOLID, ANR project Masquelspec, C’Nano, Capes, and Fondation Nanosciences de Grenoble.

9:48AM A29.00008 Coherent coupling of a superconducting flux qubit to an electron spin ensemble in diamond, XIAOBO ZHU, SHIRO SAITO, ALEXANDER KEMP, KOSUKE KAKUYANAGI, SHIN-ICHI KARIMOTO, HAYATO NAKANO, WILLIAM J. MUNRO, YASUHIRO TOKURA, NTT Basic Research Laboratories, MARK S. EVERITT, KAE NEMOTO, National Institute of Informatics, MAKOTO KASU, NTT Basic Research Laboratories, NORIKAZU MIZUOCHI, University of Osaka; PRESTO JST, KOUICHI SEMBA, NTT Basic Research Laboratories — We have experimentally demonstrated coherent strong coupling between a single macroscopic superconducting artificial atom (a gap tunable flux qubit [1]) and an ensemble of electron spins in the form of nitrogen-vacancy color centres in diamond. We have observed coherent exchange of a single quantum of energy between a flux qubit and a macroscopic ensemble consisting of about 3.0×10^7 NV- centers [2]. This is the first step towards the realization of a long-lived quantum memory and hybrid devices coupling microwave and optical systems. [1] *Coherent operation of a gap-tunable flux qubit X*. B. Zhu, A. Kemp, S. Saito, K. Semba, APPLIED PHYSICS LETTERS, Volume: 97, Issue: 10 pp. 102503 (2010) [2] *Coherent coupling of a superconducting flux qubit to an electron spin ensemble in diamond* Xiaobo Zhu, Shiro Saito, Alexander Kemp, Kosuke Kakuyanagi, Shin-ichi Karimoto, Hayato Nakano, William J. Munro, Yasuhiro Tokura, Mark S. Everitt, Kae Nemoto, Makoto Kasu, Norikazu Mizuochi, and Kouichi Semba, Nature, Volume: 478, 221-224 (2011)

10:00AM A29.00009 Hybrid qubit-resonator systems: From strong to ultrastrong coupling, from equilibrium to non equilibrium phases, DAVID ZUECO, THOMAS HÜMMER, MARK JENKINS, MARÍA JOSÉ MARTÍNEZ-PÉREZ, Universidad de Zaragoza - ICMA, GEORG REUTHER, Universitat Augsburg, JUAN JOSÉ GARCÍA-RIPOLL, CSIC, FERNANDO LUIS, Universidad de Zaragoza - ICMA, PETER HÄNGGI, Universitat Augsburg — Hybrid systems : spin ensembles coupled to superconducting circuits have received a lot of attention recently. In a seminal experiment it has been demonstrated strong coupling between a NV-center spins ensemble and a flux qubit. The ensemble maps to a bosonic mode, thus this setup is a realization of a qubit-resonator model. In this talk we propose molecular magnets, instead of NV centers, as ensembles and we show that with them it is possible to reach the ultra strong coupling (the coupling is around 40% of the qubit-resonator frequencies). Finally, we emphasize the potentiality of these architectures for exploring many body physics by building arrays made of flux qubits and crystal spins. We will discuss non equilibrium signatures of Mott insulator - Superfluid phases and its feasibility within current technology.

10:12AM A29.00010 Quantum transducer in circuit optomechanics¹, NICOLAS DIDIER, ROSARIO FAZIO, Scuola Normale Superiore, NEST and Istituto NanoScienze-CNR, Pisa, Italy — Mechanical resonators are becoming macroscopic quantum objects with great potential. It is however difficult to measure and manipulate the phonon state due to the tiny motion in the quantum regime. We show that a superconducting microwave resonator linearly coupled to the mechanical mode constitutes a powerful probe and an interesting quantum source. This coupling is rendered much stronger than the usual radiation pressure interaction by adjusting a gate voltage and gives rise to coherent oscillations between phonons and photons. The phenomenon of phonon blockade is detected from the statistics of the light field [1] and a quantum tomography of the mechanical resonator is obtained after transferring the state to the microwave cavity. Quantum phonon states can also be synthesized from the cavity and hybrid entanglement can be engineered between phonons and photons. Mechanical resonators can furthermore be coupled to a large variety of quantum systems such as spins, optical photons, cold atoms, and Bose Einstein condensates. They act as a quantum transducer between an auxiliary quantum system and a microwave resonator, which is used as a quantum bus. The quantum communications are controlled with the individual gate voltages. [1] N. Didier et al., Phys. Rev. B **84**, 054503 (2011).

¹This work is supported by the QNEMS European project.

10:24AM A29.00011 Quantum control of mechanical oscillators, KONRAD LEHNERT, JILA — No abstract available.

Monday, February 27, 2012 8:00AM - 10:48AM – Session A30 GQI: Focus Session: Qubits in Diamond I 259B

8:00AM A30.00001 Stark tuning spin qubits in diamond for quantum optical networks, VICTOR ACOSTA, CHARLES SANTORI, ANDREI FARAON, ZHIHONG HUANG, Hewlett Packard Laboratories, Palo Alto, CA, KAI-MEI FU, University of Washington, Dept. of Physics, ALASTAIR STACEY, DAVID SIMPSON, TIMOTHY KARLE, BRANT GIBSON, LIAM MCGUINNESS, KUMARAVELU GANESAN, SNJEZANA TOMLJENOVIC-HANIC, ANDREW GREENTREE, STEVEN PRAWER, University of Melbourne, School of Physics, RAYMOND BEAUSOLEIL, Hewlett Packard Laboratories, Palo Alto, CA — Integrated diamond networks based on cavity-coupled spin impurities offer a promising platform for scalable quantum computing. A key ingredient for this technology involves heralding entanglement by interfering indistinguishable photons emitted by pairs of identical spin qubits. Here we demonstrate the required control over the internal level structure of nitrogen-vacancy (NV) centers located within 100 nm of the diamond surface using the DC Stark effect. By varying the voltages applied to lithographically-defined metal electrodes, we tune the zero-phonon emission wavelength of a single NV center over a range of ~ 0.5 nm. Using high-resolution emission spectroscopy, we directly observe electrical tuning of the relative strengths of spin-altering lambda transitions to arbitrary values. Under resonant excitation, we apply dynamic feedback to stabilize the optical transition against spectral diffusion. Progress on application of gated control to single NV centers coupled to single-crystal diamond photonic crystal cavities and other nanophotonic structures will be presented. This work was supported by DARPA and the UC Regents.

8:12AM A30.00002 Decoherence-protected quantum gates for a hybrid spin register in diamond¹, V.V. DOBROVITSKI, Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands, T. VAN DER SAR, Ames Laboratory and Iowa State University, Z.-H. WANG, Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands, M.S. BLOK, Ames Laboratory and Iowa State University, Ames, Iowa 50011, USA, H. BERNIEN, T.H. TAMINIAU, Ames Laboratory and Iowa State University, D.M. TOYLI, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, D.A. LIDAR, Depts of Electrical Engineering, Chemistry, and Physics, and Center for Quantum Information Science and Technology, University of Southern California, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, R. HANSON, Ames Laboratory and Iowa State University — Protecting the dynamics of coupled quantum systems from decoherence by the environment is a key challenge for solid-state quantum information processing. An idle qubit can be efficiently insulated from the environment via dynamical decoupling, but quantum gate operations are, in general, disrupted by the decoupling. This problem is particularly salient for hybrid systems, where different types of qubits evolve and decohere at vastly different rates. Here we present an efficient scheme for combining the dynamical decoupling with the quantum gate operation, using the internal resonance in the coupled-spin system. We theoretically demonstrate and experimentally achieve high-fidelity operation of a two-spin register made of the

¹The work was supported by FOM, NWO, DARPA, AFOSR, ARO, NSF, and DOE BES.

8:24AM A30.00003 Quantum Optics with Spins and Photons in Diamond, YIWEN CHU, EMRE TOGAN, MIKHAIL LUKIN, Harvard University — Quantum control of interactions between photons and solid-state systems has important applications in quantum information, metrology, and the study of material properties. The nitrogen-vacancy (NV) color center in diamond is one such solid-state system that has shown great promise as an optically addressable spin qubit and highly sensitive magnetometer. We present recent work on coherent control of spin-photon interactions in a complex solid-state environment using coherent population trapping (CPT). The intrinsic magnetic field sensitivity of our CPT scheme allows us to measure the instantaneous Overhauser field associated with the ¹³C bath present in the diamond crystal. We show that this quantum measurement technique can be used to prepare a state of the ¹³C bath that has much reduced uncertainty in the associated Overhauser field. Such a state is verified by observing a modification and narrowing of the transmission window. The preparation of a more well-defined configuration of the nuclear spin environment could lead to an increase in the coherence times of the NV electronic spin qubit, which in turn has applications in increasing the sensitivity of NV-based magnetometers.

8:36AM A30.00004 Substitutional nickel impurities in diamond: decoherence-free subspace for quantum information processing, THOMAS CHANIER, CRAIG PRYOR, MICHAEL E. FLATTE', University of Iowa — Magnetic color centers in diamond have received interest as qubits for quantum information processing due to diamond's wide band gap and long spin lifetimes which offer the possibility to initialize, manipulate and readout the quantum state of the qubit. Ni-related impurities have been known to form various color centers in diamond and here we propose the use of a substitutional Ni impurity as a qubit. The electronic and magnetic properties of a neutral substitutional nickel impurity in diamond are studied using density functional theory in the generalized gradient approximation. The spin-one ground state consists of two electrons with parallel spins, one located on the nickel ion in the 3d⁹ configuration and the other distributed among the nearest-neighbor carbons. The exchange interaction between these spins is due to p-d hybridization and is controllable with compressive hydrostatic or uniaxial strain. For sufficient strain the antiparallel spin configuration becomes the ground state. Hence, the Ni impurity forms a controllable two-electron exchange-coupled system that should be a robust qubit for solid-state quantum information processing.

8:48AM A30.00005 Cooling Nuclear Spins in Diamond via Dark State Spectroscopy, ADI PICK, MICHAEL GULLANS, EMRE TOGAN, YIWEN CHU, Harvard University, SUSANNE YELIN, University of Connecticut, MIKHAIL LUKIN, Harvard University, CUA TEAM, ITAMP TEAM — Optical cooling methods in atomic physics, developed over the last half century, enable reaching temperatures as low as a few nK. Some of these methods can be applied for cooling spin ensembles in solid state systems. We describe a method for cooling the nuclear spins of ¹³C impurities in diamond, via optical manipulation of the electronic spin associated with an NV⁻ center. We present the physical mechanism which leads to optical pumping of the nuclear spin ensemble into particular nuclear states. The method relies on optically driving three electronic levels in the Λ configuration, and on using the formation of dark states under the conditions of Coherent Population Trapping, (CPT). The dynamics of the nuclear ensemble during this cooling process can be described analytically by using statistical tools, including anomalous random walk models and Levy flights. I survey the theoretical results of the model and discuss some predictions for experimental signatures of Levy flights in this system.

9:00AM A30.00006 Decoherence imaging of spin ensembles by a scannable single nitrogen-vacancy center in diamond, LAN LUAN, MICHAEL GRINOLDS, SUNGKUN HONG, PATRICK MALETINSKY, RONALD WALSWORTH, MIKHAIL LUKIN, AMIR YACOBY, Harvard University — Measuring the decoherence of the spin state of a single nitrogen-vacancy (NV) center in diamond has been proposed as a sensitive method for detecting ensembles of electron or nuclear spins. Using a scanning NV center magnetometer with a single NV residing about 10 nm from the scanning device surface, we explore the effect of T₂ as the device is brought in close proximity to a sample surface. We observe that the spin coherence of the NV center is strongly reduced when it comes into contact with the sample. We are able to restore the coherence by performing dynamic decoupling schemes on the NV spin, suggesting that the sample-induced decoherence originates from the fluctuating magnetic field of a surface spin ensemble. The decoherence diminishes when we increase the NV to sample surface distance by 10nm either vertically or laterally. These experiments demonstrate the potential for using the coherence of a single NV spin to locally detect and spatially map spin ensembles.

9:12AM A30.00007 Investigating spin decoherence in nanodiamonds using a multi-frequency electron spin resonance, A. DAS, V. STEPANOV, Z. KOBOS, Z.H. WANG, S. TAKAHASHI, University of Southern California — Nitrogen-vacancy (NV) centers in nanodiamonds (NDs) are extremely useful for applications of nanoscale magnetic sensing as well as for conducting fundamental science because of their unique spin properties including capability to initialize the NV spin state and their long decoherence time even at room temperature. Various sizes of nanodiamonds are commercially available. Spin properties of NV centers in NDs are often quite different from those of bulk diamonds. Possible reasons for the difference are surface defects and surface distortions and strains. In this presentation, we will discuss spin properties and spin decoherence in various NDs studied by X-band (10 GHz) and high field (230 and 115 GHz) spectrometers. We will also study properties of environmental noises in NDs using dynamical decoupling techniques.

9:24AM A30.00008 Deep Level Tight-Binding Model for Transition Metal Dopant States in Diamond, VICTORIA KORTAN, CUNEY SAHIN, MICHAEL FLATTÉ, University of Iowa Department of Physics and Astronomy — Diamond is a promising system for quantum information processing [1], providing the possibility of single-spin-photon entanglement, as well as the potential for high-speed spin manipulation at room temperature (such as has been demonstrated for the electronic spin associated with an NV center [2]). Ion implantation has been demonstrated for controllable positioning of NV centers; in principle other dopants could be so implanted as well. For example, transition-metal dopants could potentially be used as optically and electrically active single spin qubits [3]. Here we use a deep level tight binding model to study the electronic trends and defect wave functions of transition-metal dopants in diamond. Starting with the Green's functions of homogeneous diamond (within an spd^s* tight-binding model), a Koster-Slater approach is used to evaluate the defect state. This work is supported by an AFOSR MURI.

[1] A. M. Stoneham, A. H. Harker and G. W. Morley, J. Phys.: Condns. Matter 21, 364222 (2009).

[2] R. Hanson, O. Gywat and D. D. Awschalom, Phys. Rev. B. 74, 161203(r) (2006).

[3] R. Larico, et. al., Phys. Rev. B. 79, 115202 (2009).

9:36AM A30.00009 A method to measure hyperfine interaction beyond standard statistical limit¹, KILHYUN BANG, WEN YANG², L. J. SHAM, Department of Physics, University of California San Diego — We propose a method to measure the hyperfine interaction between a single electron spin and a nuclear spin and apply it to the trapped electron and the ¹⁵N nuclear spin in a diamond nitrogen-vacancy (NV) center. The electron spin is prepared in a pure quantum state and the nuclear spin acquires an unknown partial polarization as a consequence of the preparation of the electron state. The proposed quantum measurement protocol is independent of the incoherence of the initial nuclear spin state. The model utilizes the time τ of a sequence of quantum operations as well as the number N of repeated sequences to increase the accuracy and the precision of the estimation. The deleterious effect of the electron spin decoherence on the precision during time τ is included in the simulation. While in the statistical limit the standard deviation (measure of imprecision) of the estimation is proportional to $1/\sqrt{N}$, the quantum operations in time τ enables the imprecision to decrease faster as $1/\tau$ instead of the equivalent statistical limit of $1/\sqrt{\tau}$. Thus, the net imprecision of the estimation dips below the statistical limit. The robustness test of our simulation shows that experimental implementation of such a precision measurement is possible.

¹This material is based upon work supported by, or in part by the U. S. Army Research Office under contract/grant number ARO-MURI W911NF-08-2-0032.

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9:48AM A30.00010 Towards Probing Living Cell Function with NV Centers in Nanodiamonds, ALEXANDER SUSHKOV, IGOR LOVCHINSKY, NICHOLAS CHISHOLM, Harvard University, DAVID HUNGER, Ludwig-Maximilians-Universität, ALEXEY AKIMOV, P.N. Lebedev Physical Institute, PEGGY LO, AMY SUTTON, JACOB ROBINSON, NORMAN YAO, STEVEN BENNETT, HONGKUN PARK, MIKHAIL LUKIN, Harvard University — We report on recent progress in using the nitrogen-vacancy (NV) center in nanodiamonds as a local probe of paramagnetic free radical concentrations in living cells. The ability to monitor the local magnetic environment within the cell provides us a new tool to study organelle function during normal operation or in response to applied stimuli. Our approach involving biologically inert, robust sensor of local magnetic fields with nanoscale resolution opens up a new interface between quantum and biological sciences.

10:00AM A30.00011 Anomalous decoherence of a nitrogen-vacancy center in a nuclear spin bath¹, REN-BAO LIU, NAN ZHAO, ZHEN-YU WANG, Department of Physics, The Chinese University of Hong Kong — A spin loses its coherence in its noisy environment. It is generally believed that stronger noise causes faster decoherence. Here we show that in a quantum bath, the case can be the opposite. We predict that the double-transition of a nitrogen-vacancy center spin-1 in diamond can have longer coherence time than the single transitions, even though the former suffers twice stronger noise from the nuclear spin bath than the latter. This anomalous decoherence effect is due to manipulation of the bath evolution via flips of the center spin.

¹This work was supported by Hong Kong RGC/GRF CUHK402410, CUHK Focused Investments Scheme, National Natural Science Foundation of China Project 11028510, and NSFC-RGC Joint Project N-CUHK403/11.

10:12AM A30.00012 Manipulation of ¹³C nuclear spins in diamond via dynamical decoupling control of the electron spin¹, HOI-CHUN PO, REN-BAO LIU, Department of Physics, The Chinese University of Hong Kong — Utilizing the anisotropic nature of the hyperfine coupling between a negatively charged nitrogen-vacancy (NV) center spin and a moderately separated ¹³C nuclear spin, we present a scheme to efficiently control the ¹³C spin in 3 to 4 pulse cycles. This scheme uses only microwave pulses tuned to swap the NV center spin between the $m_s = 0$ and $m_s = 1$ states. With a strong magnetic field of the order of 10^3 G along the NV center symmetry axis, the nuclear spin can be flipped in approximately 10 μ s. We also numerically study the effect of various sources of errors in realistic scenario and demonstrate that the fidelity of the scheme is satisfactory. The pulse sequences can be readily generalized to perform any single qubit operation on the nuclear spin.

¹This work was supported by Hong Kong RGC/GRF CUHK402209, NSFC/RGC Joint Project N-CUHK403/11, and NSFC Project 11028510.

10:24AM A30.00013 Narrowing Overhauser field by coherent population trapping, ZHAN-FENG JIANG, REN-BAO LIU JIANG, Department of Physics, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong, China — By optical coupling to an excited state, an electron spin may be trapped to a coherent dark state when the Overhauser field has a proper value. At the same time, the fluctuation of nuclear spins is suppressed. Although the electron may jump out of the dark state due to the Fermi-contact hyperfine interaction between the electron and the nuclei, it still has a predominant probability to stay at the dark state. The narrowing of the Overhauser field prolongs the coherent time of the electron spin. The Overhauser field is always suppressed as the external magnetic field varies in a large range. A window with a long coherent time forms when we scan the external magnetic field. This work is supported by Hong Kong RGC/GRF Project CUHK402209 and NSFC/RGC Joint Project N-CUHK403/11.

10:36AM A30.00014 Spin echo probe of quantum criticality in the one-dimensional transverse-field Ising model, SHAOWEN CHEN, KE CHEN, RENBAO LIU, Department of Physics, The Chinese University of Hong Kong — We study the detection of quantum phase transition in the one dimensional transverse-field Ising model. In the model, we attach a spin-1/2 to the Ising spin chain as a probe and study the decoherence behavior of the probing spin with spin echo techniques. We evaluate the effective spectrum density of the local field that the Ising spin chain impart to the probing spin and identify the contributions from the thermal fluctuations and quantum fluctuations to the probe spin decoherence. The output of our work provides a better understanding of the quantum phase transition of this model. This work is supported by Hong Kong RGC/GRF Project CUHK 402410 and NSFC/RGC Joint Project N-CUHK403/11.

Monday, February 27, 2012 8:00AM - 11:00AM –
Session A31 GMAG DMP: Focus Session: Topological Insulators - Exotic Phases and Phase Transitions 260

8:00AM A31.00001 Quantum Anomalous Hall Effect in Magnetic Topological Insulator GdBiTe₃¹, HAI-JUN ZHANG, XIAO ZHANG, SHOU-CHENG ZHANG, Department of Physics, McCullough Building, Stanford University, Stanford, CA 94305-4045 — The quantum anomalous Hall (QAH) state is a two-dimensional bulk insulator with a non-zero Chern number in absence of external magnetic fields. Protected gapless chiral edge states enable dissipationless current transport in electronic devices. Doping topological insulators with random magnetic impurities could realize the QAH state, but magnetic order is difficult to establish experimentally in the bulk insulating limit. Here we predict that the single quintuple layer of GdBiTe₃ film could be a stoichiometric QAH insulator based on *ab-initio* calculations, which explicitly demonstrate ferromagnetic order and chiral edge states inside the bulk gap. We further investigate the topological quantum phase transition by tuning the lattice constant and interactions. A simple low-energy effective model is presented to capture the salient physical feature of this topological material.

¹This work is supported by the Army Research Office (No.W911NF-09-1-0508) and the Keck Foundation.

8:12AM A31.00002 First-principles study of magnetic ion doping in thin film Bi₂Se₃: electronic structure and topological phase¹, JINO IM, HOSUB JIN, ARTHUR J. FREEMAN, Northwestern University — We study the quantum anomalous Hall state in magnetic ion-doped Bi₂Se₃ thin films. By using first-principles density functional theory, we investigate this electronic structure and identify its topological phase. We find that magnetic ion doping induces the exchange field splitting and changes the spin-orbit coupling strength. As the doping concentration increases, the exchange field splitting strength increases and the spin-orbit coupling strength may decrease depending on the type of magnetic ion. Based on these results, we show that the quantum anomalous Hall state in the doped Bi₂Se₃ thin film emerges at a certain range of doping concentration. The Hall conductance of the doped Bi₂Se₃ thin film will also be discussed with various doping concentrations.

¹Supported by the DOE (Grant No. DE-FG02-88ER45372)

8:24AM A31.00003 Charge 4e Superconductivity from Quantum Spin Hall phase, EUN GOOK MOON, CENKE XU, University of California Santa Barbara — We present how to achieve charge 4e superconductor as a ground state studying non-relativistically induced quantum numbers of Skyrmions. It is shown that induced charge of Skyrmions interacting with fermion with quadratic band touching dispersion is twice bigger than one of Skyrmions with Dirac-like fermion. We also show that the former Skyrmions are always bosons while the latter ones are determined by the number of fermion flavors. Possible physical realization is discussed focusing on Skyrmions of quantum spin Hall order parameter in bi-layer graphene. Properties of quantum phase transition between charge 4e superconductor and quantum spin Hall phase are also discussed.

8:36AM A31.00004 Majorana fermions in semiconductor nanowires with realistic physical parameters, TUDOR STANESCU, West Virginia University — Semiconductor nanowires proximity coupled to s-wave superconductors represent a unique solid state platform for realizing and observing the elusive Majorana fermion. The existence and stability of the Majorana bound states localized at the ends of the wire depend on a set of parameters that includes the chemical potential, the external magnetic field, the spin-orbit coupling, the strength of the semiconductor-superconductor coupling, and the strengths of various types of disorder. It is critical to determine whether or not the parameter regimes that ensure the stability of the Majoranas are consistent with realistic experimental conditions. In this talk I will summarize the results of a theoretical study of multiband semiconductor nanowires that focuses on understanding the key experimental conditions required for the realization and detection of Majorana fermions. I will show that multiband occupancy not only lifts the stringent constraint of one-dimensionality, but also allows having higher carrier density in the nanowire. This significantly enhances the stability of the topologically nontrivial phase against various types of disorder, such as short-range impurities in the bulk superconductor, disorder at the semiconductor-superconductor interface, and disorder in the semiconductor nanowire. The detailed study of the parameter space for multiband semiconductor nanowires establishes the realistic likelihood of the existence of zero-energy Majorana modes within laboratory conditions.

9:12AM A31.00005 Topological States and Adiabatic Pumping in Quasicrystals¹, YAAKOV KRAUS, YOA V LAHINI, ZOHAR RINGEL, MOR VERBIN, ODED ZILBERBERG, Weizmann Institute of Science — We find a connection between quasicrystals and topological matter, namely that quasicrystals exhibit non-trivial topological phases attributed to dimensions higher than their own [1]. Quasicrystals are materials which are neither ordered nor disordered, i.e. they exhibit only long-range order [2]. This long-range order is usually expressed as a projection from a higher dimensional ordered system. Recently, the unrelated discovery of Topological Insulators [3] defined a new type of materials classified by their topology. We show theoretically and experimentally using photonic lattices, that one-dimensional quasicrystals exhibit topologically-protected boundary states equivalent to the edge states of the two-dimensional Integer Quantum Hall Effect. We harness this property to adiabatically pump light across the quasicrystal, and generalize our results to higher dimensional systems. Hence, quasicrystals offer a new platform for the study of topological phases while their topology may better explain their surface properties.

[1] Y. E. Kraus, Y. Lahini, Z. Ringel, M. Verbin, and O. Zilberberg, arXiv:1109.5983 (2011).

[2] C. Janot, *Quasicrystals* (Clarendon, Oxford, 1994), 2nd ed.

[3] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).

¹ Authors appear in alphabetical order.

9:24AM A31.00006 Skyrmion quantum numbers and quantized pumping in two dimensional topological chiral magnets¹, BOHM-JUNG YANG, NAOTO NAGAOSA, Correlated Electron Research Group (CERG), RIKEN Advanced Science Institute, Wako, Saitama 351-0198, Japan — We investigate the general conditions to achieve the adiabatic charge and spin polarizations and quantized pumping in 2D magnetic insulators possessing inhomogeneous spin structures. In particular, we focus on the chiral ferrimagnetic insulators which are generated via spontaneous symmetry breaking from correlated two dimensional topological insulators. Adiabatic deformation of the inhomogeneous spin structure generates the spin gauge flux, which induces adiabatic charge and spin polarization currents. The unit pumped charge/spin are determined by the product of two topological invariants which are defined in momentum and real spaces, respectively. The same topological invariants determine the charge and spin quantum numbers of skyrmion textures. It is found that in noncentrosymmetric systems, a new topological phase, dubbed the topological chiral magnetic insulator, exists in which a skyrmion defect is a spin-1/2 fermion with electric charge e . Considering the adiabatic current responses of generic inhomogeneous systems, it is shown that the quantized topological response of chiral magnetic insulators is endowed with the second Chern number.

¹Supported by JSPS through FIRST program.

9:36AM A31.00007 Beyond Floquet theory: new paradigms for robust topological phenomena in strongly driven systems, MARK RUDNER, Harvard/Ohio State University, MICHAEL LEVIN, University of Maryland, EREZ BERG, Harvard — The discoveries of the quantized Hall effect [1] and Thouless' quantized adiabatic pumping [2] revealed the existence of a new class of extremely robust quantum phenomena which can be observed with high fidelity, largely independent of sample details. The immunity of these remarkable effects to a variety of perturbations can be understood in terms of a topological structure associated with the systems' wave functions. The rapid development of powerful tools for controlling solid state and atomic systems over the last decade has motivated the exploration of topological phenomena in driven systems. Recently, Kitagawa and coworkers [3] discussed analogs of previously known topological phenomena in terms of the Floquet operators of periodically-driven systems. Intriguingly, this work also revealed new robust phenomena, such as the existence of robust chiral edge modes in a 2D system with vanishing Chern numbers for all bulk Floquet bands. Here we construct the topological invariant which distinguishes phases with and without chiral edge modes, and discuss generalizations to other 1D and 2D systems.

[1] K. von Klitzing, G. Dorda, and M. Pepper, Phys. Rev. Lett. 45, 494 (1980).

[2] D. J. Thouless, Phys. Rev. B 27, 6083 (1983).

[3] T. Kitagawa, et al., Phys. Rev. B 82, 235114 (2010).

9:48AM A31.00008 Emergent Topological Phases with Multiple Bands and Artificial Gauge Fields, ALEXANDRU PETRESCU, Yale University Physics Department, New Haven, CT, 06520 USA, KARYN LE HUR, Yale University Physics Department, New Haven, CT, 06520 USA and Center for Theoretical Physics (CPHT), Ecole Polytechnique, Palaiseau 91128, France — Particles on a two-dimensional Kagome lattice have attracted growing attention recently in relation to topological insulators and topological phases. Such Kagome structures can be engineered in optical lattices and can also be loaded with bosons. Similar tight-binding models might also be realized in photonic QED circuits. In this work, we investigate in detail the 3-band model emerging from such a tight-binding model on the two-dimensional Kagome lattice in the presence of artificial gauge fields and identify novel phases of matter such as bulk metals with helical edge states. We investigate the stability of edge modes inside a topological metallic phase and the role of lattice anisotropies and disorder, as well as relation to current experiments.

10:00AM A31.00009 Possible interaction driven topological phases in (111) bilayers of LaNiO_3 , YING RAN, KAI-YU YANG, Department of Physics, Boston College, Chestnut Hill, MA, 02467, WENGUANG ZHU¹, DI XIAO, SATOSHI OKAMOTO, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, ZIQIANG WANG, Department of Physics, Boston College, Chestnut Hill, MA, 02467 — We use the variational mean-field approach to systematically study the phase diagram of a bilayer heterostructure of the correlated transition metal oxide LaNiO_3 , grown along the (111) direction. The Ni^{3+} ions with d^7 (or e_g^1) configuration form a buckled honeycomb lattice. We show that as a function of the strength of the on-site interactions, various topological phases emerge. In the presence of a reasonable size of the Hund's coupling, as the correlation is tuned from intermediate to strong, the following sequence of phases is found: (1) a Dirac half-semimetal phase, (2) a quantum anomalous Hall insulator (QAH) phase with Chern number one, and (3) a ferromagnetic nematic phase breaking the lattice point group symmetry. The spin-orbit couplings and magnetism are both dynamically generated in the QAH phase.

¹Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996

10:12AM A31.00010 Quantum Phase Transitions in the Kane-Mele-Hubbard Model¹, ZI YANG MENG, Center for Computation and Technology, Louisiana State University, MARTIN HOHENADLER, Institute for Theoretical Physics and Astrophysics, University of Wuerzburg, THOMAS C. LANG, STEFAN WESSEL, Institute for Theoretical Solid State Physics, RWTH Aachen University, ALEJANDRO MURAMATSU, Institut fuer Theoretische Physik III, Universitaet Stuttgart, FAKHER F. ASSAAD, Institute for Theoretical Physics and Astrophysics, University of Wuerzburg — We study the ground state phase diagram of the Kane-Mele-Hubbard model on the two-dimensional honeycomb lattice. At half-filling the phase diagram is mapped out using projective auxiliary field quantum Monte Carlo simulations. We present a refined phase boundary for the quantum spin liquid. The topological (quantum spin-Hall) insulator at finite Hubbard interaction strength is adiabatically connected to the ground state of the Kane-Mele model. For the magnetic phase at large Hubbard interaction strength, we show that the magnetic order is restricted to the transverse direction. The transition from the topological band insulator to the antiferromagnetic Mott insulator is in the universality class of the three-dimensional XY model. The numerical data also suggest that the spin liquid to topological insulator and spin liquid to Mott insulator transitions are both continuous.

¹DFG funding through SFB/TRR 21, and WE 3639/2-1

10:24AM A31.00011 Topological Phase Transitions for Interacting Finite Systems¹, KAI SUN, University of Maryland, College Park, CHRISTOPHER VARNEY, MARCOS RIGOL, Georgetown University, VICTOR GALITSKI, University of Maryland, College Park — We investigate topological phase transitions in interacting systems via the observation of a topologically protected level crossing. This level crossing is robust and sharply defines a topological transition even in finite-size systems. For Chern insulators, this technique gives the same topological transition point as obtained in the Chern number calculation (via flux insertion). However, in the presence of space inversion symmetry, we proved that if the topological index changes by an odd integer at the topological transition, the level crossing can only arise under (some of) the four high-symmetry boundary conditions. This discovery provides a very efficient way to detect topological phase transitions, which reduces the computational load dramatically. In contrast to the standard Chern number technique, which requires to compute the ground state wave function for hundreds of different boundary conditions, our technique achieves the same result by calculating the excitation gap for only four different boundary conditions. We demonstrate this technique in the Haldane-Fermi-Hubbard model utilizing exact diagonalization. Generalization to time-reversal invariant $\mathbb{Z}_2$ topological insulators will also be discussed.

¹Supported by NSF-JQI-PFC, ONR and U.S.-ARO.

10:36AM A31.00012 Topological phases and phase transitions in a two-dimensional fermionic lattice, CRISTIANE MORAIS SMITH, WOUTER BEUGELING, Utrecht University, NATHAN GOLDMAN, Universite libre de Bruxelles — A topological state of matter is characterized by a topological invariant, which is protected against disorder effects. For the quantum Hall effect, the Hall conductivity is protected since it is carried by chiral edge states, induced by a magnetic field. Systems with large spin-orbit coupling exhibit the quantum spin Hall effect, where the protected quantity is the spin Hall conductivity, carried by helical edge states. In our theoretical study of a fermionic tight-binding model we show that the interplay between the magnetic field and the spin-orbit coupling generates spin-imbalanced chiral phases and exotic phase transitions between helical and chiral spin textures. We explore the experimental possibilities to observe these phase transitions in cold-atom systems, for which the necessary strengths of the magnetic field and spin-orbit coupling are accessible. As a second application, we investigate the spectrum of topological phases in HgTe quantum wells doped with Mn ions (in collaboration with Molenkamp's group). We show that this doping leads to interesting reentrant effects of both the Hall and spin Hall conductivities.

10:48AM A31.00013 Phase Structure of the Topological Anderson Insulator, DONGWEI XU, Oklahoma State University, VINCENT E. SACKSTEDER, JUNJIE QI, JIE LIU, Institute of Physics, Chinese Academy of Sciences, HUA JIANG, Peking University, X. C. XIE, Oklahoma State University, Peking University — We report the phase structure of disordered HgTe topological Anderson insulator in a 2-D geometry. We use exact diagonalization to calculate the spectrum and eigenstate structure, and recursive green's functions to calculate the conductance. All observables are measured at several system sizes, allowing us to determine phase transitions and two critical points. The quantized-conductance TAI phase contains two phases: TAI-I lying in a bulk band gap, and TAI-II where bulk states exist but are localized. We find that the TAI-II phase persists at disorder strengths where there is no bulk band gap; a bulk band gap is not necessary to obtain conductance quantization. In a previous work the weak-disorder edge of the TAI phase was explained as a transition into the bulk gap (TAI-I), but we find also a direct transition into the ungapped (TAI-II) quantized phase. Effective medium theory (SCBA) predicts well the boundaries and interior of the TAI-I phase, but fails at larger disorders including the interior of the TAI-II phase. When the system size is smaller than the bulk localization length, the quantized TAI region is bounded by either the bulk band edge or the localization length, but when the system size is large it is bounded by a transition of edge states.

Monday, February 27, 2012 8:00AM - 11:00AM — Session A32 DCMF: Topological Insulators: Quantum Hall Effect 261

8:00AM A32.00001 Weak antilocalization in HgTe quantum wells and topological surface states: Massive versus massless Dirac fermions¹, EVELINA HANKIEWICZ, GRIGORY TKACHOV, Wuerzburg University — HgTe quantum wells and surfaces of three-dimensional topological insulators support Dirac fermions with a single-valley band dispersion. In this work we conduct a comparative theoretical study of the weak antilocalization in HgTe quantum wells (QWs) and topological surface states. The difference between these two single-valley systems comes from a finite band gap (effective Dirac mass) in HgTe quantum wells in contrast to gapless (massless) surface states in topological insulators. The finite effective Dirac mass implies a broken internal symmetry, leading to suppression of the weak antilocalization in HgTe quantum wells and transition to the weak localization regime as a function of the gap or carrier density. In particular, we show how the difference in the behavior of the weak localization corrections for HgTe QWs allows to distinguish topological versus normal insulators. Further for the topological surface states we predict specific weak-antilocalization magnetoconductivity in a parallel magnetic field due to their exponential decay in the bulk. The relevant experiments will be discussed.

¹This work was funded through DFG Grant HA5893/1-2

8:12AM A32.00002 Topological insulators in magnetic fields: Quantum Hall effect and edge channels with non-quantized θ -term, LARS FRITZ, MATTHIAS SITTE, ACHIM ROSCH, University of Cologne/ Germany, EHUD ALTMAN, Weizmann Institute — We investigate how a magnetic field induces one-dimensional edge channels when the two-dimensional surface states of three-dimensional topological insulators become gapped. The Hall effect, measured by contacting those channels, remains quantized even in situations, where the θ -term in the bulk and the associated surface Hall conductivities, σ_{xy}^S , are not quantized due to the breaking of time-reversal symmetry. The quantization arises as the θ -term changes by $\pm 2\pi n$ along a loop around n edge channels. Model calculations show how an interplay of orbital and Zeeman effects leads to quantum Hall transitions, where channels get redistributed along the edges of the crystal. The network of edges opens new possibilities to investigate the coupling of edge channels.

8:24AM A32.00003 The topological Hubbard model and its high-temperature quantum Hall $\nu = 1$ state, TITUS NEUPERT, Condensed Matter Theory Group, Paul Scherrer Institute, Switzerland, LUIZ SANTOS, Department of Physics, Harvard University, SHINSEI RYU, Department of Physics, University of Illinois at Urbana-Champaign, CLAUDIO CHAMON, Physics Department, Boston University, CHRISTOPHER MUDRY, Condensed Matter Theory Group, Paul Scherrer Institute, Switzerland — The quintessential two-dimensional lattice model that describes the competition between the kinetic energy of electrons and their short-range repulsive interactions is the repulsive Hubbard model. We study a time-reversal symmetric variant of the repulsive Hubbard model defined on a planar lattice: Whereas the interaction is unchanged, any fully occupied band supports a quantized spin Hall effect. We show that at $1/2$ filling of this band, the ground state develops spontaneously and simultaneously Ising ferromagnetic long-range order and a quantized charge Hall effect when the interaction is sufficiently strong. We ponder on the possible practical applications, beyond metrology, that the quantized charge Hall effect might have if it could be realized at high temperatures and without external magnetic fields in strongly correlated materials.

8:36AM A32.00004 Magnetic field dependence of the edge channels in HgTe quantum wells¹, BENEDIKT SCHARF, ALEX MATOS-ABIAGUE, JAROSLAV FABIAN, Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — In recent years much attention has been devoted to topological insulators, that is, materials which are insulating in the bulk, but have conducting states at their surface. This new class of topological states has first been observed experimentally in HgTe quantum wells. In such a two-dimensional topological insulator, which is also synonymously referred to as a quantum spin Hall insulator, these surface states are one-dimensional, helical edge channels. Here we study a HgTe quantum well in the presence of a constant perpendicular magnetic field. Using tight-binding calculations as well as deriving an analytical expression to determine the electron dispersion and states, we solve the effective low-energy Hamiltonian of this system in a finite-strip geometry. Our main focus is on the behavior of these solutions with increasing magnetic field. In particular, we describe the evolution of the edge states as the system crosses from the quantum spin Hall to the quantum Hall regime.

¹This work has been supported by the Deutsche Forschungsgemeinschaft via GRK 1570 and SFB 689.

8:48AM A32.00005 Phase Diagram of Massive Dirac Fermions with Tunable Interactions in High Magnetic Fields¹, R.N. BHATT, Department of Electrical Engineering and Princeton Center for Theoretical Science, Princeton University, Princeton, NJ 08544, Z. PAPIC, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544, Y. BARLAS, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, D.A. ABANIN, Princeton Center for Theoretical Science, Princeton University, Princeton, NJ 08544 — We study the strongly correlated states of massive fermions in two dimensions with Berry's phase π and 2π , in the limit of high magnetic fields. Due to the chiral band structure and massive carriers, the effective Coulomb interactions depend on the external magnetic field, and lead to a number of phases within a single low-lying Landau level. The tunability of the interactions allows the study of the transitions between phases in a more direct manner than in GaAs-based systems where the form of the interactions is independent of the magnetic field. We map the phase diagram at partial fillings $\nu = 1/3, 1/2, 3/5$ of the low-lying Landau levels, and find transitions between fractional quantum Hall states, compressible Fermi-liquid-like states, as well as charge-density-waves. We also find a new, broad regime of the effective interactions which favor the paired non-Abelian states. Our study identifies the strongly correlated phases expected in high-mobility graphene, bilayer graphene, topological insulators, and other materials with the non-trivial Berry phases, and provides a realistic method for studying the phase transitions between them.

¹This work was supported by DOE grant DE-SC0002140

9:00AM A32.00006 Isotropic Landau levels of relativistic and non-relativistic fermions in 3D flat space, YI LI, CONGJUN WU, University of California, San Diego — The usual Landau level quantization, as demonstrated in the 2D quantum Hall effect, is crucially based on the planar structure. In this talk, we explore its 3D counterpart possessing the full 3D rotational symmetry as well as the time reversal symmetry. We construct the Landau level Hamiltonians in 3 and higher dimensional flat space for both relativistic and non-relativistic fermions. The 3D cases with integer fillings are Z_2 topological insulators. The non-relativistic version describes spin-1/2 fermions coupling to the Aharonov-Casher $SU(2)$ gauge field. This system exhibits flat Landau levels in which the orbital angular momentum and the spin are coupled with a fixed helicity. Each filled Landau level contributes one 2D helical Dirac Fermi surface at an open boundary, which demonstrates the Z_2 topological nature. A natural generalization to Dirac fermions is found as a square root problem of the above non-relativistic version, which can also be viewed as the Dirac equation defined on the phase space. All these Landau level problems can be generalized to arbitrary high dimensions systematically.

[1] Yi Li and Congjun Wu, arXiv:1103.5422.

[2] Yi Li, Ken Intriligator, Yue Yu and Congjun Wu, arXiv:1108.5650.

9:12AM A32.00007 Topological property for magnetic flux tubes in a two-dimensional electron gas, LU-YAO WANG, National Chiao Tung University, dept. of Electrophysics, ZHIGUO LV, Shanghai Jiao Tong University, dept. of Physics, CHON-SAAR CHU, National Chiao Tung University, dept. of Electrophysics — We have studied the energy spectrum in the presence of square magnetic flux-tubes in a two-dimensional electron gas. Our finding is that the Dirac-like dispersion can be formed out between the third and the fourth magnetic subbands without including the Zeeman interaction. This Dirac-like dispersion is not band-inverted type with a global gap. This Dirac-like dispersion becomes band-inverted when the Zeeman interaction is included. We expect that the inverted magnetic subbands due to the Zeeman interaction can be recognized as the topological insulator. This topology property can be supported by the Chern number from the magnetic subbands.

9:24AM A32.00008 Pi-flux as a universal probe of two-dimensional topological insulators¹, VLADIMIR JURICIC, Instituut-Lorentz for Theoretical Physics, Leiden University, The Netherlands, ANDREJ MESAROS, Department of Physics, Boston College, Chestnut Hill, MA 02467, USA, ROBERT-JAN SLAGER, JAN ZAAANEN, Instituut-Lorentz for Theoretical Physics, Leiden University, The Netherlands — We show that the existence of a Kramers pair of zero-energy modes bound to a vortex carrying π -flux is a generic feature of topologically nontrivial phases in the $M-B$ model, describing HgTe quantum wells, and therefore this vortex represents the bulk probe of the band topology [1]. We explicitly find the form of the zero-energy states by analytically solving Dirac equation which contains a momentum-dependent Schrödinger mass, besides the usual Dirac mass term. A particular regularization of the vortex potential yields the modes exponentially localized and regular at the origin that carry nontrivial charge or spin quantum number.

[1] V. Juricic, A. Mesaros, R.-J. Slager, and J. Zaanen, arXiv:1108.3337.

¹V. J. acknowledges the support of the Netherlands Organization for Scientific Research (NWO).

9:36AM A32.00009 Strongly driven Floquet topological insulator in semiconductor quantum wells, XUEDA WEN, CHING-KAI CHIU, Physics Department, UIUC, PHYSICS DEPARTMENT, UIUC COLLABORATION — Floquet topological insulator in a weak-field driven semiconductor quantum well was proposed most recently. In this article we extend the situation to strongly driving field, which can generate high-order harmonic resonances. With appropriate form of driving field, it is found that whether topological transition can happen depends on the number of resonances N we can observe. If N is odd, topological transition can happen; if N is even, topological transition cannot happen. This phenomenon may be observed in semiconductor quantum wells by applying a strongly oscillating magnetic field. In addition, our discussion can be extended to other systems such as p-wave superconductors and spin chains.

9:48AM A32.00010 Quantum Hall effect in a one-dimensional dynamical system¹, JONATHAN EDGE, JAN DAHLHAUS, Leiden University, JAKUB TWORZYDLO, University of Warsaw, CARLO BEENAKKER, Leiden University — We construct a periodically time-dependent Hamiltonian with a phase transition in the quantum Hall universality class [1]. This Hamiltonian is closely related to that of a discrete time quantum walker, but additionally it allows us to study effects of disorder. A particular choice for the form of the Hamiltonian enables us to determine the time evolution of the system in one of the dimensions exactly. Simulations of the system can thus be performed in one dimension, thereby reducing the computational effort required. We investigate the topological phase transition associated with tuning between different quantum Hall plateaux and determine the critical exponent for the divergence of the localisation length. Our scheme can in principle also be implemented in cold atoms experiments, opening the doors to investigating the quantum Hall phase transition in a one-dimensional cold atoms set up.

[1] J. P. and Edge, J. M. and Tworzydlo, J. and Beenakker, C. W. J., PRB 84 115133 (2011).

¹European Early stage researcher grant.

10:00AM A32.00011 Quarter-Filled Honeycomb Lattice with a Quantized Hall Conductance¹, EFRAT SHIMSHONI, Bar-Ilan University, GANPATHY MURTHY, University of Kentucky, RAMAMURTI SHANKAR, Yale University, HERBERT FERTIG, Indiana University, Bloomington — We study a generic two-dimensional hopping model on a honeycomb lattice with strong spin-orbit coupling, without the requirement that the half-filled lattice be a Topological Insulator. For quarter-(or three-quarter) filling, we show that a state with a quantized Hall conductance generically arises in the presence of a Zeeman field of sufficient strength. We discuss the influence of Hubbard interactions and argue that spontaneous ferromagnetism (which breaks time-reversal) will occur, leading to a quantized anomalous Hall effect. G. Murthy, E. Shimshoni, R. Shankar, and H. A. Fertig, arxiv:1108.2010[cond-mat.mes-hall]

¹NSF and BSF

10:12AM A32.00012 Berry Curvature and Phonon Hall Effect, TAO QIN, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, JUNREN SHI, International Center for Quantum Materials, Peking University, Beijing 100871, China — Abstract We establish the general phonon dynamics of magnetic solids by incorporating the Mead-Truhlar correction in the Born-Oppenheimer approximation. The effective magnetic-field acting on the phonons naturally emerges, giving rise to the phonon Hall effect. A general formula of the intrinsic phonon Hall conductivity is obtained by using the corrected Kubo formula with the energy magnetization contribution properly incorporated. The resulting phonon Hall conductivity is fully determined by the phonon Berry curvature and the dispersions. Based on the formula, the topological phonon system could be rigorously defined. In the low temperature regime, we predict that the phonon Hall conductivity is proportional to T^3 for the ordinary phonon systems, while that for the topological phonon systems has the linear T dependence with the quantized temperature coefficient.

[1] Tao Qin and Junren Shi, arXiv:1111.1322 (2011)

[2] Tao Qin, Qian Niu and Junren Shi, Phys. Rev. Lett., Accepted, (2011).

10:24AM A32.00013 Dissipationless Phonon Hall Viscosity, SUK-BUM CHUNG, MAISSAM BARKESHLI, XIAO-LIANG QI, Stanford University — We study the acoustic phonon response of crystals hosting a gapped time-reversal symmetry breaking electronic state. The phonon effective action can in general acquire a dissipationless “Hall” viscosity, which is determined by the adiabatic Berry curvature of the electron wave function. This Hall viscosity endows the system with a characteristic frequency, ω_v ; for phonons of frequency ω , it shifts the phonon spectrum by an amount of order $(\omega/\omega_v)^2$ and it mixes the longitudinal and transverse sound waves with a relative amplitude ratio of ω/ω_v and with a phase shift of $\pm\pi/2$, to lowest order in ω/ω_v . We study several examples, including the integer quantum Hall states, the quantum anomalous Hall state in $\text{Hg}_{1-y}\text{Mn}_y\text{Te}$ quantum wells, and a mean-field model for $p_x + ip_y$ superconductors. We discuss situations in which the phonon response is directly related to the gravitational response, for which striking predictions have been made. When the electron-phonon system is viewed as a whole, this provides an example where measurements of Goldstone modes may serve as a probe of adiabatic curvature of the gapped sector of a system.

10:36AM A32.00014 3D Topological Insulators in the Continuum with Nearly Flat Bands, CONGJUN WU, YI LI, University of California, San Diego, XIANGFA ZHOU, University of Science and Technology of China — We propose a three-dimensional topological insulating state in the harmonic potential with a strong spin-orbit coupling breaking the inversion symmetry. The system gives rise to Landau-level like quantization with the full 3D rotational symmetry and time-reversal symmetry. The radial quantization generates the energy gap between neighboring bands. The states inside each band are characterized by their angular momentum over which the dispersions are suppressed by spin-orbit coupling and thus nearly flat and without Bloch-wave states. Surface states exhibit helical Dirac Fermi surfaces which are described by the Z2 index. Similar analysis in 2D shows the existence of topological insulators in the harmonic potential with strong Rashba spin-orbit coupling. These topological insulating states can be achieved from the dimensional reduction of the quantum Hall states in 3D and 4D flat space.

10:48AM A32.00015 Photo-induced quantum Hall insulators without Landau levels, TAKUYA KITAGAWA, Department of Physics, Harvard University, TAKASHI OKA, Department of Physics, Faculty of Science, University of Tokyo, LIANG FU, Physics Department, Harvard University, ARNE BRATAAS, Department of Physics, Norwegian University of Science and Technology, EUGENE DEMLER, Department of Physics, Harvard University — In this talk, we demonstrate that non-equilibrium transport of graphene under the application of off-resonant light displays a near quantization of Hall conductance. While previous studies of topological phenomena under coherent drives focused on the effective topological band structure, electron occupations in the non-equilibrium systems, which are so far neglected, play a crucial role to determine the transport properties. Using the formalism that consistently take this into account, we show that the topological band structures can directly manifest themselves in the transport properties in Landauer-type configurations under the application of off-resonant light. We give an intuitive explanation of the induction of Chern numbers in the band structure, by showing that the virtual photon absorption/emissions of electrons produces an effective second-order hopping with phase accumulation, leading to the effective Haldane model. Our proposal opens the perspective to realize so-called quantum Hall systems without Landau levels in materials such as graphene and three dimensional topological insulators under coherent drives.

Monday, February 27, 2012 8:00AM - 11:00AM – Session A33 GERA: Physics of Photovoltaics 106

8:00AM A33.00001 Search of novel photovoltaic absorbers from first-principles spectroscopic screening of hundreds of materials¹, LIPING YU, National Renewable Energy Laboratory, ALEX ZUNGER, University of Colorado Boulder — Screening for candidate PV absorbers from numerous existing materials would require a good selection criterion. Initial selection criteria generally rest on the intrinsic material properties and abundance, postponing defect and contact issues to after the list of candidates has been narrowed down. The currently available Shockley-Queisser efficiency formula gives a universal efficiency vs band gap curve (no matter whether the gap is direct or indirect) and ignore all radiative recombination loss, and has proven over the years to be insufficient. Here we propose a calculable selection criterion of “spectroscopic limited maximum efficiency (SLME)” which considers the type of band gap (direct allowed, direct forbidden and indirect), the shape of absorption spectra and material-dependent radiative recombination loss by a simple model. First-principles quasiparticle calculations of SLME for ~300 generalized I-III-VI and ~500 I-V-VI materials identify over 40 candidates with higher SLME than currently used best thin-film absorbers. Analysis of the electronic structure of the top candidates reveals an interesting mechanism for high absorptivity and shows that some indirect gap materials can even be better than direct gap materials.

¹Funded by DOE through Energy Frontier Research Centers, Center for Inverse Design.

8:12AM A33.00002 ABSTRACT WITHDRAWN —

8:24AM A33.00003 First-principles electronic structure of β -FeSi₂ and FeS₂, PENGXIANG XU, TIMO SCHENA, STEFAN BLÜGEL, GUSTAV BIHLMAYER, Peter Gruenberg Institut & Institute for Advanced Simulation, Forschungszentrum Juelich and JARA, 52425 Juelich, Germany — Applying density functional theory in the framework of the full-potential linearized augmented plane-wave (FLAPW) method [1], we investigated electronic structure of potential future photovoltaic materials - β -FeSi₂ and FeS₂ in their bulk phases and for selected surface orientations and terminations. Their band gaps are examined using hybrid functionals as well as many-body perturbation theory in the GW-approximation to get insight of their photovoltaic performance. The gap nature in β -FeSi₂ changes from direct to indirect as suitable strain field is induced in the structure by epitaxially matching with Si substrate. Furthermore, we also studied the atomic and electronic structure of β -FeSi₂ and FeS₂ thin films for different orientations with different terminations. The most stable orientations are determined by comparing their cohesive energy. Detailed electronic structure calculations show that surface states originating from Fe play an important role and might determine their photovoltaic properties.

[1] www.flapw.de

8:36AM A33.00004 The effect of surface stoichiometry on the band gap of the pyrite FeS₂(100) surface¹, YANNING ZHANG, JUN HU, MATT LAW, RUQIAN WU, University of California, Irvine — Iron pyrite (FeS_2) is experiencing a resurgence of interest for use in solar photovoltaic and photoelectrochemical cells. The main hurdle to the use of pyrite is the low open-circuit voltage of pyrite devices, which may result from gap states created by surface and bulk defects. Recently, systematic spin-polarized DFT calculations were performed for a series of pyrite $\text{FeS}_2(100)$ surfaces to clarify the effect of surface stoichiometry on stability, electronic structure, and band gap. It was found that while stoichiometric and S-poor $\text{FeS}_2(100)$ surfaces are semiconductors with band gaps of 0.56-0.72 eV, S-rich surfaces are small-gap semiconductors ($E_g < 0.3$ eV) or metals. The stoichiometric $\text{FeS}_2(100)$ surface is spin polarized in the topmost layer (2 μ_B per Fe) and displays a band of Fe d_{z^2} gap states centered 0.2 eV above the valence band edge. Our calculations suggest that the low open-circuit voltage of pyrite solar cells may result from a narrowed surface band gap. S-poor surfaces may provide larger photovoltages than S-rich surfaces. The segregation process of sulfur vacancy under different surface conditions are also being studied, so as to provide useful guidelines for the design and fabrication of better pyrite photovoltaic materials and devices.

¹We thank the NSF SOLAR Program (Award CHE-1035218) and the UCI School of Physical Sciences Center for Solar Energy for support of this work. Calculations were performed on parallel computers at NERSC and at NSF supercomputer centers.

8:48AM A33.00005 Band gap engineering of Zn based II-VI semiconductors through uniaxial strain, SATYESH YADAV, RAMPI RAMPRASAD, University of Connecticut — The electronic structure of bulk wurtzitic ZnX ($X=O, S, Se, \text{ and } Te$) under uniaxial strain along the [0001] direction is investigated using hybrid density functional theory calculations and many-body perturbation theory. It is found that uniaxial tensile and large compressive strains decrease the band gap, similar to what has been predicted by semilocal density functional theory (DFT) calculations [Yadav et. al, Phys. Rev. B, **81**, 144120 (2010)]. Moreover, the change in the band gap under uniaxial strains predicted by semilocal DFT is in good quantitative agreement with the present results at all strains considered, thereby bringing a measure of redemption to conventional (semi)local DFT descriptions of the electronic structure of at least this class of insulators. The present results have important implications for band gap engineering through strain, especially for complex systems containing a large number of atoms (e.g., nanowires) for which higher-level calculations may be too computationally intensive.

9:00AM A33.00006 Searching Stable Cu_xS Structure for Photovoltaic Application, QIANG XU, BING HUANG, YUFENG ZHAO, National Renewable Energy Lab, YANGFA YAN, Department of Physics and Astronomy The University of Toledo, ROMMEL NOUFI, SU-HUAI WEI, National Renewable Energy Lab — Employing the density-functional theory (DFT) methods, we systematically search for the most energetically favorable Cu_xS compounds in a wide range of $1.2 < x \leq 2.0$ guided by the experimentally identified four minerals, i.e., the chalcocite ($x = 2$), djurite ($x = 1.94$), digenite ($x = 1.80$), and anilite ($x = 1.75$) compounds. For the chalcocite Cu_2S , all its three phases have direct band gaps of 1.3-1.4 eV, with the chalcocite low phase being more stable than other two phases, i.e., the chalcocite high and the chalcocite cubic. According to our calculation, the poor durability of the Cu_2S is mainly due to the energetically favorable formation of Cu vacancies. The calculated formation heat as a function of x shows that the anilite $Cu_{1.75}S$ is the most stable structure. Unfortunately, this material is not a good light absorber because of its metallic feature. We propose that doping of the anilite $Cu_{1.75}S$ with interstitial Sn atoms may result in a compound $Cu_{1.75}Sn_{0.125}S$ with an optimum direct band gap of 1.37 eV. Such a material has the ability of light absorption similar to the chalcocite Cu_2S .

9:12AM A33.00007 Si Nanoparticles embedded in solid matrices for solar energy conversion: electronic and optical properties from first principle calculations, STEFAN WIPPERMANN, Department of Chemistry, University of California, Davis 95616, TIANSHU LI, Department of Civil and Environmental Engineering, George Washington University, Washington, D.C. 20052, DARIO ROCCA, Department of Chemistry, University of California, Davis 95616, GERGELY ZIMANYI, Department of Physics, University of California, Davis 95616, GIULIA GALLI, Department of Chemistry, University of California, Davis 95616, MULTIPLE EXCITON GENERATION IN ALL-INORGANIC NANOSTRUCTURED SOLAR CELLS COLLABORATION¹ — In device applications for solar energy conversion, nanoparticles are often embedded in a solid matrix, either crystalline or amorphous. At present a detailed understanding of the influence exerted by the embedding matrix on absorption of sunlight by the nanoparticle, and the role of the nanoparticle-matrix interface remains elusive. Building on a previous study of Si nanoparticles embedded in SiO_2 [1], we investigate Si nanoparticles embedded in ZnS , used in recent experiments as a charge transport layer. A realistic model of the nanoparticle-matrix interface is created by performing ab-initio molecular dynamics simulations, and electronic and optical properties of the embedded Si nanocrystals, are obtained by first principles.

[1] T.Li, F.Gygi, G.Galli, Phys, Rev. Lett. 107, 206805 (2011)

¹NSF/Solar funded collaboration (grant No. DMR-1035468)

9:24AM A33.00008 Multiple exciton generation in silicon nanoparticles¹, MARTON VOROS, Department of Atomic Physics, Budapest University of Technology and Economics, ADAM GALLI, Hungarian Academy of Sciences, Research Institute for Solid State Physics and Optics, DARIO ROCCA, Department Of Chemistry, University of California, Davis, GIULIA GALLI, Department Of Chemistry, Department Of Physics, University of California, Davis, GERGELY ZIMANYI, Department Of Physics, University of California, Davis — Multiple Exciton Generation (MEG) in semiconductor nanocrystals is considered to be a promising path to improve the efficiency of solar energy conversion. Recent experimental and theoretical studies indicate that MEG is more efficient in nanoparticles (NPs) than in the bulk only on a relative energy scales in units of the gap. The primary cause of this is that quantum confinement increases the energy gap substantially in NPs. MEG will be a true breakthrough when nanocrystals are identified whose impact ionization rate is enhanced even on the absolute energy scale. For this search, we calculated impact ionization rates of silicon NPs with diameters up to 2 nm using density functional theory. Our calculations clearly demonstrate that surface reconstruction creates classes of new states at low energies, de facto lowering the NP gap and thus holding the promise of increasing MEG even on the absolute energy scale. Our calculations include static screening within the random-phase approximation. We show that a full treatment of the transition matrix elements is essential to obtain correct results due their strong energy dependence.

¹Support from Grant NSF DMR-1035468 is acknowledged.

9:36AM A33.00009 All-Carbon Photovoltaics, MARCO BERNARDI, PRIYANK KUMAR, NICOLA FERRALIS, Massachusetts Institute of Technology, SHENQIANG REN, University of Kansas, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology — We present an alternative scheme for nanostructured solar cells, where carbon nanomaterials are the only constituents of a bulk-heterojunction active layer and fulfill the role of absorbers, donors and acceptors, in the absence of conjugated polymers. Ab-initio simulations were employed to calculate the band alignment for interfaces between carbon nanotubes, fullerene derivative PCBM and reduced graphene oxide, showing the presence of Type-II and Schottky heterojunctions useful for charge separation in the active layer. Accordingly, we prepared all-carbon solar cells with optimized proportions of these three components that achieved AM1.5 efficiencies up to 1.5%, with fill factors up to 70% and increased thermal stability and lifetime compared to polymer-based devices. Our results show the potential of all-carbon solar cells as an alternative to polymer based ones: the key combination of high carrier mobility, visible and IR absorption and stability under illumination makes them suitable for next-generation flexible photovoltaics.

9:48AM A33.00010 Porous Silicon Applications for Photovoltaic Solar Cell Devices¹, GULSEN KOSOGLU, MEHMET YUMAK, UGUR DINC, OZHAN OZATAY, YANI SKARLATOS, CARLOS CARCIA CARCIA, Bogazici University Physics Department — The photovoltaic industry searches for low cost, energy competitive solar cell modules, and the usual material used is crystalline silicon, which has been covering 90% of the solar module market for a long time. Porous silicon (P-Si) is used in photovoltaic applications as an ultra efficient anti-reflection coating, while a graded layer with an expanded band gap offers increased absorption in the visible spectrum regions. We have built P-Si solar cell devices having considered different physical Si wafer parameters such as crystal orientation, resistivity, and doping levels; which crucially affect the device efficiency. Porous Si wafers, prepared after etching crystalline silicon in high HF concentrations, exhibit fluorescence in the purple wavelength region of the visible spectrum under UV illumination. We are now in the process of improving the efficiency of the device by modulating the structure of the P-Si wafer, and studying its photovoltaic characteristics.

¹Bogazici University Research Funding:5782 TUBITAK Grand Funding:209T099 Bogazici University Infrared Funding:6121

10:00AM A33.00011 Quantum-dot nanostructures for effective harvesting, detection, and conversion of IR radiation , NIZAMI VAGIDOV, ANDREI SERGEEV, ANDREI ANTIPOV, Electrical Engineering Department, University at Buffalo, SUNY, KIMBERLY SABLON, JOHN LITTLE, U.S. Army Research Laboratory, Adelphi, VLADIMIR MITIN, Electrical Engineering Department, University at Buffalo, SUNY — Our novel approach to improve harvesting, detection, and conversion of IR radiation is based on engineering of three-dimensional potential barriers introduced by quantum dots with built-in charge due to inter-dot doping. The barriers around dots exponentially suppress capture processes and increase the photoelectron lifetime. The built-in-dot charge also strongly enhances the coupling of QD structures to IR radiation. Both effects radically improve the responsivity of IR photodetectors and photovoltaic efficiency of quantum-dot solar cells. Here we report a 50% increase in photovoltaic efficiency in quantum-dot solar cells as well as 25 times increase of the photoresponse of quantum-dot infrared photodetectors when the built-in-dot charge increases up to six electrons per dot. We also present results of modeling of photoelectron kinetics and discuss perspectives of IR photodetectors and solar cells based on quantum dots with built-in charge.

10:12AM A33.00012 ABSTRACT HAS BEEN MOVED TO K1.00149 —

10:24AM A33.00013 Device analysis of vertically aligned single-core nanocoaxial solar cells , T. KIRKPATRICK, C. ANDRONACHE, M.J. BURNS, M.J. NAUGHTON, Boston College — Analytical expressions for device transport are derived and numerically calculated for an array of vertically aligned single-core nanocoaxial solar cells. Total current of the device is derived as a function of the geometrical configuration of the photovoltaic junction, and expressions for rectifying current behavior are subsequently solved for and analyzed. Fundamental differences and similarities in the physics of device performance are inferred based on the analytical expressions for planar, nanowire, and nanocoaxial solar cells. To emphasize the physical difference of device performance pertaining to geometrical configuration, a comparison between planar and nanocoaxial device performance is analyzed for an amorphous silicon p-i-n junction solar cell.

10:36AM A33.00014 ABSTRACT WITHDRAWN —

10:48AM A33.00015 ABSTRACT WITHDRAWN —

Monday, February 27, 2012 8:00AM - 10:48AM —

Session A34 DCP: Focus Session: Impact of Ultrafast Lasers I: X-rays and THz 107A

8:00AM A34.00001 Ultrafast X-ray Laser Studies of Chemical Dynamics , KELLY GAFFNEY, SLAC National Accelerator Laboratory and Stanford University — First light at the LCLS x-ray free electron laser at the SLAC National Accelerator Laboratory marked the beginning of hard x-ray laser science 2009. With pulse energies in excess of a milliJoule and pulse durations as short as 5 femtoseconds in duration, the LCLS provides a novel and potentially transformative approach for investigating chemical dynamics in complex systems. Understanding the coupled evolution of electrons and nuclei during chemical transformations remains the central and vexing challenge in the study of chemical reaction dynamics. Ultrafast optical electronic spectroscopy can monitor both the nuclear and the electronic evolution that occurs during a chemical reaction, but this joint sensitivity often impedes the robust interpretation of experimental measurement. The LCLS provides the opportunity to simultaneously measure electronic dynamics with x-ray fluorescence and nuclear dynamics with elastic x-ray scattering, providing a robust means for disentangling the coupled motions of electrons and nuclei during excited state internal conversion and intersystem crossing. These exciting new opportunities will be discussed in the context of recent studies of photo-induced spin crossover dynamics in iron(II) tris-bipyridine. $[\text{Fe}(\text{bpy})_3]^{2+}$.

8:36AM A34.00002 Coherently controlled orientation and alignment of molecules in the gas phase by intense THz fields , SHARLY FLEISCHER, YAN ZHOU, ROBERT W. FIELD, KEITH A. NELSON, Department of Chemistry, Massachusetts Institute of Technology — We report the use of intense terahertz (THz) pulses to orient polar molecules in the gas phase. Short THz fields exert torques that drive coherent molecular rotational motion, and multiple interactions with strong THz fields can yield multiple-quantum rotational coherences with the prospect of high degrees of orientation (dipoles pointing in the same direction in space) and alignment (molecular axes parallel to each other regardless of dipole orientation). THz-induced molecular orientation offers new possibilities in gas-phase x-ray diffraction, molecular orbital mapping through high harmonic generation and photoelectron angular distribution imaging, and other applications. We demonstrate significantly enhanced coherent control using two THz pulses with an optimized relative time delay. We show in the case of atmospheric water that a short, strong THz field induces long-lived coherent THz emission (free induction decay) that drives significant further rotational responses in a pre-excited polar gas sample. This class of experiments enables broad new capabilities for molecular spectroscopy and control beyond those afforded through molecular alignment by intense optical fields, which do not produce any net orientation.

8:48AM A34.00003 Capturing the Coupled Dynamics of Electrons, Atoms and Spins in Molecules and Materials using Ultrafast X-Rays , MARGARET MURNANE, JILA, University of Colorado at Boulder — No abstract available.

9:24AM A34.00004 Using time-resolved Ru L-edge X-ray absorption spectroscopy to capture photoinduced transient electronic structure in a solar cell dye molecule , BENJAMIN VAN KUIKEN, MICHAEL LYNCH, MUNIRA KHALIL, Department of Chemistry, University of Washington, Seattle, WA 98195, NILS HUSE, HANA CHO, MATTHEW STRADER, ROBERT SCHOENLEIN, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — Understanding the electronic structure of transition metal dye molecules used in dye-sensitized solar cells (DSSC) is critical for determining the functioning of these devices. Ru^{II} dyes such as Ru(dcbpy)₂(NCS)₂ (termed RuN3) have been components in some of the most effective DSSCs. We use synchrotron-based picosecond Ru L-edge X-ray absorption spectroscopy (XAS) to monitor changes the changes in the electronic structure of RuN3⁴⁻ that accompany the ¹A₁ to ³MLCT conversion initiated with a 400 nm light pulse. The results are interpreted by simulating the Ru L₃ X-ray absorption spectra of the ¹A₁ and ³MLCT states with time-dependent density functional theory (TD-DFT). We observe the formation of the Ru^{III} oxidation state of RuN3⁴⁻ within the 70 ps time resolution of our experiment. The TD-DFT simulation allows us to assign a spectral feature in the Ru L-edge spectrum as a probe of the electronic structure of the NCS ligands due to overlap between Ru 4d and NCS π^* orbitals. A 1.2 eV blue shift in this feature between ground and ³MLCT state corresponds to depletion in charge density on the NCS ligands in the excited state. We will discuss in detail the local electronic structure around the Ru atom in the transient ³MLCT state measured by time-resolved XAS.

9:36AM A34.00005 Ultrafast molecular processes mapped by femtosecond x-ray diffraction

, THOMAS ELSAESSER, Max-Born-Institute, 2 a Max-Born-St., Berlin, 12489 — X-ray diffraction with a femtosecond time resolution allows for mapping photoinduced structural dynamics on the length scale of a chemical bond and in the time domain of atomic and molecular motion. In a pump-probe approach, a femtosecond excitation pulse induces structural changes which are probed by diffracting a femtosecond hard x-ray pulse from the excited sample. The transient angular positions and intensities of diffraction peaks give insight into the momentary atomic or molecular positions and into the distribution of electronic charge density. The simultaneous measurement of changes on different diffraction peaks is essential for determining atom positions and charge density maps with high accuracy. Recent progress in the generation of ultrashort hard x-ray pulses (Cu K_{α} , wavelength $\lambda = 0.154$ nm) in laser-driven plasma sources has led to the implementation of the powder diffraction and the rotating crystal method with a time resolution of 100 fs. In this contribution, we report new results from powder diffraction studies of molecular materials. A first series of experiments gives evidence of a so far unknown concerted transfer of electrons and protons in ammonium sulfate $[(NH_4)_2SO_4]$, a centrosymmetric structure. Charge transfer from the sulfate groups results in the sub-100 fs generation of a confined electron channel along the c-axis of the unit cell which is stabilized by transferring protons from the adjacent ammonium groups into the channel. Time-dependent charge density maps display a periodic modulation of the channel's charge density by low-frequency lattice motions with a concerted electron and proton motion between the channel and the initial proton binding site. A second study addresses atomic rearrangements and charge dislocations in the non-centrosymmetric potassium dihydrogen phosphate $[KH_2PO_4]$, KDP. Photoexcitation generates coherent low-frequency motions along the LO and TO phonon coordinates, leaving the average atomic positions unchanged. The time-dependent maps of electron density demonstrate a concomitant oscillatory relocation of electronic charge with a spatial amplitude of the order of a chemical bond length, two orders of magnitude larger than the vibrational amplitudes. The coherent phonon motions drive the charge relocation, similar to a soft mode driven phase transition between the ferro- and paraelectric phase of KDP.

10:12AM A34.00006 Time-resolved X-ray fragmentation probing of molecular isomerization

, VLADIMIR PETROVIC, Department of Physics, Stanford University, MARCO SIANO, Blackett Laboratory, Imperial College London, UK, JAMES L. WHITE, Department of Applied Physics, Stanford University, PHILIP H. BUCKSBAUM, Departments of Physics and Applied Physics, Stanford University, AMO14110 COLLABORATION — Short intense X-ray pulses, now available at FELs, are already having a strong impact on the AMO science. In addition to scattering or resonant absorption, it is possible to use X-ray radiation to probe processes on molecular timescales through non-resonant absorption by initiating a molecular fragmentation in a time-resolved manner. Core-ionized molecules composed of light elements predominantly relax through Auger decay into multiply charged molecular ions, which subsequently fragment through Coulomb repulsion. The fragmentation patterns (ion time-of-flight spectra, ion-kinetic energy release, Auger spectra, etc.) encode information about instantaneous nuclear geometry and momenta. Unlike intense IR laser field fragmentation, X-ray fragmentation occurs in the weak-field regime. In order to test the potential of time-resolved X-ray fragmentation for probing isomerization, we selected the example of ring opening of 1,3-cyclohexadiene. In a time-resolved UV-pump - X-ray fragmentation-probe experiment performed at Linac Coherent Light Source at SLAC we observed an increase in the average ion-KER and an increase in the number of lighter fragments upon photoexcitation. We discuss how the evolving fragmentation patterns reflect the structural change that the molecule is undergoing.

10:24AM A34.00007 A Femtosecond Time-Resolved Transient X-ray Absorption Study of Light-Induced Coupling and Transparency in Xenon

, MING-FU LIN, UXSL/CSD Lawrence Berkeley Lab and UC Berkeley, ADRIAN PFEIFFER, UC Berkeley, DANIEL NEUMARK, STEPHEN LEONE, UXSL/CSD Lawrence Berkeley Lab and UC Berkeley, OLIVER GESSNER, UXSL/CSD Lawrence Berkeley Lab. — We have performed a femtosecond time-resolved transient x-ray absorption spectroscopy study to monitor the light induced coupling between bright and dark states in xenon exposed to infrared (780 nm) laser pulses with intensities up to 5×10^{13} W/cm². Significant transient variations in the inner-shell absorption spectra between ~ 63 eV and ~ 69 eV photon energy are observed. Near time zero, the transmission at 67 eV increases from 6(1) % (field-free) to 14(3) % (laser dressed). Transient absorption and transient transparency effects are interpreted within a picture of strong-field induced coupling between core-excited $4d^{-1}(^2D_{5/2})6p(^2P_{3/2})$ and $4d^{-1}(^2D_{3/2})6p(^2P_{1/2})$ states at 65.1 and 67 eV, respectively, and nearby dark states with *ns* and *nd* characters. The major features of the transient absorption spectra can be well described within a three-level (Autler-Townes) coupling scheme. Employing this model, a dipole-moment for the $4d^{-1}(^2D_{3/2})6p(^2P_{1/2})$ to $4d^{-1}(^2D_{3/2})6s(^2S_{1/2})$ transition of 0.4(0.1) Debye is derived.

10:36AM A34.00008 High Resolution THz Studies of Crystalline Channel Hydrates

, DAVID PLUSQUELLIC, SHIN CHOU, ZEESHAN AHMED, KEVIN DOUGLASS, JULIA SCHERSCHLIGT, National Institute of Standards and Technology — In this study, we use vibrationally state-resolved THz spectroscopy to examine the phonon mode structure of several peptides and carbohydrates co-crystallized with water. Studies are performed before and after the water is removed under vacuum on a range of systems for water in hydrophobic and hydrophilic environments. Predictions from first principles calculations are used to model the observed spectra and to obtain detailed energetic information on the dehydration processes. A new phase-coherent heterodyne method based on chirped THz pulses may be discussed.

Monday, February 27, 2012 8:00AM - 10:48AM —

Session A35 DCP: Focus Session: DFT I: Strongly Correlated Systems; GW and Many-Body Perturbation Theory 107B

8:00AM A35.00001 Real-Space DFT Models for Strong Correlation

, ERIN JOHNSON, University of California, Merced — Accurate treatment of strongly-correlated electrons remains an important challenge for density-functional theory. Most functionals underestimate the energy lowering arising from non-dynamical electron correlation, as in stretched covalent bonds, open-shell singlet states, and many transition-metal compounds, including semiconductors. We develop a new density-functional approach combining physical insight from chemical structure with real-space modeling of the exchange-correlation hole, based on the Becke-Roussel exchange functional. The method is capable of predicting correct dissociation limits and describing strong correlation in many-electron systems.

8:36AM A35.00002 DFT+DMFT versus DFT+U description of Mott insulators: DMFT restores spin and orbital symmetry and removes metastable states

, BERNARD AMADON, CEA, DAM, DIF, F 91297 Arpajon, France — In the last twenty years, the development of methods based on the coupling of Density Functional Theory in the Local Density Approximation and Hubbard-like terms has led to a successful description of many strongly correlated systems. These methods include DFT+U which contains a static description of interaction and the combination of DFT with Dynamical Mean Field Theory (DFT+DMFT) which adds fluctuations to the description of interactions. We present implementations of DFT+U and DFT+DMFT in the same framework, and with the same approximations. We show, in agreement with previous results in the literature, and even in the simple Hubbard I approximation to DMFT, that DFT+DMFT is able to describe Mott insulator without any breaking of spin and orbital symmetry. We show that this improvement simply removes the appearance of metastable states, and thus solve a practical and physical problem encountered in particular in the description of actinides oxides in DFT+U calculations.

8:48AM A35.00003 Renormalized second-order perturbation theory for the electron correlation energy: concepts and benchmarks, PATRICK RINKE, XINGUO REN, MATTHIAS SCHEFFLER, Fritz-Haber-Institute der MPG, Berlin, Germany, GUSTAVO SCUSERIA, Rice University, Houston, USA — We present a renormalized second-order perturbation theory (R2PT) for the electron correlation energy that combines the random-phase approximation (RPA), second-order screened exchange (SOSEX) [1], and renormalized single excitations (rSE) [2]. These three terms all involve a summation of certain types of diagrams to infinite order, and can be viewed as a “renormalization” of the direct, the exchange and the single excitation (SE) term of 2nd-order Rayleigh-Schrödinger perturbation theory based on an (approximate) Kohn-Sham reference state. A preliminary version of R2PT has been benchmarked for covalently-bonded molecular systems and chemical reaction barrier heights [3] and shows an overall well balanced performance. We have extended this, by including “off-diagonal” diagrams into the rSE term and expect this refined version of R2PT to be more generally applicable to electronic systems of different bonding characteristics. Extended benchmarks of van-der-Waals-bonded molecules and crystalline solids will be presented. [1] A. Grüneis *et al.*, J. Chem. Phys. **131**, 154115 (2009). [2] X. Ren *et al.*, Phys. Rev. Lett. **106**, 153003 (2011). [3] J. Paier *et al.*, arXiv:cond-mat/1111.0173.

9:00AM A35.00004 Efficient GW methods implemented in molecular orbital space: Ionization energy and electron affinity of conjugated molecules¹, SAN-HUANG KE, Department of Physics, Tongji University, 1239 Siping Road, Shanghai 200092, China — An efficient all-electron non-selfconsistent GW (G^0W^0) method is proposed, which is based on the full random-phase approximation and implemented in the molecular-orbital space with algorithms for reducing the error coming from the incompleteness of the basis set. The convergence of its result with regard to the size of the basis set is examined. Based on this, we further implement a quasiparticle self-consistent GW (QSGW) approach with Gaussian basis functions. The high computational efficiency allows us to deal with larger molecules from the first principles, and we applied our methods to calculate the ionization energy (IE) and electron affinity (EA) of ten conjugated molecules with up to 32 atoms. The G^0W^0 result improves the Hartree-Fock result significantly, especially for EA, and, furthermore, the QSGW improves the G^0W^0 and gives results of both IE and EA in very good agreement with the available experimental data and also with the results from the Δ SCF calculation using the B3LYP functional. This indicates that our all-electron *ab initio* GW calculation can describe very well molecular electronic structures, making the QSGW approach a good candidate for investigating electronic and transport properties of molecular systems.

¹Work supported by the Shanghai Pujiang Program under Grant No. 10PJ1410000 and by the MOST 973 Project under Grant No. 2011CB922204 as well as by the National Natural Science Foundation of China under Grant No. 11174220

9:12AM A35.00005 Exact DFT with the density matrix renormalization group¹, E. MILES SToudenMIRE, Dept. of Physics and Astronomy, University of California, Irvine — The density matrix renormalization group (DMRG) is a powerful, controlled numerical method traditionally applied to lattice models of strongly correlated electrons in 1D and 2D. By extending DMRG to simulate electronic structure models on a 1D quasi-continuum grid, we can compute exact Kohn-Sham (KS) potentials and even perform exact full KS calculations.² On their own, the continuum DMRG calculations provide significant insight into the structure of strongly correlated many-body wavefunctions both for smaller molecules and chains exceeding one hundred atoms. Combining DMRG with the machinery of density functional theory allows us to explore the reasons for the success or failure of standard DFT approximations and to better understand which many-body effects are faithfully reproduced by the KS system.

¹This work is funded by the U.S. Department of Energy (Grant No. DE-FG02-08ER46496)

²E.M. Stoudenmire, Lucas O. Wagner, Steven R. White, Kieron Burke, arXiv:1107.2394

9:48AM A35.00006 Exact density functionals for 1d systems¹, LUCAS WAGNER, E. SToudenMIRE, Department of Physics and Astronomy, University of California, Irvine, KIERON BURKE, Department of Physics and Astronomy and Department of Chemistry, University of California, Irvine, STEVEN WHITE, Department of Physics and Astronomy, University of California, Irvine — The success of modern density functional theory (DFT) can be attributed to the Kohn-Sham (KS) scheme, for which density functional approximations are both practical and rather simple. We are often left in the dark, however, when trying to understand why certain approximations fail, or how well they approximate the true functional. To study such questions, an exact implementation of KS-DFT is required. Though exact KS-DFT is as difficult as solving the original many-body problem, the density matrix renormalization group (DMRG) gives us a powerful tool to do this. DMRG is a highly efficient wavefunction solver in 1d, which we use to solve model continuum systems with a long-range soft-Coulomb interaction between particles. Using DMRG, we implement exact KS-DFT and investigate its inner workings. Results for some atom chains are discussed and compared to HF and LDA calculations. Preprint at arXiv:1107.2394.

¹With deep appreciation for DOE grant DE-FG02-08ER46496.

10:00AM A35.00007 Exact Kohn-Sham eigenstates versus quasi-particles in simple models of strongly correlated electrons, JAIME FERRER¹, DIEGO CARRASCAL², Departamento de Física, Universidad de Oviedo, Spain — We present analytic expressions for the exact density functional and Kohn-Sham Hamiltonian of simple tight-binding models of correlated electrons. These are the single- and double-site versions of the Anderson, Hubbard and spinless fermion models. The exact exchange and correlation potentials are fully non-local. The analytic expressions allow to compare the Kohn-Sham eigenstates of exact density functional theory with the many-body quasi-particle states of these correlated-electron systems. The exact Kohn-Sham spectrum describes correctly many of the non-trivial features of the many-body quasi-particle spectrum, as for example the precursors of the Kondo peak. However, we find that some pieces of the quasi-particle spectrum are missing because the many-body phase-space for electron and hole excitations is richer.

¹CINN (CSIC - Universidad de Oviedo), Spain and Department of Physics, Lancaster University, UK

²CINN (CSIC - Universidad de Oviedo), Spain

10:12AM A35.00008 Spectroscopic Fingerprinting of Small Molecules via Many-Body Perturbation Theory, PETER DOAK, Molecular Foundry, LBNL; Department of Chemistry, UC-Berkeley, PIERRE DARANCET, JEFFREY NEATON, Molecular Foundry, LBNL — Quantitative understanding of the photophysics of small organic molecules is an important challenge and relevant to a range of energy conversion applications. Existing first-principles methods, such as time-dependent density functional theory, coupled cluster, and other quantum chemistry-based approaches can sometimes provide onset energies with good accuracy, but agreement at higher energies - a more complete spectral fingerprint - is frequently less adequate. Here we use DFT and many-body perturbation theory, within the GW approximation and the Bethe-Salpeter Equation approach, to compute the UV-Vis absorption spectra for a range of small molecules, comparing closely to room-temperature, solution-phase measurements of onsets and spectra. First-principles molecular dynamics is used to prepare snapshots of finite temperature conformations. The effects of continuum and explicit solvation models are considered. The importance of dynamic disorder, delocalized unoccupied states, and solvation are thoroughly discussed in the context of experiments. Support: DOE via the Molecular Foundry and Helios SERC, and NSF via NCN. Computational support provided by NERSC.

10:24AM A35.00009 Going beyond DFT for Organic/Titanium Dioxide interfaces¹, LEONARDO

M. MARION JORGE, MARCELO ALVES-SANTOS, MARÍLIA J. CALDAS, Instituto de Física - Universidade de São Paulo — There is increasing interest in organic/oxide interfaces, particularly for light harvesting and light-emitting devices, and it is important to obtain theoretical information for basic quantities such as the energy-level alignment across the interface. Accurate descriptions of the electronic structure of the composite system, as e.g. [1], are however scarce. The method used should give reliable results for both organic and oxide materials, to guarantee a good description of the hybrid system. In this work we have explored different DFT functionals (PZ-LDA, and those that include a fraction of Exact-Exchange as PBE0, HSE and B3LYP [2]) and compared the results with those obtained by Many-Body Perturbation theory with the GW approximation[3]. We have chosen as prototype systems TiO₂, both bulk crystal and model surface, and Thiophene. We have found that none of the used DFT schemes give optimal results for both organic and inorganic systems at the same time, so moving beyond DFT is mandatory.

[1] C.D. Valentin et.al., Phys. Rev. Lett. 97, 166803 (2006)

[2] J.P. Perdew et.al., J. Chem. Phys. 105, 9982 (1996); J. Heyd et.al., J. Chem. Phys. 118, 8207 (2003); P.J. Stephens et.al., J. Phys. Chem. 98, 11623 (1994)

[3] A. Marini et.al., Comp. Phys. Comm. 180, 1392 (2009)

¹Work supported by FAPESP, INEO, and LCCA

10:36AM A35.00010 Accurate potential energy surfaces for transition-metal complexes with

DFT+U(R), HEATHER KULIK, Stanford University — We introduce an improvement to the Hubbard U augmented density functional approach known as DFT+U that incorporates variations in the value of self-consistently calculated, linear-response U with changes in geometry. This approach overcomes the one major shortcoming of previous DFT+U studies, i.e. the use of an averaged Hubbard U when comparing energies for different points along a potential energy surface is no longer required. While DFT+U is quite successful at providing accurate descriptions of localized electrons (e.g. d or f) by correcting self-interaction errors of standard exchange correlation functionals, we show several examples from diatomic molecules to porphyrins to surface science applications where this position-dependent DFT+U(R) provides a significant two- to four-fold improvement over DFT+U predictions. DFT+U(R) reduces errors in binding energies, frequencies, and equilibrium bond lengths by applying the linear-response, position-dependent U(R) at each point. We also propose a metric for whether a standard DFT+U approach is sufficient by determining the strength of the dependence of U on changes in coordinates.

Monday, February 27, 2012 8:00AM - 11:00AM – Session A36 DCP: Focus Session: New Energy I 107C

8:00AM A36.00001 Facing our Energy Challenges in a New Era of Science, ERIC ROHLFING, US

Department of Energy, Office of Science, Office of Basic Energy Sciences — As our nation and the world face daunting challenges in energy supply and the environmental consequences of energy use, how can basic science contribute to transforming the way in which we generate and use energy? How can we use the power of modern science, notably chemical physics, to accelerate the transition to a more sustainable energy future? In this talk, I shall present some of the current strategic thinking from the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences (BES). In particular, I shall present how the department is approaching the entire R&D spectrum for energy technologies and how BES engages the scientific community to identify basic research needs for advancing energy technologies.

8:36AM A36.00002 Semiconductor nanostructures for artificial photosynthesis, PEIDONG YANG, UC,

Berkeley — Nanowires, with their unique capability to bridge the nanoscopic and macroscopic worlds, have already been demonstrated as important materials for different energy conversion. One emerging and exciting direction is their application for solar to fuel conversion. The generation of fuels by the direct conversion of solar energy in a fully integrated system is an attractive goal, but no such system has been demonstrated that shows the required efficiency, is sufficiently durable, or can be manufactured at reasonable cost. One of the most critical issues in solar water splitting is the development of a suitable photoanode with high efficiency and long-term durability in an aqueous environment. Semiconductor nanowires represent an important class of nanostructure building block for direct solar-to-fuel application because of their high surface area, tunable bandgap and efficient charge transport and collection. Nanowires can be readily designed and synthesized to deterministically incorporate heterojunctions with improved light absorption, charge separation and vectorial transport. Meanwhile, it is also possible to selectively decorate different oxidation or reduction catalysts onto specific segments of the nanowires to mimic the compartmentalized reactions in natural photosynthesis. In this talk, I will highlight several recent examples in this lab using semiconductor nanowires and their heterostructures for the purpose of direct solar water splitting.

9:12AM A36.00003 Oxygen Evolution Electrocatalysis on Cobalt Oxide surfaces¹, MICHAL BAJDICH,

JCAP-North, LBL, Berkeley, CA 94720, JENS K. NORSKOV, SUNCAT, SLAC, Stanford, CA 94025, MONICA GARCÍA-MOTA, Department of Chemical Engineering, Stanford University, Stanford, CA 94305, ALEXIS T. BELL, JCAP-North, LBL, Berkeley, CA 94720 — The oxidation of water for hydrogen production using sunlight is of high importance to photo-fuel cell research. The electrochemical approach via heterogeneous catalysis to water splitting is a very promising route. The key challenge of this method lies in reduction of the losses, i.e., over-potential, for the oxygen evolution reaction (OER) on the anode. In this work, we investigate the dependence of theoretical over-potential of OER on type of anode by applying standard density functional theory (DFT). We attempt to explain recent experimental observation of enhanced activity on gold supported Cobalt Oxide surfaces [1]. We explore variety of possible CoO structures and associated surfaces which could emerge under operating conditions of catalyst. Finally, we also explore the influence of environment and admixtures of CoO with other elements.

[1] B.S. Yeo, A.T. Bell, AT, J. Am. Chem. Soc., 133, 5587-5593 (2011).

¹support from Joint Center for Artificial Photosynthesis (heterogeneous catalysis)

9:24AM A36.00004 High-throughput synthesis and screening of photon absorbers and photo-catalysts for solar fuel cells, SLOBODAN MITROVIC, MARTIN MARCIN, SEAN LIN, JIAN JIN, Joint Center for Artificial Photosynthesis,

California Institute of Technology — Joint Center for Artificial Photosynthesis is a D.O.E. Energy Innovation Hub conceived to develop solar fuel cell technologies by bringing together the critical mass of scientist and engineers nationwide. The High-Throughput Experimentation group at JCAP is developing pipelines for accelerated discovery of new materials - photon absorbers, photoelectrochemical and electrochemical catalysts - using combinatorial approaches (ink-jet, sol-gel, physical vapor deposition). Thin films of semiconducting metal-oxides, sulfides, nitrides and phosphides are synthesized and screened in high-throughput according to their optical and photoelectrochemical properties, as well as structure and phase. Vast libraries of materials and data are generated and made available to inside and outside research groups. Here we present data on binary, ternary and quaternary metal-oxide systems prepared by the ink-jet technology. The systems include tungsten-based photo-absorbers and nickel-iron-based catalysts for water splitting.

9:36AM A36.00005 Transport in and chemistry on transition metal oxides for energy conversion , EMILY CARTER, Princeton University — We use quantum mechanics techniques to search for robust, efficient, and inexpensive materials for solid oxide fuel cells (SOFCs) that convert fuels to electricity, photovoltaics (PVs) that convert sunlight to electricity, and photo-catalytic electrodes (PCEs) that convert sunlight, CO₂, and H₂O into fuels. In our SOFC research, we focus on cathode optimization, often considered the limiting factor. If oxide ion diffusion and electron transport can be enhanced, along with rapid dissociative adsorption of dioxygen, lower temperatures can be used, which would facilitate wider deployment. In the solar energy conversion arena, the cost-efficiency tradeoff for PV materials motivates new options. I will discuss why it is difficult to find effective PCE materials; in particular I will enumerate the very significant constraints beyond those on PVs that they must satisfy to achieve high efficiency. Limiting oneself to abundant elements further constrains the design space. As a result, we are focusing primarily on first row transition metal oxide materials. Key properties of conventional and novel materials, along with some new design principles, will be discussed. The work is revealing which dopants or mixed oxides are likely to provide the most efficient energy conversion materials.

10:12AM A36.00006 A comparison in activity between transition-metal oxides and transition metals , ALEKSANDRA VOJVODIC, Stanford University, FELIX STUDDT, FRANK ABILD-PEDERSEN, THOMAS BLIGAARD, SLAC National Accelerator Laboratory, JENS NØRSKOV, Stanford University — Transition-metal oxides are widely used materials in catalysis as substrates and promoters, but also as the active catalyst materials themselves. We compare the reactivity of transition-metal oxides with the one of transition metals. The comparison is exemplified for the ammonia synthesis reaction. First we show that there exist characteristic Brønsted-Evans Polanyi (BEP) relations (linear relations between transition state and dissociation energies) for dissociation of molecules on transition-metal oxides in the rutile and perovskite structure. It is well-known that the (211) metal surface is several orders of magnitude more reactive than the (111) metal surface due to the lower BEP line for the 211 facet. We find that both rutiles and perovskites follow BEP relations that are lower than the one of the 211 facet. Second we utilize the established BEP relations together with calculated adsorption energetics in a micro-kinetic model to obtain a volcano plot for the catalytic activity. We find that oxides have a higher turn over frequency as compared with metals. Hence, oxides intrinsically have a great advantage in terms of catalytic activity which opens up for catalyst design.

10:24AM A36.00007 Energy conversion and fuel production from electrochemical interfaces¹ , NENAD MARKOVIC, Argonne National Laboratory — Design and synthesis of energy efficient and stable electrochemical interfaces (materials and double layer components) with tailor properties for accelerating and directing chemical transformations is the key to developing new alternative energy systems – fuel cells, electrolyzers and batteries. In aqueous electrolytes, depending on the nature of the reacting species, the supporting electrolyte, and the metal electrodes, two types of interactions have traditionally been considered: (i) direct – covalent bond formation between adsorbates and electrodes, involving chemisorption, electron transfer, and release of the ion hydration shell; and (ii) relatively weak non-covalent metal-ion forces that may affect the concentration of ions in the vicinity of the electrode but do not involve direct metal-adsorbate bonding. The range of physical phenomena associated with these two classes of bonds is unusually broad, and are of paramount importance to understand activity of both metal-electrolyte two phase interfaces and metal-Nafion-electrolyte three phase interfaces. Furthermore, in the past, researcher working in the field of fuel cells (converting hydrogen and oxygen into water) and electrolyzers (splitting water back to H₂ and O₂)) seldom focused on understanding the electrochemical compliments of these reactions in battery systems, e.g., the lithium-air system. In this lecture, we address the importance of both covalent and non-covalent interactions in controlling catalytic activity at the two-phase and three-phase interfaces. Although the field is still in its infancy, a great deal has already been learned and trends are beginning to emerge that give new insight into the relationship between the nature of bonding interactions and catalytic activity/stability of electrochemical interfaces. In addition, to bridge the gap between the “water battery” (fuel cell ↔ electrolyzer) and the Li-air battery systems we demonstrate that this would require fundamentally new knowledge in several critical areas. We conclude that understanding the complexity (simplicity) of electrochemical interfaces would open new avenues for design and deployment of alternative energy systems.

¹Work done in collaboration with R. Subbaraman, D. Tripkovic, D. Strmcnik, N. Danilovic, G. Wiberg, Chao Wang, K-C Chang, D. van der Vliet, A. Paulikas, and V. Stamenkovic, Argonne National Laboratory, Materials Science Division.

Monday, February 27, 2012 8:00AM - 10:48AM –

Session A37 FEd SPS: Research Collaboration between Mentors and Undergraduate Students

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8:00AM A37.00001 Atomic, molecular and optical physics at Bethel¹ , CHAD HOYT, DAN KLEMME, Bethel University — An example of the close connection between research and advanced labs at Bethel University is the recent realization of cold lithium atoms in a magneto-optical trap (MOT). Several aspects of the cooling and trapping research took root in the laboratory components of the Optics and Lasers upper-level courses. These included a wavelength meter with sub-picometer accuracy and precision, stabilized laser diodes and molecular and atomic spectroscopy. Work on the MOT began in 2008 and has involved students (a total of 12, including several post-General Physics sophomores) working during summers, course projects and senior research. Lithium MOTs offer challenges (e.g. low vapor pressure) and advantages in an undergraduate lab with respect to the more common rubidium systems. Lasers for lithium are at 671 nm, a more practical red color that can still take advantage of inexpensive laser diodes and broadband optical coatings. Its relatively simple atomic structure makes lithium amenable for stringent comparisons between theory and experiment. Recent high precision absolute frequency measurements using an atomic beam disagree. Cold-atom spectroscopy of lithium could help resolve questions about the atomic structure of lithium.

¹NASA MN Space Grant Consortium, CID Inc.

8:12AM A37.00002 Lithium in a Magneto-Optical Trap , DAN KLEMME, CHAD HOYT, Bethel University — We recently cooled and trapped $\sim 10^7$ neutral ^7Li atoms in a magneto-optical trap. Our laser source is a home-built external cavity diode laser at 671 nm and a semiconductor tapered amplifier. Acousto-optic modulators are used to generate five different laser detunings that are necessary for repumping between hyperfine states in the trapping and slowing laser beams. The laser is locked by phase-sensitive detection of fluorescence produced by a frequency-modulated laser beam normally incident to the lithium atomic beam. The laser is tuned to the $2S_{1/2}(F=2) \rightarrow 2P_{3/2}(F')$ D2 transition. Two coils of wire with ~ 100 A of current flowing through them in an anti-Helmholtz orientation generate the magnetic field gradient whose magnitude increases from zero with distance from the center of the trap. We describe a few preliminary measurements on the trapped atoms such as temperature, atom number, and loading/unloading times. Eventually, the cold lithium will be used to demonstrate single-photon cooling in an optical dipole trap. Additionally, we plan to use the trap to do high-resolution, cold atom spectroscopy.

8:24AM A37.00003 Undergraduate Research in Theoretical Physics at Goucher College: Thermal Properties of Extreme Type-II Superconductors in High Magnetic Fields¹, SASHA DUKAN, JULIAN IRWIN, Department of Physics and Astronomy, Goucher College, MD 21204 — The subject matter of this faculty/student collaborative research involves the complex theoretical task of calculating the thermodynamic properties of strongly coupled extreme type-II superconductors starting from the high-field limit of the Landau level pairing scheme. In these systems, the low temperature and high magnetic field regime of the phase diagram fundamentally differs from the familiar low-field mixed phase, primarily by the appearance of gapless quasiparticle excitations in the energy spectrum. This theoretical/computational research was performed over the past three years in collaboration with Goucher College undergraduate students majoring in physics, mathematics and computer science. These students used their analytical and computational skills to develop computer programs and to calculate numerically the thermal properties of realistic superconducting materials. I will describe how this project created an intellectual environment where students developed an awareness of theoretical physics research and its impact on emerging technologies as well as its possible contribution to the solutions for the global energy challenge.

¹This work is supported by NSF grant no. DMR-0856415.

8:36AM A37.00004 Thermal properties of Extreme Type-II Superconductors in High Magnetic Fields¹, JULIAN IRWIN, SASHA DUKAN, Department of Physics and Astronomy, Goucher College, MD21204 — The subject matter of our investigation involves the complex theoretical task of calculating the specific heat of a two-gap extreme type-II superconductor. In extreme type-II superconductors, at low temperatures and high magnetic fields, Landau level quantization of electronic energies results in the appearance of gapless excitations at highly symmetrical points on the Fermi surface. The careful measurements of thermal properties like specific heat in the superconducting mixed state at low temperatures and high magnetic fields can reveal this novel gapless behavior. We present a detailed theoretical and numerical study of a realistic, disordered superconductor in high magnetic field and compare our calculated specific heat to available experimental data for the well-known two-gap superconductors NbSe₂ and LuNi₂B₂C. We also discuss the alterations to the location and number of gapless excitations caused by the inclusion of off-diagonal electronic pairing.

¹This work is supported by NSF grant no. DMR-0856415.

8:48AM A37.00005 Undergraduate Studies on Compressible Flows and Shock Waves¹, KEITH STEIN, JENNIFER SCHOMMER, BENJAMIN HEPPNER, Bethel University — The Bethel University physics department believes advanced lab projects and undergraduate research experiences are crucial in the development of our students, particularly those that pursue graduate studies in physics, engineering and other applied fields. Open-ended advanced lab projects are key components in several upper level physics courses. Student project work in a specific course is often enhanced by student experiences in other upper level physics courses or other research experiences. For example, projects in *Fluid Mechanics* (PHY420) are often enriched by experiences that students bring from projects in *Optics* (PHY330) and *Computer Methods in Physics* (PHY350). We present examples from recent undergraduate projects on compressible flows and shock waves. Special attention is given to a project involving the design, construction, and initial testing of a small supersonic blowdown tunnel. This facility was initially constructed as part of a project in *Fluid Mechanics* (fall 2010). Subsequent student research projects have included high-speed video shadowgraph imaging (summer 2011) and the development of a MATLAB GUI to allow for side-by-side comparisons between simulation and ongoing experiments with the tunnel (fall 2011).

¹Minnesota Space Grant Consortium

9:00AM A37.00006 Graphical User Interface for Supersonic Flow and Shock Waves in a Converging-Diverging Nozzle¹, JENNIFER SCHOMMER, KEITH STEIN, BENJAMIN HEPPNER, Bethel University — A graphical user interface (GUI) is developed to study the compressible flow in a converging-diverging (CD) nozzle. Related experiments are carried out with a small supersonic blowdown tunnel in the Bethel University physics department. The tunnel is constructed with two 5-gallon pressure tanks which are connected by a CD nozzle. Flow in the nozzle goes through three stages during the operation of the blowdown tunnel. The first stage is highly transient and culminates with the development of the quasi-static flow condition throughout the nozzle. In the second stage, flow is fully developed with sufficient driving pressure to sustain supersonic flow in the entire divergent section of the nozzle. In the final stage, the driving pressure is no longer sufficient and a normal shock recedes from the exit of the nozzle to the throat. The GUI is created with MATLAB and focuses on modeling the second and third stage of the flow in the nozzle. Modeling in stage two is based on a 1D isentropic flow assumption, whereas stage three is based on 1D isentropic flow along with normal shock relations. Additional functions of the GUI are being implemented to allow for side-by-side comparisons between simulation and ongoing experiments.

¹Minnesota Space Grant Consortium

9:12AM A37.00007 Characterization of Gold Nanoparticles for Radiotherapy Applications, YOSHI ARAKI, JAMES ROONEY, TABBETHA DOBBINS, Rowan University — Gold nanoparticles (AuNPs) are able to conjoin with biological molecules and efficiently absorb light for conversion into heat energy. Thus, they are being investigated for treatment of near surface carcinomas. In this research, we synthesize AuNPs using two different approaches to yield variation in particle size and monodispersity. Transmission electron microscopy was used to characterize particle size and shape while UV-Visible spectrophotometry characterized their absorption wavelength. Presently, fibroblast cells are being used to establish protocols for cell growth, exposure to nanoparticles, irradiation, and cell viability. The future direction of this work is to synthesize a variety of nanoparticles in order to determine the optimal shape, size and composition for photothermal radiotherapy treatment.

9:24AM A37.00008 Absorption and Agglomeration of Gold Nanoparticles as a means to Probe Cell Metabolic Activity for Radiotherapy Applications, ADAM STEFANKIEWICZ, FRANK HOLDER, TABBETHA DOBBINS, Rowan University — Poly(lactic-co-glycolic acid) (PLGA) surface treatment of gold nanoparticles (AuNPs) enable those particles to cross the cellular wall. Once within the cell, absorption spectral shifts, predicted by the Mie Theory equation, occur because the dielectric constant of the matrix differs from that surrounding the cell. This phenomena will lead to particle agglomeration (due to changes in surface energy of the particles) and shifts in the Mie absorption spectra. Both phenomena are being explored in fibroblast cells as a means to track cell type and cellular metabolic activity. UV-Vis spectrophotometry and scanning electron microscopy (SEM) are incorporated to analyze the resulting particle/cell mixtures. Early results will be presented.

9:36AM A37.00009 Research in growth, characterization, and applications of wide bandgap materials at a Primarily Undergraduate Institution¹, CHRISTOPHER MOORE, ROBERT LOUDER, Coastal Carolina University — Zinc oxide (ZnO) is a wide bandgap semiconductor that has attracted a great deal of attention with demonstrated applications in ultraviolet (UV) light detection, air-quality monitoring, missile warning systems, gas detection, and utilization as light-emitting diodes. Our undergraduate research group has been characterizing the growth of various ZnO film and nanowire systems, and we have fabricated and characterized ZnO-based devices, such as UV photodetectors, gas sensors, and photocatalysts. The materials and characterization systems with which we are working and our small niche within the broader field combine to address many of the challenges associated with undergraduate research. In this talk, we will discuss these challenges and how we have overcome them. We will also discuss how we have taken small amounts of money and crumbling facilities and produced a strong research group that involves 3-5 undergraduate students per semester, publishes approximately two peer-reviewed articles per year with undergraduate co-authors, and has achieved a steady stream of external funding.

¹Funding for this work provided by NSF DMR #1104600.

9:48AM A37.00010 Photocatalytic activity of ZnO thin films prepared by DC sputter deposition and thermal oxidation, ROBERT LOUDER, CHRISTOPHER MOORE, Coastal Carolina University — Zinc oxide (ZnO) is a wide-bandgap semiconductor with a broad range of applications, such as photocatalysis. The photocatalytic properties of ZnO result from the highly-oxidizing holes and reducing electrons that are induced on the ZnO surface by ultraviolet (UV) light. The efficiency of electron-hole pair formation is therefore critical for photocatalysis, and thus the optical quality of the films in the UV region is of critical importance. ZnO thin films have been fabricated using DC sputter deposition of Zn-metal films followed by thermal oxidation at different temperatures (300, 600, and 900°C). Characterization of the optical properties of the resulting ZnO thin films through photoluminescence indicates that increasing oxidation temperature leads to reduced UV excitonic emission. The photocatalytic activities of the films were also characterized by measuring the efficiency of degradation of Rhodamine B dye in solution. The photocatalytic efficiency of the film annealed at a temperature of 300°C was higher compared to those of the films annealed at temperatures of 600°C and 900°C. The increased photocatalytic efficiency is attributed to the increased optical quality of the films that results from lower oxidation temperatures.

10:00AM A37.00011 Investigating the Role of Disorder in the Two-Dimensional Superfluid Transition, D.R. LUHMAN, L.R. WADLEIGH, P.G. BUMCROT, Carleton College — The superfluid transition in two-dimensional helium films is an example of a Berezinskii-Kosterlitz-Thouless transition. Characteristic features of the superfluid transition, such as the abrupt onset of superfluidity, have been observed to be significantly altered in disordered two-dimensional systems. We are in the initial stages of experiments aimed at understanding the role of disorder in the two-dimensional superfluid transition. Disorder is introduced into the system by adsorbing helium films to CaF₂ surfaces with varying roughness. Quantitative characterization of the roughness of these films is crucial to understanding the superfluid transition in a disordered environment and is our current focus. The overall scope and goals of our experiments will be presented along with some of the challenges of doing low temperature physics in the undergraduate setting. The important role that undergraduates have played in these experiments will also be discussed.

10:12AM A37.00012 Characterization of CaF₂ surfaces using Adsorption-Desorption Isotherms and Atomic Force Microscopy, L.R. WADLEIGH, D.R. LUHMAN, P.G. BUMCROT, Carleton College — We are interested in using rough CaF₂ films to study the superfluid transition in two-dimensional helium systems. These experiments require quantitative information regarding the topography of the CaF₂ surfaces. The surface roughness of CaF₂ films is known to increase with film thickness as has been shown with previous atomic force microscopy (AFM) measurements [1]. We have fabricated a series of CaF₂ samples of different film thicknesses and thus different surface roughnesses. These surfaces were studied using AFM and adsorption-desorption isotherm measurements with liquid nitrogen at T=77 K. The isotherm measurements allow us to determine the pore size distribution of each CaF₂ film thickness. We find the emergence of hysteretic capillary condensation due to deep pores in the CaF₂ as the film thickness increases. The development of these deep pores is also seen in our AFM measurements. Our combined results provide a detailed description of CaF₂ surface roughness which can be utilized in the planned superfluid experiment. [1] D.R. Luhman and R.B. Hallock, Phys. Rev. E **70**, 051606 (2004).

10:24AM A37.00013 Surface plasmon microscopy with low-cost metallic nanostructures for biosensing I, NATHAN LINDQUIST, Bethel University, SANG-HYUN OH, University of Minnesota, LAUREN OTTO, Bethel University — The field of plasmonics aims to manipulate light over dimensions smaller than the optical wavelength by exploiting surface plasmon resonances in metallic films. Typically, surface plasmons are excited by illuminating metallic nanostructures. For meaningful research in this exciting area, the fabrication of high-quality nanostructures is critical, and in an undergraduate setting, low-cost methods are desirable. Careful optical characterization of the metallic nanostructures is also required. Here, we present the use of novel, inexpensive nanofabrication techniques and the development of a customized surface plasmon microscopy setup for interdisciplinary undergraduate experiments in biosensing, surface-enhanced Raman spectroscopy, and surface plasmon imaging. A Bethel undergraduate student performs the nanofabrication in collaboration with the University of Minnesota. The rewards of mentoring undergraduate students in cooperation with a large research university are numerous, exposing them to a wide variety of opportunities. This research also interacts with upper-level, open-ended laboratory projects, summer research, a semester-long senior research experience, and will enable a large range of experiments into the future.

10:36AM A37.00014 Surface plasmon microscopy with low-cost metallic nanostructures for biosensing II, LAUREN OTTO, Bethel University, SANG-HYUN OH, University of Minnesota, NATHAN LINDQUIST, Bethel University — Due to diffraction, traditional far-field optical microscopy cannot achieve the resolution necessary for applications in nano-scale imaging, sensing, and spectroscopy. However, the manipulation of surface plasmon waves in metallic nanostructures offers a solution. Surface plasmons are evanescent electromagnetic waves sustained by the oscillations of free electrons at the surface of a metal film. As plasmons propagate on the surface, they will probe the surface with high sensitivity and large field intensities. Furthermore, since plasmons are sensitive to within only 10-100 nm from the metallic surface and exhibit large electric field intensities, they have been explored for applications in biosensing and surface-enhanced Raman spectroscopy. We present the development of a microscopy setup for surface plasmon biosensing and the use of reliable, repeatable, low-cost nanofabrication techniques based on template stripping. High-quality nano-patterns are fabricated and used for proof-of-concept biosensing and surface-enhanced Raman spectroscopy experiments. In our customized microscopy setup, holographic illumination with arbitrary laser patterns is made possible by a spatial light modulator. This aids in the careful optical characterization of our nanofabricated samples.

Monday, February 27, 2012 8:00AM - 11:00AM —
Session A39 DCOMP: Electronic Structure: Theory and Numerical Methods 109B

8:00AM A39.00001 Ab initio calculation of atomic level stress in intermetallic compounds and glasses¹, MADHUSUDAN OJHA, University of Tennessee, DON M. NICHOLSON, Oak Ridge National Lab, TAKESHI EGAMI, University of Tennessee — The atomic level stress is largely unexplored as a characterization tool that is sensitive to the local atomic environment. Local quantities, such as magnetic moment and volume, are directly related to the local pressure. For example the local Voronoi volume and pressure have the expected inverse relationship and magnetic moments are reduced due to reduced volume associated with pressure. For a simple system with one atom per unit cell at equilibrium the local stresses are zero. An atom in a multicomponent system can find itself under pressure that results from its cage of surrounding atoms. The atomic level stress is calculated with the Locally Self-consistent Multiple scattering (LSMS) method for Al-Au and Cu-Zr compounds and glasses, and trends are compared to the results for simple B2 compounds with atoms of different sizes.

¹The work at the University of Tennessee and Oak Ridge National Laboratory was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Science and Engineering Division.

8:12AM A39.00002 Towards ab initio simulation of solid state materials at 10 nm scale¹, YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, G. MALCOLM STOCKS, DON M. NICHOLSON, ODBADRAKH KHORGOLKHUU, AURELIAN RUSANU, Oak Ridge National Laboratory — For the simulation of nanostructured materials and materials with structural defects, it is necessary to consider large size unit cells consisting of thousands or more atoms. It is especially true for our investigation of radiation damage effects on the structural materials. We found that for a reasonably high energy radiation, large unit cell samples at least at 10 nm scale are needed in order for allowing the thermal energy introduced into the sample by the radiation to have sufficient space to dissipate. In this presentation, we point out that, for ab initio electronic structure calculation of a system with a unit cell at such a large scale, it is essential to pay careful attention to numerical stability. We show some numerical pitfalls that will arise as a result of large number of atoms getting involved. The round-off errors accumulated in the calculation of long-range Coulomb interactions, in particular, can lead to divergence of self-consistent iterations. We discuss our approach for circumventing these numerical difficulties.

¹This research is based upon work supported as part of the Center for Defect Physics in Structural Materials (CDP), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

8:24AM A39.00003 Distributed Network-Based Verification and Validation of Electronic Structure Computations using ETEST¹, GARY YUAN, Graduate Group in Applied Science, University of California Davis, Davis CA 95616, FRANCOIS GYGI, Department of Computer Science, University of California Davis, Davis CA 95616 — ETEST is a web-based framework for verification and validation of electronic structure computations [1,2]. It enables automatic comparison and post-processing of simulation data obtained using Abinit, Quantum-Espresso, Siesta, Exciting, Qbox and VASP. We present new features of ETEST that extend its operation to a distributed network of servers. This capability enables sharing, verification, validation, comparison, and post-processing of simulations across a decentralized network of ETEST servers hosted by different institutions. Examples of cross-server operations including multiple servers will be demonstrated.

[1] G. Yuan and F. Gygi, Computational Science & Discovery 3, 015004 (2010) doi:10.1088/1749-4699/3/1/015004G

[2] <http://etest.ucdavis.edu>

¹Supported by NSF OCI 60000572 and DOE SciDAC DE-FC02-06ER25794

8:36AM A39.00004 Calculation of quasi particle energies using a spectral decomposition of the static dielectric matrix: application to molecules and nanoparticles¹, T. ANH PHAM, University of California, Davis, HUY-VIET NGUYEN, University of California, Davis and Center for Computational Physics, Institute of Physics, Vietnam, DARIO ROCCA, GIULIA GALLI, University of California, Davis — We present a novel approach to evaluate quasi particle energies within many body perturbation theory, that substantially improves both the computational efficiency and the numerical accuracy of existing techniques.² We use a spectral decomposition of the static dielectric matrix as a basis for the frequency dependent density-density response function, and density functional perturbation theory to avoid the explicit calculation of empty electronic states. A Lanczos-chain algorithm is employed that allows for the evaluation of spectra over a wide frequency range. The numerical accuracy of computed quasi particle energies is controlled by a single parameter. The efficiency and accuracy of our approach are demonstrated by computing vertical ionization potentials and electron affinities of several molecules and diamondoids. Our results are in good agreement with experiment and those reported in the literature using Quantum Monte Carlo calculations.

¹This work was supported by DOE SciDAC-e DE-FC02-06ER25777 grant and computer time was provided by NERSC. HVN was partially supported by Vietnam's National Foundation for Science and Technology Development under grant No. 103.02-2010.33

²Huy-Viet Nguyen, T. Anh Pham, D. Rocca and G. Galli (preprint).

8:48AM A39.00005 First-principles calculations of quasiparticle energies of open-shell condensed matter systems¹, JOHANNES LISCHNER, UC Berkeley and Lab Berkeley National Lab, JACK DESLIPPE, UC Berkeley, MANISH JAIN, STEVEN G. LOUIE, UC Berkeley and Lab Berkeley National Lab — We present a Green's function approach to quasiparticle excitations of open-shell systems within the GW approximation. It is shown that accurate calculations of the characteristic multiplet structure require a precise knowledge of the self energy and, in particular, its poles. We achieve this by constructing the self energy from appropriately chosen mean-field theories on a fine frequency grid. We present results for the nitrogen dioxide molecule and the negatively charged nitrogen-vacancy defect in diamond, which are in good agreement with experiment and other high-level theories.

¹This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility

9:00AM A39.00006 On the accuracy of the G^0W^0 method: From Si to ZnO ¹, PEIHONG ZHANG, ZHIJUN YI, BI-CHING SHIH, Department of Physics, University at Buffalo, State University of New York, Buffalo, New York 14260, JACK DESLIPPE, STEVEN G. LOUIE, Department of Physics, University of California, Berkeley and Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — The *ab initio* GW method has been recognized as one of the most powerful theories in predicting quasiparticle excitations in solids. Due to computational limitations, earlier GW calculations usually made use of certain generalized plasmon-pole approximations to carry out frequency integration of the electron self-energy. In addition, often the convergence of the calculated results with respect to various cutoff parameters (such as the number of conduction bands and the size of the dielectric matrix) was not investigated in details. With advances in computational methodology and technology, fully converged GW calculations with explicit frequency integration become possible. In this talk, we will discuss fully converged G^0W^0 results for a range of materials, ranging from the most “theory friendly” system Si to the widely discussed and controversial system ZnO . We will compare explicit frequency integration vs various generalized plasmon-pole models. We will also discuss effects of various cutoff parameters used in GW calculations.

¹We acknowledge the computational support provided by the Center for Computational Research at the University at Buffalo, SUNY. This work is supported by DOE under Grant No. DE-SC0002623 and by NSF under Grant No. DMR-0946404.

9:12AM A39.00007 A Comparison of Different Treatments of Spin-Orbit Coupling within the GW Approach¹, BRAD BARKER, University of California-Berkeley, Lawrence Berkeley National Laboratory, JACK DESLIPPE, Lawrence Berkeley National Laboratory, OLEG V. YAZYEV, Ecole Polytechnique Federale de Lausanne (EPFL), Switzerland, STEVEN G. LOUIE, University of California-Berkeley, Lawrence Berkeley National Laboratory — Spin-orbit coupling is responsible for the unique electronic properties of many fascinating materials such as topological insulators. We have developed and implemented an approach in which the effects of spin-orbit interactions to the quasiparticle band structure are incorporated within the GW approach, employing spinor wavefunctions computed at the DFT level with fully relativistic pseudopotentials. We compare these results to separate calculations where spin-orbit coupling is applied as a perturbation either before or after the GW calculation of the band structure. We apply these methods to the properties of materials with heavy ion cores to determine possible differences from the different schemes.

¹This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory’s NERSC facility

9:24AM A39.00008 Dielectric screening : Effects of Core Polarization on Phonons and Quasiparticle Bands¹, AMANDEEP KAUR, ERIK YLVISAKER, University of California, Davis, DEYU LU, Brookhaven National Lab, Upton, NY, GIULIA GALLI, WARREN PICKETT, University of California, Davis — We investigate the influence of core polarization on the dielectric screening of atoms, molecules and solids with focus on non metallic systems. We compare results for dielectric band structures and for the eigenvalues of the dielectric matrix obtained by varying the number of valence electrons included in our calculations. We show that (semi)-core electronic states may substantially influence the dielectric screening, even if they lie very deep in energy compared to the outermost valence electrons. We then discuss how the changes in dielectric screening observed when including (semi)-core electrons affect computed quasi particle energies at the GW level, and phonon frequencies, e.g. the LO-TO splitting. We focus on closed shell atoms, including Be, Mg, Ca, Ar, Zn, simple diatomic molecules and simple ionic solids, e.g. LiH and NaH.

¹ DE-FC02-06ER25777

9:36AM A39.00009 Novel approach to electron partitioning and definitive oxidation state assignment in solids, LAI JIANG, SERGEY LEVCHENKO¹, ANDREW RAPPE, University of Pennsylvania — Oxidation state of an atom is usually defined by partitioning electrons to the nucleus based on charge density distribution, which inherits uncertainty from the probabilistic nature of wavefunctions. Here we propose a first principle approach to electron partitioning in insulating solids based on wavefunction topology. By calculating polarization change upon shifting an atomic sublattice to its periodic image, the charge transferred during nuclei displacement can be derived. To rationalize, in Wannier representation the Berry’s phase polarization is directly related to the position of Wannier Center (WC) of each band, therefore a quantized charge flow is determined by the number of WCs that move together with (*i. e.* belong to) the nucleus. We provide both rigorous mathematical definition of oxidation states in this scheme and results from calculations of various sample systems that corroborate with oxidation states assigned by conventional chemical insight.

¹ Author has since moved to Fritz-Haber-Institut der Max-Planck-Gesellschaft, but all presented work is done at the University of Pennsylvania

9:48AM A39.00010 On the Formation of XLi_3N_2 Compounds ($X = Sc-Zn$), JAN HERBST, LOUIS HECTOR, JR., GM R&D Center — Ternary lithium nitrides XLi_3N_2 are known to form for the 3d transition elements $X = Sc, Fe$. We explore the formation of such compounds for other 3d elements by means of density functional theory using the crystal structures of $ScLi_3N_2$ and $FeLi_3N_2$ as templates. Enthalpies of formation including electronic and phonon contributions are calculated for the most stable structures. Thermodynamic stability with respect to known binary and ternary compounds is investigated in order to assess prospects for phase formation. In the case of $FeLi_3N_2$ we find an antiferromagnetic state lower in energy than the ferromagnetic state previously identified.

10:00AM A39.00011 Surface Studies with Combined Free Energy Functionals of Electronic and Liquid Densities¹, KENDRA LETCHWORTH WEAVER, RAVISHANKAR SUNDARARAMAN, TOMÁS ARIAS, Department of Physics, Cornell University — The microscopic structure of both a solid surface and a contacting liquid can be dramatically affected by the interaction between the two systems, particularly at the interface between a polar surface and a polar liquid. We present a study of oxide and metallic surfaces in an aqueous electrolyte environment with Joint Density Functional Theory (JDFT), a computationally efficient alternative to molecular dynamics simulations which replaces thermal sampling with a single variational principle for the free energy of the full system. Within the rigorous framework of JDFT, we introduce classical density-functionals for ionic species and describe how to couple them with existing functionals for liquid water and traditional electronic density-functionals. Calculations employ a liquid water functional, which captures bulk properties and microscopic structure over the entire phase diagram of the liquid, and a density-only coupling functional between the electronic and liquid systems, which can reproduce solvation free energies of small molecules to within chemical accuracy. With this microscopically accurate description of the liquid-solid interface structure, we gain physical insight which could direct future studies of catalysis and electrode stability in electrochemical systems.

¹This material is based upon work supported by the Energy Materials Center at Cornell (EMC2), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001086

10:12AM A39.00012 Origin of magnetic interactions and their influence on the structural properties of Ni₂MnGa and related compounds, BURAK HIMMETOGLU, MATTEO COCCIONI, University of Minnesota — In this work, we perform first principles DFT calculations to investigate the interplay between magnetic and structural properties in Ni₂MnGa. We demonstrate that the relative stability of austenite (cubic) and non-modulated martensite (tetragonal) phases depend critically on magnetic interactions between Mn atoms. While standard approximate DFT functionals stabilize the latter phase, a more accurate treatment of electronic localization and magnetism obtained with DFT+U suppresses the non-modulated tetragonal structure for the stoichiometric compound, in better agreement with the experiments. This observation can be explained using the Anderson impurity model, where Mn atoms are treated as periodic magnetic impurities embedded in Ga *p* and Ni *d* conduction electrons that mediate RKKY type magnetic interactions between Mn *d* electrons. Using this picture we show that the structural properties of the material are determined by the competition between super-exchange interactions mediated through Ni *d* and Ga *p* states. Finally, we show that off-stoichiometric compositions with excess Mn promote transition to a non-modulated tetragonal structure, in agreement with experiments.

10:24AM A39.00013 Redshift of excitons in carbon nanotubes caused by the environment polarizability: A BSE study, MICHAEL ROHLFING, University of Osnabrueck, Germany — Optical excitations of molecular systems can be modified by their physical environment. We analyze the underlying mechanisms within many-body perturbation theory (GW approximation and Bethe-Salpeter equation, BSE), which is particularly suited to study non-local polarizability effects on the electronic structure. Here we focus on the example of a semiconducting carbon nanotube, which observes redshifts of its excitons when the tube is touched by another nanotube or other physisorbates. We show that the redshifts mostly result from the polarizability of the attached ad-system. Electronic coupling may enhance the redshifts, but depends very sensitively on the structural details of the contact.

10:36AM A39.00014 Vibrational properties of correlated systems from ab-initio calculations, MATTEO COCCIONI, BURAK HIMMETOGLU, Department of Chemical Engineering and Materials Science, University of Minnesota, ANDREA FLORIS, Department of Physics, King's College London — In this talk I will present a recent extension of Density Functional Perturbation Theory to the DFT+U energy functional that allows to compute the vibrational properties of materials from their correlated ground state. The new computational tool, named DFPT+U, is used to investigate the phonon spectrum of MnO and NiO. The more accurate account of electronic correlation through the Hubbard-corrected functional results in a significant improvement in the agreement between the computed phonon frequencies and available experiments. In particular, we obtain a significant reduction in the splitting between the center-zone optical modes (due to the antiferromagnetic order) that confirms the importance of electronic localization in the description of magnetic couplings between metal ions. The order of the split optical modes is also shown to correlate with the occupation of the *d* states of the transition metal atoms opening for the possibility to use measurements of the vibrational frequencies to investigate certain aspects of the electronic structure of these compounds. In the last part of the talk I will also present the application of DFPT+U to Cu compounds and will discuss the possibility to use it to compute the electron-phonon coupling of high *T_c* superconductors.

10:48AM A39.00015 Effect of strong correlations on the electronic and transport properties of porphyrin wires¹, VICTOR MANUEL GARCIA SUAREZ, Departamento de Fisica, Universidad de Oviedo AND CINN (CSIC) AND Physics Department, Lancaster University, RUBEN FERRADAS, Departamento de Fisica, Universidad de Oviedo AND CINN (CSIC), JAIME FERRER, Departamento de Fisica, Universidad de Oviedo AND CINN (CSIC) AND Physics Department, Lancaster University, THEORY GROUP, CONDENSED MATTER TEAM — Recent transport experiments performed on porphyrin molecules show that wires based on these molecules could be used to design future nanoscale elements with low attenuation as a function of distance and able to work at room temperature. Apart from their rather good transport properties, which come from the conjugation of their molecular backbone, porphyrins are also very interesting due to the fact that they have a metallic element in the middle that affects their electronic properties and could also introduce magnetic effects. In this talk I will show first-principles simulations based on density functional on the electronic and transport properties of porphyrin wires between gold leads, paying special attention to the effect of using different metallic elements in the central part of the molecule (Fe, Co, Ni, Zn and Cu). Strong correlations are introduced in the form of LDA+U. The results show that the metallic element plays a crucial role in the electronic structure of the molecule around the HOMO and LUMO orbitals and introduces magnetic effects that affect the transport properties.

¹Ramon y Cajal contract RYC-2010-06053 and research project FIS2009-07081, Ministerio de Ciencia e Innovacion

Monday, February 27, 2012 8:00AM - 11:00AM —
Session A40 DBIO DPOLY: Focus Session: Protein Association I: Phase Separation, Crystallization, Self-Assembly 156A

8:00AM A40.00001 TBD, ROBERT HAYRE, UC-Davis — No abstract available.

8:36AM A40.00002 Phase Separation in Solutions of Monoclonal Antibodies¹, GEORGE BENEDEK², YING WANG, ALEKSEY LOMAKIN, Massachusetts Institute of Technology, RAMIL LATYPOV, Amgen, Inc — We report the observation of liquid-liquid phase separation (LLPS) in a solution of humanized monoclonal antibodies, IgG2, and the effects of human serum albumin, a major blood protein, on this phase separation. We find a significant reduction of phase separation temperature in the presence of albumin, and a preferential partitioning of the albumin into the antibody-rich phase. We provide a general thermodynamic analysis of the antibody-albumin mixture phase diagram and relate its features to the magnitude of the effective inter-protein interactions. Our analysis suggests that additives (HSA in this report), which have moderate attraction with antibody molecules, may be used to forestall undesirable protein condensation in antibody solutions. Our findings are relevant to understanding the stability of pharmaceutical solutions of antibodies and the mechanisms of cryoglobulinemia.

¹Work supported by Amgen Inc.

²Alfred H. Caspar Professor of Physics and Biological Physics

8:48AM A40.00003 Concentrated dispersions of equilibrium protein nanoclusters that reversibly dissociate into active monomers¹ , THOMAS M. TRUSKETT, KEITH JOHNSTON, JENNIFER MAYNARD, AMEYA BORWANKAR, MARIA MILLER, BRIAN WILSON, AILEEN DININ, TARIK KHAN, KEVIN KACZOROWSKI, The University of Texas at Austin — Stabilizing concentrated protein solutions is of wide interest in drug delivery. However, a major challenge is how to reliably formulate concentrated, low viscosity (i.e., syringeable) solutions of biologically active proteins. Unfortunately, proteins typically undergo irreversible aggregation at intermediate concentrations of 100-200 mg/ml. In this talk, I describe how they can effectively avoid these intermediate concentrations by reversibly assembling into nanoclusters. Nanocluster assembly is achieved by balancing short-ranged, cosolute-induced attractions with weak, longer-ranger electrostatic repulsions near the isoelectric point. Theory predicts that native proteins are stabilized by a self-crowding mechanism within the concentrated environment of the nanoclusters, while weak cluster-cluster interactions can result in colloidal-stable dispersions with moderate viscosities. I present experimental results where this strategy is used to create concentrated antibody dispersions (up to 260 mg/ml) comprising nanoclusters of proteins [monoclonal antibody 1B7, polyclonal sheep Immunoglobulin G and bovine serum albumin], which upon dilution in vitro or administration in vivo, are conformationally stable and retain activity.

¹We acknowledge support from the Packard Foundation (TT, JM), Welch Foundation (F-1319, KJ; F-1696, TT), National Science Foundation (NSFSTC-CHE-9876674, KJ; CBET-0968038, KJ; CBET-1065357, TT), and Gates Foundation (JM).

9:00AM A40.00004 Aggregation behavior of bovine and porcine insulin in presence of inhibitors , KIERSTEN BATZLI, BRIAN LOVE, University of Michigan — Insulin aggregation can be problematic when the insulin is in pharmaceutical solution, as well as when aggregates form in insulin pumps or subcutaneously at port sites. Pharmaceutical insulins often include an added stabilizer, such as metacresol, but even with this added compound the protein may degrade, aggregate and become less effective. With greater understanding of the kinetics of aggregation associated with insulin aggregation, a more effective stabilizer may be identified to inhibit aggregation. Bovine and porcine insulin in pharmaceutically relevant concentrations of 5 mg/ml were induced to denature and aggregate at elevated temperature and low pH and the aggregation behavior was characterized as a function of time and temperature by rheology and small angle x-ray scattering (SAXS). Aggregation behavior was probed in both neat solution and with the addition of known inhibiting compounds. The efficacy of the inhibiting compounds at retarding the protein aggregation was found to be related to the hydrophobicity of the compounds and potential inhibitors of interest were identified.

9:12AM A40.00005 Design rules for the self-assembly of a protein crystal , THOMAS HAXTON, STEPHEN WHITELAM, Lawrence Berkeley National Laboratory — The need to crystallize proteins for X-ray studies has motivated theories of protein crystallization. These theories, based largely on the behavior of isotropic spheres that form close-packed crystals, predict that assembly is enhanced near the metastable critical point associated with phase separating into a vapor of proteins (protein-poor solution) and a liquid of proteins (protein-rich solution). However, most protein crystals are open structures stabilized by anisotropic interactions, and many assemble best above the critical point. Using theory and simulation, we show that optimal assembly of one such crystal, a model surface-layer protein crystal, is not predicted by the critical point but can be predicted by a combination of two design rules: the thermodynamic driving force must be on the order of the thermal energy, and interactions must be made as nonspecific as possible without promoting liquid-vapor phase separation. In experimental terms, our results suggest adjusting solution conditions in order to impose a defined supersaturation at the liquid-vapor critical point. Our findings suggest that self-assembly of open crystals is more akin to viral capsid self-assembly than to the crystallization of spherical colloids.

9:24AM A40.00006 Protein Crystal Nucleation and Growth , SATHISH AKELLA, SETH FRADEN, Brandeis University, BRANDEIS UNIVERSITY TEAM — We have developed a microfluidic emulsion based technique to determine the homogeneous and heterogeneous nucleation rates of protein crystallization under conditions of high supersaturation. We utilize the fact that the nucleation rate is constant if no crystal nucleus is formed and count the number of protein droplets with no crystals with time, which decays exponentially with decay constant inversely proportional to nucleation rate and drop volume. We report results of experiments on nucleation and growth rates of lysozyme crystallization. The emulsions are placed on a temperature gradient stage allowing simultaneous measurement of rates as a function of temperature. We routinely scan 30,000 drops in each experiment.

9:36AM A40.00007 ABSTRACT WITHDRAWN —

9:48AM A40.00008 Water dynamics during the association of hiv capsid proteins studied by all-atom simulations¹ , NAIYIN YU, MICHAEL HAGAN, Brandeis University — The C-terminal domain of the HIV-1 capsid protein (CA-C) plays an important role in the assembly of the mature capsid. We have used molecular dynamics simulations combined with enhanced sampling methods to study the association of two CA-C proteins in atomistic detail. In this talk we will discuss the dynamics of water during the association process. In particular, we will show that that water in the interfacial region does not undergo a liquid-vapor transition (de-wetting) during association of wild type CA-C. However, mutation of some hydrophilic residues does lead to a dewetting transition. We discuss the relationship between the arrangement of hydrophilic and hydrophobic residues and dewetting during protein association. For the HIV capsid protein, the arrangement of hydrophilic residues contributes to maintaining weak interactions, which are crucial for successful assembly.

¹This work was supported by Award Number R01AI080791 from the National Institute Of Allergy And Infectious Diseases.

10:00AM A40.00009 Interfacial Microrheology of Lysozyme Layers During Formation at the Air-Water Interface , DANIEL ALLAN, DANIEL REICH, ROBERT LEHENY, Johns Hopkins University — Proteins can adsorb to the air-water interface to form viscoelastic layers. Characterizing the rheology of such layers is challenging, due to the confined geometry, the fragility of the layers, and the possibility of mesoscale spatial heterogeneity. Passive microrheology — using the thermal motion of colloidal probes to interrogate the mechanical response of the surrounding medium — is a suitable technique for addressing these difficulties. In particular, this approach sheds light on the properties of incipient protein layers that are characterized by modest interfacial viscosities. We describe microrheology studies of lysozyme layers at the air-water interface, in which we determine the evolving interfacial shear response through the viscoelastic transition that signifies layer formation. Spatial heterogeneity in the interfacial rheology is identified and discussed within the framework of layer formation as a gel transition. Layers formed by adsorption of protein from the aqueous subphase and by spreading protein directly onto the interface are compared and studied across a range of concentrations, demonstrating the sensitivity of layer properties to the rate and manner of protein accretion.

10:12AM A40.00010 Measurements of Diffusion within Concentrated Bovine α -Crystallin Suspensions¹, NUWAN KARUNARATNE, JUSTIN BERRY², LARENCE LURIO, Northern Illinois University, GEORGE THURSTON, Rochester Institute of Technology, JANAE DEBARTOLO, SURESH NARAYANAN, ALEC SANDY, JOHN WEIZEORICK, Advanced Photon Source, Argonne National Laboratory — α -Crystallin is a major protein component of the vertebrate eye lens. The chaperone-like behavior of these water soluble proteins play a key role in maintaining lens transparency by preventing condensation of other lens proteins. We report photon correlation spectroscopy measurements, both X-ray Photon Correlation Spectroscopy (XPCS) and Dynamic Light Scattering (DLS), indicating protein diffusion within suspensions of α -Crystallin. Measurements were carried out at 2°C, 10°C and 35°C, over a wide range of concentrations from the diluted limit to the regime close to the physiological lens concentration. In the diluted regime, DLS measurements can be modeled by a single exponential fit indicating a single relaxation mode and at higher concentrations two relaxation modes can be identified by fitting the data to a double exponential decay function, a clear indication of the polydispersed nature of the concentrated samples. XPCS measurements show dynamics at the highest concentration but cannot resolve the faster dynamics (below 20ms) at lower concentration. We also provide estimates for the viscosity of α -Crystallin suspensions as a function of temperature and protein volume fraction using the falling ball method.

¹NSF Grant No: DMR 0706369

²Presently at: Boston University School of Medicine, Boston, MA.

10:24AM A40.00011 Master Equation Approach to Protein Assembly – Degradation of Protein Aggregates, GEORG MEISL, University of Cambridge — Protein aggregation is dependent on several microscopic processes such as nucleation, elongation and fragmentation of aggregates. Applying simple chemical kinetics to these processes allows one to derive master equations describing the entire system. In almost all cases they take the form of highly non-linear coupled differential equations for which no exact analytical solutions can be derived. Nonetheless an analytical description of the problem is absolutely essential to determine the relative importance of different microscopic processes and develop a rational approach to finding cures. Using a self consistent approach, my group has recently made headway in finding approximate analytical solutions for several systems and successfully applied them to explain a wide range of experimental observations (Knowles et al., Science 326, 1533 (2009)). I have generalised this description to include degradation of aggregates by various cellular processes. These degradation processes are thought to play an important role in vivo in determining when aggregation speed becomes critical and leads to disease.

10:36AM A40.00012 Intermediate-range order in protein suspensions, YUN LIU, University of Delaware/NIST, LIONEL PORCAR, PETER FALUS, Institut Laue-Langevin, WEI-REN CHEN, Oak Ridge National Laboratory, EMILIANO FRATINI, University of Florence, KUNLUN HONG, Oak Ridge National Laboratory, PIERO BAGLIONI, University of Florence — Intermediate-range order (IRO) has been widely observed in vitreous silica, water ice, metallic glass, and even in ionic liquids. Our recent work demonstrates that there is IRO present in a colloidal suspension, such as protein solution, when both a short-range attraction and long-range repulsion are present. We have verified this experimentally using lysozyme solutions, where a peak (IRO peak) seen in small angle neutron scattering (SANS) has been mistakenly called a cluster peak as it has once been considered an indication of a cluster rich phase in solution. By combining both SANS and neutron spin echo (NSE) techniques, we clearly show that there is no direct relation between cluster formation and the presence of an IRO peak. By investigating the short time dynamics using NSE, we show that the formation of clusters is still indeed possible at high concentrations.

10:48AM A40.00013 An energy landscape approach to protein aggregation, ALEXANDER BUELL, TUOMAS KNOWLES, University of Cambridge, Department of Chemistry — Protein aggregation into ordered fibrillar structures is the hallmark of a class of diseases, the most prominent examples of which are Alzheimer's and Parkinson's disease. Recent results (e.g. Baldwin et al. J. Am. Chem. Soc. 2011) suggest that the aggregated state of a protein is in many cases thermodynamically more stable than the soluble state. Therefore the solubility of proteins in a cellular context appears to be to a large extent under kinetic control. Here, we first present a conceptual framework for the description of protein aggregation (see AK Buell et al., Phys. Rev. Lett. 2010) that is an extension to the generally accepted energy landscape model for protein folding. Then we apply this model to analyse and interpret a large set of experimental data on the kinetics of protein aggregation, acquired mainly with a novel biosensing approach (see TPJK Knowles et al, Proc. Nat. Acad. Sc. 2007). We show how for example the effect of sequence modifications on the kinetics and thermodynamics of human lysozyme aggregation can be understood and quantified (see AK Buell et al., J. Am. Chem. Soc. 2011). These results have important implications for therapeutic strategies against protein aggregation disorders, in this case lysozyme systemic amyloidosis.

Monday, February 27, 2012 8:00AM - 11:00AM –
Session A41 DBIO DPOLY DMP: Focus Session: Structure and Dynamics of Membranes 156B

8:00AM A41.00001 A Neutron View of Proteins in Lipid Bilayers¹, STEPHEN WHITE, University of California at Irvine, Dept. of Physiology and Biophysics — Despite the growing number of atomic-resolution membrane protein structures, direct structural information about proteins in their native membrane environment is scarce. This problem is particularly relevant in the case of the highly-charged S1-S4 voltage-sensing domains responsible for nerve impulses, where interactions with the lipid bilayer are critical for the function of voltage-activated potassium channels. We have used neutron diffraction, solid-state nuclear magnetic resonance spectroscopy, and molecular dynamics simulations to investigate the structure and hydration of bilayer membranes containing S1-S4 voltage-sensing domains. Our results show that voltage sensors adopt transmembrane orientations, cause a modest reshaping of the surrounding lipid bilayer, and that water molecules intimately interact with the protein within the membrane. These structural findings reveal that voltage sensors have evolved to interact with the lipid membrane while keeping the energetic and structural perturbations to a minimum, and that water penetrates into the membrane to hydrate charged residues and shape the transmembrane electric field.

¹Research supported in part by PO1 GM86685 from NIGMS and NINDS.

8:36AM A41.00002 Curvature Forces in Membrane Lipid-Protein Interactions¹, MICHAEL F. BROWN, Departments of Chemistry and Biochemistry and Physics, University of Arizona, Tucson AZ 85721 — Membrane protein conformational changes, folding, and stability may all involve elastic deformation of the bilayer. Non-specific properties of the bilayer play a significant role in modulating protein conformational energetics. A flexible-surface model (FSM) describes the balance of curvature and hydrophobic forces in lipid-protein interactions. The FSM describes elastic coupling of membrane lipids to integral membrane proteins. Curvature and hydrophobic matching to the lipid bilayer entails a stress field that explains membrane protein stability. Rhodopsin provides an important example, where solid-state NMR and FTIR spectroscopy characterize the energy landscape of the dynamically activated receptor. Time-resolved UV-visible and FTIR spectroscopic studies show how membrane lipids affect the metarhodopsin equilibrium due to non-specific material properties. Influences of bilayer thickness, nonlamellar-forming lipids, detergents, and osmotic stress on rhodopsin function are all explained by the new biomembrane model. By contrast, the older fluid-mosaic model fails to account for such effects on membrane protein activity. According to the FSM proteins are regulated by membrane lipids whose spontaneous curvature most closely matches the activated state within the lipid membrane.

¹Work supported by NIH Grants EY012049 and EY018891.

8:48AM A41.00003 Thickness fluctuations in pure lipid bilayers, MICHIOHRO NAGAO, NIST and Indiana University, ANDREA WOODKA, PAUL BUTLER, NIST, LIONEL PORCAR, BELA FARAGO, ILL — Recently neutron spin echo (NSE) revealed dynamical processes in a surfactant membrane system around the length scale of the membrane thickness where the classical Helfrich treatment breaks down. This excess dynamics (on top of the bending fluctuations) observed in a nonionic surfactant, water and oil system, was attributed to thickness fluctuations of the membrane. In the case of bilayers formed with the nonionic surfactant in water the thickness fluctuation amplitude was estimated to be a few angstroms. In the study presented here, we apply the technique to explore thickness fluctuations in lipid bilayers. The result shows clear evidence of thickness fluctuations above T_m , where the lipid tails display liquid ordering, while none are discernable below T_m . The estimated amplitude of the observed membrane thickness fluctuations is approximately 4 Å. These results are consistent with theoretical expectation and recent molecular dynamics simulations. Varying the lipid tail length from 14 carbons to 18 carbons per tail does not appear to affect to the dynamics very much.

9:00AM A41.00004 A Simple Analysis of Small-Angle Neutron Scattering Data to Estimate Thickness Fluctuations of the Membrane, TAKUMI HAWA, VICTOR LEE, School of Aerospace and Mechanical Engineering, The University of Oklahoma — Small-angle neutron scattering (SANS) and neutron spin echo (NSE) experiments are one of the most important laboratory techniques to investigate structure and dynamic properties of biological and nanotechnology-related membrane systems. Due to the sensitivity of about 1 100 nm length scales, these experimental techniques provide extensive information over a wide variety of technological and scientific applications. Recently, the author and his colleagues studied swollen lamellar structure systems consisting of nonionic surfactant, water, and oil using SANS/NSE and molecular dynamics (MD) simulation. They proposed a new experimental technique to measure the thickness fluctuations of surfactant layers and verified their approach using MD simulations. In this talk a possible simpler approach to estimate the membrane thicknesses and fluctuations directly from the isotropic scattering intensities in the two-dimensional SANS profile will be proposed. Generally, this characteristic feature is reproduced using various scattering theories to estimate the membrane thickness; however, the thickness fluctuation amplitude has never been estimated from the SANS profile. The results obtained from the approach will be compared with the experimental results obtained by Nagao and co-workers.

9:12AM A41.00005 High-resolution Structures of Protein-Membrane Complexes by Neutron Reflection and MD Simulation: Membrane Association of the PTEN Tumor Suppressor, MATHIAS LOESCHE, Carnegie Mellon University — The lipid matrix of biomembranes is an in-plane fluid, thermally and compositionally disordered leaflet of 5 nm thickness and notoriously difficult to characterize in structural terms. Yet, biomembranes are ubiquitous in the cell, and membrane-bound proteins are implicated in a variety of signaling pathways and intra-cellular transport. We developed methodology to study proteins associated with model membranes using neutron reflection measurements and showed recently that this approach can resolve the penetration depth and orientation of membrane proteins with Ångström resolution if their crystal or NMR structure is known. Here we apply this technology to determine the membrane binding and unravel functional details of the PTEN phosphatase, a key player in the PI3K apoptosis pathway. PTEN is an important regulatory protein and tumor suppressor that performs its phosphatase activity as an interfacial enzyme at the plasma membrane-cytoplasm boundary. Acting as an antagonist to phosphoinositide-3-kinase (PI3K) in cell signaling, it is deleted in many human cancers. Despite its importance in regulating the levels of the phosphoinositoltriphosphate $PI(3,4,5)P_3$, there is little understanding of how PTEN binds to membranes, is activated and then acts as a phosphatase. We investigated the structure and function of PTEN by studying its membrane affinity and localization on in-plane fluid, thermally disordered synthetic membrane models. The membrane association of the protein depends strongly on membrane composition, where phosphatidylserine (PS) and phosphatidylinositol diphosphate ($PI(4,5)P_2$) act synergetically in attracting the enzyme to the membrane surface. Membrane affinities depend strongly on membrane fluidity, which suggests multiple binding sites on the protein for $PI(4,5)P_2$. Neutron reflection measurements show that the PTEN phosphatase “scoots” along the membrane surface (penetration < 5 Å) but binds the membrane tightly with its two major domains, the C2 and phosphatase domains. In the bound state, PTEN's regulatory C-terminal tail is displaced from the membrane and organized on the far side of the protein, ~ 60 Å away from the bilayer surface, in a rather compact structure. The combination of binding studies and neutron reflection allows us to distinguish between PTEN mutant proteins and ultimately may identify the structural features required for membrane binding and activation of PTEN. Molecular dynamics simulations, currently in progress, refine this structural picture further.

9:48AM A41.00006 Application of Small-Angle Neutron and X-ray Scattering in Determining Lipid Bilayer Structure¹, JIANJUN PAN, FREDERICK A. HEBERLE, Neutron Scattering Science Division, Oak Ridge National Laboratory, NORBERT KUCERKA, Canadian Neutron Beam Centre, National Research Council, Chalk River, Ontario, Canada, STEPHANIE TRISTRAM-NAGLE, Department of Physics, Carnegie Mellon University, MICHELLE SZYMANSKI, MARY KOEPFINGER, Douglass Residential College, Rutgers University, JOHN KATSARAS, Neutron Scattering Science Division, Oak Ridge National Laboratory — Accurately determining lipid structure in biologically relevant fluid bilayers is not straightforward. We have recently developed a hybrid experimental/computational technique (i.e., the scattering density profile, or SDP model), which exploits the fact that neutron and X-ray scattering are sensitive to different bilayer thicknesses - the large difference in neutron scattering length density (SLD) between prolated lipid and deuterated water defines the overall bilayer thickness, while X-ray scattering resolves the headgroup-headgroup distance due to the large scattering contrast between the electron-rich phosphate groups and the hydrocarbon/aqueous medium. A key step in the SDP analysis is the use of MD simulations to parse the lipid molecule into fragments whose volume probability distributions follow simple analytical functional forms. Given the appropriate atomic scattering lengths, these volume probabilities can simultaneously predict both the neutron and X-ray SLD profiles, and hence the scattering form factors. Structural results for commonly used phosphatidylcholine and phosphatidylglycerol lipids will be given.

¹This work acknowledges the support of ORNL, NIST, and Cornell High Energy Synchrotron Source.

10:00AM A41.00007 Growth Mechanism of Lipid-Based Nanodiscs – a Model Membrane for Studying Kinetics of Particle Coalescence¹, ANDREW HU, University of Connecticut, Mechanical Engineering, MU-PING NIEH, University of Connecticut, Institute of Materials Science, Chemical Materials & Biomolecular Engineering, ANTHONY DIZON, University of Connecticut, Chemical Materials & Biomolecular Engineering, MING LI, University of Connecticut, Institute of Materials Science, TAI-HSI FAN, University of Connecticut, Mechanical Engineering — Lipid-based nanodiscs composed of long- and short- chain lipids [namely, dimyristoyl phosphatidylcholine (DMPC), dimyristoyl phosphatidylglycerol (DMPG) and dihexanoyl phosphatidylcholine (DHPC)] constantly form at high lipid concentrations and at low temperatures (i.e., below the melting transition temperature of DMPC, T_m). The initial size of these nanodiscs (at high total lipid concentration, $C_L > 20$ wt.%) is relatively uniform and of similar dimension (according to dynamic light scattering and small angle neutron scattering experiments), seemingly independent of thermal history. Upon dilution, the nanodiscs slowly coalesce and grow in size with time irreversibly. Our preliminary result shows that the growth rate strongly depends on several parameters such as charge density, C_L and temperature. We have also found that the nanodisc coalescence is a reaction limit instead of diffusion limit process through a time-resolved study.

¹Funding supported by NSF CMMI - 1131587.

10:12AM A41.00008 Swellable Model POPC/POPG/DHPC Membrane with a Lamellar Long-Range Order¹, MING LI, MU-PING NIEH, Department of Chemical, Materials & Biomolecular Engineering, Institute of Materials Science, University of Connecticut, Storrs, CT 06269, USA — A physiological relevant biomimetic model membrane is of great necessity for the structural characterization of membrane protein. This presentation will report a small-angle neutron scattering (SANS) result on two lipid bicellar series composed of 1-palmitoyl-2-oleoyl-*sn*-glycero-3-phosphocholine (POPC)/1,2-dihexanoyl-*sn*-glycero-3-phosphocholine (DHPC) and POPC/DHPC/1-palmitoyl-2-oleoyl-*sn*-glycero-3-phospho-(1'-*rac*-glycerol) (POPG). Instead of the multi-lamellae vesicle (MLV) structure observed in zwitterionic POPC/DHPC mixture, the perforated lamellae (PL) structure is found in POPC/POPG/DHPC upon addition of small amount of charged lipid, POPG $\{R=[\text{POPG}]/([\text{POPC}]+[\text{POPG}])=0.01\}$. The PL phase exists from 10 to 60 degree C and the interlamellar spacing (d-spacing) varies from 12.9 to 49.0 nm as the lipid concentration changes from 25 to 7.5% wt where the lamellae still indicate long-range order. The effect of temperature and charge density (R) on structural variation will be discussed in this presentation.

¹We gratefully acknowledge the support from National Science Foundation (NSF-CMMI1131589).

10:24AM A41.00009 Mobility of water and selected atoms in bilayer DMPC membranes¹, F.Y. HANSEN, Technical University of Denmark, H. TAUB, M. BAI, A. MISKOWIEC, University of Missouri-Columbia — Molecular dynamics simulations have been used to determine the mobility of water molecules as a function of their positions in a fully hydrated free standing DMPC membrane at 303 K. In a 10 Å thick water layer with bulk density just outside the membrane, the mobility of the water molecules is reduced by about a factor of two relative to bulk. For water molecules penetrating deeper into the membrane there is an increasing reduction in the mobility with up to two orders of magnitude for those deepest into the membrane. A comparison with the mobility of selected atoms in the lipid molecules shows that about 5 water molecules/lipid molecule move on the same time scale as the lipid molecules and may therefore be considered to be so tightly bound to them that they essentially follow their motion. The simulation results are quantitatively compared with quasielastic neutron scattering results on single-supported bilayer DMPC membranes.

¹Supported by NSF Grant Nos. DMR-0705974 and DGE-1069091

10:36AM A41.00010 Structure of single-supported DMPC lipid bilayer membranes as a function of hydration level studied by neutron reflectivity and Atomic Force Microscopy¹, A. MISKOWIEC, P. SCHNASE, M. BAI, H. TAUB, U. Mo., F.Y. HANSEN, Tech. U. of Denmark, M. DUBEY, S. SINGH, J. MAJEWSKI, LANSCE — We have recently been investigating the diffusion of water on single-supported DMPC lipid bilayer membranes at different levels of hydration, using high-resolution quasielastic neutron scattering (QNS). To aid in the interpretation of these QNS studies, we have conducted neutron reflectivity (NR) measurements on SPEAR at LANSCE to characterize the structure of similarly prepared samples. Protonated DMPC membranes were deposited onto SiO₂-coated Si(100) substrates and characterized by Atomic Force Microscopy (AFM) at different levels of hydration. We find reasonable agreement between the membrane thickness determined by NR and AFM at room temperature. We also find consistency between the scattering length density (SLD) profile in the vicinity of the upper leaflet of the supported DMPC membrane and that found in a molecular dynamics simulation of a freestanding membrane at 303 K. However, the fit to the reflectivity curve can be improved by modifying the SLD profile near the leaflet closest to the SiO₂ surface.

¹Supported by NSF Grant Nos. DMR-0705974 and DGE-1069091.

10:48AM A41.00011 Cholesterol Flip-Flop Dynamics in a Phospholipid Bilayer: A 10 Microsecond All-Atom Molecular Dynamics Simulation, KEN-ICHI NOMURA, AMIT CHOUBEY, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, Collaboratory for Advanced Computing and Simulations, University of Southern California, Los Angeles, California 90089-0242, USA — Cholesterol (CHOL) molecules play a key role in modulating the rigidity of cell membranes, and controlling intracellular transport and signal transduction. Using all-atom molecular dynamics and the parallel replica approach, we study the effect of CHOL molecules on mechanical stresses across a dipalmitoylphosphatidylcholine (DPPC)-CHOL bilayer, and the mechanism by which CHOL molecules migrate from one bilayer leaflet to the other (flip-flop events). On average, we observe a CHOL flip-flop event in half-a-microsecond. Once a CHOL flip-flop event is triggered, the inter-leaflet migration occurs in about 62 nanoseconds. The energy barrier associated with flip-flop events is found to be 73 kJ/mol. Results for membrane rigidity as a function of CHOL concentration will also be presented.

Monday, February 27, 2012 8:00AM - 10:48AM –
Session A42 DBIO DPOLY: Focus Session: Cytoskeleton and Biomechanics - Biochemical mechanisms 156C

8:00AM A42.00001 Stochastic simulations of the growth dynamics and organization of lamellipodia-like actin networks, LONGHUA HU, GAREGIN PAPOIAN, Department of Chemistry and Biochemistry, University of Maryland — Cell migration is essential to many biological processes such as embryonic development, wound healing and immune response. The crawling movement of cells is a complex process that involves the protrusion of the leading edge of a cell, adhesion to the substrate, generation of the traction force to move cell body and the subsequent release of adhesions. Lamellipodia are flat sheet-like membrane protrusions at the leading edge of the crawling cells. The dynamic remodeling of the dendritically branched actin network in lamellipodia generates force to drive the movement of cells. We have developed a simplified, three-dimensional computational model to study the growth of lamellipodia-like actin networks. Our model integrates the essential biochemical regulation processes as well as the mechanical aspect of actin polymerization, where the interactions between the semi-flexible filaments and the plasma membrane are taken into account. Using stochastic simulations, we study how membrane tension and external resistance on membrane affect the growth dynamics and organization of the actin network.

8:12AM A42.00002 How ion binding affects actin filament stability and flexural rigidity, HYERAN KANG, MICHAEL BRADLEY, BRANNON MCCULLOUGH, Yale University, ANAËLLE PIERRE, ENS de Cachan, France, ELENA GRINTSEVICH, UCLA, ENRIQUE DE LA CRUZ, Yale University — Actin filaments are semi-flexible biopolymers essential for the mechanical support and cell motility. Ions strongly affect actin polymerization and the flexibility of actin filaments; however, the molecular basis for how ions are coupled to the mechanics of actin filaments remains elusive. Here, we demonstrate a linkage between cation binding and both actin filament polymerization and flexural rigidity. Our results show that the thermodynamic stability and flexural rigidity of actin filament increase with cation concentration in a manner that implicates specific cation binding as opposed to general electrostatic screening. Using structural bioinformatics, we identify two distinct cation-binding sites within the F-actin structure that help explain how specific cation binding is linked to actin polymerization and flexural rigidity. Site-specific substitution of a charged amino acid residue at one of the sites modulates the cation concentration-dependence of filament bending stiffness, consistent with a bound cation at this site increasing the flexural rigidity of actin filaments. Mutation of a charged amino acid at the other site causes "polymerization incompetent" G-actin.

8:24AM A42.00003 Mechanotransduction through the plasma membrane & cytoskeleton, KRISTINA HAASE, ANDREW PELLING, University of Ottawa — Mechanical forces initiate immediate and long-term changes in cells; however the exact mechanisms remain unclear, albeit crucial for understanding the pathology of disease. We used combined confocal and atomic force microscopy (AFM) to investigate changes in cell morphology and elasticity in response to a mechanical stimulus. The AFM was used as a nano-indentor to gauge the response of the membrane and cytoskeleton (CSK) of HeLa cells. We observed their viscoelastic nature by probing cells transfected with a green fluorescent protein localized at the plasma membrane. Inhibition of acto-myosin contractility (AMc) resulted in a significant decrease of cellular elasticity, and a corresponding increase in mean deformation. We also investigated the rate at which the membrane and CSK deform and relax in response to a local force. The response to a local perturbation is nearly instantaneous for control cells and shows no statistical difference when compared to cells treated with CSK-inhibiting drugs. Inhibition of AMc affects the rate of recovery, in comparison to control cells which recover quite quickly (30-60s). Overall, we demonstrated short and long-term deformation and subsequent recovery of both the cell membrane and actin network in response to a local force.

8:36AM A42.00004 Leading at the Front: How EB Proteins Regulate Microtubule Dynamics, TAVIARE HAWKINS, University of Massachusetts-Amherst — Microtubules are the most rigid of the cytoskeletal filaments, they provide the cell's scaffolding, form the byways on which motor proteins transport intracellular cargo and reorganize to form the mitotic spindle when the cell needs to divide. These biopolymers are composed of alpha and beta tubulin monomers that create hollow cylindrical nanotubes with an outer diameter of 25 nm and an inner diameter of 17 nm. At steady state concentrations, microtubules undergo a process known as dynamic instability. During dynamic instability the length of individual microtubules is changing as the filament alternates between periods of growth to shrinkage (catastrophe) and shrinkage to growth (rescue). This process can be enhanced or diminished with the addition of microtubule associated proteins (MAPs). MAPs are microtubule binding proteins that stabilize, destabilize, or nucleate microtubules. We will discuss the effects of the stabilizing end-binding proteins (EB1, EB2 and EB3), on microtubule dynamics observed in vitro. The EBs are a unique family of MAPs known to tip track and enhance microtubule growth by stabilizing the ends. This is a different mechanism than those employed by structural MAPs such as tau or MAP4.

9:12AM A42.00005 Redundancy and cooperativity in the mechanics of compositely crosslinked cytoskeletal networks, J.M. SCHWARZ, Physics Department, Syracuse University, D.Q. QUINT, School of Natural Sciences, University of California-Merced, MOUMITA DAS, Physics Department, Syracuse University — The cytoskeleton contains many types of crosslinkers. Some crosslinkers allow free rotations between filaments and others do not. The mechanical interplay between different crosslinkers is an open issue in cytoskeletal mechanics. Therefore, we develop a theoretical framework based on rigidity percolation to study a generic filamentous system containing both stretching and bond-bending forces to address this issue. The framework involves both analytical calculations via effective medium theory and numerical simulations on a percolating triangular lattice with very good agreement between both. We find that the introduction of angle-constraining crosslinkers to a semiflexible filamentous network with freely-rotating crosslinks can cooperatively lower the onset of rigidity to the connectivity percolation threshold—a result speculated for years but never before obtained via effective medium theory. In other words, the system can attain rigidity at the lowest concentration of material possible. We further demonstrate that introducing angle-constraining crosslinks results in mechanical behaviour similar to just freely-rotating crosslinked semiflexible filaments, indicating redundancy. Our results also impact upon collagen and fibrin networks in biological and bio-engineered tissues.

9:24AM A42.00006 The origins of strain stiffening in fibrin networks, LOUISE JAWERTH, Harvard University, STEFAN MUENSTER, University of Erlangen, Nuremberg, DAVID WEITZ, Harvard University — Fibrin networks form the structural scaffold of blood clots; their non-linear mechanical properties are crucial to stem the flow of blood at a site of vascular injury. A hallmark of these networks is strain stiffening: a stiffness that increases non-linearly as a network is strained. Deformations of the fibers and the network combine to control the mechanical properties of the bulk and must lead to the strain stiffening behavior of the networks; however, the details of this process are unknown. Here, we study fibrin networks undergoing shear on a confocal microscope and compare this to bulk rheological measurements. We track individual fiber branchpoints as function of system strain. We characterize the non-affinity of the motion and show that the low strain, linear regime corresponds to highly non-affine motion while the high strain, nonlinear regime corresponds to affine motion. Moreover, we show that the non-linear bulk response can be well approximated by considering the fibers to be linear elastic elements with soft compressive behavior and, therefore, is a result of the topology of the network itself rather than nonlinearity of its constituents.

9:36AM A42.00007 Semiflexible filament networks viewed as fluctuating beam frames, TIANXIANG SU¹, PRASHANT PUROHIT, University of Pennsylvania — We present a new method combining structural and statistical mechanics to study the entropic elasticity of semiflexible filament networks. We view a filament network as a frame structure and use structural mechanics to determine its static equilibrium configuration under applied loads in the first step. To account for thermal motion around this static equilibrium state, we then approximate the potential energy of the deformed frame structure up to the second order in kinematic variables and obtain a deformation-dependent stiffness matrix characterizing the flexibility of the network. Using statistical mechanics, we then evaluate the partition function, free energy and thermo-mechanical properties of the network in terms of the stiffness matrix. We show that penalty methods commonly used in finite elements to account for constraints, are applicable even when statistical and structural mechanics are combined in our method. We apply our framework to understand the expansion, shear, uniaxial tension and compression behavior of some simple filament networks. We are able to capture the stress-stiffening behavior due to filament reorientation and stretching out of thermal fluctuations, as well as the reversible stress-softening behavior due to filament buckling.

¹Currently at Harvard University

9:48AM A42.00008 Spindle Assembly and Architecture: From Laser Ablation to Microtubule Nucleation, DANIEL NEEDLEMAN, JAN BRUGUES, VALERIA NUZZO, ERIC MAZUR, Harvard University — Spindles are arrays of microtubules that segregate chromosomes during cell division. It has been difficult to validate models of spindle assembly due to a lack of information on the organization of microtubules in these structures. Here we present a novel method, based on femtosecond laser ablation, capable of measuring the detailed architecture of spindles. We used this method to study the metaphase spindle and find that microtubules are shortest near poles and become progressively longer towards the center of the spindle. These data, in combination with mathematical modeling, high resolution imaging, and biochemical perturbations, are sufficient to reject previously proposed mechanisms of spindle assembly. Our results support a new model of spindle assembly in which microtubule polymerization dynamics are not spatially regulated, microtubule transport locally sorts microtubules – determining their proper organization in the spindle without moving them appreciable distances –, and the profile of microtubule nucleation controls the length of the spindle.

10:00AM A42.00009 Coupling stochastic kinetics and mechanics uncovers new dynamics induced by focal adhesions in filopodia, MARIA MINAKOVA, GAREGIN PAPOIAN, University of Maryland at College Park — Cell motility recently became a target for physical chemists and biophysicists. It is generally understood that in real biological systems, chemical and mechanical processes are coupled, sometimes in a very complex manner. Focal adhesions (FAs) represent a biologically relevant example of multi molecular assemblies that serve a mechanical function and have intriguing biochemical properties. FAs and their role in filopodial dynamics have been extensively studied experimentally from a biological standpoint. Although there are many biochemical studies of FAs kinetics in the literature, only a few works study FA dynamics from a physical perspective. In our work we developed a robust stochastic model of the filopodia coupled to mechanical properties of FAs, retrograde flow and the substrate. We carried out extensive simulations of the filopodial stochastic growth on the timescales of minutes, as well as a detailed theoretical description of a steady state, mapping multi dimensional phase space of mechanical and kinetic parameters onto various dynamics regimes. The combination of mean field analyses with detailed microscopic simulations provides a united platform for treating mechanochemical processes underlying complex behavior of the filopodial system.

10:12AM A42.00010 Growth Cone Biomechanics in Peripheral and Central Nervous System

Neurons , JEFFREY URBACH, DANIEL KOCH, WILL ROSOFF, Georgetown University, HERBERT GELLER, NIH — The growth cone, a highly motile structure at the tip of an axon, integrates information about the local environment and modulates outgrowth and guidance, but little is known about effects of external mechanical cues and internal mechanical forces on growth-cone mediated guidance. We have investigated neurite outgrowth, traction forces and cytoskeletal substrate coupling on soft elastic substrates for dorsal root ganglion (DRG) neurons (from the peripheral nervous system) and hippocampal neurons (from the central) to see how the mechanics of the microenvironment affect different populations. We find that the biomechanics of DRG neurons are dramatically different from hippocampal, with DRG neurons displaying relatively large, steady traction forces and maximal outgrowth and forces on substrates of intermediate stiffness, while hippocampal neurons display weak, intermittent forces and limited dependence of outgrowth and forces on substrate stiffness. DRG growth cones have slower rates of retrograde actin flow and higher density of localized paxillin (a protein associated with substrate adhesion complexes) compared to hippocampal neurons, suggesting that the difference in force generation is due to stronger adhesions and therefore stronger substrate coupling in DRG growth cones.

10:24AM A42.00011 An Atomic Force Microscopy based investigation of specific biomechanical properties for various types of neuronal cells

, ELISE SPEDDEN, Physics and Astronomy, Tufts University, JAMES WHITE, Physics and Astronomy and Biomedical Engineering, Tufts University, DAVID KAPLAN, Biomedical Engineering and Chemical Engineering, Tufts University, CRISTIAN STAIL, Physics and Astronomy, Tufts University — Here we describe the use of Atomic Force Microscope (AFM) based techniques to characterize and explore the influence of biochemical and biomechanical cues on the growth and interaction of neuronal cells with surrounding guidance factors. Specifically, we use AFM topography and AFM force spectroscopy measurements to systematically investigate the morphology, elasticity, and real time growth of neuronal processes in the presence of different types of extracellular matrix proteins and growth factors. We therefore create a series of systems containing specified neuron densities where the type of the underlying growth promoting protein is different from sample to sample. For each system we measure key biomechanical parameters related to neuronal growth such as height and elastic modulus at multiple growth points on several types of neurons. We show that systematic measurements of these parameters yield fundamental information about the role played by substrate-plated guidance factors in determining elastic and morphological properties of neurons during growth.

10:36AM A42.00012 Nuclear Physics in a biological context

, DENNIS DISCHER, Univ. Pennsylvania — A solid tissue can be soft like fat or brain, stiff like striated muscle and heart, or rigid like bone – and of course every cell has a nucleus that contributes in some way small or large to tissue mechanics. Indeed, nuclei generally exhibit rheology and plasticity that reflects both the chromatin and the nuclear envelope proteins called lamins, all of which change in differentiation. Profiling of tissue nuclei shows that the nuclear intermediate filament protein Lamin-A/C varies over 30-fold between adult tissues and scales strongly with micro-elasticity of tissue, while other nuclear envelope components such as Lamin-B exhibit small variations. Lamin-A/C has been implicated in aging syndromes that affect muscle and fat but not brain, and we find nuclei in brain-derived cells are indeed dominated by Lamin-B and are much softer than nuclei derived from muscle cells with predominantly Lamin-A/C. In vitro, matrix elasticity can affect expression of nuclear envelope components in adult stem cells, and major changes in Lamin-A/C are indeed shown to direct lineage with lower levels favoring soft tissue and higher levels promoting rigid tissue lineage. Further molecular studies provide evidence that the nucleus transduces physical stress. References: (1) J.D. Pajerowski, K.N. Dahl, F.L. Zhong, P.J. Sammak, and D.E. Discher. Physical plasticity of the nucleus in stem cell differentiation. PNAS 104: 15619-15624 (2007). (2) A. Buxboim, I. Ivanova, and D.E. Discher. Matrix Elasticity, Cytoskeletal Forces, and Physics of the Nucleus: how deeply do cells 'feel' outside and in? Journal of Cell Science 123: 297-308 (2010).

Monday, February 27, 2012 8:00AM - 10:24AM –

Session A43 FPS: Invited Session: Broader Impacts of Research-NSF Policy and Individual Responsibility 157AB

8:00AM A43.00001 Science, the Scientists and Values

, ALAN LESHNER, AAAS — Although individual scientists engage in research for diverse reasons, society only supports the enterprise because it benefits humankind. We cannot always predict how that will happen, or whether individual projects will have clear and direct benefits, but in the aggregate, there is widespread agreement that we are all better off because of the quality and diversity of the science that is done. However, what scientists do and how it benefits humankind is often unclear to the general public and can at times be misunderstood or misrepresented. Moreover, even when members of the public do understand what science is being done they do not always like what it is showing and feel relatively free to disregard or distort its findings. This happens most often when findings are either politically inconvenient or encroach upon issues of core human values. The origins of the universe can fit into that latter category. This array of factors contributes to the obligation of scientists to reach out to the public and share the results of their work and its implications. It also requires the scientific community to engage in genuine dialogue with the public and find common ground where possible.

8:36AM A43.00002 The APS and the Impact on Physics and Society

, BARRY C. BARISH, California Inst of Technology, LIGO 18-34 — No abstract available.

9:12AM A43.00003 Why Physicists Have a Responsibility to Society

, CHARLES FERGUSON, Federation of American Scientists — The debate and controversy over the NSF criterion on broader societal impacts of NSF-funded research have served the important function of challenging the physics community to reexamine why public money should support pure and applied physics research and what is the role of physicists in society. I will argue that the criterion, while well intentioned, appears ill informed and runs the risk of creating a check list of activities that will seemingly fulfill physicists' responsibility to connect their work to larger societal issues. Moreover, I will argue in favor of having a portion of government-funded research for scientific investigations based primarily, if not solely, on the intellectual and scientific merits of the proposals. Most government-funded research is already connected to larger societal impacts such as national defense, energy research, and economic issues. While I will call for reassessment of the NSF criterion on broader societal impacts, my talk will explain why physicists, as citizens and scientists, must reenergize their efforts to positively effect society and will offer advice about how they can do so.

9:48AM A43.00004 The Broader Impact Criteria- What's the solution? A panel discussion

, DON PROSNITZ, None — The need for social control of science—especially 20th and now 21st century science—has been debated for decades. Science is supported by society, and research results ultimately have large societal impacts. Physicists arguing for increased research budgets invariably point out the collateral benefits to society—often economic—of their discovery-based research. Congress agreed, and attempted to institutionalize this metric in the 'America COMPETES Reauthorization Act of 2010' by insisting that researchers illustrate how their work will provide for (among other things) increased economic competitiveness of the United States and increased National Security. Is such a metric inevitable in these days of constrained resources? Is it desirable or even implementable? Can benefits be predicted, or are the most important societal consequences of basic research serendipitous? This talk will examine these questions, including looking at how other nations are attempting to deal with the issue, and present some suggestions for satisfying both society's insistence on a return on their investment and scientists' need for unfettered exploration. The program will conclude with a Q and A and panel discussion with all of the session's speakers.

Monday, February 27, 2012 8:00AM - 11:00AM –

Session A44 DPOLY DBIO: Focus Session: Hydrophobic Interactions and Hydrogen Bonding Networks in Polymeric and Soft Matter Systems 157C

8:00AM A44.00001 More than one dynamic crossover in protein hydration water¹, GIANCARLO FRANZESE, Universitat de Barcelona, Spain, MARCO G. MAZZA, TU Berlin, Germany, KEVIN STOKELY, Center for Polymer Studies, Boston University, MA, SARA PAGNOTTA, Centro de Física de Materiales, Donostia-San Sebastian, Spain, FABIO BRUNI, Università di Roma Tre, Italy, H. EUGENE STANLEY, Center for Polymer Studies, Boston University, MA — We study by theory, simulations and experiments, the dynamics of the hydrogen bond (HB) network of a percolating layer of water hydrating lysozyme powder. Using dielectric spectroscopy we measure the temperature dependence of the relaxation time of proton charge fluctuations. These fluctuations are associated with the dynamics of the HB network of water molecules adsorbed on the protein surface. Using Monte Carlo simulations and mean-field calculations, we study the dynamics and thermodynamics of a coarse-grained model that successfully reproduces the properties of hydration water. Both experimental and model analyses are consistent with the interesting possibility of two dynamic crossovers, (i) at ≈ 252 K, and (ii) at ≈ 181 K. Because the experiments agree with the model, we can relate the two crossovers to the presence at ambient pressure of two specific heat maxima. The first is caused by fluctuations in the HB formation, and the second, at a lower temperature, is due to the reordering of the HB network.

¹NSF Grant CHE 0908218, MICINN-FEDER (Spain) grant FIS2009-10210

8:12AM A44.00002 The effect of salt solutes on the relaxation dynamics of water from 65 to 720 GHz, NGUYEN VINH, MARK SHERWIN, JIM ALLEN, ITST, Department of Physics, University of California, Santa Barbara, KEVIN PLAXCO, Department of Chemistry and Biochemistry, University of California, Santa Barbara — During the past decade, a variety of measurement techniques have provided evidence that ions and other solute molecules effect the structure and dynamics of the water molecules directly surrounding them. Most of these experiments have employed infrared spectroscopy which explores vibrational relaxation of the hydration shell by observing intramolecular vibrations. Terahertz spectroscopy, in contrast is sensitive to intermolecular dynamics. Here we use a vector network analyzer based *terahertz dielectric relaxation spectrometer* operating over the frequency range from 65 to 720 GHz. The literature on relaxation dynamics of water is extensive and variable. But these measurements clarify the situation and confirm that the dynamics of water over this regime are best described in terms of three Debye relaxation processes with the characteristic times of 8.56, 1.1 ps and 179 fs (at 25.0 °C). Remarkably, while the relaxation times themselves are not sensitive to salt concentration, the relative strength of the relaxation modes depends in a systematic way on the solute molarity. We discuss these results by relating the salt concentration dependent strength of the three processes to the dynamics and structure of first three hydration shells. Our measurements shed light on the dynamics of hydration shells around solute molecules in a biologically relevant environment.

8:24AM A44.00003 Investigating How Contact Angle Effects the Interaction between Water and a Hydrophobic Surface, ADELE POYNOR, CAITLYN NEIDIG, Allegheny College — By definition hydrophobic substances hate water. What happens when water is forced into contact with a hydrophobic surface? One theory is that an ultra-thin low-density region forms near the surface. Contact angle is a measure of how hydrophobic a surface is. We have employed an automated home-built Surface Plasmon Resonance (SPR) apparatus to investigate the effect of varying the contact angle on the depletion layer

8:36AM A44.00004 Mesoscale inhomogeneities in an aqueous ternary system, DEEPA SUBRAMANIAN, STEPHEN HAYWARD, ELIA ALTABET, Department of Chemical and Biomolecular Engineering, University of Maryland, College Park, MD 20742, PETER COLLINGS, Department of Physics and Astronomy, Swarthmore College, Swarthmore, PA 19081, MIKHAIL ANISIMOV, Department of Chemical and Biomolecular Engineering, University of Maryland, College Park, MD 20742 — Aqueous solutions of certain low-molecular-weight organic compounds, such as alcohols, amines, or ethers, which are considered macroscopically homogeneous, show the presence of mysterious mesoscale inhomogeneities, order of a hundred nm in size. We have performed static and dynamic light scattering experiments in an aqueous ternary system consisting of tertiary butyl alcohol and propylene oxide. Tertiary butyl alcohol is completely soluble in water and in propylene oxide, and forms strong hydrogen bonds with water molecules. Based on results of the study, we hypothesize that the mesoscale inhomogeneities are akin to a micro phase separation, resulting from a competition between water molecules and propylene oxide molecules, wanting to be adjacent to amphiphilic tertiary butyl alcohol molecules. Coupling between two competing order parameters, super-lattice binary-alloy-like (“antiferromagnetic” type) and demixing (“ferromagnetic” type) may explain the formation of these inhomogeneities. Long-term stability investigation of this supramolecular structure has revealed that these inhomogeneities are exceptionally long-lived non-equilibrium structures that persist for weeks or even months.

8:48AM A44.00005 Statistical Mechanics of Thermosensitive Nanoparticle Binding: Quantifying Hydrophobic Interactions in Bulk Solution, ALESSIO ZACCONE, Cavendish Laboratory, University of Cambridge, JEROME CRASSOUS, University of Lund, BENJAMIN BERI, Cavendish Laboratory, University of Cambridge, MATTHIAS BALLAUFF, Helmholtz Zentrum Berlin — We present a novel method which allows one to quantify the binding energy between complex hydrophobic nanoparticles in bulk aqueous solutions by means of light scattering. We tested the method on the case of thermosensitive nanoparticles made of a solid polymeric core onto which a thermosensitive p-NIPAM microgel shell is grafted. The microgel shrinks above a critical T at which the hydrophobic attraction sets in. By means of a novel statistical mechanics model to interpret the data, we manage to demonstrate that the binding energy as a function of T of thermosensitive nanoparticles behaves like in the case of neat two-level systems, with a rather sharp transition from hard-sphere (hydrophilic) to attractive (hydrophobic) at the critical temperature. The model allows us to make a clear quantitative connection between the binding energy and the entropy change of the grafted microgel upon going from hydrophilic to hydrophobic (in turn related to the microgel structure). The methods presented in this work can be applied to quantify the binding energy of complex biomolecules in bulk solution, which is a major challenge in biophysics nowadays. Reference: A. Zaccane, J.J. Crassous, B. Beri, and M. Ballauff, Phys. Rev. Lett. 107, 168303 (2011).

9:00AM A44.00006 Effect of Valence of Counterions on the Structure of Charged Membranes, a Computer Simulation Study, BAOFU QIAO, MONICA OLVERA DE LA CRUZ, Department of Materials Science, Northwestern University — Phospholipids have been investigated for a long period, due to its ability of self-assembling into bilayer structures which resemble biological membranes. But most of the studies have been limited on the neutral phosphatidylcholine based lipids. The understanding of charged membranes (e.g., phosphatidylserine) is very limited due to the repulsion between the charged groups on lipids. In the present work, we investigated the effect of different counter-ions on the structures of charged membranes formed by 1,2-dilauroyl-sn-glycero-3-phospho-L-serine. Three kinds of counterions were investigated, from monovalent, to divalent, to trivalent ions. Molecular dynamics simulations were performed at all-atom level. We have calculated the area per lipid. And the interaction between counterions and COO⁻ groups was found to dominate over that between counterions and PO₄⁻ groups.

9:12AM A44.00007 Deconstructing Classical Water Models at Interfaces and in Bulk: Hydrophobic Interactions and Hydrogen Bonding¹

, JOHN D. WEEKS, Institute for Physical Science and Technology and Department of Chemistry and Biochemistry University of Maryland, College Park, MD — Using concepts from perturbation and local molecular field theories of liquids we divide the potential of the SPC/E water model into short and long ranged parts. The short ranged parts define a minimal reference network model that captures very well the structure of the local hydrogen bond network in bulk water while ignoring effects of the remaining long ranged interactions. This deconstruction can provide insight into the different roles that the local hydrogen bond network, dispersion forces, and long ranged dipolar interactions play in determining a variety of solvation and other properties of SPC/E and related classical models of water. We use these short ranged models along with local molecular field theory to quantify the influence of these interactions on the structure of hydrophobic interfaces and the crossover from small to large scale hydration behavior. The implications of our findings for theories of hydrophobicity and possible refinements of classical water models will also be discussed.

¹This work was supported by the National Science Foundation (grants CHE0628178 and CHE0848574)

9:48AM A44.00008 A SAFT-based classical density functional for water

, DAVID ROUNDY, JESSICA HUGHES, ERIC KREBS, Oregon State University — We present a new classical density functional for water based on a combination of Statistical Associating Fluid Theory (SAFT-VR) with the Fundamental Measure Theory (FMT) functional for the hard-sphere fluid. In the homogeneous limit, our functional reduces to the published optimal SAFT model of Clark *et al* [1]. By adding a single fitting parameter, we reproduce the bulk surface tension of water within a wide temperature range. We will present results for hydrophobic hard rods and spheres, including the temperature dependence of the hydrophobic interaction.

[1] G. Clak, A. Haslam, A. Galindo, and G. Jackson, *Molecular Physics* **104**, 3561 (2006).

10:00AM A44.00009 Morphology and chirality control self-assembly of sickle hemoglobin inside red blood cells¹

, XUEJIN LI, HUAN LEI, Division of Applied Mathematics, Brown University, Providence, RI 02912, BRUCE CASWELL, School of Engineering, Brown University, Providence, RI 02912, GEORGE KARNIADAKIS, Division of Applied Mathematics, Brown University, Providence, RI 02912 — Sickle cells exhibit abnormal morphology and membrane mechanics in the deoxygenated state due to the polymerization of the interior sickle hemoglobin (HbS). In this study, the dynamics of self-assembly behavior of HbS in solution and corresponding induced cell morphologies have been investigated by dissipative particle dynamics approach. A coarse-grained HbS model, which contains hydrophilic and hydrophobic particles, is constructed to match the structural properties and physical description (including crowding effects) of HbS. The hydrophobic interactions are shown to be necessary with chirality being the main driver for the formation of HbS fibers. In the absence of chain chirality, only the self-assembled small aggregates are observed whereas self-assembled elongated step-like bundle microstructures appear when we consider the chain chirality. Several typical cell morphologies (sickle, granular, elongated shapes), induced by the growth of HbS fibers, are revealed and their deviations from the biconcave shape are quantified by the asphericity and elliptical shape factors.

¹This work was supported by the National Institutes of Health (NIH) Grant R01HL094270 and the National Science Foundation (NSF) Grant CBET-0852948.

10:12AM A44.00010 Secondary structure formation in peptide amphiphile micelles

, MATTHEW TIRRELL, Institute for Molecular Engineering, University of Chicago — Peptide amphiphiles (PAs) are capable of self-assembly into micelles for use in the targeted delivery of peptide therapeutics and diagnostics. PA micelles exhibit a structural resemblance to proteins by having folded bioactive peptides displayed on the exterior of a hydrophobic core. We have studied two factors that influence PA secondary structure in micellar assemblies: the length of the peptide headgroup and amino acids closest to the micelle core. Peptide length was systematically varied using a heptad repeat PA. For all PAs the addition of a C12 tail induced micellization and secondary structure. PAs with 9 amino acids formed beta-sheet interactions upon aggregation, whereas the 23 and 30 residue peptides were displayed in an alpha-helical conformation. The 16 amino acid PA experienced a structural transition from helix to sheet, indicating that kinetics play a role in secondary structure formation. A p53 peptide was conjugated to a C16 tail via various linkers to study the effect of linker chemistry on PA headgroup conformation. With no linker the p53 headgroup was predominantly alpha helix and a four alanine linker drastically changed the structure of the peptide headgroup to beta-sheet, highlighting the importance of hydrogen bonding potential near the micelle core.

10:24AM A44.00011 Friction and Hydration Repulsion Between Hydrogen-Bonding Surfaces

, ROLAND NETZ, Free University Berlin, Germany — The dynamics and statics of polar surfaces are governed by the hydrogen-bonding network and the interfacial water layer properties. Insight can be gained from all-atomistic simulations with explicit water that reach the experimentally relevant length and time scales. Two connected lines of work will be discussed: 1) On surfaces, the friction coefficient of bound peptides is very low on hydrophobic substrates, which is traced back to the presence of a depletion layer between substrate and water that forms a lubrication layer. Conversely, friction forces on hydrophilic substrates are large. A general friction law is presented and describes the dynamics of hydrogen-bonded matter in the viscous limit. 2) The so-called hydration repulsion between polar surfaces in water is studied using a novel simulation technique that allows to efficiently determine the interaction pressure at constant water chemical potential. The hydration repulsion is shown to be caused by a mixture of water polarization effects and the desorption of interfacial water.

Monday, February 27, 2012 8:00AM - 11:00AM —

Session A45 DPOLY: Focus Session: Thin Film Block Copolymers - Directed Assembly 159

8:00AM A45.00001 Directed Ordering of Block Copolymer Thin Films with Flexible Interfaces for Functional Materials¹

, ALAMGIR KARIM, University of Akron — Orientation control of block copolymer (BCP) films is important for advanced technological applications. We present studies on directed ordering of block copolymer thin films on rigid substrates such as quartz to elastomeric PDMS and flexible Kapton substrates for tunable orientation of microphase separated poly(styrene) – block -poly(methylmethacrylate) (PS-PMMA) cylinder and lamellae forming BCP films. Although the crosslinked PDMS has low surface energy, its surface energy can be tuned by exposing to UV-Ozone (UVO) that presents an opportunity to change BCP-PDMS interfacial energy to control BCP orientation across full range of orientation and film wettability. On the other hand, Kapton offers a near neutral surface for PS-PMMA without surface modification. Via a modified version of a dynamic thermal processing termed cold zone annealing-sharp (CZA-S), we obtain a wide range of orientations of the block copolymer films in unfilled and nanoparticle filled systems with an interest in photovoltaic systems. With CZA-S, vertical orientation of PS-PMMA can be obtained in films as thick as 1 micron with etchable PMMA domains for membrane applications. GISAXS characterization of these etched BCP membranes reveals up to 5 orders of diffraction indicating hexagonally packed vertical nanopores that extend throughout the film. Under similar thermal gradient, but static conditions, temporally stable vertical cylinders form only within a narrow zone of maximum temperature gradient. Primary CZA-S ordering mechanism thus involves propagating this narrow vertically oriented zone of BCP cylinders created at the maximum thermal gradient section, across the film. An optimal speed is needed since the process competes with preferential surface wetting dynamics that favors parallel orientation. These results are reproduced on large area flexible films on a prototype dynamic R2R assembly platform with incorporated multi-CZA gradient for thin (100 nm) BCP films currently.

¹Acknowledgements: NSF-DMR and DOE-BES

8:36AM A45.00002 Facile Route to Vertically Aligned High-Aspect Ratio Block Copolymer Films via Dynamic Zone Annealing¹, GURPREET SINGH, MANISH KULKARNI, Department of Polymer Engineering, University of Akron, Akron OH 44325, KEVIN YAGER, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973, DETLEF SMILGIES, 3Cornell High Energy Synchrotron Source, Cornell University, Ithaca, New York 14853, DAVID BUCKNALL, Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332, ALAMGIR KARIM, Department of Polymer Engineering, University of Akron, Akron OH 44325 — Directed assembly of block copolymers (BCP) can be used to fabricate a diversity of nanostructures useful for nanotech applications. The ability to vertically orient etchable high aspect ratio (~30) ordered BCP domains on flexible substrates via continuous processing methods are particularly attractive for nanomanufacturing. We apply sharp dynamic cold zone annealing (CZA-S) to create etchable, and predominantly vertically oriented 30nm cylindrical domains in 1 μ m thick poly(styrene-*b*-methylmethacrylate) films on low thermal conductivity rigid (quartz) and flexible (PDMS & Kapton) substrates. Under similar static conditions, temporally stable vertical cylinders form within a narrow zone above a critical temperature gradient. Primary ordering mechanism of CZA-S involves sweeping this vertically orienting zone created at maximum thermal gradient. An optimal speed is needed since the process competes with preferential surface wetting dynamics that favors parallel orientation. GISAXS of etched BCP films confirms internal morphology.

¹ Acknowledgement: Work supported by NSF DMR-1006421

8:48AM A45.00003 Controlling Domain Orientation in Thin Films of Lamellar AB and ABA Block Copolymers, NIKHILA MAHADEVAPURAM, THAI VU, GILA STEIN, University of Houston — Thin films of block copolymers are very popular for low cost, large area nanopatterning. To generate a nanoporous template, the domains must be oriented perpendicular to the substrate. This talk will discuss the effects of copolymer architecture on surface energetics and domain orientations. We consider lamellar copolymers based on polystyrene (PS) and poly(methyl methacrylate) (PMMA) blocks. All films are cast on “neutral” substrates, and the resulting structures are evaluated with microscopy and grazing-incidence small-angle X-ray scattering. For PS-PMMA diblock copolymers, domain orientations are very sensitive to process conditions. The desired perpendicular orientation is most reliably obtained at high annealing temperatures where PS and PMMA have similar melt surface tensions. For PMMA-PS-PMMA triblock copolymers, the perpendicular domain orientation is stable for all film thicknesses and annealing temperatures that were studied, consistent with recent works that consider architectural effects when calculating the copolymer surface tension. These data suggest that triblocks are easier to use for nanopatterning. However, we also find that diblock and triblock films contain a high density of tilted domains, and such defects should be minimized for most applications.

9:00AM A45.00004 Diblock and Triblock Copolymer Thin Films on a Substrate with Controlled Selectivity¹, YONG-BIAO YANG, JAEUP KIM, UNIST, JUNHAN CHO, Dankook University — We study the morphology developments in linear ABC triblock and also AB diblock copolymer films on neutral and selective substrates, using a self-consistent field theory (SCFT). For the ABC copolymer films, various nanopatterns with tunable square morphologies evolved due to the effects of the substrate preferable to interior (B) block. The domain patterns became diversified from those parallel to the substrate with substrate selectivity for end-block or those vertical to the substrate without substrate selectivity. Furthermore, in order to figure out an economical and efficient way to fabricate useful passive pattern transfer layers potentially applicable to microelectronic processes and ultrahigh density storage media, we scrutinized conditions for generating square symmetries using symmetric AB diblock copolymers deposited on substrates created from ABC triblock copolymer films. It was found that a thinner film with relatively weak incompatibility can produce square patterns.

¹ This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MEST) (No. 2011-0027260 and 2011-0005403).

9:12AM A45.00005 Microdomain Orientation of PS-*b*-PMMA Thin Films on the PS grafted Substrates, DU YEOL RYU, RUI GUO, EUNHYE KIM, Yonsei University — The phase transitions and morphologies, specifically the orientation of lamellar microdomains of symmetric polystyrene-*b*-poly(methyl methacrylate) (PS-*b*-PMMA) were investigated with grazing incidence small-angle x-ray scattering (GISAXS) and transmission electron microscopy (TEM). The microdomain orientation in thin films of PS-*b*-PMMA on the substrates with brushed (or grafted) polymers was influenced by the interfacial interactions, where grafting density of underlying PS layers are controlled by the reaction parameters such as time and temperature during grafting to the substrates. When grafting density range of PS brush is adjusted, such a simple and facile route provides the perpendicular orientation of cylindrical and lamellar microdomains in PS-*b*-PMMA films.

9:24AM A45.00006 Orientation control of cold zone annealed Block copolymer films on tunable gradient surface energy substrates using combinatorial methods, MANISH KULKARNI, GURPREET SINGH, ALAMGIR KARIM, The University of Akron — Microphase morphologies of poly(styrene)-block-poly(methylmethacrylate) (PS-PMMA) block co-polymer (BCP) films coated on various tunable surface energy gradient (SEG) substrates were compared. Substrates were prepared by coating silane self assembled monolayer (SAM) and hydrophobic sol-gel based layer of silica (xerogel) on quartz and exposed to UV-ozone radiation by placing them on an accelerating stage that oxidizes the surface to generate SEG. The combinatorial thickness gradient samples of BCP film were prepared by flow coating the BCP solution orthogonal to the SEG. Samples were annealed using novel cold zone annealing (CZA) method with a sharp thermal gradient (50 °C/mm) to obtain highly ordered BCP morphologies. Effect of CZA annealing rate and film thickness on BCP morphologies of the SAM treated and untreated quartz as well as xerogel substrates were compared. It was observed that BCP films coated on the untreated quartz substrates exhibited hexagonally packed perpendicular cylindrical morphologies whereas higher area fraction of parallel cylinders was observed for SEG xerogel substrates for higher surface energies (>40 mJ/m²). BCP 2D surface morphologies studied using AFM, were confirmed to extend to the interior of the film (3D) by GISAXS.

9:36AM A45.00007 Block Copolymer Ordering on Soft, Patternable and Flexible Substrates, ARZU HAYIRLIOGLU, GURPREET SINGH, ALAMGIR KARIM, Department of Polymer Engineering, The University of Akron, Akron, 44325, OH — Directed assembly of cylinder and lamellae forming block copolymer films via flexible PDMS substrate is examined to investigate the ordering properties of polystyrene-*b*-poly(methyl methacrylate) (PS-*b*-PMMA) films. We study the cases where the PS-*b*-PMMA films are either directly coated on patterned PDMS flexible substrates, or coated on a flat PDMS substrate with a top patterned and flexible PDMS confinement. The surface energy of the PDMS substrates was modified to vary from 20 to 68 mJ/m² by exposing them to UV-ozone (UVO) for controlled wettability and orientation control. We replicated different patterned media and observed perpendicular lamellar orientation and parallel cylindrical orientation on patterned flexible substrate at higher surface energies in preliminary measurements. Characterization of orientation was investigated with Grazing-Incidence Small Angle X-ray Scattering (GISAXS) measurement as well as with Atomic Force Microscope (AFM) results. Optical Microscope (OM) was also used to study of the surface morphology of the BCP films.

9:48AM A45.00008 Controlling the alignment and the morphology of bilayer BCP films using templated self-assembly, AMIR TAVAKKOLI K. G., MIT, Dept. of Electrical Engineering and Computer Science, KEVIN W. GOTRIK, ADAM F. HANNON, ALFREDO ALEXANDER-KATZ, CAROLINE A. ROSS, MIT, Dept. of Materials Science and Engineering, KARL K. BERGGREN, MIT, Dept. of Electrical Engineering and Computer Science — Templated self-assembly of block copolymer (BCP) thin films can control the alignment of BCP microdomains in a single layer using chemical and topographical methods. However, controlling the alignment and the morphology of BCP microdomains in two different layers simultaneously and fabricating complicated three-dimensional (3D) structures is relatively unexplored. This control is useful for the fabrication of multilevel thin film devices. Also, the forces and energetics governing BCP self-assembly are better understood at the bulk scale. This paper discusses how to control the BCP in two different layers by using a majority-block-functionalized post template. We showed by using an array of majority block functionalized posts, we could fabricate very complicated three-dimensional structures and we were able to control the BCP in two different layers. We fabricated three dimensional junctions and bends in two different levels of the BCP, bottom and top. Moreover, we showed we could fabricate periodic superstructures as well as changing the morphology of the BCP in one of the layers from the original cylinders to ellipsoids, spheres, and bicontinuous cylinders and having two different morphologies on top of each other.

10:00AM A45.00009 Controlling the Block Copolymer Patterns via Combining Graphoepitaxy and Surface Guidance¹, HYUNJUNG JUNG, Korea University, SUMI LEE, EUN AE KWAK, Samsung Electronics, SANGHOON WOO, Korea University, FRANK LEIFARTH, CRAIG HAWKER, University of California, Santa Barbara, JUNE HUH, DU YEOL RYU, Yonsei University, JOONA BANG, Korea University — One of the key issues for the block copolymer patterning is controlling the pattern array. Using directed assembly of block copolymer on the chemically patterned surfaces guarantee highly uniform array or controlled non-regular array. In this system, the chemically patterned surface can induce well resisted array over arbitrary large areas. However, this method requires expensive and complicated e-beam lithography and thus is not readily applicable to mass production process. Alternatively, another method is the graphoepitaxy method. In this case, the self-assembly of block copolymer is guided by the topographical wall of lithographically pre-patterned substrates. But, it has limitation on the pitch size of wall to obtain the highly ordered patterns. In this work, we demonstrate a new type of fabrication method to achieve highly controlled and uniform block copolymer patterns. Our approach is to combine the graphoepitaxy method and hexagonally surface guiding patterns from crosslinkable block copolymers. When the lamellar forming block copolymers were prepared on hexagonal patterns, a highly aligned stripe was obtained and the alignment was significantly improved comparing to the case when no hexagonal surface patterns were used.

¹Samsung Electronics

10:12AM A45.00010 Macroscopic Ordering of Block Copolymers into Sequenced Patterns on Topographically Corrugated Surface, SUNGJUNE PARK, LARISA TSARKOVA, STEPHANIE HILT, DWI an der RWTH Aachen e. V., Lehrstuhl für Makromolekulare Materialien und Oberflächen, RWTH Aachen University, Germany, STEFAN ROITSCH, JOACHIM MAYER, Gemeinschaftslabor für Elektronenmikroskopie, RWTH Aachen University, Germany, ALEXANDER BÖKER, DWI an der RWTH Aachen e. V., Lehrstuhl für Makromolekulare Materialien und Oberflächen, RWTH Aachen University, Germany — For the guided block copolymer assembly we used corrugated SiCN ceramic substrates which were fabricated by a facile replication process using non-lithographic PDMS masters. During thermal annealing of polystyrene-b-polybutadiene diblock copolymer, the material transport was guided by the wrinkled substrate to form regular modulations in the film thickness. As a consequence of the thickness-dependent morphological behavior of block copolymers, the film surface appears as sequenced patterns of alternative microphase separated structures. The ordering process is attributed to the formation of reverse terraces which match the substrate topography, so that the resulting surface patterns are free from the surface relief structures within macroscopically-large areas. The issues of the film thickness, the substrate surface energy and the pattern geometry are addressed. Our approach demonstrates an effective synergism of external confinement and internal polymorphism of block copolymers towards complex hierarchically-structured patterned surfaces.

10:24AM A45.00011 Block copolymer thin films with long-range lateral order, ILJA GUNKEL, Lawrence Berkeley National Laboratory, TING XU, University of California, Berkeley, ALEXANDER HEXEMER, Lawrence Berkeley National Laboratory, THOMAS RUSSELL, University of Massachusetts, Amherst — We investigated thin block copolymer films on silicon wafers as well as faceted surfaces of sapphire. Thin films were prepared by spin-coating block copolymer solutions on the corresponding substrates. Subsequent annealing in organic solvent vapors served as a means to induce lateral long-range order in the thin films. The resulting block copolymer structures were analyzed by AFM and GISAXS.

10:36AM A45.00012 Combining block copolymer lithography with nano-imprinting lithography: Mass-producing sub-20nm unidirectional line patterns, XIAODAN GU, SUNG WOO HONG, THOMAS P. RUSSELL, University of Massachusetts Amherst, UMASS AMHERST TEAM — A facile, simple pathway for mass production of highly aligned sub 20 nm unidirectional line patterns over arbitrarily large areas is reported. The directed self-assembly of block copolymers and nano-imprint lithography technique are combined together for this purpose. Polystyrene-b-poly(4-vinylpyridine) (PS-b-P4VP) was self-assembled on the faceted sapphire substrates to generate unidirectionally aligned cylindrical microdomains oriented parallel to the substrate. The nanoporous trench patterns were achieved by selective reconstruction of the cylindrical P4VP microdomains followed by oxygen plasma etching. The resulting 1D trench nanopatterns were characterized by scanning force microscopy, scanning electron microscopy, and grazing incident small angle x-ray scattering (GISAXS), yielding an orientation parameter of 0.974. A cyclic-siloxane was cast onto the polymeric trench nanopatterns and cured to make a negative replica. After demolding, the cross-linked siloxane replica was used as a second master to mass-produce unidirectionally aligned nanolines on various substrates with high fidelity, quality, and yield by nano-imprinting lithography technique. Importantly, this strategy works for both thermal and UV-assisted imprinting. The methodology may afford an easy approach for mass production of ideal templates for the fabrication of magnetic storage media, optical devices, and arrays of conducting wires.

10:48AM A45.00013 Offset block copolymer printing using brushless substrates and elastomeric stamps, HYO SEON SUH, University of Wisconsin - Madison, HYUNSIK YOON, DO KYEONG KWON, KOOKHEON CHAR, Seoul National University, M. SERDAR ONSES, JEONG IN LEE, PAUL NEALEY, University of Wisconsin - Madison — The block copolymer (BCP) films have been utilized as the useful templates for the nanopatterning because of their ability to form quite small feature size with a relatively easy and cheap method. Recently, the control of orientation as well as the perfect registration with long range order of nanostructures in BCP films has been achieved by directing the assembly of BCP films with the chemical or topographical templates. However, such control of nanostructures and utilization of BCP films are limited on Si wafers since the templates are usually prepared by the semiconductor fabrication process. In this study, we will introduce a technique that overcomes such limitation on the application of BCP films. The chemical pattern prepared by e-beam lithography on the substrate without polymer brushes or mats was used as a template for the directed assembly of BCP films. Because the adhesion between this template and a BCP film is fairly weak, the directed assembled BCP films on this template could be easily transferred to the other substrates with adhesion-controlled elastomeric stamps. We believe that this transfer method, or printing method, would expand the applications of BCP films to areas where the nanotemplates are required.

Monday, February 27, 2012 8:00AM - 11:00AM –

Session A46 DPOLY: Invited Session: Inherently Strained Polymers and Soft Materials 160AB

8:00AM A46.00001 Switching Shape of Nematic Elastomers, KENJI URAYAMA, Department of Materials Chemistry, Kyoto University — Nematic elastomers (NEs) are a novel class of materials. NEs possess both the elastic properties of rubbers and the orientational properties of liquid crystals. The combination of these two properties makes the shape of NEs very sensitive to external stimuli. We focus on the thermally induced deformation of the NE films inherently possessing the two types of inhomogeneous director alignments, i.e., hybrid and twist alignments. In the NEs with hybrid alignments (HNEs), the director continuously changes by 90 degree from planar alignment to vertical alignment between the top and bottom surfaces. In the twist NEs, the director parallel to the surfaces smoothly rotates by 90 degree around the thickness axis, and the director at the mid-plane is parallel to the long or short axis of the film. In the HNEs and TNEs, the director change along the normal of the films causes the planes at different depth to respond differently to temperature variation, and the films are thus expected to change shape. We experimentally demonstrate that (i) depending on the width/thickness ratio, the TNE ribbons form the spiral ribbons or helicoids whose spiral or helical pitch markedly depends on temperature [1], and (ii) the HNE ribbons exhibit giant bending in response to temperature variation [2]. We theoretically interpret these experimental observations on the basis of the elastic models with the data of thermally induced uniaxial deformation of the corresponding NEs with globally planar alignment.

[1] Sawa, Ye, Urayama, Takigawa, Gimenez-Pinto, Selinger, R., Selinger, J., Proc. Natl. Acad. Sci., USA, 108, 6364 (2011).

[2] Sawa, Urayama, Takigawa, DeSimone, Teresi, Macromolecules, 43, 4362 (2010).

8:36AM A46.00002 Surface shape memory in polymers, PATRICK MATHER, Syracuse University — Many crosslinked polymers exhibit a shape memory effect wherein a permanent shape can be prescribed during crosslinking and arbitrary temporary shapes may be set through network chain immobilization. Researchers have extensively investigated such shape memory polymers in bulk form (bars, films, foams), revealing a multitude of approaches. Applications abound for such materials and a significant fraction of the studies in this area concern application-specific characterization. Recently, we have turned our attention to surface shape memory in polymers as a means to miniaturization of the effect, largely motivated to study the interaction of biological cells with shape memory polymers. In this presentation, attention will be given to several approaches we have taken to prepare and study surface shape memory phenomenon. First, a reversible embossing study involving a glassy, crosslinked shape memory material will be presented. Here, the permanent shape was flat while the temporary state consisted of embossed parallel grooves. Further the fixing mechanism was vitrification, with T_g adjusted to accommodate experiments with cells. We observed that the orientation and spreading of adherent cells could be triggered to change by the topographical switch from grooved to flat. Second, a functionally graded shape memory polymer will be presented, the grading being a variation in glass transition temperature in one direction along the length of films. Characterization of the shape fixing and recovery of such films utilized an indentation technique that, along with polarizing microscopy, allowed visualization of stress distribution in proximity to the indentations. Finally, very recent research concerning shape memory induced wrinkle formation on polymer surfaces will be presented. A transformation from smooth to wrinkled surfaces at physiological temperatures has been observed to have a dramatic effect on the behavior of adherent cells. A look to the future in research and applications for surface shape memory in polymers will round out the talk.

9:12AM A46.00003 Cell Forces and Cytoskeletal Order Parameters, DENNIS DISCHER, Univ. Pennsylvania — Nematic, Smectic and Isotropic Order parameters have found wide-spread use in characterizing all manner of soft matter systems, but have not yet been applied to characterize and understand the structures within living cells, particularly cytoskeletal structures. Several examples will be used to illustrate the utility of such analyses, ranging from experiments on stem cells attached to or in various elastic matrices to embryonic heart tissue and simulations of membrane cytoskeletons under all manner of stressing. Recently developed theory will be shown to apply in general with account of cell contractility, matrix elasticity and dimensionality as well as cell shape and a newly defined "cytoskeletal polarizability." The latter property of cells is likely different between different cell types due to different amounts of key cytoskeletal components with some types of stem cells being more polarizable than others. Evidence of coupling to the nucleus as a viscoelastic inclusion will also be presented.

References: (1) P. Dalhaimer, D.E. Discher, T. Lubensky. Crosslinked actin networks exhibit liquid crystal elastomer behavior, including soft-mode elasticity. Nature Physics 3: 354-360 (2007). (2) A. Zemel, F.Rehfeldt, A.E.X. Brown, D.E. Discher, and S.A. Safran. Optimal matrix rigidity in the self-polarization of stem cells. Nature Physics 6: 468 - 473 (2010).

9:48AM A46.00004 Tension in Highly Branched Polymers¹, MICHAEL RUBINSTEIN, University of North Carolina — We propose a systematic method of designing branched macromolecules capable of building up high tension in their covalent bonds, which can be controlled by changing solvent quality. This tension is achieved exclusively due to intramolecular interactions by focusing lower tensions from its numerous branches to a particular section of the designed molecule. The simplest molecular architecture, which allows this tension amplification, is a so-called pom-pom macromolecule consisting of a relatively short linear spacer and two z -arm stars at its ends. Tension developed in the stars due to crowding of their branches is amplified by a factor of z and focused to the spacer. There are other highly branched macromolecules, such as molecular brushes - comb polymers with high density of side branches, that have similar focusing and amplification properties. In addition molecular brushes transmit tension along their backbone. Adsorption or grafting of these branched molecules on a substrate results in further increase in tension as compared to molecules in solution. Molecular architectures similar to pom-pom and molecular brushes with a high tension amplification parts can be used in numerous sensor applications. Unique conformations of molecular brushes in a pre-wetting layer allow direct visualization by atomic force microscope. Detailed images of individual molecules spreading along the surface enable critical evaluation of theories of chain dynamics in polymer monolayer. Strong spreading of densely branched macromolecules on a planar substrate can lead to high tension in the molecular backbone sufficient to break covalent bonds.

¹This work was done in collaboration with S. Panyukov, S. Sheiko, J. Brock, and A. Bacanu

10:24AM A46.00005 New strategies in adaptive polymer gels, EUGENIA KUMACHEVA, University of Toronto — Plants possess a remarkable ability to change their shape in response to the changes in ambient conditions. These transitions are believed to be governed by the non-uniform accumulation of elastic energy and the release of localized stresses. The self-shaping behaviour of plants offers a new paradigm for creating adaptable materials by-design, however currently prediction of three-dimensional transformations in soft matter remain a challenge. Here we report on the nature-inspired strategy for the generation of complex three-dimensional structures by programming stimuli-responsive deformations of a composite planar polymer gel sheet. This work constitutes a major step towards the preprogrammed design of adaptable soft materials with applications in sensing and actuation.

Monday, February 27, 2012 8:00AM - 11:00AM —
Session A47 DPOLY: Focus Session: Gelation and Glass Transition in Colloids and Soft Matter Systems I 160C

8:00AM A47.00001 Gelation kinetics of gelatin using particle tracking microrheology, JOSEPH HARDCASTLE, Boston University, RAMA BANSIL, Boston University — Previous studies with gelatin have observed four distinct stages during the physical gelation process [Normand et al. Macromolecules, 2000, 33, 1063]. In this presentation we report measurements of microrheology in an effort to examine the time evolution of the gel on short length scales and time scales. By tracking latex particles in gelatin solution at different temperatures we can follow the microrheological changes and kinetics of the gelation process. Using the generalized Stokes-Einstein relation viscoelastic properties of these quasi-static gel states the evolution of the storage and loss moduli, G' and G'' , are examined as functions of both time and temperature. The data show that both G' and G'' exhibit power law scaling versus frequency with the same exponent. The temperature and concentration dependence of the frequency at which the system crosses over from viscous to elastic behavior will be presented.

8:12AM A47.00002 Temperature Dependent Dynamics and Structure of Soft Colloids, PRAVEEN AGARWAL, SAMANVAYA SRIVASTAVA, LYNDEN ARCHER, Cornell University — We have investigated the effect of temperature on the structure and dynamics of a particular class of soft colloids created by densely grafting polymer chains to the nanoparticle surface. These materials are able to display fluid like properties even in the absence of any external solvent and are termed as self-suspended fluids. Temperature dependent rheology of these materials has displayed several interesting features including increased solid like response with increase in temperature. Tethered polymer chain in this particular system is *cis* 1-4 polyisoprene, which is a type-A dielectric and allows the effect of temperature change on the global dynamics of the tethered chain to be separately investigated with broadband dielectric spectroscopy. Furthermore, we have investigated the effect of temperature change on the nanoparticle structure and dynamics with the help of small angle X-ray scattering (SAXS) and X-ray photon correlation spectroscopy (XPCS). Based on our finding, we have provided an alternative description of the jamming phase diagram applicable to this system.

8:24AM A47.00003 Confinement-induced solidification of attractive colloidal suspensions, JACINTA CONRAD, MELISSA SPANNUTH, Chemical and Biomolecular Engineering, University of Houston — Using a model colloidal-polymer suspension, we show that confinement induces solidification in attractive colloidal suspensions via a fundamentally different route from that active in hard sphere colloidal suspensions. For a range of polymer concentrations, the suspensions undergo a phase transition from a colloidal fluid with clusters to a colloidal gel with increasing confinement while polymer and particle concentration are held constant. Surprisingly, the effects of confinement appear at much larger thicknesses in attractive colloidal suspensions than in hard sphere suspensions. We find that solidification in confined attractive suspensions is not driven by structuring of the colloids at the walls or by shear-induced migration or clustering. Instead, by analyzing the cluster size distributions in the fluid phase as a function of confinement, we find that the strength of the interparticle attraction increases as the samples are confined. We further demonstrate that this change in the strength of attraction leads to increasingly arrested particle dynamics as colloidal gels are confined.

8:36AM A47.00004 Gelation of self-assembled bile acid-PEG conjugates, SATU STRANDMAN, FRANTZ LE DEVEDEC, X.X. ZHU¹, University of Montreal — The aggregation of macromolecules and low-molar-mass compounds into elongated self-assemblies such as wormlike micelles, fibers, or tubules increases the viscosity of the solutions and often leads to gelation due to network formation, even in organic solvents. Such one-dimensional nanostructures are promising candidates for drug delivery vehicles, packing materials for separation, templates for metal nanowires, biocides, and photo- or biocatalysis. An interesting group of compounds capable of this type of self-organization are bile acids, which are endogenous steroids known to form gels at high concentrations and appropriate pH conditions. Grafting poly(ethylene oxide) on bile acids via anionic polymerization brings along thermoresponsiveness represented by lower critical solution temperature (LCST), while self-assembling occurs below another threshold temperature leading to a gelation at high concentrations, as shown by rheological experiments. The latter transition is assigned to the nanotube formation of pegylated bile acids, visualized by electron microscopy.

¹corresponding author

8:48AM A47.00005 The Role of Charge Interactions in Colloidal Gelation, EMILY RUSSELL, Harvard University, JORIS SPRAKEL, Wageningen University, THOMAS KODGER, DAVID WEITZ, Harvard University — We demonstrate the gelation of a novel system of oppositely charged colloidal particles. The particles are charged by grafting a polyelectrolyte brush from the surface, and suspended in a polar solvent with added monovalent salt. Confocal microscopy allows us to study in detail the three-dimensional structure and dynamics of these binary gels as we vary the particle volume fraction, interaction strength, and relative number ratio of the two particle species, and we find a transition between a gel and a fluid state with each of these parameters. We find that the mean contact number of particles in the gel decreases as we approach the gel line, in contrast to what has been reported in the literature for depletion gels.

9:00AM A47.00006 Anomalous Phase Transitions in Soft Colloid-Polymer Binary Mixtures¹, JAYDEEP BASU, AJAY KANDAR, Department of Physics, Indian Institute of Science, Bangalore, India, SURESH NARAYANAN, ALEC SANDY, XSD, APS, Argonne National Laboratory, USA — We have shown earlier [1] that these PGNPs resemble star polymers or spherical brushes in terms of their morphology in the melt. However, these particles show dynamics in melt which is quite different from other soft colloidal particles. Since most of the work on soft colloidal particles have been performed in solutions we have now explored the phase behavior of the PGNPs in good solvent using microscopic structural and dynamical measurements on binary mixtures of homopolymers and soft colloids consisting of polymer grafted nanoparticles. We observe anomalous structural and dynamical phase transitions of these binary mixtures, including appearance of spontaneous orientational alignment and logarithmic structural relaxations, as a function of added homopolymers of different molecular weights. Our experiments points to the possibility of exploiting the phase space in density and homopolymer size, of such hybrid systems, to create new materials with unique properties. Reference: 1. Sivasurender Chandran, Sarika C. K., A. K. Kandar, J. K. Basu, S. Narayanan, and A. Sandy, J. Chem. Phys. **135**, 134901 (2011).

¹We acknowledge DST, India for funding. AK acknowledges CSIR, India for fellowship

9:12AM A47.00007 Injectable Solid Peptide Hydrogel as Cell Carrier: Effects of Shear Flow on Hydrogel and Cell Payload¹, DARRIN POCHAN, University of Delaware — Peptides were designed to intramolecularly fold into β -hairpins once they are exposed to physiological conditions and then consequently self-assemble into a rigid hydrogel with a network structure of branched and entangled, 3nm-wide fibrils. These physical hydrogels can be injected as preformed solids, because they can shear-thin and consequently flow under an appropriate shear stress but immediately recover back into solids on removal of the stress with gel stiffness restoring over time. In this work, mechanisms of gel shear-thinning and immediate recovery were elucidated by investigating gel behavior during and after flow via mechanical and structural characterizations. Importantly, hydrogel flow behavior was studied in a capillary geometry that mimicked the actual situation of syringe injection. Hydrogel flow profiles were obtained via fluorescent particle tracking and the profile shape was found dependent on flow rate and gel stiffness. Hydrogel nanostructure was probed with small angle neutron and x-ray scattering. The results demonstrate that these hydrogels can be excellent candidates for tissue regeneration substrates and injectable therapeutic delivery vehicles.

¹Funding from the UD-NIST Center for Neutron Science and the NIH is acknowledged

9:24AM A47.00008 Shear-driven gelation of dilute colloidal suspensions, EMANUELA DEL GADO, ETH Zurich, ALESSIO ZACCONE, University of Cambridge, DANIELE GENTILI, HUA WU, MASSIMO MORBIDELLI, ETH Zurich, MICROSTRUCTURE AND RHEOLOGY, ETH ZURICH TEAM, CHEMISTRY AND APPLIED BIOSCIENCES, ETH ZURICH TEAM — Shear-driven solidification of dilute colloidal suspensions has dramatic impact on their applications, ranging from industrial making of paints to artificial or natural microfluidic devices and is a prototype of far from equilibrium transitions. In a set of experiments on a dilute charge-stabilized colloidal suspension, we have monitored shear-induced aggregation in a fully controlled way and rationalized the effect of the shear stress from the initially liquid suspension to the final solid. By combining light scattering, rheology and microscopy images, we show that the suspension changes, under shear, into a suspension of non-Brownian aggregates whose packing fraction increases with the shearing time. Upon flow cessation, these aggregates can eventually form cohesive random packings where each inter-aggregate bond involve a large number of colloidal bonds. Such solidification mechanism is thus a hybrid between colloidal gelation and the packing-driven jamming of non-Brownian suspensions.

9:36AM A47.00009 Aggregation and network formation in aqueous methylcellulose near the sol-gel transition, SARA ARVIDSON, JOHN MCALLISTER, JOSEPH LOTT, FRANK BATES, TIMOTHY LODGE, University of Minnesota — Methylcellulose (MC) is a semi-flexible polymer which can be soluble in water at low temperatures, depending on the average number of methoxyl groups on each repeat unit. Upon heating, soluble MCs pass through a lower critical solution temperature (LCST) and undergo thermoreversible gelation, which is well described by Winter-Chambon critical gelation theory. The relaxation exponent (n) exhibits a smooth variation with concentration, approaching $n = 1$ at low concentration and $n = 0.5$ high concentration. We selected a set of commercial MC for materials with similar degrees of substitution, but known for their significant variations in gelation temperature in water. MCs which gel at higher temperatures also exhibit a plateau in elastic modulus at low frequencies, which indicates two relevant length scales coexist just below the gel point. Scattering experiments (static, dynamic, and small angle x-ray and neutron) are compared to rheological measurements to reveal the MC chain structures and aggregation associated with phase separation and gelation and enable a mechanistic understanding of these phenomena.

9:48AM A47.00010 Effect of particle stiffness on glassy dynamics of dense colloidal liquids, RAYMOND SEEKELL, Notre Dame University, PRASAD SARANGAPANI, MedImmune, LLC, Y. ÉLAINE ZHU, Notre Dame University — “Fragile” glassy materials show a non-Arrhenius dependence of relaxation time with temperature close to the glass transition and have been extensively studied for molecular glass formers as model “hard-sphere” colloidal suspensions, but we lack a complete understanding of “strong” glass formers which show an Arrhenius dependence on temperature approaching the glass transition. In this work, we investigate the glassy dynamics of microgels of varied particle stiffness in dense aqueous suspensions using confocal microscopy. Poly(N-isopropylacrylamide) (PNIPAM) microgel particles of variable stiffness in aqueous media are synthesized by precipitation polymerization varying the cross-linking density to resemble “strong” glass forming liquids owing to their directional elastic interparticle interactions at increased microgel volume fraction. The fragility effect on the glassy dynamics in dense colloidal suspension is investigated as we tune the behavior from “soft-sphere” to “hard-sphere” limits. We find that dynamic heterogeneity, specifically string-like motion, is more pronounced as stiffness increases.

10:00AM A47.00011 Thermo-adjustable mechanical properties of polymer, lipid-based complex fluids, MILLICENT FIRESTONE, SUNGWON LEE, Argonne National Laboratory — Combined rheology (oscillatory and steady shear) and SAXS studies reveal details on the temperature-dependent, reversible mechanical properties of nonionic polymer, lipid-based complex fluids. Compositions prepared by introduction of the polymer as either a lipid conjugate or a triblock copolymer form an elastic gel as the temperature is increased to 18 °C. The network is produced from PEO chain entanglement and physical crosslinks confined within the intervening aqueous layers of a multilamellar structured lyotropic mesophase. Although the complex fluids are weak gels, tuning of the gel strength can be achieved by temperature adjustment. The sol state formed at reduced temperature arises as a consequence of the well-solvated PEO chains adopting a non-interacting, conformational state. Complex fluids prepared with the triblock copolymers exhibit greater tunability in viscoelasticity than those containing the PEGylated-lipid conjugate because of the temperature-dependent water solubility of the central PPO block. The water solubility of PPO at reduced temperatures results in the polymer being expelled from the self-assembled amphiphilic bilayer, causing collapse of the swollen lamellar structure and loss of the PEO network. At elevated temperatures, the triblock reinserts into the bilayer producing an elastic gel. These studies identify macromolecular architectures for the facile preparation of dynamic soft materials possessing a range of mechanical properties that can be tuned by modest temperature control.

10:12AM A47.00012 Mechanics of networks of aliphatic fibers in aqueous surfactant media¹, GIULIANO ZANCHETTA, Department of Physics, University of Fribourg, MARCO CAGGIONI, VINCENZO GUIDA, Procter & Gamble, VERONIQUE TRAPPE, Department of Physics, University of Fribourg — We investigate the structural and rheological properties of aliphatic fibers dispersed in aqueous solutions of anionic surfactants, typically used in liquid detergents to provide yield stress. This system displays an onset to solid-like properties that depends on fiber concentration. In this contribution we will discuss how tuning the state of the surfactant background influences the fiber-fiber interactions and the mechanical properties of the gel.

¹We acknowledge funding from Procter & Gamble.

10:24AM A47.00013 Elimination of branching in self- assembled beta hairpin peptide fibrils, SAMEER SATHAYE, DARRIN POCHAN, Department of Materials Science and Engineering, University of Delaware, POCHAN GROUP TEAM — Hydrophobic collapse of amphiphilic -hairpin peptides (e.g. MAX1 VKVKVKVKV^DPPTKVKVKVKV-NH₂) into fibrils and their hierarchical assembly into branched, hydrogel networks has been extensively studied. A physically crosslinked hydrogel network is formed due to fibrillar entanglement and branched defects in hydrophobic collapse during fibril formation. Alternating valine residues with side chains of the same size are responsible for the hydrophobic collapse of the molecule into a b-hairpin and fibril nanostructure with branching. In a new sequence LNK1 (LNK1 (Nal)K(Nal)KAKAKV^DPPTKAKAK(Nal)K(Nal)-NH₂) the non-beta turn valines were replaced with Naphthylalanine and alanine amino acid residues, with hydrophobic side chains of larger and smaller volume, respectively, than valine. Thus, formation of a “lock and key” type structure was attempted in the hydrophobic core of the peptide fibrils that would eliminate fibril branching. The folding and network formation of LNK1 has been studied by Circular Dichroism spectroscopy (CD), Transmission Electron Microscopy (TEM) and Oscillatory Rheology. Preliminary rheological characterization suggests the elimination of branching in the fibrils and also a possibility that LNK1 networks, unlike MAX1, are just nanofibrillar suspensions rather than permanently physically crosslinked hydrogels.

10:36AM A47.00014 Bond orientational order in randomly-packed colloidal spheres¹, ELI SLOUTSKIN, ALEXANDER BUTENKO, Physics Department, Bar-Ilan University — Systems of jammed particles are abundant, yet poorly understood. These systems are often naively assumed to be disordered, such that only short-range correlations are present and all spatial directions are equivalent. Yet, the mechanical stability of these materials implies that a network of mechanical forces percolates through the sample, which may give rise to long-range correlations and symmetry breaking. We directly measure, by confocal microscopy, the positions of hard colloids, which are sedimented by centrifugation, to form a jammed matter. We follow the centrifugation process in motion, measuring the density profile of our particles along the sample. Strikingly, while only short-range positional order exists in our system, both in the fluid and in the jammed state, the orientations of the bonds between the nearest neighbors are correlated in the jammed state, throughout the system. This breaks the rotational symmetry of the jammed state. Moreover, the rotational symmetry is correlated with the direction of gravity, suggesting that the mechanical network of forces plays an important role in our system. This breaking of rotational symmetry, observed in our system, must have an impact on a wide range of properties in other, more complex, randomly packed systems.

¹This research was supported by the Israel Science Foundation (#85/10, #1668/10) and Kahn Foundation.

10:48AM A47.00015 Anharmonicity in Amino Acids¹, HERCULANO MARTINHO, THAMIRES LIMA, MARIANA ISHIKAWA, Universidade Federal do ABC — Two special dynamical transitions of universal character have been recently observed in macromolecules (lysozyme, myoglobin, bacteriorhodopsin, DNA, and RNA) at $T^* \sim 100 - 150$ K and $T_D \sim 180 - 220$ K. The underlying mechanisms governing these transitions have been subject of debate. In the present work it is reported a survey on the temperature dependence of structural, vibrational and thermodynamical properties of a nearly anhydrous amino acid (orthorhombic polymorph of the amino acids L-cysteine and L-proline at a hydration level of 3.5%). The temperature dependence of X-Ray diffraction, Raman spectroscopy, and specific heat were considered. The data were analyzed considering amino acid-amino acid, amino acid-water, and water-water phonon-phonon interactions, and molecular rotors activation. Our results indicated that the two referred temperatures define the triggering of very simple and specific events that govern all the interactions of the biomolecule: activation of CH_2 rigid rotors ($T < T^*$), phonon-phonon interactions between specific amino acid and water dimer vibrational modes ($T^* < T < T_D$), and water rotational barriers surpassing ($T > T_D$).

¹We would like to thank the Brazilian agencies CNPq (301018/2006-5) and FAPESP (2011/06618-0) for their financial support

Monday, February 27, 2012 8:00AM - 11:00AM – Session A48 DPOLY: Charged and Ion-Containing Polymers 161

8:00AM A48.00001 Influence of Plasticizer on Ion Aggregation in Single-ion Polymer Conductors, HANQING ZHAO, DAN KING, PAUL PAINTER, RALPH COLBY, JAMES RUNT, Penn State University — In this study, we add a miscible small molecule plasticizer to a polyester copolymer ionomer. The latter is synthesized from oligomeric polyethylene oxide (molecular weight = 600) separated by the lithium salt of 85 percent sulfonated dimethyl isophthalate units. Materials with different plasticizer contents are systematically investigated by FTIR spectroscopy, X-ray scattering and dielectric spectroscopy. Decreased T_g and a corresponding Increase in cation mobility are expected in these plasticized systems. Ionic conductivity depends on both the number of ions and their mobility, which in turn depends on the relationship between ion states (free ions, ion pairs and ion aggregates). With FTIR, we characterize and quantify the ionic structures in order to investigate how their ratio changes with plasticizer content. X-ray scattering reveals the change in ion aggregation. Further, dielectric spectroscopy is used to study ion conductivity and polymer dynamics of these materials.

8:12AM A48.00002 Atomistic molecular dynamics simulations of model ionomers, DAN BOLINTINEANU, MARK STEVENS, AMALIE FIRSCHKNECHT, Sandia National Laboratories — Ionomers are polymers that contain a small fraction of ionic groups. Due to their unique electrical properties, ionomers are being investigated as potential solid electrolytes in mobile battery applications. However, a lack of fundamental understanding of the relationship between ionomer chemistry, morphology and ion transport have hindered such efforts. To this end, we report atomistic molecular dynamics (MD) simulations of a model ionomer (polyethylene-co-acrylic acid) neutralized with different ions at various neutralization levels. The structure factor computed from the simulations is in good agreement with experimental X-ray scattering data, which provides strong validation of the simulation methods. Our simulations provide additional insight into the shape and size distribution of ionic clusters; in particular, we observe large networks of string-like clusters, and report quantitative features of these structures as a function of ionic group spacing in the polymer backbone, counterion type and neutralization level. We also investigate several features of ion transport in these systems. Since ion diffusion is slow relative to the time scales accessible to our simulations, we limit discussion to local, qualitative features of the ion transport mechanism.

8:24AM A48.00003 Weak polyelectrolytes grafted to nanoparticles and flat surfaces, STEPHEN BARR, ATHANASSIOS PANAGIOTOPOULOS, Chemical and Biological Engineering, Princeton University — The charge distribution on polyelectrolytes is a key factor which controls their conformation and interactions. In weak polyelectrolytes, this distribution is determined by a number of factors, including the solvent conditions and the local environment. We investigate this using grand canonical titration Monte Carlo simulations of a coarse grained polymer model. In this method, each polymer bead is able to change its ionization state based on its dissociation constant, the pH of the solution, and interactions with other particles in the system. We focus on a system of polymers with one end tethered to the surface of a nanoparticle and determine both the charge and the polymer conformation as the pH and solvent quality are varied. We compare the results to both a fixed charge model and to polyelectrolytes grafted to a flat surface.

8:36AM A48.00004 Large scale molecular dynamics study of polymer-surfactant complex, MONOJOY GOSWAMI, BOBBY SUMPTER, Oak Ridge National Laboratory, Oak Ridge, TN — In this work, we study the self-assembly of cationic polyelectrolytes mediated by anionic surfactants in dilute or semi-dilute and gel states. The understanding of the dilute system is a requirement for the understanding of gel states. The importance of polyelectrolyte with oppositely charged colloidal particles can be found in biological systems, such as immobilization of enzymes in polyelectrolyte complexes or nonspecific association of DNA with protein. With the same understanding, interaction of surfactants with polyelectrolytes shows intriguing phenomena that are important for both in academic research as well as industrial applications. Many useful properties of PE surfactant complexes come from the highly ordered structures of surfactant self-assembly inside the PE aggregate. We do large scale molecular dynamics simulation using LAMMPS to understand the structure and dynamics of PE-surfactant systems. Our investigation shows highly ordered ring-string structures that have been observed experimentally in biological systems. We will investigate many different properties of PE-surfactant complexation which will be helpful for pharmaceutical, engineering and biological applications.

8:48AM A48.00005 Near Edge X-ray Absorption Fine Structure Studies of Cu Ion-Containing PAMAMOS Dendrimer Networks, ROBERT BUBECK, PETAR DVORNIC, Michigan Molecular Institute, DANIEL FISCHER, NIST — There is continuing interest in the development of nanocomposites containing metal ions based on the use of dendrimers as the host matrix. One may utilize functionalized dendrimer interiors to complex the added constituent and serve as a template for the organization of the resulting nanoscale structures. Potential applications of include: catalysts, biotechnology, functional membranes, molecular sensors, etc. We report on recent results obtained using near edge X-ray absorption fine structure (NEXAFS) to characterize $\text{Cu}(2+)$ covalent interactions in three-dimensionally cross linked dendrimer networks. These networks were made from radially-layered poly(amidoamine-organosilicon), PAMAMOS, dendrimers having generation 4 (G4) polyamidoamine (PAMAM) interiors surrounded by one layer of organosilicon, OS, exterior branch cells. Lower generation homologues (i.e., G1 through G3) were also examined on a more limited basis. The nitrogen and carbonyl moieties contained in the PAMAM dendrimer interior were shown to be highly interactive with metallic cations, in large measure because of the dendrimer geometry. Similar measurements on chemically similar but much less physically constraining hyperbranched polymers indicated very limited interaction with the amine and carbonyl moieties.

9:00AM A48.00006 Mean-Field Modeling of the Encapsulation of Weakly Acidic Particles in Polyelectrolyte Dendrimers, THOMAS LEWIS, VENKAT GANESAN, University of Texas at Austin — The unique architecture of dendrimers has attracted interest in a wide-variety of biomedical applications such as drug delivery. Dendrimers act as covalent micelles and have been shown experimentally to internalize hydrophobic molecules inside their cavities. Moreover, many drugs of low water solubility are weakly acidic and have been shown to form complexes with polybasic dendrimers, with the encapsulation ability being dependent upon the solution pH. Furthermore, the grafting of neutral water soluble chains such as polyethylene glycol (PEG) have shown to increase the encapsulation of poorly soluble drug molecules. In order to gain insight into the equilibrium behavior of drug-dendrimer complexes, we have developed and numerically solved a Self-Consistent Field Theory approach for both grafted and non-grafted annealed charged dendrimer molecules in the presences of drug molecules. Specifically, this work examines the effect of drug size, dendrimer generation, grafting chain length, and solution pH upon dendrimer encapsulation abilities.

9:12AM A48.00007 Structure-Property Relationships in Precise Acid-Containing Polymers ,

FRANCISCO BUITRAGO, University of Pennsylvania, KATHLEEN OPPER¹, KENNETH WAGENER, University of Florida, KAREN WINEY, University of Pennsylvania, KAREN WINEY'S LAB TEAM, KENNETH WAGENER'S LAB TEAM — Acid-containing polymers have specific interactions that produce complex and hierarchical morphologies providing a remarkable combination of mechanical properties, namely being both dissipative and resilient. Despite the widespread industrial use of such materials, rigorous structure-property relationships remain elusive due to structural heterogeneity in the available copolymers. Recently, linear polyethylenes with pendent acid groups separated by a precisely controlled number of carbon atoms have been synthesized by acyclic diene metathesis (ADMET) polymerization. X-ray scattering shows that the molecular uniformity of these acid copolymers results in morphologies with nearly monodisperse acid aggregates and polyethylene crystals assembled in highly organized hierarchical structures. Taking advantage of these ordered morphologies to obtain well-defined mechanical data, we probe the elastic modulus, yield stress and second yield stress of precise acid-containing polymers as a function of the number of carbon atoms between acid groups, acid type (acrylic and phosphonic), and mono- or geminal acid functionalization.

¹Currently at DuPont, Wilmington, DE

9:24AM A48.00008 ABSTRACT HAS BEEN MOVED TO S1.00320 —

9:36AM A48.00009 Block copolymer ion gels for gas separation , YUANYAN GU, Department of Chemistry,

University of Minnesota, TIMOTHY LODGE, Department of Chemistry and Department of Chemical Engineering and Materials Science, University of Minnesota — Carbon dioxide removal from light gases (eg. N₂, CH₄, and H₂) is a very important technology for industrial applications such as natural gas sweetening, CO₂ capture from coal-fire power plant exhausts and hydrogen production. Current CO₂ separation method uses amine-absorption, which is energy-intensive and requires frequent maintenance. Membrane separation is a cost-effective solution to this problem, especially in small-scale applications. Ionic liquids have recently received increasing interest in this area because of their selective solubility for CO₂ and non-volatility. However, ionic liquid itself lacks the persistent structure and mechanical integrity to withstand the high pressure for gas separation. Here, we report the development and gas separation performances of physically crosslinked ion gels based on self-assembly of ABA-triblock copolymers in ionic liquids. Three different types of polymers was used to achieve gelation in ionic liquids. Specifically, a triblock copolymer ion gel with a polymerized ionic liquid mid-block shows performances higher than the upper bound of well-known "Robeson Plot" for CO₂/N₂.

9:48AM A48.00010 Transport and phase behavior in anion-conducting diblock copolymers ,

GUILLAUME SUDRE, Lawrence Berkeley National Laboratory, SEBNEM INCEOGLU, University of California, Berkeley , NITASH BALSARA, UC Berkeley and LBNL — Anion-exchange membranes can be used in various applications such as direct methanol fuel cells or devices for artificial photosynthesis. Consequently, these membranes have to conduct the anions efficiently, remain insoluble in water or methanol, and be impermeable to various gases. Block copolymers are good candidates to reach these aims. Their ability to self-assemble, particularly into bi-continuous phases, makes it possible to use one polycationic block that would conduct the anions, while a second neutral block can be designed as a structural block to insure the mechanical stability of the system. Our study focuses on the relationship between phase behavior and anion conductivity of diblock copolymers as a function of molecular weight, composition and cationic groups. We have chosen to use a model system made of styrene for the neutral block, and of chloromethylstyrene for the second block since it is easily cationizable with various functionalities, reacting easily with e.g. trimethylamine or n-butylimidazole. This model system is synthesized by nitroxide-mediated radical polymerization with molecular weights between 2 to 40 kg/mol and fractions of chloromethylstyrene in the range of 15-40 mol%. The results obtained from small-angle X-ray scattering showed lamellar morphologies for most systems. The temperature-dependence of the conductivity was assessed by performing measurements on membranes that were either immersed in water or in a controlled atmosphere at 98% of relative humidity.

10:00AM A48.00011 Polyelectrolyte Uptake by PEMs at High Salt¹ , DAVID HOAGLAND, Dept. of Polymer

Sci. and Eng., Univ. of Massachusetts Amherst, ZHAOHUI SU, BO PENG, XINGJIE ZAN, State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry — Upon a jump in salt concentration, a polyelectrolyte multilayer (PEM) constructed by the layer-by-layer process will swell, and in consequence, uptake from solution a large additional mass of the capping polyelectrolyte. Here, swelling and uptake are monitored in time by the quartz crystal microbalance with dissipation (QCM-D) method as a function of elevated salt concentration (0.75M<[NaCl]<2.5 M) during the uptake of poly(styrene sulfonate) (PSS, MW~70,000 g/mol) by poly(diallyldimethylammonium chloride)/PSS PEMs made at [NaCl]=0.5M. For [NaCl] less than ~1 M, PSS adds only at/near the PEM surface, while for higher [NaCl], PSS fully permeates the PEM, contributing a PSS mass approaching, even exceeding, that already present; higher salt concentration leads to faster and greater PSS uptake. Above [NaCl]=1.0 M, uptake is diffusive, characterized by surprisingly large and sharply [NaCl]-dependent diffusion coefficients (~10⁻¹⁴ – 10⁻¹² cm²/s). This uptake process opens a general opportunity for facile bulk and surface modifications of PEMs.

¹D.H. acknowledges support of the NSF-sponsored Univ. of Massachusetts MRSEC and Z.S. acknowledges support of the National Natural Science Foundation of China (50921062)

10:12AM A48.00012 Polyelectrolytes in Salt Solutions: Molecular Dynamics Simulations ,

ANDREY DOBRYNIN, JAN-MICHAEL CARRILLO, University of Connecticut — We performed MD simulations of polyelectrolyte solutions in the presence of salt. Polyelectrolyte solutions were modeled as an ensemble of chains of charged LJ particles with explicit counterions and salt ions. Our simulations have shown that in dilute and semidilute polyelectrolyte solutions the electrostatic chain persistence length scales with ionic strength as $I^{-1/2}$. This is due to counterion condensation on the polymer backbone. In dilute polyelectrolyte solutions the chain size decreases with increasing salt concentration as $R \propto I^{-1/5}$, which is in line with the scaling of the persistence length on the ionic strength, $l_p \propto I^{-1/2}$. In semidilute solution at low salt concentrations the chain size decreases with increasing polymer concentration, $R \propto c_p^{-1/4}$, while at high salt concentrations it is, $R \propto I^{-1/8}$. Our simulations confirmed that the peak position in the polymer scattering function scales with the polymer concentration in dilute polyelectrolyte solutions as $c_p^{1/3}$. In semidilute polyelectrolyte solutions at low salt concentrations the peak shifts towards larger values of $q^* \propto c_p^{1/2}$ while at high salt concentrations the peak location depends on the ionic strength as $I^{-1/4}$. The simulations confirmed a general scaling relations between a quantity $X(I)$ in salt solutions and corresponding quantity $X(I_0)$ in salt-free solutions, $X(I) = X(I_0)(I/I_0)^\beta$ with exponents; $\beta=-1/2$ for persistence length l_p , $\beta=1/4$ for solution correlation length, $\beta=-1/5$ and $\beta=-1/8$ for chain size R in dilute and semidilute solution, respectively.

10:24AM A48.00013 Electrostatic persistence length of flexible polyelectrolytes: resolving the controversy between theory and experiments , WEI QU, ERIK LUIJTEN, Northwestern University — The salt concentration

dependence of the electrostatic persistence length l_e of flexible polyelectrolytes has been the subject of extensive debate over the past two decades. Although theoretically a consensus has been reached regarding the correctness of the extension by Khokhlov and Khachaturian (KK) of the well-known Odijk-Skolnick-Fixman (OSF) theory to flexible polyelectrolytes, one crucial question remains: the strong disagreement between the OSF-KK prediction and various experimental observations. We present the results of extensive simulations of a flexible polyelectrolyte in solution to elucidate the origin of this discrepancy, and demonstrate that it originates from neglecting ionic excluded volume in the theoretical treatment.

10:36AM A48.00014 Layer-by-Layer Assembly of Charged Nanoparticles on Porous Substrates: Molecular Dynamics Simulations¹, JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, Institute of Materials Science and Department of Physics, University of Connecticut — We performed molecular dynamics simulations of multilayer assembly of oppositely charged nanoparticles on porous substrates with cylindrical pores. The film was constructed by sequential adsorption of oppositely charged nanoparticles in layer-by-layer fashion from dilute solutions. The multilayer assembly proceeds through surface overcharging after completion of each deposition step. There is almost linear growth in the surface coverage and film thickness during the deposition process. The multilayer assembly also occurs inside cylindrical pores. The adsorption of nanoparticles inside pores is hindered by the electrostatic interactions of newly adsorbing nanoparticles with the multilayer film forming inside the pores and on the substrate. This is manifested in saturation of the average thickness of the nanoparticle layers formed on the pore walls with increasing number of deposition steps. The distribution of nanoparticles inside cylindrical pore was nonuniform with significant excess of nanoparticles at the pore entrance.

¹NSF # DMR-1004576

10:48AM A48.00015 Diffusion of Polyelectrolyte Chains within Multilayer Films, SVETLANA SUKHISHVILI, LI XU, ALIAKSANDR ZHUK, Stevens Institute of Technology, NJ 07030, JOHN ANKNER, Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — Using a series of polycations synthesized by atom transfer radical polymerization, we investigate the relative importance of the effects of hydrophobicity, polymer charge density, and steric hindrance to charge pairing on chain dynamics within polyelectrolyte complexes (PECs) and within polyelectrolyte multilayer (PEM) films. First, by applying fluorescence correlation spectroscopy (FCS), ellipsometry and fluorescence recovery after photobleaching (FRAP), we found that the dynamics of chain exchange within PECs is directly correlated with the mode (linear vs. exponential) of PEM film growth. Second, through a combination of neutron reflectometry (NR) and FRAP techniques to the same PEM types, we found that diffusion of polyelectrolyte chains within multilayer films is highly anisotropic, with diffusion coefficients being 10^4 - 10^5 higher in a direction parallel to the substrate compared to that perpendicular. Chain mobility was also controlled by ionic strength of annealing solutions and steric hindrance to ionic pairing of interacting polyelectrolytes.

This work was supported by the National Science Foundation under Award DMR-0906474 (S.S.). Neutron measurements were performed at the Spallation Neutron Source at the Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the DOE under contract No. DE-AC05-00OR22725.

Monday, February 27, 2012 8:00AM - 11:00AM –
Session A49 DPOLY: Focus Session: Long-time, Entangled Dynamics in Polymers - Linear, Transient, Non-linear Rheology, Tubes 162A

8:00AM A49.00001 Microscopic theory of the tube confinement potential and relaxation of entangled needle liquids under stress, DANIEL SUSSMAN, KEN SCHWEIZER, University of Illinois at Urbana-Champaign — We have developed a first-principles theory of the transverse confinement potential in an entangled needle fluid based on exactly enforcing uncrossability at the two-rod level while self-consistently renormalizing many-particle effects [Sussman & Schweizer PRL 107, 078102 (2011); J. Chem. Phys. 135, 131104 (2011)]. The predicted tube radius and long-time diffusion constant are consistent with the asymptotic reptation scaling laws under quiescent conditions, but in contrast with the usual tube model strong anharmonicities soften the confinement potential in a manner that quantitatively agrees with experiments on heavily entangled F-actin solutions. This weakening of entanglement constraints has multiple dramatic consequences under applied deformation: tube dilation, accelerated reptation, reduction of the transverse entropic barrier, and a critical stress or strain beyond which tube localization is destroyed. The degree-of-entanglement-dependent competition between reptative and transverse-hopping relaxation is established as a function of stress and strain. A mapping between rigid rods and flexible chain systems is also proposed, allowing predictions to be made for the tube diameter, entanglement onset, and transport properties of chain polymer liquids.

8:12AM A49.00002 Rheology of linear monodisperse polyethylene melts from atomistic Molecular Dynamics simulations¹, NIKOS KARAYIANNIS, Institute of Optoelectronics and Microsystems (ISOM) and ETSII, Polytecnic University of Madrid (UPM), Spain, JORGE RAMIREZ, Department of Chemical Engineering, ETSI Industriales, Polytecnic University of Madrid (UPM), Spain, ALEXEI LIKHTMAN, Department of Mathematics, University of Reading, United Kingdom — In our contribution we present results from very long, Molecular Dynamics simulations of linear monodisperse polyethylene (PE) chains with lengths ranging from 0.5 to 18 entanglements. We adopt a hierarchical modeling approach: in the first step we employ Monte Carlo simulations consisting of chain-connectivity altering algorithms to ensure full scale equilibration. Secondly, massive parallel MD simulations are conducted in the canonical ensemble. Besides the standard dynamical information, the stress relaxation curves are calculated for all PE systems. By bridging present atomistic results with the tube theory through the newly-introduced slip-spring model [Likhtman, Macromolecules 38, 6128 (2005)] we are able to calculate the plateau modulus and viscosity for well entangled, industrially relevant PE melts. In all cases, comparison between available experimental data and present simulation findings reveals a very good to excellent agreement. The proposed multi-scale methodology is generally applicable and can be extended to polymers of different molecular architecture and chemical constitution, as well as blends and more complex interfacial systems.

¹We acknowledge support by MICINN through project MAT2010-15482. NCK acknowledges support through projects “Ramon y Cajal” and “I3.”

8:24AM A49.00003 Intermolecular constraints in the dynamics of semiflexible entangled polymer melts, MARINA GUENZA, University of Oregon — We present a Langevin equation for the contemporary dynamics of a group of interpenetrating semiflexible entangled polymer chains. The theory explicitly accounts for the intermolecular intermonomer repulsion between a pair of chains, generated by their inability to cross each other, i.e. the phenomenon of entanglements. The “effective” potential experienced by the chains arises from the repulsion between two monomers belonging to different chains, propagating through the chain connectivity, and the dynamics of chain interdiffusion and relaxation. With time the local hard-core potential is overcome by the relative motion of the polymers and the system relaxes. The same formalism applies to both unentangled and entangled melts. Short chains do not experience entanglements, because their relaxation process is faster than the average time that is necessary for the chain to diffuse a distance comparable to the mesh size, or length between two entanglements. Finally no a priori hypothesis has to be made about the processes that drive relaxation as the formalism is simply the conventional Rouse approach, generalized to treat the motion of interacting macromolecules, whose chains cannot cross each other.

8:36AM A49.00004 Long-Time Dynamics in Polymers: Experimental Results¹ , SINDEE SIMON, Department of Chemical Engineering, Texas Tech University — The long-time dynamics in several polymeric systems have been investigated with a focus on the relationship between the bulk and shear viscoelastic responses. Materials studied include polystyrene, a three-arm star polystyrene, and two polycyanurates of different crosslink densities. A custom-built pressurizable dilatometer has been used to measure the time-dependent bulk modulus, as well as the pressure-volume-temperature behavior in these materials. The temperature-dependent shift factors are used to test the TV⁷ thermodynamic scaling law proposed in the literature for segmental relaxation times. The thermodynamic scaling law successfully reduces the data for all of the materials; however, $T - T_g$ scaling also successfully reduces the data and differences in implications of the two scaling approaches will be discussed. Comparison of the retardation spectra for the bulk and shear responses shows that at extremely long times, the chain mechanisms available to the shear response are not available to the bulk; for times related to the glassy dynamics, the two responses have similar slopes, indicating that they may have similar underlying molecular mechanisms, but the magnitudes are different, a finding that remains to be explained.

¹Funding from the National Science Foundation DMR-0606500

9:12AM A49.00005 Tube Dynamics of Mildly Entangled Polymers: Semiflexibility Effects , JIAN QIN, SCOTT MILNER, Dept. of Ch. E. at Penn. State Univ., USA, PAVLOS STEPHANOPOULOS, Dept. of Math. & Stat. at Univ. of Cyprus, Cyprus, VLASIS MAVRANTZAS, Dept. of Ch. E. at Univ. of Patras, Greece — The prevailing theory of polymer rheology rests on a careful analysis of tube dynamics, tested by comparing predicted rheological response functions to experimental measurements. We provide a direct test of this theory by analyzing the tube dynamics of recently simulated mildly entangled polyethylene melt. The tube dynamics is obtained by defining the tube primitive path, *i.e.*, the tube center line, as the short-time average of molecular dynamics trajectories, and by monitoring how the tangent-tangent correlations evolve with time. It was found that the tube is semiflexible, and that the tube relaxation rate obtained from simulation results cannot be accounted for by the prevailing theory, since the effect of contour length fluctuations built into the theory is too strong. This discrepancy is particularly relevant to the mildly entangled system. To fix this, we incorporated semiflexibility into the theory, which was originally designed for flexible tubes, and found that the corrected theory describes the simulation results nearly quantitatively.

9:24AM A49.00006 A critical analysis of typical assumptions in the theory of entangled polymer dynamics in elongational flows , MARAT ANDREEV, RENAT KHALIULLIN, JAY SCHIEBER, Illinois Institute of Technology, Department of Chemical and Biological Engineering — The discrete slip-link model (DSM) was developed to describe the dynamics of entangled polymer melts of arbitrary chain architecture in arbitrary deformation. The model is able to predict linear viscoelasticity of monodisperse linear, polydisperse linear and star-branched systems. The model also shows good agreement with dielectric relaxation experiments. In this work we apply DSM to non-linear flows of monodisperse linear polystyrene and polyisoprene melts without any adjustable parameters. Model predictions for shear flow agree very well with experimental results. The DSM is able to capture the transient response as well as the steady state viscosity. However, for elongational flow, agreement is unsatisfactory at large strains. We explore a number of simplifications of the model and their effect on flow predictions, including: finite extensibility, convective constraint release and activation of dangling ends. Only after discarding all approximations and assumptions as a source of discrepancy between DSM predictions and experimental data can we conclude whether additional physics concepts are necessary to describe non-linear rheology of entangled polymer melts.

9:36AM A49.00007 Exploring the role of long-chain branching in large deformation of entangled melts , GENGXIN LIU, Department of Polymer Science , University of Akron, Akron, OH, United States, KWSTAS NTETSIKAS, APOSTOLOS AVGEROPOULOS, Department of Materials Science and Engineering, University of Ioannina, Ioannina, Greece, SHI-QING WANG, Department of Polymer Science , University of Akron, Akron, OH, United States, UNIVERSITY OF AKRON COLLABORATION, UNIVERSITY OF IOANNINA COLLABORATION — Most of our past studies have focused on nonlinear responses to large deformation of entangled polymers made of linear flexible chains. Little is known about nonlinear rheological behavior of entangled polymers containing long-chain branching (LCB), apart from the literature work on low-density polyethylene (LDPE). In this work, we present a first study to compare linear polyisoprene with a well-defined dendritic polyisoprene. Consistent with the extensional rheological behavior of LDPE, we find LCB to impede shear yielding so that the entanglement network could extend significantly more before failure during uniaxial extension. This study also investigated its shear deformation behavior to explain the absence of necking like failure in uniaxial extension. The research is funded, in part, by a grant from the National Science Foundation (DMR-1105135).

9:48AM A49.00008 Similarity and difference between simple shear and uniaxial extension of entangled polymers¹ , HAO SUN, SHI-QING WANG, Department of Polymer Science, University of Akron — There is ample evidence to show that the essential physics governing yielding of entangled polymers is the same, independent of the mode of deformation, *e.g.*, shear versus extension. In either of these two most commonly studied forms of deformation, the elastic retraction force associated with the chain deformation cannot grow without bound during continuous deformation. In practice, a transition from the initial dominantly elastic deformation to flow (irreversible deformation) inevitably takes place. Such yielding can produce strain localization in large deformation of well entangled polymer melts. Apart from the superficial difference related to the confusion about the “strain hardening” behavior, a true difference in the respective responses of entangled melts to shear and extension arises when the strain rate is sufficiently high. The entanglement network can still yield on its path to the eventual flow state upon startup shear. However, startup extension could cause the entanglements to lock in, and the melt undergoes rubber-like rupture instead of yielding. This presentation raises the question of whether shear is an intrinsically different deformation from uniaxial extension in the extremely high rate limit.

¹The research is funded, in part, by a grant from the National Science Foundation (CMMI-0926522).

10:00AM A49.00009 Large-deformation and long-time behavior of entangled melts in complex geometries , XIANGYANG ZHU, SHI-QING WANG, University of Akron — Recent particle-tracking velocimetric (PTV) observations have revealed strain localization either during startup shear beyond the stress overshoot or after a large step shear of entangled polymers [*e.g.*, *Macromolecules*, **42**, 6261 (2009)]. The physical pictures leading to these decohesion events have been put forward [J. Chem. Phys. **127**, 064903(2007); J. Rheol. **53**, 1389 (2009)]. In this presentation we apply the particle-tracking velocimetric method [Macromol. Mater. Engr. **292**, 15 (2007)] to study similar strain localization phenomena originating from yielding of the entanglement network in other forms of deformation including uniaxial extension, “squeeze flow” and extrusion of polymers from a wide open space into a narrow opening. The striking discontinuities in the velocity profile can all be understood in terms of a shear yielding criterion. The research is funded, in part, by a grant from the National Science Foundation (CMMI-0926522)

10:12AM A49.00010 Barrier to chain retraction: where we are six years after the first report of shear inhomogeneity in entangled polymers?¹, SHI-QING WANG, POUYAN BOUKANY, YANGYANG WANG, SHIWANG CHENG, Polymer Science, University of Akron — At APS2006, we reported the first PTV observations of macroscopic motions after shear cessation from step strain on an entangled polybutadiene solution (Macromolecules **2007**, 40, 8031). Since then we have shown that the classical polystyrene solutions display similar non-quiescent relaxation, invalidating the agreement between the data based on PS solutions and the Doi-Edwards damping function. Based on polymer melts we found that this network breakup phenomenon also occurs after a step strain produced with a rate that according to the tube model is too low to generate chain stretching (Macromolecules **2009**, 42, 6261). Does the current tube model possess the necessary ingredients to depict these findings? Here we present new experimental data that further supports the concept of a finite cohesion level for the entanglement network: There is a finite confining force that keeps chains engaged in the network, ensures the structural integrity and allows linear response behavior to take place. In contrast, the tube model perceives barrier-free chain retraction on the Rouse time for any amount of imposed strain, which would necessarily lead to destruction of the original network. Our experiments show that this does not appear to be the case.

¹This work is supported, in part, by a grant from NSF (DMR-0804726).

10:24AM A49.00011 Neutron Reflectivity Study of Interdiffusion of Ionomers into Van der Waals Polymer Thin Films, THUSITHA ETAMPAWALA, DILRU RATNAWEERA, SIDATH WIJESINGHE, DVORA PERAHIA, Department of Chemistry, Clemson University, Clemson, SC, JAROSLAW MAJEWSKI, Lujan Neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, NM — The slow dynamic processes in amorphous ionic polymers are affected by physical cross-links resulting from clustering of the ionic groups. Therefore in addition to entanglement barriers, the motion of the polymers is coupled to the dynamics of the ionic clusters where the resulting dynamics is an interplay between the effects of the two types of barriers. Using neutron reflectometry we have probed a model system where interfacial diffusion of a Van der Waals polymer, polystyrene, into its sulfonated analogs. Results controlling the molecular weights that determine the overall number of entanglements as well as the degree of sulfonation which affects the strength and number of the ionic clusters will be presented. Comparison to the diffusion of polystyrene into polystyrene will resolve the effects of the ionic clusters from those of entanglements. The presence of the physical cross-links slows down the dynamics significantly with respect to that of polystyrene and an asymmetric process where the non-ionic blocks migrate into the ionic one is observed. Further rearrangements take place at a later stage.

10:36AM A49.00012 Development of Interfacial Strength and Entanglements During Welding of Polymers, TING GE, MARK O. ROBBINS, Johns Hopkins University, FLINT PIERCE, GARY S. GREEST, Sandia National Laboratories, DVORA PERAHIA, Clemson University — Thermal welding is a common means of joining polymer parts. Interfacial strength increases with welding time t_w as polymer chains diffuse across the interface. The microscopic origin of this interfacial strength enhancement was investigated with large scale molecular simulations employing a coarse-grained bead-spring model. Polymer surfaces were held together at a temperature well above the glass transition temperature T_g . States at t_w up to 10^9 time steps were then quenched to a temperature below T_g for mechanical tests. We test the interfacial strength by shearing the weld along a direction parallel to the interface. The maximum shear stress $\sigma_{\max}$ before failure is used to characterize the interfacial strength. We find that $\sigma_{\max}$ increases as $t_w^{1/4}$ before saturating to its bulk value. This agrees with previous experiments by a lap-joint shear method [1]. In addition, our analysis shows that the dominant shear failure mode changes from chain pull-out at the interface for small t_w , to chain scission for large t_w . We examine the average contour length $\langle l \rangle$ of chains that have diffused across the interface. As predicted by the reptation dynamics, $\langle l \rangle$ increases as $t_w^{1/4}$. We also track the evolution of entanglements using the *Primitive Path Analysis* (PPA) algorithm [2]. Our results show that the total number of interfacial entanglements is directly related to interfacial strength and also increases as $t_w^{1/4}$.

[1] D. B. Kline, R. P. Wool, *Polym. Eng. Sci.* 1988, 28(1), 52–57.

[2] R. Everaers *et al.*, *Science*, 303, 823–826, 2004

10:48AM A49.00013 Using the parallel plates geometry for nonlinear rheological measurements, ZAHRA FAHIMI, Institute for Complex Molecular Systems and Department of Mechanical Engineering, Eindhoven University of Technology, 5600 MB Ein, The Netherlands, CHASE P. BROEDERSZ, Lewis-Sigler Institute for Integrative Genomics and the Department of Physics, Princeton University, Princeton, NJ 08544, USA, HANS M. WYSS, Institute for Complex Molecular Systems and Department of Mechanical Engineering, Eindhoven University of Technology, 5600 MB Ein, The Netherlands — Conventional wisdom dictates that studying the mechanical response of viscoelastic materials in the nonlinear regime should be done either with a cone-plate or a Couette geometry, where the applied strain is homogeneous in the measuring volume. However, the use of parallel plates would have important advantages in a wide range of applications. For instance solid-like hydrogel materials can often be processed readily into flat films. We show that the nonlinear viscoelastic behavior can also be obtained from measurements in a parallel plate geometry. By tracing the torque response and its derivative with respect to the applied strain, we obtain a general stress strain relation, which indeed captures the proper material behavior. The approach does not require any assumptions for the material's viscoelastic behavior. We show practical examples different classes of soft materials to illustrate that our approach enables access to the full nonlinear response of these materials, including the detailed shape of the stress response in large amplitude oscillatory shear measurements. Our approach should be applicable to a wide range of soft materials, including hydrogels, colloidal suspensions, or biological tissues.

Monday, February 27, 2012 8:00AM - 10:48AM –

Session A50 DPOLY: Liquid Crystalline Order in Polymers, Soft Matter, and Complex Fluids

162B

8:00AM A50.00001 Shape Memory as a Process: Optimizing Polymer Design for Shape Recovery, RICHARD VAIA, HILMAR KOERNER, KYUNGMIN LEE, ROBERT STRONG, MATTEW SMITH, HUABIN WANG, TIM WHITE, LOON-SENG TAN, Air Force Research Laboratory — Shape memory is a process that enables the reversible storage and recovery of mechanical energy through a change in shape. Polymers provide a unique alternative to kinematic designs and other materials (e.g. metallic alloys) for applications requiring large deformation and novel control options. The effect control of storage and relaxation of strain energy associated with chain deformation depends on the nonlinear visco-elastic behavior and glassy dynamics of the polymer network. Considering the molecular understanding of rubbery elasticity, chain entanglements in concentrated polymer liquids, affine deformation of networks, and glass fragility, heuristic guidelines can be formulated to optimize the molecular design of a polymer for shape memory. These are applied to the development of a polymer system for shape memory processes at high-temperature (200°C). The low-crosslink density polyimide exhibits very rapid shape recovery, excellent fixity, high creep resistance, and good cyclability. Furthermore, the molecular design affords a very narrow temperature range for programming and triggering shape change that can also be accessed by photo-isomerization of the cross-link nodes.

8:12AM A50.00002 Shape and Memory in Liquid Crystalline Elastomers, ANSELM GRIFFIN, WANTING REN, PHILIP MCMULLAN, WHITNEY KLINE, MOHAN SRINIVASARAO, Georgia Tech — As part of an ongoing effort to understand the origins of shape memory in liquid crystalline elastomers (LCE), we have synthesized and examined a series of SmC main-chain LCEs. Uniaxial stretching of these polydomain films at room temperature produces a monodomain structure that can, upon removal of load, retain the monodomain and a significant level of strain. Although these films show ordinary elastic response at temperatures near the isotropization (clearing) temperature, at room temperature – far below the clearing temperature – the mechanical response is anelastic. Experimental studies of isothermal strain recovery vs time after unloading will be presented along with details of the temperature profile for strain recovery of these LCEs. A rationale for the shape memory behavior is proposed that involves moving of crosslink points in the smectic lamellar arrangement during the stretching event and trapping of these crosslinks in different positions at low temperatures. This trapping is driven by the chemical segregation of the crosslink points from the mesogenic unit which can be thermally overcome at elevated temperatures allowing full elastic recovery.

8:24AM A50.00003 Phase Behavior of Disk-Coil Macromolecules, YONGJOO KIM, EDWARD HA, ALFREDO ALEXANDER-KATZ, MIT — We explore the self-assembly of disk-coil macromolecules using Monte Carlo simulations in the NPT ensemble. Our study focuses on the role that coil length compared to the size of the disk has on the phase behavior of the system as well as the effect of stacking interactions between the disks. As a function of temperature T , we find a disordered phase at high T and lamellar, perforated lamellar, and cylinder phases at intermediate T . If we further lower the temperature, the disk-rich regions spontaneously order, and we find ordered lamellar, ordered perforated lamellar, and ordered cylinder phases depending on the strength of the stacking interactions. The appearance of any of these phases is, however, strongly dependent on the length of the coil. In addition to constructing a comprehensive phase diagram, we further analyze the correlations in the system, as well as the director vector field of the disks, and use it to construct an order parameter. We show that the latter changes drastically at the ordering transition points. We find that the ordered cylinder phase has a high degree of parallel packing. Our results are important to understand the self-assembly of supramolecular structures of disk-coil amphiphiles that are ubiquitous in nature, such as the chlorophyll molecule.

8:36AM A50.00004 Liquid Crystal Phases of Semiflexible Polymers, IAN MACKAY, DON SULLIVAN, University of Guelph — Liquid crystal polymers exhibit orientational order (nematic phase) and position order (smectic phase). Previous work on semiflexible polymers using self-consistent field theory studied the isotropic-nematic and nematic-smectic transition for homogenous and diblock copolymers. The nematic phase is stabilized by excluded-volume effects between wormlike cylindrical segments. The smectic phase is further stabilized by excluded-volume effects between terminal end segments. Because models of semiflexible polymers include orientational degrees of freedom, in addition to the usual positional degrees of freedom, they are computationally more demanding to study. Spectral decomposition applied to segment orientations has previously been used to make computation feasible. However this method does not converge well for strongly ordered states, which arise in many real systems. I describe a Crank-Nicolson finite difference method applied to the orientations which is expected to converge well for highly ordered systems. This method also exhibits better numerical stability and accuracy and may thus serve as a better foundation for further studies of highly ordered systems. I also describe a modification to the spectral method which can compute the tilted Smectic C phase.

8:48AM A50.00005 Photomechanical mechanism and structure-property considerations in the generation of photomechanical work in glassy, azobenzene liquid crystal polymer networks, KYUNG MIN LEE, Air Force Research Laboratory, Wright-Patterson AFB, NELSON TABIRYAN, BEAM Engineering for Advanced Measurements Company, TIMOTHY BUNNING, TIMOTHY WHITE, Air Force Research Laboratory, Wright-Patterson AFB — Azobenzene-containing polymeric materials have shown shape adaptive responses when irradiated with light. We contrast the photogenerated mechanical response of glassy, polydomain azobenzene liquid crystal polymer networks (azo-LCN) upon exposure to either UV or blue-green irradiation. The profound differences in the fundamental photomechanical response to exposure to light in these wavelength regimes are dictated by distinctive photochemical mechanisms, elucidated through UV/VIS spectroscopic examination of the materials before and after irradiation with UV and blue-green light. The glassy, photoresponsive polymeric materials were subjected to structure-property examination to ascertain the role of crosslink density, azobenzene concentration, and azobenzene connectivity (crosslinked or pendant) on the photomechanical output.

9:00AM A50.00006 Surface wrinkling in liquid crystal elastomer bilayers¹, ADITYA AGRAWAL, Rice University, PAUL LUCHETTE, Kent University, WALTER CHAPMAN, Rice University, PETER MUHORAY, Kent University, RAFAEL VERDUZCO, Rice University — Mechanically-induced surface wrinkling patterns, also known as strain-induced elastic buckling instability for mechanical measurements (SIEBIMM), represent a versatile and high throughput technique for thin film metrology. However, the technique requires clamping and mechanically straining bilayer samples, which can introduce errors and present challenges with small samples. Here, we present a modified approach in which thin films are deposited on top of a stimuli-responsive liquid crystal elastomer (LCE). Temperature changes induce a spontaneous and controllable shape-change in the LCE substrate, without the need for clamping or mechanically straining. We show that LCE bilayers can be used to accurately measure the modulus of nanoscale poly(styrene) films, down to 20 nm thick films. Furthermore, the surface wrinkle orientation can be controlled using different preparation methods and reoriented in a single sample with temperature changes only. In the case of thick (over 500 nm) PS films, the bilayer flexes in response to temperature changes. This work shows that LCE bilayers are useful systems for thin film metrology and controlled assembly using well-defined surface structures.

¹This work was supported by the Welch Foundation for Chemical Research

9:12AM A50.00007 Field-induced orientational order of liquid crystals in random environments¹, LENA LOPATINA, JONATHAN SELINGER, Liquid Crystal Institute, Kent State University — Over the last twenty years, there has been extensive theoretical and experimental work on liquid crystals in disordered polymer networks and other random environments. It was shown that the disordered environment disrupts the long-range order of the liquid crystal. Recently, D.-K. Yang has performed new experiments, in which an electric field is applied to the polymer-disordered liquid crystal, leading to a large Kerr effect, i.e. field-induced long-range orientational order [1]. This experimental approach offers new opportunities for liquid-crystal displays. To understand the experiments and improve the applications, we perform Monte Carlo simulations of a nematic liquid crystal in a disordered polymer network. These simulations show the formation of randomly oriented domains of uniform directors. We study the response to an applied field by calculating the Kerr coefficient for variable system parameters. Furthermore, using an Imry-Ma-like approach we predict the domain size as a function of temperature and material properties of the system, and estimate the induced orientational order parameter due to an electric field. The simulations and analytic results agree well with each other and with the experiments.

[1] Y.-C. Yang and D.-K. Yang, Appl. Phys. Lett. 98, 023502 (2011).

¹This work was supported by NSF DMR-1106014.

9:24AM A50.00008 Highly viscous liquid crystalline mixtures: the alternative to liquid crystalline elastomers, PETR SHIBAIEV, CRISTINA SCHLESIER, LEAH NEWMAN, SCOTT MCDONALD, Fordham University, Department of Physics — Novel highly viscous liquid crystalline materials based on mixtures of glass forming oligomers and low molar mass liquid crystals were recently designed [1, 2] and studied. In this communication the novel data are presented, the analysis and discussion are extended. It is shown that viscoelastic properties of the materials are due to the physical entanglements between cyclic oligomers and low molar mass mesogens, not due to the chemical crosslinks between molecular moieties. However, the mechanical properties of these viscoelastic materials resemble those of chemically crosslinked elastomers (elasticity and reversibility of deformations). The properties of chiral and non-chiral materials loaded with ferromagnetic nanoparticles are discussed in detail. Cholesteric materials undergo gigantic color changes in the wide spectral range under the deformation that allows distant detection of deformation and determination the anisotropy of deformation and its type. The materials doped with laser dyes become mechanically tunable lasers themselves and emit coherent light while pumped by external laser. A simple model is suggested to account for the observed effects; physical properties of the novel materials and liquid crystalline elastomers are compared and discussed.

[1] P.V. Shibaev, C. Schlesier, R. Uhrlass, S. Woodward, E. Hanelt, Liquid Crystals, 37:12, 1601-1604

[2] P.V. Shibaev, P. Riverra, D. Teter, S. Marsico, M. Sanzari, V. Ramakrishnan, E. Hanelt, Optics Express, 16, 2965 (2008)

9:36AM A50.00009 Linear aggregation and liquid crystalline ordering: from semi-flexible polymers to rigid rods¹, TATIANA KURIAKOVA, Brown University, ZACH KOST-SMITH, M.D. BETTERTON, MATTHEW A. GLASER, Colorado University, Boulder — Reversible self-assembly of filamentous aggregates is ubiquitous in soft matter and biophysics. Examples include worm-like micelles, patchy colloids, chromonic liquid crystals, DNA and RNA, and protein polymers and fibrils. These rod-like aggregates can form liquid-crystal (LC) phases; the liquid-crystal order then couples to the aggregation, promoting the formation of longer aggregates in the LC phases. We study the coupled aggregation and liquid crystalline ordering of a minimal system of sticky cylinders that interact primarily by hard-core interactions but can stack and bind end to end, making use of both analytic theory and Monte Carlo simulation. Accurate treatment of aggregate flexibility is essential for quantitative comparison of theoretical and experimental phase diagrams and other properties. Our analytic model describes aggregates as wormlike chains in an effective aligning nematic field, and allows self-consistent determination of this field within a density functional theory formalism over a broad range of aggregate flexibilities. We compare the analytic results for isotropic-nematic phase equilibrium with simulations performed in our group as well as similar work from the Sciortino group [De Michele et al., arXiv:1108.6135].

¹This work was supported by NSF MRSEC Grant DMR-0820579, NSF Grant DMR-087685, and by the ICAM Branches Cost Sharing Fund.

9:48AM A50.00010 Liquid Crystal Elastomer Motors¹, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University, XIAOYU ZHENG, Dept. of Mathematical Sciences, Kent State University — Motors produce motion due to the transfer of energy, but not of momentum, to the device. In LCE motors, motion arises due to changes in the shapes of solid samples. Here we consider motors where the shape change is a bend, rather than an elongation or contraction. We focus on the light-driven motor of Ikeda et al.; we analyze in detail the physical mechanisms which bring about the motion, and discuss the momentum current which is generated. We present the results of numerical simulations, and compare these with experimental observations.

¹This work was supported under NSF DMR- 0606357.

10:00AM A50.00011 Orientational fluctuations of amorphous nematogenic solids, FANGFU YE, Georgia Institute of Technology, BING LU, University of Illinois at Urbana-Champaign, PAUL GOLDBART, Georgia Institute of Technology — Amorphous nematogenic solids (ANS) are media comprising rod-like nematogens that have been randomly linked to form elastically deformable macroscopic networks. Classes of ANS include chemical nematogen gels (i.e., networks of small molecules) and liquid crystalline elastomers (built from crosslinked nematogen-containing macromolecules), as well as biophysical networks such as those composed of actin filaments. We use a method inspired by the cavity approach to construct a replica free energy for these random systems, and investigate the correlations of the thermal fluctuations of the orientational alignment of the nematogens at spatially separated points. We identify two qualitatively distinct regimes: (a) a weakly localized regime, in which the correlations decay exponentially with separation; and (b) a strongly localized regime, characterized by correlations that also decay but oscillate as they do.

10:12AM A50.00012 ABSTRACT WITHDRAWN —

10:24AM A50.00013 Non-Monotonic Concentration Effects in the Phase Behavior and Nematic Orders: Mixtures of Side-Chain Liquid Crystalline Polymers and Low-Molecular-Weight Liquid Crystals¹, BILIN ZHUANG, ZHEN-GANG WANG, California Institute of Technology — Mixtures of side-chain liquid crystal polymers (SCLCPs) and low-molecular-weight liquid crystals (LMWLCs) are novel materials with applications such as optical data storage, non-linear optics, solid polymer electrolytes, chromatography and display materials. Recent experiments showed that the nematic-isotropic transition temperature and the nematic orders of each component vary non-monotonically with concentration. Existing theories, which combine the Flory-Huggins theory for isotropic mixing and the Maier-Saupe theory for nematic order, cannot explain such non-monotonicity. Here, we extend the existing theories by, first, incorporating the local steric constraints between the side-chain and the polymer backbone on the SCLCPs, and second, accounting for the crowding effects at high SCLCP concentrations. The new extended theory is able to resolve the discrepancies between the predictions of existing theories and the experimental observations.

¹This work is supported by an A*STAR fellowship.

10:36AM A50.00014 Effect of blending on nematic order in semiflexible polymers, KIRAN KHANAL, JUTTA LUETTNER-STATHMANN, Departments of Physics and Chemistry, University of Akron — Semiflexible polymers of sufficient stiffness exhibit liquid crystalline order at sufficient polymer concentrations. In this work, we investigate blends of flexible and semiflexible polymers with the aid of Monte Carlo simulations of a bond-fluctuation model. The model is an extension of Shaffer's bond-fluctuation model, where chain stiffness is controlled by including different forms of bending penalties, and includes attractive interactions between monomers. From simulations for a range of values of the bending energy, density, and temperature, we determine the effect of concentration of the flexible polymer on liquid crystalline order and domain formation.

Monday, February 27, 2012 8:00AM - 11:00AM —

Session A51 DCMP DFD: Colloids I: Beyond Hard Spheres Boston Convention Center 154

8:00AM A51.00001 Photonic Droplets Containing Transparent Aqueous Colloidal Suspensions with Optimal Scattering Properties, JIN-GYU PARK, SOFIA MAGKIRIADOU, Department of Physics, Harvard University, YOUNG-SEOK KIM, Korea Electronics Technology Institute, VINOTHAN MANOHARAN, Department of Physics, Harvard University, HARVARD UNIVERSITY TEAM, KOREA ELECTRONICS TECHNOLOGY INSTITUTE COLLABORATION — In recent years, there has been a growing interest in quasi-ordered structures that generate non-iridescent colors. Such structures have only short-range order and are isotropic, making colors invariant with viewing angle under natural lighting conditions. Our recent simulation suggests that colloidal particles with independently controlled diameter and scattering cross section can realize the structural colors with angular independence. In this presentation, we are exploiting depletion-induced assembly of colloidal particles to create isotropic structures in a millimeter-scale droplet. As a model colloidal particle, we have designed and synthesized core-shell particles with a large, low refractive index shell and a small, high refractive index core. The remarkable feature of these particles is that the total cross section for the entire core-shell particle is nearly the same as that of the core particle alone. By varying the characteristic length scales of the sub-units of such 'photonic' droplet we aim to tune wavelength selectivity and enhance color contrast and viewing angle.

8:12AM A51.00002 Curvature-Induced Capillary Interaction between Spherical Particles at a Liquid Interface¹, NESRIN SENBIL, CHUAN ZENG, BENNY DAVIDOVITCH, ANTHONY D. DINSMORE, University of Massachusetts Amherst — Capillary interactions among particles adsorbed at a fluid interface are important in a variety of natural and technological systems but still pose many mysteries. Capillary interactions induced by buoyancy, referred to as the "Cheerios" effect, have been studied for years. Here, we experimentally investigate how anisotropic interfacial shape affects capillary forces among millimeter-sized spheres. The Cheerios model predicts that particles with densities that are higher and lower compared to the fluids adsorbed at an initially flat interface will repel. Our experiments, however, clearly show that they can attract one another at the short range. We explain our results with a model, in which each sphere creates an anisotropic curvature at the position of the other sphere. To satisfy the constant contact-angle boundary condition, the interface is deformed with quadrupolar symmetry around each sphere. This quadrupolar deformation creates a short-ranged, attractive capillary force. The range of size and density ratios at which we observe a dominant short-range attraction is consistent with the model. Our results show how interfacial shape may be used to direct the assembly of interfacial particles.

¹Funded by the NSF-supported MRSEC on Polymer at UMASS(DMR-0820506)and NSF CBET-0967620.

8:24AM A51.00003 Using Micron-Sized Ellipsoids as a New Tool for Microrheology, DAVID C. KILGORE, KENNETH W. DESMOND, ERIC R. WEEKS, Emory University — Microrheology is a well-established technique, and in its simplest form it allows you to measure the viscosity of a fluid by examining the diffusion of microspheres, provided the diameter of the microspheres is known. We are developing a similar technique using ellipsoids, where the viscosity can be calculated without prior knowledge of the length and width of the ellipsoid. The asymmetry of ellipsoids provides a distinct advantage, allowing for the diffusion to be decomposed into two translational motions and one rotational motion. For each of these diffusive motions, we can measure a diffusion constant and relate the constant to the three unknowns: the length and width of the ellipsoid, and the viscosity. By measuring the three diffusion constants, we can determine the three unknowns. To verify this technique, we produce ellipsoids in the lab and suspend them in a viscous solution for three-dimensional imaging of the diffusion with a confocal microscope. We are able to get good agreement between the microrheological measurements and macroscopic viscosity measurements.

8:36AM A51.00004 Non-capillary binding of colloidal particles to liquid interfaces, DAVID KAZ, UC Berkeley, RYAN MCGORTY, UC San Francisco, VINOTHAN MANOHARAN, Harvard University — We observe colloidal polystyrene particles binding reversibly to an oil-water interface through the combination of a repulsive electrostatic force and an attractive van der Waals force. Previously studied interactions of an aqueous colloidal particle and a liquid interface have generally fallen into two categories: 1) electrostatic repulsion indicated by the dependence on salt and 2) capillary adsorption where surface tension brings the particle in contact with both phases and is indicated by practically irreversible binding. With our technique of pushing individual colloidal particles towards a planar oil-water interface and observing their motion in three-dimensions with holographic microscopy we have observed both interactions. However, our observations indicate that under certain conditions the electrostatic repulsion, which is due to repulsive image charges, is weak enough for a particle to experience a van der Waals attraction while strong enough to prevent a particle from penetrating the interface and becoming bound through capillary action. We observe individual particles transition between repulsive and attractive interactions with the interface suggesting that these colloidal particles have a heterogeneous surface charge.

8:48AM A51.00005 Memory effects in soap film arrangements, NICOLAS VANDEWALLE, STEPHANE DORBOLO, GEOFFROY LUMAY, JULIEN SCHOCKMEL, MARTIAL NOIRHOMME, GRASP, Institute of Physics B5a, University of Liege, B4000 Liege — We report experiments on soap film configurations in a triangular prism for which the shape factor can be changed continuously. Two stable configurations can be observed for a range of the shape factor h . A hysteretic behaviour is found, due to the occurrence of another local minima in the free energy. Experiments demonstrate that soap films can be trapped in a particular configuration being different from a global surface minimization. This metastability can be evidenced from a geometrical model based on idealized structures. Depending on the configuration, providing clues on the structural relaxations taking place into 3D foams, such as T1 rearrangements. The composition of the liquid is also investigated leading to dynamical picture of the transition. (Phys. Rev. E 83, 021403 (2011))

9:00AM A51.00006 Droplet-based microfluidics and the dynamics of emulsions, JEAN-CHRISTOPHE BARET, QUENTIN BROSSEAU, BENOIT SEMIN, XIAOPENG QU, Max-Planck Institute for Dynamics and Self-Organization, DROPLETS, MEMBRANES AND INTERFACES TEAM — Emulsions are complex fluids already involved for a long time in a wide-range of industrial processes, such as, for example, food, cosmetics or materials synthesis [1]. More recently, applications of emulsions have been extended to new fields like biotechnology or biochemistry where the compartmentalization of compounds in emulsion droplets is used to parallelise (bio-) chemical reactions [2]. Interestingly, these applications pinpoint to fundamental questions dealing with surfactant dynamics, dynamic surface tension, hydrodynamic interactions and electrohydrodynamics. Droplet-based microfluidics is a very powerful tool to quantitatively study the dynamics of emulsions at the single droplet level or even at the single interface level: well-controlled emulsions are produced and manipulated using hydrodynamics, electrical forces, optical actuation and combination of these effects. We will describe here how droplet-based microfluidics is used to extract quantitative informations on the physical-chemistry of emulsions for a better understanding and control of the dynamics of these systems [3].

[1] J. Bibette et al. Rep. Prog. Phys., 62, 969-1033 (1999)

[2] A. Theberge et al., Angewandte Chemie Int. Ed. 49, 5846 (2010)

[3] J.-C. Baret et al., Langmuir, 25, 6088 (2009)

9:12AM A51.00007 Pseudo-Steady Liquid Transport in Aqueous Foams during Filling of a Container, MICHAEL CONROY¹, RAMAGOPAL ANANTH², Naval Research Laboratory — Various applications of aqueous foams involve filling a container or a column (e.g., fractionation), where the foam is formed and processed. However, existing studies in the literature do not treat the filling stage and only describe liquid transport within a static foam bed. We developed a theory that predicts liquid loss from the foam and the liquid distribution within its interior during the filling and post-filling stages. During the filling stage, the theory predicts that the foam reaches a pseudo-steady state characterized by a time-independent drainage rate and liquid fraction. The pseudo-steady-state liquid fraction appears above a thin, liquid-saturated boundary layer that exists at the bottom of the foam bed. During the post-filling stage, the theory predicts that the drainage rate decreases with time, similar to static foams beds studied by others. The theory compares well with our previously reported volume-averaged macroscopic model and drainage measurements for dry (high-expansion) foams. We will show that drainage during the filling stage is significant when the fill time is comparable to the intrinsic drainage time scale of the foam.

¹This work was performed while M. W. Conroy was a NRC Postdoctoral Associate at NRL.

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9:24AM A51.00008 Coarsening of Two Dimensional Foams on a Curved Surface, ADAM ROTH, University of Pennsylvania, CHRIS JONES, Cornell University, DOUG DURIAN, University of Pennsylvania — We report on foam coarsening and statistics of bubble distributions in a closed, two dimensional, hemispheric cell of constant curvature. Using this cell it is possible to observe individual bubbles and measure their coarsening rates. Our results are consistent with the modification to von Neumann's law predicted by Avron and Levine. We observed the relative frequencies of bubbles with a given number of sides and found a shortage of bubbles with few sides as compared to a flat two dimensional cell. We also measured the value of $m(n)$, the average number of sides of an n sided bubble, and found general agreement with the Aboav-Weaire law, although there was greater deviation than for a flat cell.

9:36AM A51.00009 Analysis of emulsion stability in acrylic dispersions¹, SURESH AHUJA, Retired — Emulsions either micro or nano permit transport or solubilization of hydrophobic substances within a water-based phase. Different methods have been introduced at laboratory and industrial scales: mechanical stirring, high-pressure homogenization, or ultrasonics. In digital imaging, toners may be formed by aggregating a colorant with a latex polymer formed by batch or semi-continuous emulsion polymerization. Latex emulsions are prepared by making a monomer emulsion with monomer like Beta-carboxy ethyl acrylate (β -CEA) and stirring at high speed with an anionic surfactant like branched sodium dodecyl benzene sulfonates, aqueous solution until an emulsion is formed. Initiator for emulsion polymerization is 2-2'-azobis isobutyramide dehydrate with chain transfer agent are used to make the latex. If the latex emulsion is unstable, the resulting latexes produce a toner with larger particle size, broader particle size distribution with relatively higher latex sedimentation, and broader molecular weight distribution. Oswald ripening and coalescence cause droplet size to increase and can result in destabilization of emulsions. Shear thinning and elasticity of emulsions are applied to determine emulsion stability.

¹Xerox Corporation

9:48AM A51.00010 ABSTRACT WITHDRAWN —

10:00AM A51.00011 Dynamics of charged particles in nonpolar solvent in response to an electric field, TINA LIN, DAVID WEITZ, Harvard University — In nonpolar solvent, surfactant molecules aggregate to form charge-stabilizing reverse micelles. This enables surface charging of colloidal particles suspended in nonpolar solvent. We investigate the dynamics of such charged particles in response to an externally applied electric field. By combining microfluidics and confocal microscopy, we directly visualize the transport of particles between two parallel electrodes. We use direct visualization to measure the electrophoretic mobility of each particle and determine the effect of added surfactant on the measured mobility. In addition, we find that the presence of surfactant has a significant effect on the transport dynamics of the charged particles.

10:12AM A51.00012 Controlling Aggregation in Non-Polar Asphaltene Suspensions Through Electrostatics, SARA HASHMI, ABBAS FIROOZABADI, Yale University — Asphaltenes, the most aromatic and largest molecular weight components of petroleum fluids, can undergo a liquid-liquid phase transition in conditions including highly non-polar environments. Phase separation begins with molecular association and proceeds to and through the colloidal length-scale until complete sedimentation or deposition. Non-ionic polymeric dispersants can stabilize asphaltenes at the colloidal scale in non-polar suspensions. We perform a variety of experiments which suggest that stabilization occurs by adsorption of dispersant onto the asphaltenes, truncating the progress of precipitation. In particular, dynamic light scattering (DLS) and phase-analysis light scattering (PALS) measurements indicate that electrostatic repulsion is responsible for stabilizing asphaltene colloids against further aggregation. Aggregation time increases exponentially with dispersant concentration, as expected for particles interacting through a combination of attractive dispersion forces and repulsive electrostatics. However, contrary to current understandings of electrostatic stabilization in non-polar systems, the charges in colloidal asphaltene suspensions seem to arise from the asphaltene colloids themselves rather than from dispersant micelles.

10:24AM A51.00013 The Electric Double Layer Structure Around Charged Spherical Interfaces¹, ZHENWEI YAO, MARK BOWICK, XU MA, Syracuse University — We derive a formally simple approximate analytical solution to the Poisson-Boltzmann equation for the spherical system via a geometric mapping. Its regime of applicability in the parameter space of the spherical radius and the surface potential is determined, and its superiority over the linearized solution is demonstrated. In addition, the influence of nonuniform surface potential on the electric double layer structure is studied for large spheres in the weak potential limit.

¹This work was supported by the National Science Foundation grant DMR-0808812 and by funds from Syracuse University

10:36AM A51.00014 ABSTRACT WITHDRAWN —

10:48AM A51.00015 First experimental determination of permanent and induced electric dipolar moments of colloidal cellulose nanocrystals dispersed in apolar solvents¹, BRUNO FRKA-PETESIC, BRUNO JEAN, LAURENT HEUX, CERMAV-CNRS — Scientists and industrialists show a growing interest for cellulose nanocrystals (CNCs) since these rod-like nanoparticles display excellent mechanical properties that make them perfect candidates for the design of high performance biobased composites. Furthermore, CNCs can be obtained as colloidal suspensions in apolar solvents that form chiral nematic (cholesteric) liquid crystals. Our aim is to obtain homogeneous unidimensional structures to enhance the optical and/or mechanical properties of CNCs-based architectures at a macroscopic scale. Using electric fields, CNCs suspensions from either cotton or tunicate were successfully oriented in the direction of an electric field, in both AC and DC configurations. To probe the electric field induced orientation of the CNCs, a birefringence experimental set-up has been developed. While applying short electric DC field pulses, static and transient birefringence has been measured in diluted isotropic suspensions. From these measurements, we determined both the permanent and induced electric dipolar moments of the CNCs, whose effects appeared to be of the same order of magnitude. The results are discussed regarding to the CNC type and the apolar solvent used.

¹This work was supported by ANR-08-NANO-P235 BIOSELF

Monday, February 27, 2012 8:00AM - 11:00AM – Session A52 GSNP: Using Chaos to Control Quantum Systems 153C

8:00AM A52.00001 Regularization of tunneling rates in quantum chaotic systems, LOUIS PECORA, Naval Research Laboratory — Prototypical systems of two potential wells separated by a tunneling barrier exhibit the unexpected and counter-intuitive results that regular, non-chaotic systems have tunneling rates that fluctuate with energy dramatically over several orders of magnitude whereas the fully chaotic wells have orders of magnitude smaller fluctuations. All calculations were found from the Schrodinger equation using the Boundary Element Method. A random, plane wave theory explains the magnitude of the average tunneling rates as well as their fluctuations. We show that we can tune the amount of variance in tunneling rates by changing the shape of the quantum wells implying possible device design capabilities for nanodevices that operate in the electron ballistic regime.

8:36AM A52.00002 Relativistic quantum Darwinism in Dirac fermion and graphene systems, XUAN NI, Arizona State University, LIANG HUANG, Arizona State University; Lanzhou University, Gansu, China, YING-CHENG LAI, Arizona State University, LOUIS PECORA, Naval Research Laboratory — We solve the Dirac equation in two spatial dimensions in the setting of resonant tunneling, where the system consists of two symmetric cavities connected by a finite potential barrier. The shape of the cavities can be chosen to yield both regular and chaotic dynamics in the classical limit. We find that certain pointer states about classical periodic orbits can exist, which are signatures of relativistic quantum Darwinism (RQD). These localized states suppress quantum tunneling, and the effect becomes less severe as the underlying classical dynamics in the cavity is chaotic, leading to regularization of quantum tunneling. Qualitatively similar phenomena have been observed in graphene. A physical theory is developed to explain relativistic quantum Darwinism and its effects based on the spectrum of complex eigenenergies of the non-Hermitian Hamiltonian describing the open cavity system.

8:48AM A52.00003 Relativistic quantum chaos—an analytic Dirac equation approach¹, LIANG HUANG, HONGYA XU, School of Physical Science and Technology, Lanzhou University, YING-CHENG LAI, School of Electrical, Computer, and Energy Engineering, Arizona State University — Relativistic quantum chaos has attracted much attention since the discovery of graphene in 2004. Using graphene billiard as an apparatus of relativistic quantum particles, relativistic quantum scars, level spacing statistics, and relativistic quantum scattering have been widely investigated recently. However, since graphene has two non-equivalent Dirac points which can be coupled together by various processes, it has been wondered that whether the observed phenomena are inherent to the relativistic movement or caused by the discrete graphene lattice structure and boundary terminations. Based on Berry et al.'s work on neutrino billiards, we developed a conformal transformation method to solve the 2D Dirac equation in a confined region resembling chaotic billiards in the classical limit. This method solves both the eigen-energies and the eigen-wavefunctions of the 2D massless Dirac fermions. Level spacing statistics and relativistic quantum scars for a heart-shaped billiard are investigated and comparisons with graphene billiards are made.

¹This work was supported by AFOSR under Grant No. FA9550-09-1-0026 and NSF of China under Grant No. 11005053.

9:00AM A52.00004 Using Local Perturbations To Manipulate and Control Pointer States in Quantum Dot Systems, RICHARD AKIS, GIL SPEYER, DAVID FERRY, Arizona State University, ROLAND BRUNNER, University of Leoben, Austria — Recently, scanning gate microscopy (SGM) was used to image scarred wave functions in an open InAs quantum dot[1]. The SGM tip provides a local potential perturbation and imaging is performed by measuring changes in conductance. Scarred wave functions, long associated with quantum chaos, have been shown in open dots to correspond to pointer states[2], eigenstates that survive the decoherence process that occurs via coupling to the environment. Pointer states modulate the conductance, yielding periodic fluctuations and the scars, normally thought unstable, are stabilized by quantum Darwinism [3]. We shall show that, beyond probing, pointer states can be manipulated by local perturbations. Particularly interesting effects occur in coupled quantum dot arrays, where a pointer state localized in one dot can be shifted over into another with a perturbation in a completely different part of the system. These nonlocal effects may perhaps be exploited to give such systems an exotic functionality. [1] A. M. Burke, R. Akis, T. E. Day, Gil Speyer, D. K. Ferry, and B. R. Bennett, Phys. Rev. Lett. 104, 176801 (2010). [2] D. K. Ferry, R. Akis, and J. P. Bird, Phys. Rev. Lett. 104, 176801 (2004). [3] R. Brunner, R. Akis, D. K. Ferry, F. Kuchar, and R. Meisels, Phys. Rev. Lett. 101, 024102 (2008).

9:12AM A52.00005 Periodic Orbit Scar in Propagation of Wave Packet, MITSUYOSHI TOMIYA, HIROYOSHI TSUYUKI, SHOICHI SAKAMOTO, Faculty of Science and Technology, Seikei University, ERIC HELLER, Department of Physics, Harvard University — The scar-like enhancement is found in the accumulation of the time-evolving wave packet in stadium billiard. The time-average of the absolute square of the time-evolving wave functions in the stadium billiard is investigated numerically and semiclassically. Nowadays nano- or subnano-sized devices are getting more and more available. This kind of dynamical properties is essential, when the devices actually work. The enhancement appears along an unstable periodic orbit, when the Gaussian wave packet is launched as the initial state along the orbit. Introducing the window function which is closely related to the eigenfunction expansion coefficients of the wave packet, the localization around the periodic orbit is clarified by the semiclassical approximation that it is due to essentially the same mechanism of the scar states in stationary states. The “smooothed” window function is well estimated by the intensity spectrum in Prof. Heller’s theory of the long-time semiclassical dynamics. The key parameters that determine its shape are actually classical quantities: the size of the initial wave packet and the Lyapunov exponent.

9:24AM A52.00006 Chaotic Ionization of Bidirectionally Kicked Rydberg Atoms, KORANA BURKE, Boston University, KEVIN MITCHELL, UC Merced, SHUZHEN YE, F. BARRY DUNNING, BRENDAN WYKER, Rice University — A highly excited quasi one-dimensional Rydberg atom exposed to periodic alternating external electric field pulses exhibits chaotic behavior. The ionization of this system is governed by a geometric structure of phase space called a homoclinic tangle and its turnstile. We present and explain the results from an experiment designed to probe the structure of the phase space turnstile. We create time-dependent Rydberg wave packets, subject them to alternating applied electric fields (kicks), and measure the survival probability. We show that the survival probability of the electron depends not only on the initial electron energy, but also on the phase space position of the electron with respect to the turnstile—the portion of the electron wave packet inside the turnstile ionizes quickly, after one period of the applied field, while that portion outside the turnstile ionizes after multiple kicking periods. Finally, we use the turnstile geometry to explain the dependence of ionization on the kicking period. This procedure describes a very robust yet simple way to control chaotic ionization of an atomic system.

9:36AM A52.00007 Quantized Intrinsically Localized Modes¹, PETER RISEBOROUGH, Physics Department — We have calculated the quantized $n = 2$ breather spectra of both the β and the α Fermi-Pasta-Ulam lattices. The breather spectra are composed of resonances in the two-phonon continuum and branches of infinitely long-lived excitations. The non-linear attributes of these excitations become more pronounced at elevated temperatures. The calculated $n = 2$ breather and the resonance of the β -lattice hybridize and exchange identity at the zone boundary, and are in reasonable agreement with the results of previous calculations using the number conserving approximation. However, by contrast the breather spectrum the α -lattice couples resonantly with the single-phonon spectrum and cannot be calculated within a number conserving approximation. Furthermore we show that, for sufficiently strong non-linearity, the α -lattice breathers can be observed directly through the single-phonon inelastic neutron scattering spectrum. As the temperature is increased, the single-phonon dispersion relation for the α -lattice becomes progressively softer as the lattice instability is approached. We compare our theoretical results with the recent experimental observation of breathers in NaI by Manley *et al.*

¹US Department of Energy, Office of Basic Energy Sciences, Materials Science, Grant DEFG02-84ER4587

9:48AM A52.00008 Using quantum chaos to control the production of bipartite entangled states, LOCK CHEW, Nanyang Technological University, NING CHUNG, National University of Singapore — Recently, we have shown that it is possible for the entanglement dynamics to depend on the global classical dynamical regime instead of the local classical behavior. We observe that as the corresponding classical system becomes more chaotic, the rate of entanglement production increases with the emergence of larger entanglement entropy in the steady state. This suggests that quantum chaos can be used to control the generation of highly entangled quantum states, which are typically more robust against the effects of decoherence from the environment. Furthermore, the dependence of our system on the global classical dynamical regime indicates that the mode of production is insensitive to errors in the preparation of the initial separable coherent states. In this talk, I will present our recent results of using the additional control of quantum squeezing to further enhance the entanglement of the dynamically generated quantum states. I will show that the concomitant application of quantum squeezing and quantum chaos leads to a more entangled state at a faster production rate relative to squeezing without quantum chaos.

10:00AM A52.00009 Entanglement Entropy and Entanglement Spectrum for Two-Dimensional Classical Spin Configuration, HIROAKI MATSUEDA, Sendai National College of Technology — In quantum spin chains at criticality, two types of scaling for the entanglement entropy exist: one comes from conformal field theory (CFT), and the other is for entanglement support of matrix product state (MPS) approximation. On the other hand, quantum spin-chain models can be mapped onto two-dimensional (2D) classical ones. Motivated by the scaling and the mapping, we introduce new entanglement entropy for 2D classical spin configuration as well as entanglement spectrum, and examine their basic properties in the Ising and the three-state Potts models on the square lattice. They are defined by the singular values of the reduced density matrix for a Monte Carlo snapshot. We find scaling relations of the entropy analogous to the CFT and the MPS results. At criticality, the spin configuration is fractal, and various sizes of ordered clusters coexist. Then, the original snapshot can be decomposed into a set of images, and they have different length scales, respectively. This is the origin of the scaling. Based on these observations as well as calculation of the entanglement spectrum, we conclude that the amount of information of only one snapshot at criticality is equal to that of 1D quantum critical systems.

10:12AM A52.00010 Fluctuation theorem for a double quantum dot coupled to a point-contact electrometer, YASUHIRO UTSUMI, Department of Physics Engineering, Faculty of Engineering, Mie University, DMITRI GOLUBEV, MICHAEL MARTHALER, GERD SCHOEN, Karlsruhe Institute of Technology, MIE UNIVERSITY, JAPAN COLLABORATION, KARLSRUHE INSTITUTE OF TECHNOLOGY, GERMANY COLLABORATION — We study the fluctuation theorem in single-electron sequential tunneling regime. We consider single-electron transport through a double quantum dot (DQD) monitored by a capacitively coupled quantum point-contact (QPC) electrometer. In this setup it is possible to perform a direction resolved real-time electron counting experiment. We derive the full counting statistics for the coupled DQD - QPC system and obtain the joint probability distribution of the charges transferred through the DQD and the QPC. We show that the joint probability distribution satisfies the fluctuation theorem for 4-terminal system. For two-terminal DQD, the effective temperature should be introduced to recover the fluctuation theorem. The system can be described by a master equation with tunneling rates depending of the counting fields and satisfying a generalized local detailed-balance relation. Furthermore, we derive universal relations between the non-linear corrections to the current and noise, which can be verified in experiment.

10:24AM A52.00011 Electromagnetic fluctuations in non-equilibrium: Casimir forces and heat transfer, MATTHIAS KRUGER, MIT, Department of Physics, 77 Massachusetts Ave, Cambridge, MA 02139, THORSTEN EMIG, Laboratoire de Physique Theorique et Modeles Statistiques, CNRS UMR 8626, Universite Paris-Sud, 91405 Orsay cedex, France, GIUSEPPE BIMONTE, Dipartimento di Scienze Fisiche, Universita di Napoli Federico II, Complesso Universitario MSA, Via Cintia, I-80126 Napoli, Italy and INFN Sezione, VLADYSLAV GOLYK, ALEXANDER MCCAULEY, MEHRAN KARDAR, MIT, Department of Physics, 77 Massachusetts Ave, Cambridge, MA 02139 — It is well known that quantum Casimir forces play an important role in micro- or nanostructures. Recently, the role of temperature in thermal non-equilibrium raised theoretical as well as experimental interest. If the objects are held at different temperatures, the interactions depend on all temperatures in the system, and show many effects which are absent in equilibrium. Additionally, the objects exchange thermal energy by electromagnetic fields, known as radiative heat transfer, which is fundamentally different from macroscopic cases described by the well known laws of Planck or Stefan-Boltzmann. We discuss recent theoretical progress describing such effects, and illustrate the dependence of both quantities on the shapes as well as the distances of the objects.

10:36AM A52.00012 A First-Principles Method of Determining van der Waals Forces in Dissipative Media¹, YI ZHENG, ARVIND NARAYANASWAMY, Department of Mechanical Engineering, Columbia University — Lifshitz theory of van der Waals (vdW) force and energy between two planar objects is strictly valid when the medium separating two planar objects is vacuum. Generalization of Lifshitz theory to the case when intervening medium is a dissipative material, as opposed to vacuum, is a surprisingly difficult undertaking because there is no expression for the electromagnetic stress tensor in dissipative materials. Here, we derive the expression for vdW energy and pressure in planar multilayered dissipative media by computing the work done in assembling the multilayered structure from its constituent thin films. In doing so, we avoid any calculations of the Maxwell stress tensor in any medium but vacuum. Even though this work has proven to be a corroboration of Dzyaloshinskii, Lifshitz, and Pitaevskii, it has thrown new light on our understanding of vdW forces and suggests that it should be possible to achieve the similar result for objects with arbitrary shapes.

¹This work has been funded partially by the National Science Foundation through Grant CBET-0853723.

10:48AM A52.00013 Heat radiation from long cylindrical objects, VLADYSLAV GOLYK, MATTHIAS KRUGER, MEHRAN KARDAR, Massachusetts Institute of Technology — The heat radiated by objects small or comparable to the thermal wavelength can be very different from the classical blackbody radiation as described by the laws of Planck and Stefan-Boltzmann. We derive methods based on scattering of electromagnetic waves to explore the dependence on size, shape, as well as material properties. In particular, we discuss the radiation from a long cylinder at uniform temperature, describing in detail the degree of polarization of the emitted radiation by nanowires and carbon nanotubes.

Monday, February 27, 2012 8:00AM - 11:00AM — Session A53 GSNP: Disordered and Glassy Systems I 153B

8:00AM A53.00001 The dependence of fragility of glass forming liquids on interparticle interactions and density, SRIKANTH SASTRY, SHILADITYA SENGUPTA, Jawaharlal Nehru Centre for Advanced Scientific Research, FREDERIC AFFOUARD, FILIPE VASCONCELOS, Universite Lille, JNCASR COLLABORATION — The fragility of a glass forming liquid quantifies the rapidity of the change in viscosity and relaxation times with temperature and is an important material property. We study the influence of interparticle interactions on the fragility of a set of model glass formers using computer simulations. We consider both the kinetic fragility, given by the temperature variation of relaxation times, and the thermodynamic fragility obtained by the temperature variation of the configurational entropy. The Adam-Gibbs relation describes the temperature variation of relaxation times in terms of the variation of the configurational entropy, and thus we expect the kinetic and thermodynamic fragilities to be consistent with each other. We however find that the kinetic fragility increases with increasing softness of the interaction potential, with thermodynamic fragility showing the opposite trend. We rationalize our results by considering the full form of the Adam-Gibbs relation, which requires knowledge in addition of the high temperature activation energies, and explore the role of recent ideas on the scaling of temperature and density in systems exhibiting behavior akin to those with inverse power law interactions.

8:12AM A53.00002 Frequency and Wavevector Dependence of the Atomic Level Stress-Stress Correlation Function in a Model Supercooled Liquid¹, VALENTIN A. LEVASHOV, JAMES R. MORRIS, TAKESHI EGAMI, University of Tennessee and Oak Ridge National Laboratory — Temporal and spatial correlations among the local atomic level shear stresses were studied for a model liquid iron by molecular dynamics simulation [PRL 106,115703]. Integration over time and space of the shear stress correlation function $F(r, t)$ yields viscosity via Green-Kubo relation. The stress correlation function in time and space $F(r, t)$ was Fourier transformed to study the dependence on frequency, E , and wave vector, Q . The results, $F(Q, E)$, showed damped shear stress waves propagating in the liquid for small Q at high and low temperatures. We also observed additional diffuse feature that appears as temperature is reduced below crossover temperature of potential energy landscape at relatively low frequencies at small Q . We suggest that this additional feature might be related to dynamic heterogeneity and boson peaks. We also discuss a relation between the time-scale of the stress-stress correlation function and the alpha-relaxation time of the intermediate self-scattering function $S(Q, E)$.

¹This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering

8:24AM A53.00003 Measuring Dynamical Facilitation in Supercooled Liquids and Related Materials, Yael Elmatad, Center for Soft Matter, Physics Department, New York University, New York NY USA, AARON KEYS, Chemistry Department, University of California, Berkeley, Berkeley CA USA and Lawrence Berkeley National Laboratory, Berkeley, CA USA — We provide a physical interpretation for excitation dynamics in kinetically constrained lattice models in the context of supercooled liquids and granular materials. Several physical quantities such as instanton times, onset temperatures, and particle displacement fields are derived. These quantities are used to interpret measurements of dynamical facilitation previously performed for atomistic and molecular supercooled liquids and granular materials. We show that these previous measurements provide strong evidence that dynamical facilitation plays a key role in glassy materials.

8:36AM A53.00004 Excitations are localized and relaxation is hierarchical in glass-forming liquids, AARON KEYS, LESTER HEDGES, Lawrence Berkeley National Laboratory, JUAN GARRAHAN, University of Nottingham, SHARON GLOTZER, University of Michigan, DAVID CHANDLER, University of California, Berkeley — For several atomistic models of glass formers, at conditions below their glassy dynamics onset temperatures, T_o , we use importance sampling of trajectory space to study the structure, statistics and dynamics of excitations responsible for structural relaxation. Excitations are detected in terms of persistent particle displacements of length a . At supercooled conditions, for a of the order of or smaller than a particle diameter, we find that excitations are associated with correlated particle motions that are sparse and localized, occupying a volume with an average radius that is temperature independent and no larger than a few particle diameters. We show that the statistics and dynamics of these excitations are facilitated and hierarchical. Excitation energy scales grow logarithmically with a . Excitations at one point in space facilitate the birth and death of excitations at neighboring locations, and space-time excitation structures are microcosms of heterogeneous dynamics at larger scales. This nature of dynamics becomes increasingly dominant as temperature T is lowered. We show that slowing of dynamics upon decreasing temperature below T_o is the result of a decreasing concentration of excitations and concomitant growing hierarchical length

8:48AM A53.00005 Anomalous properties of liquids for a family of models with short range tetrahedral interactions, SERGEY BULDYREV, Yesiva University, GIANCARLO FRANZESE, University of Barcelona — Liquids with tetrahedral symmetry of the first coordination shell often display anomalous thermodynamic and dynamic behavior. The main reason for these anomalies is that pressurizing such liquids leads to the disordering of this local symmetry by the particles migrating from the second to the first coordination shell. This in some case may lead to the increase of entropy upon pressurizing and consequently to the volume increase upon cooling. Molecular simulations of various models with tetrahedral symmetry are able to reproduce this anomalous behavior. We study a family of simple models in which we can gradually change the degree of tetrahedrality and investigate the associated changes of the phase diagram by discrete molecular dynamics. A molecule in these models consist of a hard sphere and four point particles attached to the center of the hard sphere by directional bonds arranged in tetrahedral geometry. Each of these four particles has a narrow attractive square well so that the particles belonging to different molecules can attract to each other. We also impose a condition which does not allow a point particle in one molecule to include in its attractive well more than one point particle belonging to different molecules. We investigate how the phase diagram of the system depends on the parameters of the models. None of these models has a liquid-liquid phase transition in the accessible region of the phase. However, adding weak attractive square well to the hard sphere, or wider weak attractive square wells to the point particles can create a liquid-liquid critical point. A comparison with other simple models of the anomalous liquids is made.

9:00AM A53.00006 Stretched-exponential relaxation and hidden power laws in a solidifying 2D liquid¹, ALEXANDER PATASHINSKI, Northwestern University, RAFAL ORLIK, Orlik-software LLC, Poland, ANTONI MITUS, Polytechnic University, Wroclaw, Poland, BARTOSZ GRZYBOWSKI, MARK RATNER, Northwestern University — In a 2D Lennard-Jones liquid, the number of particles keeping their memorized nearest neighbors is found to decay stretched-exponentially; the probability for a particle to keep the same 6 nearest neighbors for a time t can be fitted with a power law. Using the lists of nearest neighbors (nn -lists) as a topological order parameter, we studied the dynamics of the structure underlying these signature features of complexity in materials. The nn -changes randomly appear along the boundaries of better ordered blocks at a time scale of the order of particles vibration period; these boundaries, and the shapes of the blocks, perform a next time-scale random motion. Particles diffusion includes periods of slow and fast diffusion. We discuss the feed-back interactions between nn -changes, block boundaries motion, and orientation relaxation in the system.

¹This work was supported by the Non-equilibrium Energy Research Center (NERC) which is an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0000989

9:12AM A53.00007 Sheared athermal soft-particle suspensions near jamming: dependence of effective diffusion on packing density and system size, KAMRAN KARIMI, CRAIG MALONEY, Carnegie Mellon University — We perform numerical simulations to study diffusion in a model bi-disperse frictionless athermal soft-particle suspension of disks in two dimensions (2D) using the so-called “mean field” version of Durian’s bubble model. We measure the effective transverse diffusion coefficient D_{eff} in shear flows at various volume fraction ϕ and shearing rate $\dot{\gamma}$. For $\phi > \phi_c$, where ϕ_c is identified with the random close packing limit, in the quasi-static limit, D_{eff} shows a pronounced linear system size dependence with very weak dependence on ϕ . For $\phi < \phi_c$, D_{eff} , in the quasi-static limit, increases with increasing ϕ and shows very little system size dependence. We discuss how the behavior of D_{eff} is related to non-trivial correlations in the spatial structure of the displacement fields *at long times* in the Fickian regime.

9:24AM A53.00008 Decoupling of Rotational and Translational Diffusion in Supercooled Colloidal Fluids¹, KAZEM V. EDMOND², Emory University, MARK T. ELSESSER³, New York University, GARY L. HUNTER, Emory University, HYUNJOO PARK, DAVID J. PINE, New York University, ERIC R. WEEKS, Emory University — Using high-speed confocal microscopy, we directly observe the three-dimensional rotational dynamics of rigid clusters of microspheres suspended in dense colloidal suspensions. The clusters are highly ordered packings of fluorescently-labeled PMMA particles, fabricated using a recently developed emulsification technique. Our colloidal suspensions serve as an excellent model of hard spheres, perhaps the simplest system with a glass transition, while the clusters probe the system’s local rotational and translational dynamics. Far from the colloidal liquid’s glass transition, both rotational and translational motion of the clusters are purely Brownian. However, in the liquid’s supercooled regime, we observe a decoupling between the two types of motion: as the glass transition is approached, rotational diffusion slows down even more than translational diffusion. The nature of the decoupling is in good agreement with theoretical predictions and experiments with molecular glass formers. Our observation supports the notion that supercooled liquids are not merely liquids with large viscosities but that diffusion takes place by fundamentally changed mechanisms.

¹NSF Grant No. CHE-0910707

²Currently at the Center for Soft Matter Research at New York University.

³Currently at the University of North Carolina.

9:36AM A53.00009 Thermodynamics versus network topology of network glasses, LE YAN, MATTHIEU WYART, Center for Soft Matter Research, Physics Department, New York University — Under cooling, the thermodynamics and the dynamics of super-cooled liquids are strongly correlated. The thermal evolutions of these quantities, characterizing the liquid fragility, depend greatly on the specific liquid considered. To date, there is no understanding of what controls these properties at a microscopic level. In chalcogenide glasses, the coordination of the covalent network can be changed continuously by varying their composition. Experiments show that as the coordination is increased, the jump of specific heat varies non-monotonically and is minimal at coordination near the Maxwell threshold where the covalent network becomes rigid. At such a composition the liquid is strong. We introduce a simplified model for the thermal evolution of networks that captures this observation.

9:48AM A53.00010 Elastic properties of compressed emulsions, IVANE JORJADZE, JASNA BRUJIC, NYU — Visualizing the packing of a dense emulsion in 3D as a function of the external pressure allows us to characterize the geometry and the local stress distribution inside this jammed system. We first test the scaling laws of the pressure and average coordination number over two orders of magnitude in density. We find deviations from theoretical exponents due to the non-affine motion of the particles. Second, we observe that the distribution of forces changes from a broad exponential at the jamming point to a narrower Gaussian-like distribution under high compression. Finally, we calculate the density of states from the measured force network in the approximation of a harmonic potential. Close to jamming, the number of low frequency modes is high, while the application of pressure shifts the distribution to higher frequencies, indicative of a rigid network. The confocal images reveal the structural features associated with the low frequency modes, as well as their localization within the packing. These data are then compared with published results from numerical simulations.

10:00AM A53.00011 Glassy Dynamics of Charge Density Waves in Chromium¹, HYEKYUNG KIM, JONATHAN LOGAN, University of Chicago, OLEG SHPYRKO, University of California San Diego, ERIC ISAACS, Argonne National Laboratory; University of Chicago — Charge-density waves provide theoretically tractable systems for exploring longstanding questions posed by the physics of elastic media in the presence of quenched disorder. Interaction of quenched pinning fields and phase elasticity of CDWs results in a complex energetic landscape of metastable states, which in turn gives rise to “glassy” phenomena such as aging and hysteresis. Using synchrotron x-rays we have observed aging of CDW order parameter Q in bulk chromium following thermal quench to out-of-equilibrium configuration. Although temperature stabilization occurs in under two minutes, Q relaxes exponentially over the course of hours toward metastable configurations that depend on sample history.

¹Argonne National Laboratory; University of Chicago

10:12AM A53.00012 Local collapse of the atomic cage in a liquid flow, TAKUYA IWASHITA, TAKESHI EGAMI, University of Tennessee — The local structure of a model glass under steady shear was studied by molecular dynamics simulation for both high ($T > T_g$) and low ($T < T_g$) temperature ranges. The local structure was presented in terms of the anisotropic pair-density function (PDF). We found that the local structure was strained over a limited range of distances, and the length-scale of the strained region was dependent on the strain rate, extrapolating to zero at a critical strain rate. A strong correlation between the local collapse, represented by cutting of the atomic bond, and the structural strain in the PDF was found. At low temperatures local failure happens in a serrated manner, caused mechanically by shear. At high temperatures the local failure occurs more randomly, which is governed by thermal fluctuation. An anomalous behavior was observed as temperature approaches to T_g . The results suggest that except for the supercooled state above T_g local failure occurs by cutting of a single bond. Only in the supercooled state multiple bonds have to be cut for flow to occur. A possible relation to the dynamic heterogeneity is discussed.

10:24AM A53.00013 Local Perturbation of Quasi Two-Dimensional Colloidal Glasses¹, KEVIN APTOWICZ, West Chester University, TIM STILL, KE CHEN, PETER YUNKER, ARJUN YODH, University of Pennsylvania — Colloids are promising and widely used model systems to investigate the phase behavior of matter at length scales and timescales accessible to optical microscopy. We utilize disordered quasi two-dimensional colloidal systems in the jammed state to study the properties of glasses. It was recently found in simulation and experiment that so-called 'soft spots', where low frequency quasi-localized modes concentrate, are the locations in glasses prone to rearrangements. Therefore, we utilize short laser pulses to perturb colloidal glasses locally. By varying the pulse intensity of the laser, the strength of the perturbation is tunable, which allows us to induce either elastic or plastic deformations in the glasses. With this experimental geometry in combination with video microscopy, we investigate the correlation between locally induced rearrangements in the colloidal glass and the location of soft spots determined from analysis of the system's vibrational eigenmodes. The dependence of the mechanical response of a glass on the local environment in terms of these dynamic heterogeneities and their persistence is discussed.

¹We acknowledge financial support from Research Corporation (KBA), MRSEC DMR11-20901 (AGY), and DAAD (TS).

10:36AM A53.00014 X-ray investigation of colloidal glasses under shear, DMITRY DENISOV, TRIET DANG, Van der Waals-Zeeman Institute, University of Amsterdam, Netherlands, BERND STRUTH, Deutsches Elektronen-Synchrotron, Hamburg, Germany, PETER SCHALL, Van der Waals-Zeeman Institute, University of Amsterdam, Netherlands — Understanding glassification or dynamical arrest is one of the grand challenges of material science and is a topic of great current interest. It is a central observation in soft matter systems as well as glass forming molecular systems that – with increasing density or decreasing temperature – the motion of the particles or molecules slows down and eventually becomes arrested. Understanding this dynamical arrest as well as relaxations in the arrested state are fundamental problems, which to a large degree remain unanswered. We use a novel combination of rheological measurement and small angle x-ray scattering (at the synchrotron DESY in Hamburg) to study structure factor of dense suspensions under shear and during relaxation. The suspensions consist of silica particles 50nm in diameter. We observe clear changes of inter particles distances and configurations due to the different shear rates. Together with future dynamic x-ray measurements we aim to develop a universal scale-bridging understanding of dynamic arrest.

10:48AM A53.00015 Boundaries Matter for Confined Colloidal Glasses, GARY L. HUNTER, Emory University, KAZEM V. EDMOND, New York University, ERIC R. WEEKS, Emory University — We confine dense colloidal suspensions within emulsion droplets to examine how confinement and properties of the confining medium affect the colloidal glass transition. Samples are imaged via fast confocal microscopy. By observing a wide range of droplet sizes and varying the viscosity of the external continuous phase, we separate finite size and boundary effects on particle motions within the droplet. Suspensions are composed of binary PMMA spheres in organic solvents while the external phases are simple mixtures of water and glycerol. In analogy with molecular super-cooled liquids and thin-film polymers, we find that confinement effects in colloidal systems are not merely functions of the finite size of the system, but are strongly dependent on the viscosity of the confining medium and interactions between particles and the interface of the two phases.

Monday, February 27, 2012 8:00AM - 10:48AM –

Session A54 GSNP: Focus Session: Complex and Co-evolving Networks - Cascades in Networks

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8:00AM A54.00001 Percolation of Double-Layer Networks with Different Topologies Under Random Attacks, DI ZHOU, JIANXI GAO, Center for Polymer Studies and Department of Physics, Boston University, SHLOMO HAVLIN, Mineva Center and Department of Physics, Bar-Ilan University, H.EUGENE STANLEY, Center for Polymer Studies and Department of Physics, Boston University — We report on the effects of topology on failure propagation models for systems consisting of two interdependent networks, which are either SF networks with different parameters, or different types of networks. Pairs of interdependent networks are known to exhibit a percolation transition upon failure accumulation. The topology of the nets significantly change the critical density of failure for the total disruption of the two net composite system. When the system is not fully coupled, the existence of a very small fraction of SF network will hold the system from fragment. When the critical threshold p_c doesn't change, robustness measure R is introduced. The consequences of the study may provide insights for future network architectures and their evolution to improve their robustness and enhancing the protection of critical infrastructure.

8:12AM A54.00002 Statistics of interacting networks with extreme preferred degrees: Simulation results and theoretical approaches¹, WENJIA LIU, BEATE SCHMITTMANN, R.K.P. ZIA, Virginia Tech Physics Dept — Network studies have played a central role for understanding many systems in nature - e.g., physical, biological, and social. So far, much of the focus has been the statistics of networks in isolation. Yet, many networks in the world are coupled to each other. Recently, we considered this issue, in the context of two interacting social networks. In particular, We studied networks with two different preferred degrees, modeling, say, introverts vs. extroverts, with a variety of "rules for engagement." As a first step towards an analytically accessible theory, we restrict our attention to an "extreme scenario": The introverts prefer zero contacts while the extroverts like to befriend everyone in the society. In this "maximally frustrated" system, the degree distributions, as well as the statistics of cross-links (between the two groups), can depend sensitively on how a node (individual) creates/breaks its connections. The simulation results can be reasonably well understood in terms of an approximate theory.

¹NSF DMR-1005417 and ICTAS Virginia Tech

8:24AM A54.00003 Correlated multiplexity in random and co-evolving multiplex networks, JUNG YEOL KIM, KYU-MIN LEE, K.-I. GOH, I.-M. KIM, Korea Univ. — Nodes in a complex networked system often engage in multiple types of interactions among them; they form a *multiplex* network with multiple layers that can be interdependent and co-evolve. In many real-world complex systems, such multiple network layers are not randomly coupled but correlated. Such a correlated multiplexity can imprint nontrivial structural correlations in the multiplex network, which in turn can impact the dynamical processes on it. Here we present some recent results on the correlated multiplexity in multiplex networks. First we show how the correlated multiplexity can dramatically alter the giant component properties of multiplex random networks. Secondly we introduce an evolution model of co-evolving multiplex networks by generalizing the well-known Barabási-Albert-type model, to show how the co-evolution of network layers can induce and modulate the degree of correlated multiplexity.

8:36AM A54.00004 Cascades of overload failures in spatial networks¹, ANDREA ASZTALOS, SAMEET SREENIVASAN, BOLESŁAW SZYMANSKI, GYORGY KORNISS, Rensselaer Polytechnic Institute — Our daily life imposes increasing demands on infrastructural networks such as the power grid, transportation network, water supply, etc. Understanding the vulnerabilities of these systems is crucial to securing them. To this end, we study the effect of spatial constraints on network resilience against cascading overloads. Specifically, we consider distributed and shortest path flows on spatially embedded networks and study the model of cascading failures (Motter and Lai (2002)) triggered by the removal of a single or multiple nodes. We present results of intentional attacks on highly loaded and high degree nodes as well as a comparison between spatially concentrated and randomly distributed, multiple attacks.

¹Supported in part by DTRA.

8:48AM A54.00005 Multiplexity-facilitated cascade dynamics in networks, KYU-MIN LEE, Department of Physics and Institute of Basic Science, Korea University, CHARLES BRUMMITT, Department of Mathematics and Complexity Sciences Center, University of California, Davis, KWANG-IL GOH, Department of Physics and Institute of Basic Science, Korea University — Most complex network studies thus far have been focused on single-layer framework. It becomes increasingly clear, however, that many real-world complex systems are *multiplex* —nodes interact with multiple types of interactions (links) which coexist, co-depend, and co-evolve. The interplay of such multiplex interactions may confer nontrivial consequences on network dynamics. Here we present recent results on how such multiplexity affects cascade dynamics on networks. We found the cascade progression is greatly facilitated by multiplexity. Layers that are unable to achieve global cascades in isolation can cooperatively achieve them by multiplex coupling. Therefore, the multiplex network can be dramatically more vulnerable to global cascades than single-layer or simplex networks. Implication of these results on cascade prediction and control in social and economic dynamics is also discussed.

9:00AM A54.00006 Cascades of failures in various models of interdependent networks, SERGEY BULDYREV, BENJAMIN KADISH, NATHANIEL SHERE, MITCHEL AHARON, GABRIEL CWILICH, Yeshiva University — Complex networks appear in almost every aspect of science and technology. Recently an analytical framework for studying the percolation properties of interacting networks has been developed [1]. These studies however have several limitations. The real networks do are not randomly connected. They are often embedded into two dimensional space. The dependency links are not connecting nodes at random but have tendency to connect nodes with similar degrees, or nodes which are close to each other in Euclidian space. Moreover, the network failures may occur not only to the loss of connectivity but also due to overload of nodes with high betweenness. We have study these situations analytically and by computer simulations and found the conditions at which networks collapse in an abrupt first order like transition when the entire network becomes non-functional or fail gradually like in a second order transition as a greater fraction of nodes is removed in the initial attack or failure.

[1] **S. V. Buldyrev**, R. Parshani, G. Paul, H. E. Stanley, and S. Havlin, “Catastrophic cascade of failures in interdependent networks,” *Nature* **464**, 1025-1028 (2010)

9:12AM A54.00007 Robustness of a Network of Networks¹, JIANXI GAO², Boston University, SERGEY V. BULDYREV³, Department of Physics, Yeshiva University, H. EUGENE STANLEY, Boston University, SHLOMO HAVLIN⁴, Department of Physics, Bar-Ilan University, Israel — Network research has been focused on studying the properties of a single isolated network, which rarely exists. We develop a general analytical framework for studying percolation of n interdependent networks. We illustrate our analytical solutions for three examples: (i) For any tree of n fully dependent Erdős-Rényi (ER) networks, each of average degree $\bar{k}$, we find that the giant component $P_\infty = p[1 - \exp(-\bar{k}P_\infty)]^n$ where $1 - p$ is the initial fraction of removed nodes. This general result coincides for $n = 1$ with the known second-order phase transition for a single network. For any $n > 1$ cascading failures occur and the percolation becomes an abrupt first-order transition. (ii) For a starlike network of n partially interdependent ER networks, P_∞ depends also on the topology—in contrast to case (i). (iii) For a looplike network formed by n partially dependent ER networks, P_∞ is independent of n .

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³SVB acknowledges the partial support of this research through the Dr. Bernard W. Gamson Computational Science Center at Yeshiva College.

⁴SH thanks the European EPIWORK project, Deutsche Forschungsgemeinschaft (DFG), and the Israel Science Foundation for financial support.

9:24AM A54.00008 Robustness of interdependent networks under targeted attack, XUQING HUANG, Center for Polymer Studies and Department of Physics, Boston University, JIANXI GAO, Department of Automation, Shanghai Jiao Tong University, SERGEY BULDYREV, Department of Physics, Yeshiva University, SHLOMO HAVLIN, Minerva Center and Department of Physics, Bar-Ilan University, H. EUGENE STANLEY, Center for Polymer Studies and Department of Physics, Boston University — When an initial failure of nodes occurs in interdependent networks, a cascade of failure between the networks occurs. Earlier studies focused on random initial failures. Here we study the robustness of interdependent networks under targeted attack on high or low degree nodes. We introduce a general technique which maps the targeted-attack problem in interdependent networks to the random-attack problem in a transformed pair of interdependent networks. We find that when the highly connected nodes are protected and have lower probability to fail, in contrast to single scale-free (SF) networks where the percolation threshold $p_c = 0$, coupled SF networks are significantly more vulnerable with p_c significantly larger than zero. The result implies that interdependent networks are difficult to defend by strategies such as protecting the high degree nodes that have been found useful to significantly improve robustness of single networks.

9:36AM A54.00009 Information Spreading in Context, DASHUN WANG, Center for Complex Network Research, Northeastern University, ZHEN WEN, HANGHANG TONG, CHING-YUNG LIN, IBM T.J. Watson Research Center, CHAOMING SONG, ALBERT-LASZLO BARABASI, Center for Complex Network Research, Northeastern University — Information spreading processes are central to human interactions. Despite recent studies in online domains, little is known about factors that could affect the dissemination of a single piece of information. In this paper, we address this challenge by combining two related but distinct datasets, collected from a large scale privacy-preserving distributed social sensor system. We find that the social and organizational context significantly impacts to whom and how fast people forward information. Yet the structures within spreading processes can be well captured by a simple stochastic branching model, indicating surprising independence of context. Our results build the foundation of future predictive models of information flow and provide significant insights towards design of communication platforms.

9:48AM A54.00010 Power-grid Network Partitioning and Cluster Optimization with Applications to Florida and Texas¹, PER ARNE RIKVOLD, IBRAHIM ABOU HAMAD, BRETT ISRAELS, Florida State University, SVETLANA V. POROSEVA, University of New Mexico — Cascading power-grid failures pose serious threats to lives and property, and it is desirable to contain them within a limited geographical area. One method to achieve this is Intelligent Intentional Islanding (I3): the purposeful partitioning of a grid into weakly connected “islands” of closely connected generators and loads. If such islands can be quickly isolated, the spread of faults can be limited. An additional constraint is that generating capacity and power demand within each island should be closely balanced to ensure self-sufficiency. I3 thus corresponds to constrained community detection in a network. After a matrix-based initial agglomeration of nearby loads and generators, we implement Monte Carlo simulated annealing to simultaneously optimize load-balance and internal connectivity of the resulting islands. The optimized network of islands is treated as a new network with the first-generation islands as the new nodes (“supergenerators” and “superloads”), and the same agglomeration and MC procedures are iteratively applied, reminiscent of real-space renormalization. Applications to the Floridian [1] and Texan high-voltage grids are demonstrated.

[1] I. Abou Hamad et al., Phys. Proc. 4, 125-129 (2010); Phys. Proc. 15, 2-6 (2011).

¹Supported in part by NSF DMR-1104829.

10:00AM A54.00011 Computational Analysis of Topological Survivability of Large-Scale Engineering Networks with Heterogeneous Nodes, SVETLANA POROSEVA, Mechanical Engineering, University of New Mexico — The scale and complexity of modern networks, their integration, and the size of population and businesses they have impact on, make their massive damage catastrophic for the society and economy. Such damage is usually caused by adverse events and is not considered by traditional design practices. In the modern society, the likelihood of adverse events has substantially increased. Therefore, there is a need in evaluating the ability of a network to survive such damage. As the network topology is a key factor to consider, the goal of our research is to develop computational tools for quantifying its effect on the network survivability. “Selfish” algorithm will be presented that addresses exponential-time complexity associated with the problem of generation and analysis of all fault combinations possible in a given network. The reduction of computational complexity is achieved by mapping an initial network topology with multiple sources and sinks onto a set of simpler smaller topologies with multiple sources and a single sink. Application to the Texas power grid will be considered.

10:12AM A54.00012 Cascading failures in interdependent lattice networks: from first order to second order phase transition¹, WEI LI, Center for Polymer Studies and Department of Physics, Boston University, Boston, MA 02215 USA, AMIR BASHAN, Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel, SERGEY BULDYREV, Department of Physics, Yeshiva University, 500 West 185th Street, New York, New York 10033, USA, EUGENE STANLEY, Center for Polymer Studies and Department of Physics, Boston University, Boston, MA 02215 USA, SHLOMO HAVLIN, Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel — We study a system composed of two interdependent lattice networks A and B, where nodes in network A depend on a node within a certain shuffling distance r of its corresponding counterpart in network B and vice versa. We find, using numerical simulation that percolation in the two interdependent lattice networks system shows that for small r the phase transition is second order while for large r it is a first order.

¹We wish to thank DTRA for financial support and Dr. Robin Burk for encouraging discussions. We acknowledge the partial support of this research through the Dr. Bernard W. Gamson Computational Science Center at Yeshiva College.

10:24AM A54.00013 Cascading behaviors in random directed dependency networks¹, YANQING HU, City College of New York Levich Institute and Department of Physics, AMIR BASHAN, SHLOMO HAVLIN, Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel, HERNAN MAKSE, City College of New York Levich Institute and Department of Physics — Cascading behaviors have been studied only for some specific dependency network systems. In this paper, we present a more general and realistic network system with both random connectivity and directed dependency links. Using percolation approach, we obtained the universal boundaries among first order transition, second order transition and unstable regimes, which depend only on less than fourth moment of degree distribution and the fractions of zero and one directed dependency link nodes. Moreover, besides the connectivity degree distribution, we also find the final state of dynamical cascading process is determined by out degree distribution of directed dependency links, and the in degree distribution only influence cascading speed.

¹This work is partially supported by ONR, DFG, DTRA, EU project Epi- work and the Israel Science Foundation. Y. Hu is supported by NSFC under Grant No. 60974084, 60534080.

10:36AM A54.00014 Loops in hierarchical channel networks¹, ELENI KATIFORI, MARCELO MAGNASCO, Rockefeller University — Nature provides us with many examples of planar distribution and structural networks having dense sets of closed loops. An archetype of this form of network organization is the vasculature of dicotyledonous leaves, which showcases a hierarchically-nested architecture. Although a number of methods have been proposed to measure aspects of the structure of such networks, a robust metric to quantify their hierarchical organization is still lacking. We present an algorithmic framework that allows mapping loopy networks to binary trees, preserving in the connectivity of the trees the architecture of the original graph. We apply this framework to investigate computer generated and natural graphs extracted from digitized images of dicotyledonous leaves and animal vasculature. We calculate various metrics on the corresponding trees and discuss the relationship of these quantities to the architectural organization of the original graphs. This algorithmic framework decouples the geometric information from the metric topology (connectivity and edge weight) and it ultimately allows us to perform a quantitative statistical comparison between predictions of theoretical models and naturally occurring loopy graphs.

¹This work was supported in part by the NSF under Grant PHY-1058899.

Monday, February 27, 2012 11:15AM - 2:15PM — Session B1 DAMOP: Atom Interferometry and New Techniques with Ultracold Atoms 203

11:15AM B1.00001 Low-temperature, high-density magneto-optical trapping of potassium using the open $4S \rightarrow 5P$ transition at 405 nm, DYLAN JERVIS, DAVID MCKAY, DAN FINE, GRAHAM EDGE, University of Toronto, JOHN PORCO-SIMPSON, University of California Santa Barbara, JOSEPH THYWISSEN, University of Toronto — We report the laser cooling and trapping of neutral potassium on an open transition. Fermionic ^{40}K is captured using a magneto-optical trap (MOT) on the closed $4S_{1/2} \rightarrow 4P_{3/2}$ transition at 767 nm and then transferred, with unit efficiency, to a MOT on the open $4S_{1/2} \rightarrow 5P_{3/2}$ transition at 405 nm. Because the $5P_{3/2}$ state has a smaller line width than the $4P_{3/2}$ state, the Doppler limit is reduced. We observe temperatures as low as $63(6) \mu\text{K}$, the coldest potassium MOT reported to date. The density of trapped atoms also increases, due to reduced temperature and reduced expulsive light forces. We measure a two-body loss coefficient of $\beta = 2 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$, and estimate an upper bound of $8 \times 10^{-18} \text{ cm}^2$ for the ionization cross section of the $5P$ state at 405 nm. The combined temperature and density improvement in the 405 nm MOT is a twenty-fold increase in phase space density over our 767 nm MOT, showing enhanced pre-cooling for quantum gas experiments. A qualitatively similar enhancement is observed in a 405 nm MOT of bosonic ^{41}K .

11:27AM B1.00002 Four techniques to achieve deeper Fermi degeneracy in Fermi-Bose mixtures, ROBERTO ONOFRIO, Department of Physics and Astronomy, University of Padova and ITAMP, Harvard-Smithsonian Center for Astrophysics — The study of exotic superfluid phases of ultracold atoms requires the achievement of deeper Fermi degeneracy with respect to the one already available. I will describe four techniques for efficient sympathetic cooling of Fermi gases with a different species Bose gas: bichromatic optical dipole [1] and light-assisted magnetic trapping [2], quasi one-dimensional Fermi-Bose mixtures [3], and fast adiabatic cooling [4].

[1] R. Onofrio and C. Presilla, Phys. Rev. Lett. 89, 100401 (2002);

[2] M. Brown-Hayes and R. Onofrio, Phys. Rev. A 70, 063614 (2004); [3] M. Brown-Hayes et al., Phys. Rev. A 78, 013617 (2008);

[4] S. Choi, R. Onofrio, and B. Sundaram, arXiv 1109.4908.

11:39AM B1.00003 Optimized sympathetic cooling of atomic mixtures via fast adiabatic strategies, STEPHEN CHOI, Department of Physics, University of Massachusetts, Boston, MA 02125, ROBERTO ONOFRIO¹, Dipartimento di Fisica Galileo Galilei, Universit  di Padova, Via Marzolo 8, Padova, Italy, BALA SUNDARAM, Department of Physics, University of Massachusetts, Boston, MA 02125 — The talk will explore the extent to which frictionless cooling techniques may be useful in sympathetic cooling of Fermi gases. It is argued that optimal cooling of an atomic species may be obtained by means of sympathetic cooling with another species whose trapping frequency is dynamically changed to maintain constancy of the Lewis-Riesenfeld adiabatic invariant, which in turn determines the temporal-profile of the changing frequency. An important motivating factor is that an usually undesired feature of these techniques, i.e., the fact that the atomic cloud does not increase its phase-space density and therefore its degeneracy, turns into a crucial asset when viewed from the perspective of maintaining the gas in the nondegenerate regime, thus making it an optimal coolant. Advantages and limitations of this cooling strategy are discussed, with particular regard to the possibility of cooling Fermi gases to a deeper degenerate regime. We also show that the links between the suggested method and quantum squeezing.

¹1) Department of Physics, University of Massachusetts, Boston, MA 02125; 2) ITAMP, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138

11:51AM B1.00004 Quantum degenerate Bose-Fermi mixture of chemically different atomic species with widely tunable interactions¹, JEE WOO PARK, CHENG-HSUN WU, IBON SANTIAGO, Massachusetts Institute of Technology, TOBIAS TIECKE, Harvard University, PEYMAN AHMADI, MARTIN ZWIERLEIN, Massachusetts Institute of Technology — We have created a quantum degenerate Bose-Fermi mixture of ²³Na and ⁴⁰K with widely tunable interactions via broad interspecies Feshbach resonances. Twenty Feshbach resonances between ²³Na and ⁴⁰K were identified. The large and negative triplet background scattering length between ²³Na and ⁴⁰K causes a sharp enhancement of the fermion density in the presence of a Bose condensate. As explained via the asymptotic bound-state model (ABM), this strong background scattering leads to a series of wide Feshbach resonances observed at low magnetic fields. Our work opens up the prospect to create chemically stable, fermionic ground state molecules of ²³Na-⁴⁰K where strong, long-range dipolar interactions will set the dominant energy scale.

¹Work was supported by the NSF, AFOSR-MURI and -PECASE, ARO-MURI, ONR YIP, DARPA YFA, a grant from the Army Research Office with funding from the DARPA OLE program and the David and Lucille Packard Foundation.

12:03PM B1.00005 Condensate Fraction in a BEC Dimer, DAVID CAMPBELL, Boston University, HOLGER HENNIG, Harvard University, DIRK WITTHAUT, Max Planck Institute for Dynamics and Self-Organization, Goettingen — Recent experiments studying a Bose Einstein Condensate (BEC) in a two-mode system, equivalent to a “dimer,” have shown that many qualitative dynamical features of the BEC can be understood from motions in the underlying classical (two-dimensional) phase space (ϕ , z). Using a Bose-Hubbard model for the dimer, we focus on quantum deviations from motions in the classical phase space. We introduce a “quantum” phase space (QPS), which we define as the minimum condensate fraction $c(\tau; \phi, z)$ of initial coherent states (ϕ, z) in the time interval $[0, \tau]$. We find that lines of equal condensate fraction in the QPS do mimic the classical trajectories of constant energy in many respects, such that the QPS clearly reflects Josephson oscillations and self-trapping. However, novel quantum features beyond the classical description appear at finite time τ . These include symmetry breaking and enhanced $c(\tau; \phi, z)$ near the classical hyperbolic fixed point and along a ridge near the classical separatrix. These features of the QPS can be readily studied in current experiments.

12:15PM B1.00006 Resonant Hawking radiation in Bose-Einstein condensates¹, FERNANDO SOLS, IVAR ZAPATA, Universidad Complutense de Madrid (Spain), MATHIAS ALBERT, Universite de Geneve (Switzerland), RENAUD PARENTANI, Universite Paris-Sud, Orsay (France) — We study double-barrier interfaces separating regions of asymptotically subsonic and supersonic flow of Bose-condensed atoms [1]. These setups contain at least one black hole sonic horizon from which the analogue of Hawking radiation should be generated and emitted against the flow in the subsonic region. Multiple coherent scattering by the double-barrier structure strongly modulates the transmission probability of phonons, rendering it very sensitive to their frequency. As a result, resonant tunneling occurs with high probability within a few narrow frequency intervals. This gives rise to highly non-thermal spectra with sharp peaks. We find that these peaks are mostly associated with decaying resonances and only occasionally with dynamical instabilities. Even at achievable non-zero temperatures, the radiation peaks can be dominated by spontaneous emission, i.e. enhanced zero-point fluctuations, and not, as is often the case in analogue models, by stimulated emission.

[1] I. Zapata, M. Albert, R. Parentani, F. Sols, New J. Phys. 13, 063048 (2011).

¹Supported by MICINN, FIS2010-21372, and Comunidad de Madrid, MICROSERES-CM

12:27PM B1.00007 Momentum Resolved Optical Lattice Modulation Spectroscopy for Bosons in Optical Lattice¹, RAJDEEP SENSARMA, Condensed Matter Theory Center, University of Maryland, College Park, KRISHNENDU SENGUPTA, Indian Association for cultivation of Science, Kolkata, India, SANKAR DAS SARMA, Condensed Matter Theory Center, University of Maryland, College Park — We propose a new method of optical lattice modulation spectroscopy for studying the spectral function of ultracold bosons in an optical lattice. We show that different features of the single particle spectral function in different quantum phases can be obtained by measuring the change in momentum distribution after the modulation. In the Mott phase, this gives information about the momentum dependent gap to particle-hole excitations as well as their spectral weight. In the superfluid phase, one can obtain the spectrum of the gapless Bogoliubov quasiparticles as well as the gapped amplitude fluctuations. The distinct evolution of the response with modulation frequency in the two phases can be used to identify these phases and the quantum phase transition separating them.

¹R.S. and S.D.S. acknowledge support from CNAM (UMD), ARO-DARPA-OLE, ARO-MURI and. JQI-NSF-PFC. K.S. acknowledges DST, INDIA project no. SR/S2/CMP-001/2009

12:39PM B1.00008 Population of atoms in the output of an atom Michelson interferometer, EBUBECHUKWU ILO-OKEKE, ALEX ZOZULYA, Worcester Polytechnic Institute — A cloud of Bose-Einstein condensate (BEC) sitting at the center of a weakly confining trap in an atom Michelson interferometer is split into two clouds that travel along different paths. The two clouds evolve and accumulate relative phase between them due to field of interest, confining potential and interatomic interactions. At the end of the interferometric cycle, the two clouds are recombined and the population of atoms found in the cloud at rest and the moving clouds depends on the relative phase. We derive an expression for the probability of counting any number of atoms within each cloud after recombination, study the dependence of the probability on the relative phase and relate our findings with experiments.

12:51PM B1.00009 Prototyping method for Bragg-type atom interferometers¹, BRANDON BENTON, MICHAEL KRYGIER, JEFFREY HEWARD, Georgia Southern University, MARK EDWARDS, Georgia Southern University and NIST, CHARLES CLARK, Joint Quantum Institute and NIST — We present a method for rapid modeling of new Bragg ultracold atom-interferometer (AI) designs useful for assessing the performance of such interferometers. The method simulates the overall effect on the condensate wave function in a given AI design using two separate elements. These are (1) modeling the effect of a Bragg pulse on the wave function and (2) approximating its evolution during the intervals between the pulses. The actual sequence of these pulses and intervals is then followed to determine the approximate final wave function from which the interference pattern can be calculated. The exact evolution between pulses is assumed to be governed by the Gross-Pitaevskii equation (GPE). We have developed both 1D and 3D versions of this method and have determined their validity by comparing their predicted interference patterns with those obtained by numerical integration of the 1D GPE and with the results of an experiment performed at NIST. We find good agreement between the 1D interference patterns predicted by this method and those found by the GPE. We show that we can reproduce the results of the NIST experiment and that this method provides estimates of 1D interference patterns 10,000 times faster than direct integration of the GPE.

¹This work supported by NSF grant number PHY-0758111

1:03PM B1.00010 Applications of chirped Raman adiabatic rapid passage to atom interferometry¹, KRISH KOTRU, DAVID L. BUTTS, C. S. Draper Laboratory, Inc., and MIT Dept. of Aeronautics and Astronautics, JOSEPH M. KINAST, DAVID M.S. JOHNSON, ANTONIJE M. RADOJEVIC, BRIAN P. TIMMONS, RICHARD E. STONER, C. S. Draper Laboratory, Inc. — We present robust atom optics, based on chirped Raman adiabatic rapid passage (ARP), in the context of atom interferometry. Such ARP light pulses drive coherent population transfer between two hyperfine ground states by sweeping the frequency difference of two fixed-intensity optical fields with large single photon detunings. Since adiabatic transfer is less sensitive to atom temperature and non-uniform Raman beam intensity than standard Raman pulses, this approach should improve the stability of atom interferometers operating in dynamic environments. In such applications, chirped Raman ARP may also provide advantages over the previously demonstrated stimulated Raman adiabatic passage (STIRAP) technique, which requires precise modulation of beam intensity and zeroing of the single photon detuning. We demonstrate a clock interferometer with chirped Raman ARP pulses, and compare its stability to that of a conventional Raman pulse interferometer. We also discuss potential improvements to inertially sensitive atom interferometers. Copyright © 2011 by The Charles Stark Draper Laboratory, Inc. All rights reserved.

¹This work was supported by the Draper Laboratory IR&D program. KK and DB acknowledge support from Draper Laboratory Fellowships.

1:15PM B1.00011 Berry-gauge tuned Bose-Einstein condensate gyroscope¹, RUDRA KAFLE, Worcester Polytechnic Institute, Worcester, MA 01609, EDDY TIMMERMANS, T- 4, Los Alamos National Laboratory, Los Alamos, NM 87544 — If stable, the many-body ground state of a dilute gas of ultra-cold, bosonic atoms occupying a superposition of two internal (hyperfine) states is a Bose-Einstein condensate (BEC) of effective spin 1/2 bosons. The superfluid BEC dynamics admits long-lived quantized vortex states in which the complex phase of the superfluid order parameter, which we call the charge phase, undergoes an integer number of 2π windings along a multiply connected path - a closed trajectory that encloses a region in which the superfluid density vanishes. In response to an overall rotation of the ring, a quantization event can occur that can be used to sense rotation. Unfortunately, the sensitivity of the ring BEC gyroscope would be limited as the quantization event sets in at a rotation frequency that is not as low as the frequencies measured by other devices such as ring laser gyroscopes. We show that the recently realized synthetic magnetic fields, in which the controlled position dependence of the spin results in an effective gauge field, can tune the BEC ring gyroscope to trigger a quantization event at much smaller rotation frequency. In addition, the effective gauge field can undergo its own quantization events in which the spin vector undergoes an integer number of 2π or 4π windings.

¹LDRD program and CNLS, LANL

1:27PM B1.00012 Frustration and glassiness in spin models with cavity-mediated interactions, SARANG GOPALAKRISHNAN, University of Illinois at Urbana-Champaign, BENJAMIN LEV, Stanford University, PAUL GOLDBART, Georgia Institute of Technology — Optical cavity photons can mediate interatomic interactions that are both long-ranged and sign-changing, thus enabling the realization of models and phases (such as supersolids [1]) that are inaccessible in conventional optical lattices. Here, we introduce a general scheme for realizing frustrated magnetic models possessing spin-glass states, using three-level atoms trapped at fixed positions inside a transversely pumped multimode cavity. We show that the effective Hamiltonian for such a system is analogous to the Hopfield associative-memory model [2], and, like the Hopfield model, possesses a spin glass phase for a sufficiently large ratio of the number of cavity modes to atoms. We argue that the spin glass phase should be accessible with realistic experimental parameters, discuss experimental signatures of the spin glass phase, and address the impact of dissipative processes such as cavity photon decay on the realizable phases and phase transitions.

[1] K. Baumann et al., *Nature* 464, 1301 (2010); S. Gopalakrishnan et al., *Nat. Phys.* 5, 845 (2009).

[2] J.J. Hopfield, *Proc. Nat. Acad. Sci* 79, 2554 (1982).

1:39PM B1.00013 Manipulation of ultracold rubidium atoms using a single linearly chirped laser pulse¹, SVETLANA MALINOVSKAYA, THOMAS COLLINS, Stevens Institute of Technology — At ultracold temperatures, atoms are free from thermal motion, which makes them ideal objects of investigations in the fields of high precision spectroscopy, metrology, quantum computation, producing Bose condensates, etc. The quantum state of ultracold atoms may be created and manipulated by optical pulses of rather low intensity and by making use of quantum control methods. Here, we discuss how the field phase variation, pulse duration and intensity, when perform in conformity, may yield a desired population distribution within the hyperfine structure of alkali atoms. We theoretically investigate ultracold Rb vapor using picosecond chirped pulses of kW/cm^2 beam intensity and show a possibility of controllable population transfer between hyperfine levels of $5^2S_{1/2}$ state through Raman resonances. Satisfying the one-photon resonance condition with the $5^2P_{1/2}$ or $5^2P_{3/2}$ state allows us to enter the adiabatic region of population transfer at very low field intensities, such that corresponding Rabi frequencies are less or equal to the hyperfine split. This methodology provides with a robust way to create a specifically designed superposition state in Rb in the basis of the hyperfine levels and perform state manipulation.

¹This research is partially supported by the National Science Foundation.

1:51PM B1.00014 Optical response of dark exciton Bose-Einstein condensate, MIKHAIL EREMENTCHOUK, MICHAEL LEUENBERGER, University of Central Florida — We study the optical response of Bose-Einstein condensate (BEC) formed by dark excitons in semiconductors. We consider the example of GaAs, where dark excitons are formed by heavy-holes and electrons with opposite signs of projections of their spins resulting in natural fragmentation of the condensate. Direct coupling of such excitons is dipole prohibited and, therefore, the optical response of semiconductor with dark condensate is provided through interaction of light with bright exciton states. We show that the Coulomb interaction of optically excited bright excitons with dark excitons residing in the BEC leads to effective renormalization of characteristics of bright excitons — e.g. their mass decreases — depending on the density of the condensate. As a result the exciton resonances experiences red-shift with decreasing amplitude. This provides an opportunity for indirect spectroscopy of dark exciton BEC.

2:03PM B1.00015 Electron field noise sensing with a scanning ion, ZACHARY FISHER, MICHAEL GUTIERREZ, MOLU SHI, DANIEL LI, YUFEI GE, PETER HERSKIND, ISAAC CHUANG, Research Laboratory of Electronics, Massachusetts Institute of Technology — Controlled shuttling of ions in a planar ion trap can serve as highly sensitive method for probing the electric field.¹ We apply this idea to the measurement of field noise effects on a microfabricated planar trap as a function of ion position. In particular, by shuttling an ion between different trapping zones, the field noise can be determined near different material surfaces, in particular dielectric materials. Surface effects on these materials are suspected to cause field fluctuations that decohere the motional state of trapped ions. By shuttling the ion to a determined location and measuring the electric field noise, a measure of the electric field noise can be determined as a function of proximity to dielectrics. A systematic examination of field noise due to dielectric versus metallic surfaces is valuable in, for example, a trapped-ion cavity QED system, where the high-reflectivity mirrors used in the optical cavities are large, exposed dielectric regions.²

¹G. Huber et al. A trapped-ion local field probe. *Appl Phys B* **100**, 725-730 (2010).

²P. Herskind, S. Wang, M. Shi, Y. Ge, M. Cetina and I. Chuang, *Optics Letters*, Vol. 36, Issue 16, 3045-3047 (2011).

Monday, February 27, 2012 11:15AM - 2:15PM – Session B2 FIP: Invited Session: Science Diplomacy: Africa and the Middle East 204AB

11:15AM B2.00001 ASP2012: Fundamental Physics and Accelerator Sciences in Africa, CHRISTINE DARVE¹, European Spallation Source — Much remains to be done to improve education and scientific research in Africa. Supported by the international scientific community, our initiative has been to contribute to fostering science in sub-Saharan Africa by establishing a biennial school on fundamental subatomic physics and its applications. The school is based on a close interplay between theoretical, experimental, and applied physics. The lectures are addressed to students or young researchers with at least a background of 4 years of university formation. The aim of the school is to develop capacity, interpret, and capitalize on the results of current and future physics experiments with particle accelerators; thereby spreading education for innovation in related applications and technologies, such as medicine and information science. Following the worldwide success of the first school edition, which gathered 65 students for 3-week in Stellenbosch (South Africa) in August 2010, the second edition will be hosted in Ghana from July 15 to August 4, 2012. The school is a non-profit organization, which provides partial or full financial support to 50 of the selected students, with priority to Sub-Saharan African students.

¹on behalf of the ASP2012 organizing committees

11:51AM B2.00002 The African Laser Centre: Transforming the Laser Community in Africa, SEKAZI MTINGWA, Massachusetts Institute of Technology — We describe the genesis and programs of the African Laser Centre (ALC), which is an African nonprofit network of laser users that is based in Pretoria, South Africa. Composed of over thirty laboratories from countries throughout the continent of Africa, the ALC has the mission of enhancing the application of lasers in research and education. Its programs include grants for research and training, equipment loans and donations, student scholarships, faculty grants for visits to collaborators' institutions, conferences, and technician training. A long-term goal of the ALC is to bring a synchrotron light source to Africa, most probably to South Africa. One highly popular program is the biennial conference series called the US-Africa Advanced Studies Institute, which is funded by the ALC in collaboration with the U.S. National Science Foundation and the International Center for Theoretical Physics in Trieste. The Institutes typically bring about thirty faculty and graduate students from the U.S. to venues in Africa in order to introduce U.S. and African graduate students to major breakthroughs in targeted areas that utilize lasers. In this presentation, we will summarize the ALC achievements to date and comment on the path forward.

12:27PM B2.00003 SESAME – A light source for the Middle East¹, HERMAN WINICK, SLAC National Accelerator Laboratory — Developed under UNESCO and modelled on CERN, SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East) is an international research centre in construction in Jordan, enabling world-class research while promoting peace through scientific cooperation. Its centerpiece, a new 2.5 GeV 3rd Generation Electron Storage Ring (133m circumference, 26nm-rad emittance, 12 places for insertion devices), will provide intense light from infra-red to hard X-rays. The Council (Bahrain, Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, Palestinian Authority, Turkey), provides the annual budget. Concrete shielding is complete, and a staff of 21 is installing the refurbished 0.8 GeV BESS Y I injector system, a gift from Germany. The facility can serve 25 simultaneous experiments. Beamline equipment has been provided by Daresbury (UK), the Helmholtz Assoc. (Germany), the Swiss Light Source, LURE (France), the Univ. of Liverpool, Elettra (Italy) and US labs. Jordan has contributed \$3.3M, in addition to a building and land. The EU has contributed \$4.8M. Commitments confirmed by Members look set to provide most of \$35M needed to complete construction of the ring and 3 beamlines. A training program has been underway since 2000. See www.sesame.org.jo

¹Support by the Office of Basic Energy Sciences, Office of Science, US Department of Energy

1:03PM B2.00004 Marshak Lectureship: The Turkish Accelerator Center, TAC, OMER YAVAS¹, Accelerator Technologies Institute, Ankara University, Ankara, Turkey — The Turkish Accelerator Center (TAC) project is comprised of five different electron and proton accelerator complexes, to be built over 15 years, with a phased approach. The Turkish Government funds the project. Currently there are 23 Universities in Turkey associated with the TAC project. The current funded project, which is to run until 2013 aims

1. To establish a superconducting linac based infra-red free electron laser and Bremsstrahlung Facility (TARLA) at the Golbasi Campus of Ankara University,
 - (a) To establish the Institute of Accelerator Technologies in Ankara University, and
2. To complete the Technical Design Report of TAC. The proposed facilities are a 3rd generation Synchrotron Radiation facility, SASE-FEL facility, a GeV scale Proton Accelerator facility and an electron-positron collider as a super charm factory.

In this talk, an overview on the general status and road map of TAC project will be given. National and regional importance of TAC will be expressed and the structure of national and international collaborations will be explained.

¹On behalf of TAC Collaboration

1:39PM B2.00005 Andrei Sakharov Prize Lecture: Physics and Freedom in Ethiopia, MULUGETA BEKELE, Department of Physics, Addis Ababa University — I will highlight my forty years involvement in physics education and research in Ethiopia and draw lessons that could be learnt from it.

Monday, February 27, 2012 11:15AM - 2:15PM –

Session B3 DCMP: Invited Session: Superconducting Coherence, Fluctuations & Inhomogeneity in Mesoscopic & Low-Dimensions 205AB

11:15AM B3.00001 Emergence of h/e -period oscillations in the critical temperature of small superconducting rings and critical velocity in one-dimensional superconductors, TZU-CHIEH WEI, CN Yang Institute for Theoretical Physics, Stony Brook University — When a large ring of superconductor is threaded by a magnetic flux, the resistance and the critical temperature exhibit oscillations in a flux quantum of $h/2e$. The flux quantum of an electron circling a thread flux on a clean metallic ring is on the contrary h/e . When the radius starts to shrink, electrons that compose of Cooper pairs may be able to roam around the ring individually without costing too much energy. An h/e period should thus arise. We discuss the emergence of h/e -period oscillations in the critical temperature of small superconducting rings and a few scenarios of superconducting-normal metal transitions. Interestingly, a threading flux is equivalent to a momentum boost in the circumferential direction of the ring. We also discuss a related issue as to how high a flow velocity one-dimensional superconductors can sustain before superconductivity gives way to this instability and the system becomes normal.

11:51AM B3.00002 Manipulating superconducting fluctuations in ultrasmall loops and quasi one-dimensional wires of Al¹, NEAL STALEY, The Pennsylvania State University — Superconducting fluctuations and the control of these fluctuations have been a problem of long-standing interest, with recent impetus provided by its relevance to the pursuit of very high temperature superconductivity through the engineering of global phase coherence. In quasi one-dimensional superconductors, fluctuations due to thermal or quantum processes lead to phase slips, and the appearance of a finite electrical resistance. We found that the critical current in mesoscopic quasi one-dimensional wires of Al is influenced by the bulk measurement electrodes, and in fact increases with magnetic field at low fields, suggesting that the phase slips are suppressed by the loss of superconductivity in the bulk electrodes. Manipulation of superconducting fluctuations is also possible in ultrasmall loops, where the strength of the fluctuations is controlled by the loop's size in comparison with ξ and the enclosed flux. For ultrasmall loops with a circumference $\sim \pi\xi(0)$, de Gennes predicted more than three decades ago that superconductivity could be completely destroyed near half-integer-flux quanta even to zero temperature. Furthermore, the resulting destructive regime, likely dominated by quantum fluctuations at low temperatures, was predicted to be suppressed with the addition of a superconducting side branch. We observed this Little-Parks-de Gennes effect in ultrasmall Al loops prepared by e-beam lithography and we found that the addition of a superconducting side branch restores the lost phase coherence. We will present our most recent data and discuss the implications of our experimental observations.

¹Work done in collaboration with Ying Liu, and supported by NSF under Grant DMR 0908700 and Penn State MRI Nanofabrication Lab under NSF Cooperative Agreement 0335765, NNIN with Cornell University.

12:27PM B3.00003 Magnetic-field-induced superconductivity and damping of phase slips in Zn nanowires¹, YU CHEN², Department of Physics, University of California-Santa Barbara — We report an observation that Zn nanowires connected with Zn electrodes, after being driven resistive by the current, re-entered their superconducting state upon the application of a small magnetic field [1, 2]. A detailed experimental investigation was carried out, with variation of parameters such as magnetic field orientation, wire length, etc.. The results provide solid evidence that this is a nonequilibrium effect associated the coupling with the boundary electrodes. There are two characteristic length scales involved, approaching either of which weakens the effect. Most importantly, we demonstrated that it is more appropriate to consider the effect to be a stabilization of superconductivity that has been suppressed by an applied current. Although we do not present a formal theory to explain all of our results here, the effect is most likely a consequence of the damping of phase fluctuations by quasiparticles which are created in the electrodes by small magnetic fields.

[1] Yu Chen, S. D. Snyder, and A. M. Goldman, Phys. Rev. Lett. 103, 127002(2009).

[2] Yu Chen, Yen-Hsiang Lin, S. D. Snyder, and A. M. Goldman, Phys. Rev. B 83, 054505(2011)

¹This work was supported by the U.S.Department of Energy under Grant No. DE-FG02-02ER46004.

²The work was done at the School of Physics and Astronomy in the University of Minnesota.

1:03PM B3.00004 Quantum liquid crystals: spontaneously modulated Fermi superfluids¹, YEN LEE LOH, University of North Dakota — What happens to a BCS superconductor when the numbers of up and down fermions are unequal? This is a fascinating and difficult problem in many-body physics. The most exciting possibility is that pairing and polarization compete to produce a modulated superfluid state, known as an Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase. This is a quantum liquid crystal exhibiting microscale phase separation, in which the excess fermions self-organize into domain walls where the pairing amplitude changes sign. There is a growing body of indirect evidence for the existence of FFLO states. As an example, I present our recent work on Al thin film superconductors in parallel magnetic fields [1]. Just below the Chandrasekhar-Clogston spin paramagnetic transition, our tunneling density of states measurements reveal a significant population of subgap states. These excess states cannot be explained in terms of conventional superconductivity, but they are a natural consequence of disordered FFLO physics. There is also hope for realizing FFLO in ultracold gases of neutral fermionic atoms. Continuum FFLO states are very fragile, but our calculations suggest that FFLO states are greatly stabilized by an optical lattice. For a cubic lattice with suitable parameters, up to 80% of the fermions participate in the FFLO phase [2]. Furthermore, we propose an interferometric technique to detect pairing amplitude modulations, which may provide the first *direct* evidence of FFLO [3].

[1] Y. L. Loh, N. Trivedi, Y. M. Xiong, P. W. Adams, and G. Catelani, "Origin of Excess Low-Energy States in a Disordered Superconductor in a Zeeman Field," PRL 107, 067003 (2011)

[2] Y. L. Loh and N. Trivedi, "Detecting the Elusive Larkin-Ovchinnikov Modulated Superfluid Phases in Imbalanced Fermi Gases in Optical Lattices," PRL 165302 (2010)

[3] M. Swanson, Y. L. Loh, and N. Trivedi, "Proposal for interferometric detection of topological defects in modulated superfluids," arXiv:1106.3908

¹Acknowledgments: DOE #DE-FG02-07ER46423, ARO, DARPA #W911NF-08-1-0338.

1:39PM B3.00005 Superconductivity in one-atomic-layer films and ultrasmall island of Pb and In grown on Si(111) by molecular beam epitaxy, JINFENG JIA, Department of Physics, Shanghai Jiao Tong University — No abstract available.

Monday, February 27, 2012 11:15AM - 2:15PM –

Session B4 DAMOP: Hybrid Systems, Optomechanics and Macroscopic Systems at the Quantum Limit I 205C

11:15AM B4.00001 Observing quantum phenomena in cavity optomechanics¹, NATHANIEL BRAHMS, DAN W. C. BROOKS, SYDNEY SCHREPPLER, THIERRY BOTTER, DAN M. STAMPER-KURN, Univ of California - Berkeley — Recent efforts have produced optomechanical systems whose mechanical elements are prepared at or near their quantum ground state. But what manifestly quantum effects can be measured with these new systems? Here we present results from our experiment, using the collective motion of an ultracold atom ensemble as a mechanical oscillator. The motion is driven by shot noise in the light's radiation pressure, allowing us to observe the production of nonclassical states of light by optomechanics – here, quadrature-squeezed light. Notably, this nonlinear optical effect occurs with only 40 pW of pump power. We also measure the quantization of the oscillator, by observing a 3:1 asymmetry in the light it scatters to low- and high-energy optical sidebands. Analyzing the light emitted from the cavity moreover provides a spectroscopic record of the energy exchanged between light and motion, allowing us to directly quantify the necessary diffusive heating of a quantum backaction-limited position measurement.

¹Support from NSF and AFOSR

11:27AM B4.00002 Cryogenic optomechanics with a 261kHz mechanical oscillator, DONGHUN LEE, ANDREW JAYICH, Yale University, JACK SANKEY, McGill University, CHEN YANG, LILY CHILDRESS, MITCHELL UNDERWOOD, KJETIL BORKJE, STEVE GIRVIN, JACK HARRIS, Yale University — Mechanical motion can interact with light via radiation pressure force. With recent experimental advances over the last few years, such optomechanical coupling has been used to reach quantum ground state of mechanical oscillators, which opens interesting new regime of observing quantum mechanics in macroscopic objects. The optomechanical devices used in this talk consist of a dielectric SiN membrane located inside a high finesse optical cavity. Combining cryogenic cooling in He3 refrigerator and resolved sideband laser cooling enables us to cool the membrane's mechanical mode (whose mechanical frequency is 261kHz) to less than 60 phonons. We will describe some technical challenges in our experiments such as the role of classical phase noise of the cooling laser at the mechanical frequency and our efforts to significantly reduce it via a filter cavity.

11:39AM B4.00003 Ultraefficient Cooling of Resonators: Beating Sideband Cooling with Quantum Control, XIAOTING WANG, SAI VINJANAMPATHY, University of Massachusetts at Boston, FREDERICK STRAUCH, Williams College, KURT JACOBS, University of Massachusetts at Boston — There is presently a great deal of interest in cooling high-frequency micro- and nano-mechanical oscillators to their ground states. The present state of the art in cooling mechanical resonators is a version of sideband cooling, which was originally developed in the context of cooling trapped ions. Here we present a method based on quantum control that uses the same configuration as sideband cooling—coupling the resonator to be cooled to a second microwave (or optical) auxiliary resonator—but will cool significantly colder. This is achieved by applying optimal control and varying the strength of the coupling between the two resonators over a time on the order of the period of the mechanical resonator. As part of our analysis, we also obtain a method for fast, high-fidelity quantum information transfer between resonators.

11:51AM B4.00004 Postselected optomechanical superpositions¹, BRIAN PEPPER, UC Santa Barbara, ROOHOLLAH GHOBADI, University of Calgary / Sharif University of Technology, EVAN JEFFREY, University of Leiden, CHRISTOPH SIMON, University of Calgary, DIRK BOUWMEESTER, UC Santa Barbara / University of Leiden — We present a scheme for achieving macroscopic quantum superpositions in weakly coupled optomechanical systems by using single photon postselection. This method allows the creation of macroscopic superpositions with currently achievable device parameters, and allows observation of decoherence on a timescale unconstrained by the system's optical decay time. This method relieves many of the challenges associated with previous optical schemes for measuring macroscopic superpositions, and only requires the devices to be in the weak coupling regime. Prospects for observing novel decoherence mechanisms are also discussed.

¹ The authors gratefully acknowledge support from NSF PHY-0804177 and Marie Curie EXT-CT-2006-042580

12:03PM B4.00005 Coupling a single spin in diamond to the quantum motion of a mechanical cantilever, STEVEN BENNETT, SHIMON KOLKOWITZ, QUIRIN UNTERREITHMEIER, Harvard University, PETER RABL, IQOQI-University of Innsbruck, ANIA BLESZYNSKI-JAYICH, University of California, Santa Barbara, JACK HARRIS, Yale University, MIKHAIL LUKIN, Harvard University — We present theoretical considerations for a magnetized mechanical cantilever coupled to a single electronic spin associated with a nitrogen-vacancy (NV) defect center in diamond. This coupled system has recently been implemented in an experiment where the NV spin was used to detect the thermal motion of a magnetic force microscope cantilever at room temperature, reading out the spin state optically using the spin-selective fluorescence of the NV. The possibility to extend this system to the quantum regime opens the door to applications such as readout and transfer of quantum information, as well as interesting theoretical questions. For example, it should be possible to reach the regime of strong coupling between the spin and the motion of the cantilever, in analogy to cavity quantum electrodynamics. We discuss the prospects for reaching the strong coupling regime and the conditions for measuring the onset of quantum effects, such as measuring the zero point motion of the cantilever using the spin as a detector.

12:15PM B4.00006 Thermally induced parametric instability in back-action evading measurement of micromechanical quadrature near the zero-point level, JUNHO SUH, MATT SHAW, AARON WEINSTEIN, KEITH SCHWAB, California Institute of Technology — Back-action evading (BAE) measurement of mechanical resonators allows, in principle, detection of a single quadrature of motion with sensitivity far below the standard quantum limit, limited in practice only by the non-idealities in the measurement. We report the results of experiments utilizing two-tone BAE in a tightly coupled cavity quantum electro-mechanical system ($\omega_c=7.1\text{GHz}$, $\omega_m=10\text{MHz}$, $g=14\text{MHz/nm}$). Due to excess dissipation in the microwave cavity, we observe a parametric instability induced by the thermal shift of mechanical resonance frequency. This bounds the minimum position imprecision on one quadrature and we measure the imprecision reaching twice the zero-point motion. We discuss the device requirements to avoid this thermal mechanism and perform measurements below the zero-point level.

12:27PM B4.00007 Mechanical squeezing via parametric amplification and feedback control¹, ANDREW DOHERTY, Centre for Engineered Quantum Systems, University of Sydney, A. SZORKOVSKY, G.I. HARRIS, W.P. BOWEN, Centre for Engineered Quantum Systems, The University of Queensland — We discuss the mechanical squeezing that can result from position measurement and feedback applied to a parametrically driven mechanical oscillator. If the parametric drive is optimally detuned from resonance, correlations between the quadratures of motion allow unlimited steady-state squeezing. This contrasts to a parametric drive alone, which is limited to 3dB of squeezing. Compared to back-action evasion, we demonstrate that the measurement strength, temperature and efficiency requirements for quantum squeezing are significantly relaxed.

¹Supported by the Australian Research Council Centre of Excellence CE110001013 and Discovery Project DP0987146.

12:39PM B4.00008 Asymmetric absorption and emission of energy by a macroscopic mechanical oscillator in a microwave circuit optomechanical system, JENNIFER HARLOW, TAUNO PALOMAKI, JOSEPH KERCKHOFF, JILA, University of Colorado and NIST, JOHN TEUFEL, RAYMOND SIMMONDS, NIST Boulder, KONRAD LEHNERT, JILA, University of Colorado and NIST — We measure the asymmetry in rates for emission and absorption of mechanical energy in an electromechanical system composed of a macroscopic suspended membrane coupled to a high-Q, superconducting microwave resonant circuit. This asymmetry is inherently quantum mechanical because it arises from the inability to annihilate the mechanical ground state. As such, it is only appreciable when the average mechanical occupancy approaches one. This measurement is now possible due to the recent achievement of ground state cooling of macroscopic mechanical oscillators [1,2]. Crucially, we measure the thermal cavity photon occupancy and account for it in our analysis. Failure to correctly account for the interference of these thermal photons with the mechanical signal can lead to a misinterpretation of the data and an overestimate of the emission/absorption asymmetry.

[1] J. D. Teufel, T. Donner, Dale Li, J. W. Harlow, M. S. Allman, K. Cicak, A. J. Sirois, J. D. Whittaker, K. W. Lehnert, R. W. Simmonds, "Sideband Cooling Micromechanical Motion to the Quantum Ground State," *Nature*, 475, 359363 (2011).

[2] Jasper Chan, et al, "Laser cooling of a nanomechanical oscillator into its quantum ground state," *Nature*, 478, 89-92 (2011).

12:51PM B4.00009 Quantum many-body system based on phonons and donors in silicon, Ö. O. SOYKAL, CHARLES TAHAN, Laboratory for Physical Sciences, College Park, MD — Cold atoms in optical lattices have become an indispensable tool for the study of many-body physics. Here, we introduce a novel many-body quantum system based on phonons with potentially useful properties. Theoretical results will be presented on the possibility of interacting systems based on phonitons, hybrid composite objects of a matter excitation and a cavity phonon. We discuss experimentally accessible regimes in silicon phoniton systems involving Mott insulator and superfluid phases. We consider experimental tools to probe these many-body states and give explicit designs for devices where they can be observed.

1:03PM B4.00010 Development of a dispersive read-out technique for quantum measurements of nanomechanical resonators¹, FRANCISCO ROUXINOL, MATT LAHAYE, Syracuse University — The development of techniques to observe non-classical behavior of micro- and nano- scale mechanical structures has received considerable attention in recent years because of the potential to use these systems for fundamental studies of quantum mechanics as well as their possible role as new technologies for applications ranging from the sensing of weak forces to quantum communication. One important route for observing such behavior is the coupling of micro- and nanomechanical resonators with superconducting qubits. Under certain conditions, qubit-coupled mechanical devices are formally analogous to Jaynes-Cummings systems which have been used in fields such as cavity QED for explorations of matter-radiation interactions and the quantum nature of light. Correspondingly, experiments in the last couple of years have begun to develop superconducting qubits as tools to manipulate and measure quantum states of mechanics. In this talk, we will discuss our efforts to integrate charge-type superconducting qubits as elements for dispersive (non-resonant) read-out and control of nanomechanical resonators, including preliminary system design and the prospects of implementing this system for read-out of the number-state statistics of nanomechanical modes.

¹This work is supported by NSF-DMR Career Award 1056423 and funding from the College of Arts and Sciences at Syracuse University.

1:15PM B4.00011 Measuring Quantum Optomechanical Self-induced Oscillations: Photon Correlation and Homodyne Tomography¹, JIANG QIAN, School of Engineering, Case Western Reserve University, FLORIAN MARQUARDT, Department of Physics, FAU Erlangen-Nuremberg, AASHISH CLERK, Department of Physics, McGill University, KLEMENS HAMMERER, Institute for Theoretical Physics, University of Hannover — Motivated by recent experimental advances in fabricating systems with large optomechanical couplings, we study the self-induced mechanical oscillations in the strong quantum regime for a single cell optomechanical system. We show that, under strong optomechanical coupling $g_M \geq \kappa$, the *persistent* state of the mechanical oscillator can have non-classical, *strongly negative* Wigner density, which can be measured by non-destructive homodyne tomography. We further propose to detect the onset of the quantum self-induced oscillation using the easier-to-measure photon two-point correlation functions $g^{(2)}(t)$. We show that there are two distinct signatures in the long-term time-average and the line-shape of $g^{(2)}(t)$ at the onset of self-induced oscillations. We show that $g^{(2)}(t)$ exhibits long-term coherence extending much beyond the optical decay time $1/\kappa$, the decay of which in the red- and blue-detune regime we explain using models of optomechanical cooling and phase noise.

¹J.Q. acknowledge the support of LRZ and Anordl Sommerfeld center for Theoretical Physics for the duration of this work, and the support of NIM and DFG through SFB631

1:27PM B4.00012 Controllable Coherent Transfer between a Superconducting Resonator and a Mechanical Oscillator, TAUNO PALOMAKI, JENNIFER HARLOW, JOSEPH KERCKHOFF, REED ANDREWS, JILA, NIST and the University of Colorado, Boulder, JOHN TEUFEL, RAYMOND SIMMONDS, National Institute of Standards and Technology, Boulder, KONRAD LEHNERT, JILA, NIST and the University of Colorado, Boulder — We report experimental results of controllable coupling between a 7.5 GHz superconducting resonator and a 10 MHz mechanical oscillator. Through time domain measurements, we demonstrate controlled coherent energy transfer between these two systems. Furthermore, by utilizing a Josephson parametric amplifier we have been able to verify coherent transfer of small amplitude states. We compare these results to frequency domain measurements and discuss experimental limitations.

1:39PM B4.00013 Using interference for high fidelity quantum state transfer in optomechanics¹, YING-DAN WANG, AASHISH A. CLERK, McGill University — We present a theoretical study of a two-cavity optomechanical system (e.g. a single mechanical resonator coupled to both a microwave and an optical cavity), investigating how interference can be used to perform mechanically-mediated quantum state transfer between the two cavities. We show that this optomechanical system possesses an effective "mechanically-dark" mode which is immune to mechanical dissipation; utilizing this feature allows highly efficient transfer of intra-cavity states, as well as of itinerant photon states. Simple analytic expressions for the fidelity of transferring both Gaussian and non-Gaussian states are provided. Our work has relevance to ongoing experimental efforts in quantum optomechanics (e.g., C. A. Regal and K. W. Lehnert, *J. Phys.: Conf. Ser.* 264, 012025 (2011); A. H. Safavi-Naeini and O. Painter, *New J. Phys.* 13, 013017 (2011)).

¹This work was supported by the DARPA ORCHID program under a grant from the AFOSR.

1:51PM B4.00014 Adiabatic State Conversion and Photon Transmission in Optomechanical Systems¹, LIN TIAN, University of California, Merced — Light-matter interaction in optomechanical systems in the strong coupling regime can be explored as a tool to transfer cavity states and to transmit photon pulses. Here, we show that quantum state conversion between cavity modes with different wavelengths can be realized with high fidelity by adiabatically varying the effective optomechanical couplings. During this adiabatic process, the quantum state is preserved in the dark mode of the cavities, similar to the adiabatic transfer schemes in EIT systems. The fidelity for gaussian states is derived by solving the Langevin equation in the adiabatic limit and shows negligible dependence on the mechanical noise. We also show that an input pulse can be transmitted to an output channel with a different wavelength via the effective optomechanical couplings. The condition for optimal transmission is derived in the frequency domain. Input pulses with a narrow spectral width can be transmitted with high fidelity. For input pulses with a large spectral width, the shape of the output pulses can be manipulated by applying time-dependent effective couplings. (1) L. Tian, arXiv:1111.2119. (2) L. Tian and H. L. Wang, Phys. Rev. A 82, 053806 (2010).

¹This work is supported by DARPA-ORCHID, NSF-DMR-0956064, NSF-CCF-0916303, and NSF-COINS.

2:03PM B4.00015 Single atom array to form a Rydberg ring¹, MINGSHENG ZHAN, PENG XU, XIAODONG HE, MIN LIU, JIN WANG, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences — Single atom arrays are ideal quantum systems for studying few-body quantum simulation and quantum computation [1]. Towards realizing a fully controllable array we did a lot of experimental efforts, which include rotating single atoms in a ring optical lattice generated by a spatial light modulator [2], high efficient loading of two atoms into a microscopic optical trap by dynamically reshaping the trap with a spatial light modulator [3], and trapping a single atom in a blue detuned optical bottle beam trap [4]. Recently, we succeeded in trapping up to 6 atoms in a ring optical lattice with one atom in each site. Further laser cooling the array and manipulation of the inner states will provide chance to form Rydberg rings for quantum simulation.

[1] M. Saffman et al., Rev. Mod. Phys. 82, 2313 (2010)

[2] X.D. He et al., Opt. Express 17, 21014 (2009)

[3] X.D. He et al., Opt. Express 18, 13586 (2010)

[4] P. Xu et al., Opt. Lett. 35, 2164 (2010)

¹This work was supported by the National Basic Research Program of China under grant No.2012CB922101

Monday, February 27, 2012 11:15AM - 2:15PM —
Session B5 DCMP DMP: Surface Electronic & Lattice Properties: Interfaces, Spin Effects, Etc. 206A

11:15AM B5.00001 Spatially Resolved Nano-Scale Characterization of Electronic States in SrTiO₃(001) Surfaces by STM/STS, KATSUYA IWAYA, TAKEO OHSAWA, RYOTA SHIMIZU, Tohoku University, TOMIHIRO HASHIZUME, Hitachi, Ltd., TARO HITOSUGI, Tohoku University, TOHOKU UNIVERSITY COLLABORATION, HITACHI, LTD. COLLABORATION, TOKYO INSTITUTE OF TECHNOLOGY COLLABORATION, JAPAN SCIENCE AND TECHNOLOGY AGENCY COLLABORATION — We have performed low temperature scanning tunneling microscopy/spectroscopy (STM/STS) measurements on TiO₂-terminated SrTiO₃(001) thin film surfaces. The conductance map exhibited electronic modulations that were completely different from the surface structure. We also found that the electronic modulations were strongly dependent on temperature and the density of atomic defects associated with oxygen vacancies. These results suggest the existence of strongly correlated two-dimensional electronic states near the SrTiO₃ surface, implying the importance of electron correlation at the interfaces of SrTiO₃-related heterostructures.

11:27AM B5.00002 The Structure of High Polarization Surface of the Antiferromagnet Cr₂O₃, NING WU, XIN ZHANG, KEISUKE FUKUTANI, XI HE, CHRISTIAN BINEK, PETER DOWBEN, Department of Physics and Astronomy and the Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, Lincoln, NE 68588, USA, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182-0266, USA, ZHAOXIAN YU, School of Physics and Engineering, Zhongshan University, Guangzhou 510275, Peoples Republic of China, UNL TEAM, UNO COLLABORATION, ZHONGSHAN COLLABORATION — Manipulation of magnetically ordered states by electrical means is among the most promising approaches towards novel spintronic devices. Electric control of the exchange bias can be realized when the passive antiferromagnetic pinning layer is replaced by a magneto-electric antiferromagnet, like the prototypical magneto-electric Cr₂O₃(0001), so long as there is also a finite remanent magnetization at the surface or boundary. We have demonstrated that a very unusual high polarization surface magnetic order exists at the surface of the Cr₂O₃(0001) surface and is robust against surface roughness from spin polarized inverse photoemission, and X-ray magnetic circular dichroism. We have also performed LEED (low energy electron diffraction) I(V) analysis to explore the surface structure above and below Neel Temperature (308 K). Temperature dependent LEED was also carried out at several different electron kinetic energies and Debye temperature was extracted. The surface and bulk Debye temperatures were obtained by fitting Debye temperature as a function of electron kinetic energy.

11:39AM B5.00003 Resonance Photoemission and Spin Polarization of Fe_xCo_{1-x}S₂¹, XIN ZHANG, NING WU, PETER DOWBEN, Nebraska Center for Materials and Nanoscience, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, NE 68588-0299, CHRIS LEIGHTON, MICHAEL MANNO, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455, USA, ELIO VESCOVO, Brookhaven National Laboratory, National Synchrotron Light Source, Upton, New York 11973, USA — The electronic structure in the region of the Fe/Co 3d band for Fe_xCo_{1-x}S₂ has been investigated by photoemission and spin polarized photoemission. The comparison between the results for different content of doped Fe was made, specifically x=0, 0.05, 0.10, 0.15 and 1. While the surface spin polarization of Fe_xCo_{1-x}S₂, measured by spin polarized ultraviolet photoemission, was reduced compared with the bulk value, we see that the spin polarization increases with Fe doping level for textured thin films. The resonance photoemission spectroscopy shows that sulfur bands have strong resonance at the photon energy of the Co 2p core level, indicating strong hybridization between Co and sulfur bands in Fe_xCo_{1-x}S₂ (small x) however, the ultraviolet photoelectron spectroscopy (UPS) of FeS₂ exhibits a slightly different d-band density of states than Fe_xCo_{1-x}S₂.

¹Work at UNL and UMN was supported by their respective NSF MRSEC's.

11:51AM B5.00004 Theoretical Band Offsets in c-Si/Si-XII Heterojunctions¹, JAMAL MUSTAFA, BRAD MALONE, MARVIN COHEN, STEVEN LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — Many different phases of silicon can be formed under pressure, with some being metastable at standard temperatures and pressures. For one such phase, Si-XII, experiments have recently suggested it to be a semiconductor, confirming theoretical predictions that it has a narrow gap in its electronic band structure. Current-voltage measurements show rectifying behavior in c-Si/Si-XII heterojunctions, indicative of a band discontinuity at the interface. We present computations that quantify this band discontinuity using bulk band structures obtained with Density Functional Theory within the Local Density Approximation. In particular, we demonstrate the use of a semiconductor's intrinsic charge neutrality level to determine band lineups.

¹This work was supported by National Science Foundation Grant No. DMR10-1006184 and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by the DOE at LBNL's NERSC facility.

12:03PM B5.00005 Band Alignment in Transparent Conducting Oxide Schottky Junctions, RAFAEL JARAMILLO, SHRIRAM RAMANATHAN, Harvard University — Better understanding and control of band alignment in oxide-semiconductor heterostructures is essential for improving the performance of devices such as sensitized solar cells and quantum dot based light emitting devices. We will present studies of Schottky junctions formed between Al-doped ZnO (AZO) conducting oxide thin films and lightly doped silicon. AZO films with varying oxygen content have been synthesized by control of oxygen pressure during growth. Transport measurements (I-V and C-V) on devices are used to illustrate the degree to which the oxide stoichiometry can be used to engineer the junction characteristics.

12:15PM B5.00006 Interface Band Structure Effects upon Hot Electron Transport Across Non-Epitaxial Metal-Semiconductor Interfaces, JOHN GARRAMONE, Department of Materials Science & Engineering, McCormick School of Engineering & Applied Science, Northwestern University, Evanston, IL 60208-3108, JOE ABEL, College of Nanoscale Science and Engineering, University at Albany, SUNY, Albany, New York 12203, USA, SALVADOR BARRAZA-LOPEZ, Department of Physics, University of Arkansas, Fayetteville, AR 72710, USA, VINCENT LABELLA, College of Nanoscale Science and Engineering, University at Albany, SUNY, Albany, New York 12203, USA — The interface band structure of a semiconductor is shown to affect the transport of hot electrons across a non epitaxial metal-semiconductor interface. This is observed by measuring the hot electron attenuation length of Ag utilizing ballistic electron emission microscopy (BEEM). The attenuation length is observed to increase sharply for energies approaching the Schottky barrier height when deposited upon Si(001) substrates and decrease slightly when deposited upon Si(111) substrates. A theoretical description demonstrates that this is due to conservation of parallel momentum and differences in interface band structure of the two silicon orientations. At higher tip biases the attenuation lengths converge allowing extraction of the inelastic and elastic scattering lengths in the silver.

12:27PM B5.00007 A numerical simulation study of inverse doped surface layer in Schottky barrier modification, SUBHASH CHAND, PRIYANKA KAUSHAL, Department of Physics, National Institute of Technology, Hamirpur-177 005 (HP) — The Poisson's and continuity equations are solved by iterative method to obtain the potential and electron and hole concentrations inside the semiconductor near the metal semiconductor interface for different inverse layer thickness and doping concentrations. The barrier height (BH) and ideality factor (IF) obtained by fitting of simulated current voltage data into thermionic emission diffusion current equation. The derived BH increases with increase in inverse layer thickness as well as with increase in the inverse layer doping concentration and then saturates at maximum value. The IF first rises with increase in inverse layer thickness and then attaining a maximum value at a particular thickness it decreases approaching unity value for large inverse layer thickness. It is observed that for large inverse layer thickness the BH attains a maximum value with unity IF. Thus, there are two regimes, namely, non-ideal regime corresponding to less inverse layer thickness where the BH has increased less and IF is more than unity and ideal regime corresponding to large inverse layer thickness where the BH attains maximum value with unity IF.

12:39PM B5.00008 Density functional calculations of the Schottky barrier height and effective work function in Ni/oxide interfaces, HYEON-KYUN NOH, YOUNG JUN OH, ALEX TAEKYOUNG LEE, K.J. CHANG, Department of Physics, Korea Advanced Institute of Science and Technology — In high-k/metal gate stacks of complementary metal-oxide semiconductor devices, it is important to control the effective work functions of metals such that they should match to the doping levels of poly-Si gates. However, it is known that metal work functions are strongly affected by interface dipoles and defects. In this work, we perform first-principles density-functional calculations to study the Schottky barrier heights and the effective metal work functions in Ni/SiO₂ and Ni/HfO₂ interface structures. We use the advanced approaches such as hybrid density functional and quasi-particle GW calculations for the exchange-correlation potential and discuss the limitations of GGA calculations. We also examine the effects of O-vacancy defects introduced at the interface on the Schottky barrier height and the effective work function. We find that, in the Ni/HfO₂ interface, the *p*-type Schottky barrier height tends to increase with increasing of the defect density due to the charge transfer at the interface, whereas it is little affected in the Ni/SiO₂ interface.

12:51PM B5.00009 Models for (001) epitaxial interfaces between CdTe and ZnO¹, JOHN JAFFE, TIFFANY KASPAR, TIMOTHY DROUBAY, Pacific Northwest National Laboratory — Epitaxial interfaces between ZnO and CdTe appear difficult to achieve given their different crystal structures (CdTe is zinc blende with conventional lattice constant $a = 6.482$ Å, ZnO is hexagonal wurtzite with $a = 3.253$ Å and $c = 5.213$ Å.) However, ZnO also occurs in a metastable zinc-blende structure with an fcc primitive lattice constant close to the hexagonal a value. Since this value is close to half of the CdTe conventional (simple cubic) lattice constant, (001)-oriented cubic ZnO films might grow epitaxially on a CdTe (001) surface in an $R45^\circ \sqrt{2} \times \sqrt{2}$ configuration. Many alignments of the interfacial layers are possible, and we describe density-functional calculations on several of these to identify the most likely, and to predict valence-band offsets between CdTe and ZnO for each. Growth of ZnO on Te-terminated CdTe (001) is predicted to produce small or even negative (CdTe below ZnO) valence band offsets, resulting in a Type I band alignment. Growth on Cd-terminated CdTe is predicted to produce large positive offsets for a type II alignment as needed, for example, in solar cells. Calculations with the GGA + U method (with $U = 7.5$ eV for Zn 3d states) gave a valence band offset of +1.8 eV while a hybrid HSE06 + U calculation gave +2.6 eV. An experimental measurement on a ZnO film grown on CdTe (001) yielded a value of +2.2 eV for the valence band offset.

¹Supported by PNNL LDRD funding.

1:03PM B5.00010 The crystalline Si₃N₄/Si interface; the electronic structure of defects, ESPEN FLAGE-LARSEN, ESPEN SAGVOLDEN, OLE MARTIN LOEVVIK, DAN MICHAEL OLSEN HEGGOE, JESPER FRIIS, SINTEF Materials and Chemistry, P.O. Box 124 Blindern, Forskningsveien 1, N-0314 Oslo, Norway, CHANG-MING FANG, University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria — A semiconducting beta-Si₃N₄(0001)/Si(111) interface model without dangling bonds is presented, and its geometric and electronic structure is compared to previous models based on calculations in a density functional theory framework. Furthermore nitrogen and phosphorus defects in the silicon layer are investigated, in particular how these defects modify the electronic structure and the electronic properties of the interface as a function of their distance to it. The local geometric structure of the nitrogen and phosphorus defects is also investigated close to the interface.

1:15PM B5.00011 Epitaxial n-ZnO on p-Si with native SiO_x reduced by Al buffer¹, C.F. CHANG, J.H. WANG, H.J. HUANG, Z.W. HUANG, P.V. WADEKAR, K.H. HUANG, C.W. LIN, J.J. LIN, S.C. SHENG, L.W. TU, S.W. YEH, N.J. HO, Q.Y. CHEN², National Sun Yat-Sen University, C.H. LIAO, R.O.C. Military Academy — RF sputtering was employed to deposit n-type zinc oxide epitaxial thin films on p-type silicon substrates to form p-i-n diodes. A buffer layer of crystalline metal oxide was introduced by redox reaction between an aluminum layer and the native SiO₂. The aluminum layer was sputtered to various thicknesses and then annealed in situ for different times. The epitaxial relations follow (111) *S_i*/(0001) *ZnO* and [110] *S_i*/[1120] *ZnO*, though certain degree of mosaicity was observed wavering around the [112] *S_i* axis. Cross-sectional TEM observations of the interfaces, x-ray crystallography via ω -2 θ and rocking scans in regards to the perfection of the structures and orientations are agreeable. The current-voltage characteristics of the p-i-n diodes show promising outlooks for light emitting and photovoltaic applications.

¹Supported by the NSC and Ministry of Education, Taiwan, through the Center for Nano Science and Technology, NSYSU.

²Corresponding author, also at Texas Center for Superconductivity, University of Houston

1:27PM B5.00012 Emergence of orbital angular momentum due to broken inversion symmetry and its contribution to Rashba-type splitting, CHOONG H. KIM, Seoul National University, Seoul, Korea, JIN-HONG PARK, Sungkyunkwan University, Suwon, Korea, SEUNG RYONG PARK, University of Colorado at Boulder, Boulder, Colorado, USA, BEOM YOUNG KIM, Yonsei University, Seoul, Korea, JAEJUN YU, Seoul National University, Seoul, Korea, CHANGYOUNG KIM, Yonsei University, Seoul, Korea, JUNG HOON HAN, Sungkyunkwan University, Suwon, Korea — We demonstrate that the chiral orbital angular momentum (OAM) structure can emerge as a result of broken inversion symmetry especially at the metal surfaces. The surface-normal electric field is responsible for chiral OAM states even if spin-orbit interaction is negligible. Such chiral OAM structure can be measured by a circular dichroism (CD) in angle-resolved photoemission spectroscopy (ARPES). To confirm the existence of OAM and its detection by CD-ARPES, we perform simulation of CD-ARPES for Cu surface states by first-principles calculation and the results agree well with our CD-ARPES experiment. Addition of the spin-orbit interaction to the chiral OAM structure produces a chiral spin angular momentum (SAM) pattern and the corresponding Rashba-type band splitting. We assert that OAM polarization should be a more widespread feature than the chiral spin structure which requires strong spin-orbit coupling.

1:39PM B5.00013 Chiral Orbital Angular Momentum and Circular Dichroism ARPES in p- and d-orbital Bands, JIN-HONG PARK, JUNG HOON HAN, Sungkyunkwan University — We derive explicit formulas relating the circular dichroism angle-resolved photoemission (CD-ARPES) signal to the existence of nonzero chiral orbital angular momentum (OAM) in the band structure. The existence of nonzero chiral OAM is a generic feature of surface states that break inversion symmetry, as pointed out in several recent articles [1-3]. We propose that CD-ARPES setup is an effective probe of the OAM of quasi-particles occupying the surface states. Explicit formulas for the *p*- and *d*-orbital bands are derived to show that the CD-ARPES signal is proportional to the OAM in the momentum space.

[1] S. R. Park, C. H. Kim, J. Yu, J. H. Han and C. Kim, Phys. Rev. Lett. **107**, 156803 (2011).

[2] S. R. Park *et al.*, arXiv:1103.0805 (2011).

[3] Choong H. Kim *et al.*, arXiv:1107.3285 (2011).

1:51PM B5.00014 A first principles study of water adsorption on α -Pu (020) surface¹, JIANGUANG WANG, ASOK K. RAY, Department of Physics, University of Texas at Arlington, Arlington, Texas 76019, USA — Adsorptions of water in molecular (H₂O) and dissociative (OH+H, H+O+H) configurations on the α -Pu (020) surface have been studied using *ab initio* methods. The full-potential FP/LAPW+lo method has been used to calculate the adsorption energies at the scalar relativistic with no spin-orbit coupling (NSOC) and fully relativistic with spin-orbit coupling (SOC) theoretical levels. It is found that the SOC effect increases the adsorption energies by ~ 0.30 eV for the two dissociative adsorptions. Weak physisorptions have been observed for the molecule H₂O on the α -Pu (020) surface with primarily a covalent bonding, while the two dissociative adsorptions are chemisorptive with ionic bonding. At the SOC level, the most stable adsorption energy is 0.58eV, the corresponding values being 5.44 eV and 5.73 eV for the partial dissociation and complete dissociation cases, respectively. Completely dissociative adsorption at a long bridge site for the dissociated O atom and two short bridge sites for the two dissociated H atoms is the most stable adsorption site. Hybridizations of O(2p)-H(1s)-Pu(5f)-Pu(6d) are observed for the two dissociative adsorptions, implying that some of the Pu-5f electrons become further delocalized and participate in chemical bonding.

¹This work is partially supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525) and by the Department of Energy.

2:03PM B5.00015 Characterization of Hydrogen Interactions with δ -Pu using Electronic Structure Theory¹, CHRISTOPHER D. TAYLOR, Los Alamos National Laboratory, SARAH C. HERNANDEZ, University of Texas at Arlington — The generalized gradient approximation to density functional theory was used to study surface, bulk, defect, and reaction states of hydrogen in δ -Pu. The quasi-disordered anti-ferromagnetic arrangement gave a volume of 24.1 Å³ and a bulk modulus of 48.1 GPa for δ -Pu, in reasonable agreement with the experimental values of 24.9 Å³ and 30-35 GPa. This arrangement was thus subsequently used for all calculations. We have determined that hydrogen interactions with δ -Pu are exothermic in character at all levels ranging from dissociative chemisorption to interstitial absorption, the formation of hydrogen-vacancy complexes, and generation of a hydride phase. The exothermic character of these interactions appears to be the reason for the rapid hydriding reaction, which has been determined experimentally to be essentially a barrierless process. The anionic character is observed to be retained. Our studies also indicate that vacancies do not appear to be strong traps for hydrogen, since the interstitial absorption sites are exothermic in nature. We will propose a scheme by which hydrogen interacts with Pu. Results will be compared with previous studies in the literature where available.

¹This work is partially supported by the Los Alamos National Laboratory - Laboratory Directed Research & Development program (C.D.T) and by the Seaborg Institute Summer Research Fellowships Program (S.C.H).

Monday, February 27, 2012 11:15AM - 2:15PM —
Session B6 DCMP DMP: Thermal Properties of Graphene and Graphene Derivatives 206B

11:15AM B6.00001 Nanoscale Thermal Transport in Graphene Interfaces, RUI MAO, BYOUNGDON KONG, North Carolina State University, THUSHARI JAYASEKERA, Southern Illinois University, MARCO BUONGIORNO-NARDELLI, KI WOOK KIM, North Carolina State University, NORTH CAROLINA STATE UNIVERSITY TEAM — We have investigated nanoscale thermal transport in epitaxial graphene systems using first-principles calculations and the Landauer formalism for phonon transport. Two types of interfaces are investigated: graphene-dielectric and graphene-metal heterojunctions. Hexagonal boron nitride (h-BN), SiC and SiC with hydrogen passivation (SiC-H) are studied as potential dielectric substrate materials for graphene devices. As for graphene-metal contacts, we have considered Au and Ti as prototypical systems for physisorbed and chemisorbed metal contacts, respectively. The interfacial thermal resistances of h-BN/G system is $5.3 \cdot 10^{-9} \text{ Km}^2/\text{W}$ at room temperature, which is approximately one order of magnitude smaller than that of SiC/G system ($55\text{-}79 \cdot 10^{-9} \text{ Km}^2/\text{W}$). Further analysis shows that heat conduction at the graphene interfaces is dominated by low-lying acoustic phonons and the thermal resistances strongly depend on atomic details at the interface such as lattice mismatch, disorder and surface reconstruction. Our work demonstrates the importance of developing a microscopic description of phonon dynamics at heterogeneous interfaces to engineer and design devices with optimal thermal management.

11:27AM B6.00002 Isotope impurity doping in graphene, JOAQUIN RODRIGUEZ-NIEVA, MIT, RIICHIRO SAITO, Tohoku University, Japan, MILDRED S. DRESSELHAUS, MIT — Isotope impurities provide a powerful technique to study phonon related properties of graphene. The advantage of this approach is that phonon frequencies or thermal properties can be modified so that we can identify the origin of the interaction in the unknown optical spectra without changing either the electrical or chemical properties. In the presence of a ^{13}C isotope impurity in a normally ^{12}C lattice, the phonon wavefunction of graphene becomes localized. When we discuss the electron-phonon interaction of graphene, we treat phonons in terms of a delocalized wavefunction. However, in real graphene, we know that 2% of the atoms are ^{13}C and thus phonons have a finite lifetime, which results in a natural width in the Raman spectra. Many experimental results were obtained recently related to isotopic doping of graphene and carbon nanotubes and its effect on Raman spectra. In this work, we calculate the localization length of the phonons as well as the power law dependence for this effect. At the same time, we calculate the phonon lifetime of the different phonon modes within first order perturbation theory to elucidate the physical mechanisms behind isotope doping and to provide further insight into the experimental results.

11:39AM B6.00003 Polarization and electric field dependent electron-phonon interaction in graphene and graphene oxide, SATYAPRAKASH SAHOO, RAM S. KATIYAR, Department of Physics, University of Puerto Rico, San Juan, PR 00936-837 — Raman spectroscopy has been emerged as one of the important tool to understand various physical properties of graphene and graphene oxide. In this study, polarized Raman scattering has been performed to understand the electron-phonon interaction in connection with the second order Raman scattering process (2D band) in monolayer, bilayer and suspended bilayer graphene. The 2D Raman band shows strong polarization dependent irrespective of number of graphene layers. This effect has been explained on the basis of anisotropic photon scattering through the nodes at the K-point of the Brillouin zone in graphene during optical absorption. We also explored the electron-phonon interaction in graphene oxide in presence of electric field. The in-situ Raman studies show significant changes in the D and G Raman bands. In particular, the splitting of G band was observed with increase in voltage which indicates the electric field can alter the deformation-potential mediated electron-phonon interaction in graphene oxide. The electrical conductivity of graphene oxide was also found to increase dramatically with increase in voltage.

11:51AM B6.00004 High-fidelity phonon transport simulation in graphene devices using efficient, variance-reduced Monte Carlo methods, COLIN LANDON, NICOLAS HADJICONSTANTINO, Mechanical Engineering, MIT — In this talk we consider thermal transport in graphene at sufficiently small scales that diffusive transport (Fourier's law) is no longer valid. In this regime, the Boltzmann transport equation may be used to describe thermal transport, and Monte Carlo is the typical solution method, especially in the context of device simulation. Unfortunately, due to the slow rate of convergence of Monte Carlo solutions with the number of samples, such simulations can be prohibitively costly. By employing a recently developed variance-reduced Monte Carlo method, we are able to efficiently simulate the Boltzmann equation for phonon transport without resorting to approximations for reducing the problem complexity or dimensionality, such as neglecting phonon-phonon scattering events, or modeling boundary scattering as a homogeneous relaxation (scattering) process. We use our simulations to characterize the error associated with these approximations in the context of thermal transport in graphene devices, but also to study thermal transport in novel two-dimensional geometries.

12:03PM B6.00005 Thermal transport in graphene-based nanostructures¹, ZLATAN AKSAMIJA, IRENA KNEZEVIC, University of Wisconsin-Madison — Thermal conductivity of graphene and graphene-based nanostructures, such as graphene nanoribbons (GNRs), CVD-grown polycrystalline graphene (PCG), and nano-patterned single-layer graphene (SLG), is of great interest due to their potential applications as logic devices, high-frequency amplifiers, and heat spreaders in future nanoelectronic circuits. Both line edge roughness (LER) and substrate scattering have been shown to impact thermal transport and reduce graphene's record thermal conductivity; however, the combination of these two mechanisms, which will both be present simultaneously in supported nanostructures, has not been explored previously, and their combined impact on thermal transport has not been assessed. We solve the phonon Boltzmann transport equation and calculate the thermal conductivity tensor in a variety of suspended and supported graphene nanostructures. We show that there is a competition between LER and substrate scattering processes, leading to a high degree of directional anisotropy of thermal conductivity. We demonstrate that transport in narrow ribbons ($W < 100 \text{ nm}$) and PCG or nano-SLG with small feature sizes is dominated by roughness scattering and highly anisotropic. We discuss different avenues of controlling thermal transport in graphene-based devices.

¹This work has been supported by the Computing Innovation Fellows Project (NSF award No. 0937060 to the Computing Research Association, sub-award CIF-146 to the University of Wisconsin) and by the AFOSR YIP program (award No. FA9550-09-1-0230).

12:15PM B6.00006 Measurements of Thermal Conductivity and Thermopower in Suspended Single and Few Layer Graphene, INSUN JO, Department of Physics, The University of Texas at Austin, Austin, TX78712, USA, MICHAEL PETTES, Department of Mechanical Engineering, The University of Texas at Austin, Austin, TX78712, USA, ZHEN YAO, Department of Physics, The University of Texas at Austin, Austin, TX78712, USA, LI SHI, Department of Mechanical Engineering, The University of Texas at Austin, Austin, TX78712, USA — Detailed study on thermal conductivity and thermopower in suspended single and few layer graphene has been hampered by experimental challenges mainly due to the difficulty of obtaining suspended samples larger than a few micrometers. Here, we report on a high-yield process for the fabrication of suspended graphene samples of one to few atomic layers on micro-thermometer devices, which allow us to investigate electrical and thermal conductivity, and thermopower from 4 K to 500 K. We find that the thermal conductivity values in suspended graphene are largely limited by scattering with surface residues in as-made devices, and they can reach values comparable to those of bulk graphite after thorough cleaning of the sample surfaces. In addition, temperature-dependent thermopower results in suspended graphene are reported.

12:27PM B6.00007 Thermal Transport in Graphene from Large-scale Molecular Dynamics Simulations, LUIZ FELIPE PEREIRA, DAVIDE DONADIO, Max Planck Institute for Polymer Research — Carbon-based materials display exceptional thermal properties. The thermal conductivity of carbon allotropes can range five orders of magnitude. In the bulk, amorphous carbon is a very poor heat conductor, with $\kappa \approx 0.01$ W/m/K, whereas diamond has the highest thermal conductivity among elemental solids, $\kappa \approx 2000$ W/m/K at room temperature. Even broader ranges can be achieved by considering carbon nanostructures. Thermal conductivities as large as 5000 W/m/K have been measured for suspended graphene and carbon nanotubes. In spite of intense investigations, there is much controversy over the actual value of the thermal conductivity of graphene, both experimentally and theoretically. Here, we present results from equilibrium and non-equilibrium molecular dynamics simulations aimed at understanding the mechanism of heat transport in graphene. In particular, we investigate the influence of finite-size and uniaxial strain on the thermal conductivity of graphene, performing large scale molecular dynamics simulations of micrometer-size models containing up to 10^6 atoms.

12:39PM B6.00008 Tunable thermal transport and negative differential thermal conductance in graphene nanoribbons, JIUNING HU, YAN WANG, AJIT VALLABHANENI, XIULIN RUAN, YONG CHEN, Purdue University — We have studied thermal transport in graphene nanoribbons (GNRs) using classical nonequilibrium molecular dynamics simulations. We show that the calculated thermal conductivity of GNRs can be dramatically tuned by the shape, isotope composition, defects, and chirality and hydrogen passivation of the edges [1-2]. For GNRs under large temperature bias beyond the linear response, we have studied negative differential thermal conductance (NDTC) [3]. The NDTC is found to vanish for a sufficiently long GNR whose temperature is fixed at one end. Furthermore, for diffusive thermal transport obeying differential Fourier's law in a generic one-dimensional system, we analytically show that NDTC requires temperature dependent thermal conductivity and simultaneously varying temperatures at both ends. We have also studied asymmetrical GNRs and observed thermal rectification [1] and direction dependent NDTC [3]. Our studies may be useful for nanoscale thermal managements and thermal signal processing using GNRs and understanding low dimensional thermal transport in general.

[1] J. Hu et. al., **Nano Letters** **9**, 2730 (2009)
 [2] J. Hu et. al., **Applied Physics Letters** **97**, 133107 (2010)
 [3] J. Hu et. al., **Applied Physics Letters** **99**, 113101 (2011)

12:51PM B6.00009 Heat Transport in Graphene, SERAP YIGEN, VAHID TAYARI, JOSHUA O. ISLAND, JAMES PORTER, A.R. CHAMPAGNE, Department of Physics, Concordia University, Montreal, QC, Canada — We fabricated suspended graphene devices and measured their thermal conductivity, κ , as a function of both temperature, T, and charge carrier density, n. Heat transport is a powerful tool to obtain information about both the phononic and electronic properties of graphene. Recent heat transport experiments in graphene have shown a high κ , but a detailed mapping of graphene's heat conductivity versus T and n is not yet available. The measurement technique we developed is a two-point method which uses graphene as its own heat source (Joule heating) and thermometer (resistivity). We report κ at temperatures ranging from 6 to 350 Kelvin, and at charge carrier densities close to the Dirac point up to about $1.5 \times 10^{11}/\text{cm}^2$, in graphene crystals whose length varies from 250 nm up to one micron. We observed that the thermal conductivity increases by over two orders of magnitude over the temperature range, and that it also increases with the crystal's length. κ can be tuned by an order of magnitude with gate voltage, opening the possibility of creating room temperature heat transistors.

1:03PM B6.00010 Raman Measurements of Thermal Transport in Suspended Monolayer Graphene of Variable Sizes in Vacuum and Gaseous Environments, SHANSHAN CHEN, ARDEN MOORE, WEIWEI CAI, JI WON SUK, JINHO AN, COLUMBIA MISHRA, CHARLES AMOS, CARL MAGNUSON, University of Texas at Austin, JUNYONG KANG, Xiamen University, Xiamen, China, LI SHI, RODNEY RUOFF, University of Texas at Austin, XIAMEN UNIVERSITY TEAM — Using micro-Raman spectroscopy, the thermal conductivity of a graphene monolayer grown by chemical vapor deposition and suspended over holes with different diameters ranging from 2.9 to 9.7 μm was measured in vacuum, thereby eliminating errors caused by heat loss to the surrounding gas. The obtained thermal conductivity values of the suspended graphene range from (2.6 ± 0.9) to $(3.1 \pm 1.0) \times 10^3 \text{ Wm}^{-1} \text{ K}^{-1}$ near 350 K without showing the sample size dependence predicted for suspended, clean, and flat graphene crystal. The lack of sample size dependence is attributed to the relatively large measurement uncertainty as well as grain boundaries, wrinkles, defects, or polymeric residue that are possibly present in the measured samples. Moreover, from Raman measurements performed in air and CO_2 gas environments near atmospheric pressure, the heat transfer coefficient for air and CO_2 was determined and found to be $(2.9 \pm 5.1 / -2.9)$ and $(1.5 \pm 4.2 / -1.5) \times 10^4 \text{ Wm}^{-2} \text{ K}^{-1}$, respectively, when the graphene temperature was heated by the Raman laser to about 510 K.

1:15PM B6.00011 Effect of electron-electron interactions in thermoelectric power in graphene, FERESHTE GHAHARI, YURI ZUEV, Columbia University, Department of Physics, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, Japan, PHILIP KIM, Columbia University, Department of Physics — Thermoelectric power (TEP) of graphene is previously measured in the disorder limited transport regime where the semiclassical Mott relation agrees with experimental data. In this presentation, we report the TEP measurement on graphene samples deposited on hexa boron nitride substrates where drastic suppression of disorder is achieved. Our results show that at high temperatures where the inelastic scattering rate due to electron-electron (e-e) interactions is higher than the elastic scattering rate by disorders, the measured TEP exhibit a large enhancement compared to the expected TEP from the Mott relation. We also investigated TEP in the quantum Hall regime at a high magnetic fields, where we observed symmetry broken integer quantum Hall and fractional quantum Hall states due to the strong e-e interactions.

1:27PM B6.00012 Derivative relations between electrical and thermoelectric quantum transport coefficients in graphene¹, XINFEI LIU, Department of Physics and Astronomy, University of California, Riverside, ZHONGSHUI MA, School of Physics, Peking University, JING SHI, Department of Physics and Astronomy, University of California, Riverside — We find that the empirical relation between the longitudinal and Hall resistivities (i.e. R_{xx} and R_{xy}) and its counterpart between the Seebeck and Nernst coefficients (i.e. S_{xx} and S_{xy}), both originally discovered in conventional two-dimensional electron gases [1,2], hold surprisingly well for graphene in the quantum transport regime except near the Dirac point. These empirical relations can be described by the following equations:

$$R_{xx} = \alpha_r \cdot \frac{B}{n} \frac{dR_{xy}}{dB}, \quad S_{yx} = \alpha_s \cdot \frac{B}{n} \frac{dS_{xx}}{dB}$$

Here R and S are electrical resistivity and thermoelectric conductivity tensor respectively. The validity of the relations is cross-examined by independently varying the magnetic field and the carrier density in graphene. We demonstrate that the pre-factor, α_s , does not depend on carrier density in graphene. By tuning the carrier mobility therefore the degree of disorders, we find that the pre-factor stays unchanged. Our experimental results validate both derivative relations for massless Dirac fermions except near the Dirac point.

- [1] A. M. Chang and D. C. Tsui, Solid State Commun. **56**, 153 (1985).
 [2] B. Tiekamp et al, Phys. Rev. Lett. **78**, 4621 (1997).

¹This work is supported in part by DMEA/CNN, DOE and NSF.

1:39PM B6.00013 Ultra-sensitive thermal measurements of graphene: pathway to single microwave photon detector, KIN CHUNG FONG, KEITH SCHWAB, Caltech — As a result of the linear energy spectrum and low dimensionality, electrons in graphene have astoundingly small thermal conductance and heat capacitance. By developing a large bandwidth, high sensitivity Johnson noise measurement technique at microwave frequency, we can measure the temperature of graphene electrons down to a precision of 0.1 mK within 1 second. This enables us to study the thermal properties of this wonder material: for instance, we have measured the energy transfer from electrons to phonons at 1 pW/K μm^2 level and a record-low heat capacity, only about 100 kJ/ μm^2 , at low temperature. We have applied these exotic thermal quantities to make a graphene bolometer and mixer. Our measurement data agree well with the theory that the proposed graphene calorimeter should have single photon sensitivity from IR down to microwave regime at ultra-low temperature.

1:51PM B6.00014 Nano Peltier cooling device from geometric effects using a single graphene nanoribbon, WAN-JU LI, Purdue University, DAO-XIN YAO, Sun Yat-sen University, ERICA CARLSON, Purdue University — Based on the phenomenon of curvature-induced doping in graphene we propose a class of Peltier cooling devices, produced by geometrical effects, without gating. We show how a graphene nanoribbon laid on an array of curved nano cylinders can be used to create a targeted cooling device. Using theoretical calculations and experimental inputs, we predict that the cooling power of such a device can approach $1\text{ kW}/\text{cm}^2$, on par with the best known techniques using standard lithography methods. The structure proposed here helps pave the way toward designing graphene electronics which use geometry rather than gating to control devices.

2:03PM B6.00015 Electrical breakdown of graphene and few-layer graphene structures, ABHISHEK SUNDARARAJAN, D. PATRICK HUNLEY, DOUGLAS R STRACHAN, University of Kentucky — The electrical breakdown of graphene and few-layer graphene (FLG) structures are investigated. To better understand the dynamics of these nano-scale thermal effects, we investigate graphene and FLG structures of various dimensions and find that significant joule heating occurs inducing the structures to evolve. A distinct change in the behavior during electrical stressing indicates that different mechanisms and geometrical effects occur at the various stages of evolution. The results could have implications on the development of high current carrying nanoscale graphene devices. Supported in part by NSF Award No. DMR-0805136, the Kentucky NSF EPSCoR program through award EPS-0814194, and the University of Kentucky Center for Advanced Materials.

Monday, February 27, 2012 11:15AM - 2:15PM –
Session B7 DCOMP DMP: Focus Session: Computational Design of Materials - Nanostructured and Energy Materials 207

11:15AM B7.00001 The Harvard Clean Energy Project: High-throughput screening of organic photovoltaic materials using first-principles electronic structure theory, JOHANNES HACHMANN, ROBERTO OLIVARES-AMAYA, SULE ATAHAN-EVRENK, Harvard University, CARLOS AMADOR-BEDOLLA, Universidad Nacional Autonoma de Mexico, ALAN ASPURU-GUZZIK, Harvard University — We present the Harvard Clean Energy Project (CEP) which is concerned with the computational screening and design of new organic photovoltaic materials. CEP has established an automated, high-throughput, in silico framework to study millions of potential candidate structures. This presentation discusses the CEP branch which employs first-principles computational quantum chemistry for the characterization of molecular motifs and the assessment of their quality with respect to applications as electronic materials. In addition to finding specific structures with certain properties, it is the goal of CEP to illuminate and understand the structure-property relations in the domain of organic electronics. Such insights can open the door to a rational, systematic, and accelerated development of future high-performance materials. CEP is a large-scale investigation which utilizes the massive computational resource of IBM's World Community Grid. In this context, it is deployed as a screensaver application harvesting idle computing time on donor machines. This cyberinfrastructure paradigm has already allowed us to characterize 3.5 million molecules of interest in about 50 million DFT calculations.

11:27AM B7.00002 The Harvard Clean Energy Project: High-throughput screening of organic photovoltaic materials using cheminformatics, machine learning, and pattern recognition, ROBERTO OLIVARES-AMAYA, JOHANNES HACHMANN, Harvard University, CARLOS AMADOR-BEDOLLA, Universidad Nacional Autónoma de México, AIDAN DALY, ADRIAN JINICH, SULE ATAHAN-EVRENK, Harvard University, SERGIO BOIXO, University of Southern California, ALAN ASPURU-GUZZIK, Harvard University — Organic photovoltaic devices have emerged as competitors to silicon-based solar cells, currently reaching efficiencies of over 9% and offering desirable properties for manufacturing and installation. We study conjugated donor polymers for high-efficiency bulk-heterojunction photovoltaic devices with a molecular library motivated by experimental feasibility. We use quantum mechanics and a distributed computing approach to explore this vast molecular space. We will detail the screening approach starting from the generation of the molecular library, which can be easily extended to other kinds of molecular systems. We will describe the screening method for these materials which ranges from descriptor models, ubiquitous in the drug discovery community, to eventually reaching first principles quantum chemistry methods. We will present results on the statistical analysis, based principally on machine learning, specifically partial least squares and Gaussian processes. Alongside, clustering methods and the use of the hypergeometric distribution reveal moieties important for the donor materials and allow us to quantify structure-property relationships. These efforts enable us to accelerate materials discovery in organic photovoltaics through our collaboration with experimental groups.

11:39AM B7.00003 Thermodynamic Stability of Semiconductors for Photocatalytic Water Splitting¹, SHIYOU CHEN, LIN-WANG WANG, Lawrence Berkeley National Laboratory, MATERIALS SCIENCES DIVISION TEAM — Band structure engineering design of the light-absorbing semiconductors for water splitting has attracted wide attention recently. One of such design is to use the Z-scheme where a photocathode is connected with photoanode to reduce (generate H₂) and oxidize (generate O₂) water respectively. This requires the conduction band of photocathode and valence band of photoanode to straddle the redox levels of water. However, equally important in this design is the thermodynamic stability of the semiconductors in the aqueous solution upon illumination, i.e., the semiconductors may be oxidized (or reduced) before the water is oxidized (or reduced), causing the corrosion of the photoanode (photocathode). We will present our theoretical study on the thermodynamic stability of a series of photocatalytic semiconductors, including metal oxides, sulfides and nitrides, through the combination of phenomenological models for the semiconductor corrosion and the first-principles total energy and band alignment calculations. We find that almost all sulfides and nitrides are unstable as photoanode, while most of oxides are stable. This limits the choice of the photoanode materials for oxygen evolution. In contrast, for photocathode, most of the considered semiconductors are stable and resistant to reduction, indicating a much wider choice of the photocathode materials for hydrogen evolution.

¹The work is supported by the Joint Center of Artificial Photosynthesis and the BES/SC of DOE under the contract No. DE-AC02-05CH11231, and the computation is performed using the NERSC and NCCS supercomputers.

11:51AM B7.00004 Rational design of competitive electrocatalysts for the oxygen reduction reaction in hydrogen fuel cells, SERGEY STOLBOV, University of Central Florida Physics Department, MARISOL ALCÁNTARA ORTIGOZA, Karlsruher Institut für Technologie, Institut für Festkörperphysik, Karlsruhe, Germany — The large-scale application of one of the most promising clean and renewable sources of energy, hydrogen fuel cells, still awaits efficient *and* cost-effective electrocatalysts for the oxygen reduction reaction (ORR) occurring on the cathode. We demonstrate that truly rational design renders electrocatalysts possessing both qualities. By unifying the knowledge on surface morphology, composition, electronic structure and reactivity, we solve that sandwich-like structures are an excellent choice for optimization. Their constituting species couple synergistically yielding reaction-environment stability, cost-effectiveness and tunable reactivity. This cooperative-action concept enabled us to predict two advantageous ORR electrocatalysts. Density functional theory calculations of the reaction free-energy diagrams confirm that these materials are more active toward ORR than the so far best Pt-based catalysts. Our designing concept advances also a general approach for engineering materials in heterogeneous catalysis.

12:03PM B7.00005 First principles design of the Pd/Co/Pd sandwich-like structure as a promising electrocatalyst for the oxygen reduction reaction on hydrogen fuel cell cathode, SEBASTIAN ZULUAGA, SERGEY STOLBOV, University of Central Florida — In the search of Pt free catalytic materials, experiments have shown an enhancement in the catalytic activity of Pd-Co alloys over Pd surfaces, comparable to the one obtained with Pt, as well as a Pd enrichment of the topmost layers. In this work we present the rational design of a new catalyst material towards the oxygen reduction reaction (ORR) consisting on Pd(111) surface sandwiched with Co as the second layer (Pd/Co/Pd). The calculated reaction free energy diagrams confirm that the proposed sandwich-like structure is highly active towards ORR. The higher catalytic activity of the Pd/Co/Pd system is traced to the change in the electronic local density of states of the Pd surface atoms. Namely the hybridization of the Pd d-states with the Co majority-spin band causes a low-energy shift of the Pd d-band. This results in a reduction of surface reactivity which is favorable for ORR. We have also studied from first principles the stability of the system and evaluated the dissolution potential of Pd in Pd/Co/Pd. The results suggest that the system will be stable in the reaction environment.

12:15PM B7.00006 Computational Design of Co-Doping Method for Indium-Reduced Chalcopyrite-Type Photovoltaic Materials, KAZUNORI SATO, Graduate School of Engineering Science, Osaka University, PRESTO-JST, YOSHIMASA TANI, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University — Chalcopyrite-type semiconductor CuInSe_2 (CIS) is one of the most promising materials for low cost photovoltaic solar-cells. However, from the point of resource security, high concentration of In in CIS is serious disadvantage. In this paper, we propose co-doping method to reduce the concentration of In in CIS-based photovoltaic materials, i.e., 2In are replaced by Zn and Sn. According to the electronic structure calculations by the KKR-CPA-LDA [1] with the self-interaction correction [2], the substitution of Zn and Sn for In does not alter the electronic structure of CIS so much. We extend our co-doping method to enhance the efficiency of solar energy conversion. In addition to Zn+Sn co-doping, we introduce S impurities at Se sites. Due to the phase separation it is found that nano-structures with high concentration of S are self-organized under the layer-by-layer crystal growth condition. Since type-II band alignment is expected between $\text{Cu}(\text{Zn}, \text{Sn})\text{Se}_2$ and $\text{Cu}(\text{Zn}, \text{Sn})\text{S}_2$, we can expect efficient electron-hole separation in decomposed $\text{Cu}(\text{Zn}, \text{Sn})(\text{Se}, \text{S})_2$ [3].

[1] H. Akai, <http://sham.phys.sci.osaka-u.ac.jp/kkr/>

[2] A. Filippetti and N. A. Spaldin, Phys. Rev. B 67 (2003) 125109.

[3] Y. Tani et al., Appl. Phys. Express 3 (2010) 101201.

12:27PM B7.00007 Effect of carbon and nitrogen doping on the structure of amorphous GeTe phase change material¹, JEAN-YVES RATY, Physics Department B5, University of Liege, 4000 Sart-Tilman Belgium, GIADA GHEZZI, SYLVAIN MAITREJEAN, PIERRE NOÉ, ANNE ROULE, CEA-Leti, Minattec, 17 rue des Martyrs, 38054 Grenoble, France, CHRISTOPHE BICHARA, CINAM-CNRS, Campus de Luminy, Case 913, 13288 Marseille Cedex 9, France, FRANÇOISE HIPPERT, LMPG-Grenoble, Minattec 3, Parvis L. Néel, 38016 Grenoble, France — Carbon and Nitrogen-doped GeTe are promising materials for use in phase change memories since the addition of C or N increases the stability of the amorphous phase. By combining ab initio molecular dynamics and X-ray scattering experiments, we show that carbon deeply modifies the structure of the amorphous phase through long carbon chains, tetrahedral and triangular units centred on carbon. A clear signature of these units is the appearance of an additional interatomic distance around 3.3 Å in the pair correlation function. Besides, the first Ge-Ge and Ge-Te distances are almost not affected by doping. The implications for the vibrational and thermal properties are finally discussed.

¹JYR acknowledges support from the FNRS and from the University of Liège (ARC).

12:39PM B7.00008 Towards Efficient Solar Cells: Optimizing Non-Equilibrium Hyperdoping Methods, TOBIAS M. SCHNEIDER, MICHAEL P. BRENNER, Harvard School of Engineering and Applied Sciences — Electrical and optical properties of semiconductors are mainly controlled by the concentration of dopants. While the highest dopant concentrations reachable in most traditional doping methods are limited by the equilibrium solubility of the dopant in the pure semiconductor material, much higher concentrations are observed after femtosecond laser treatment of silicon in a sulfur containing atmosphere. Due to altered optical properties *laser-hyperdoped* silicon is considered a promising material for next generation photovoltaic cells. To control the dopant concentration distribution and thereby tune physical properties of the material, we apply advanced adjoint based optimization techniques to the models describing the laser induced melting and diffusion processes. This allows to determine optimal process protocols generating a desired concentration distribution. Applying advanced PDE-constrained optimization techniques to laser hyperdoping thereby opens new avenues for improving the efficiency of photovoltaic cells.

12:51PM B7.00009 First-Principles Materials Design of Chalcopyrite-Type Photovoltaic Materials with Self-Organized Nano-Structures, YOSHIMASA TANI, Graduate School of Engineering Science, Osaka University, KAZUNORI SATO, Graduate School of Engineering Science, Osaka University, PRESTO-JST, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University — $\text{Cu}(\text{In}, \text{Ga})\text{Se}_2$ (CIGS) is a chalcopyrite-type semiconductor and one of the most promising materials for low cost photovoltaic solar-cells. In this paper, based on first-principles calculations, we propose that spinodal decomposition will enhance the conversion efficiency in CIGS. Our calculations are based on the KKR-CPA-LDA [1] with the self-interaction correction [2]. From the calculated mixing energy of CIGS, it is found that the system favors the spinodal decomposition. We also perform Monte Carlo simulations and find that quasi-one-dimensional nano-structures with high concentration of impurities are formed under the layer-by-layer crystal growth condition in CIGS [3]. It is expected that the photo-generated electron-hole pairs are efficiently separated by the type-II interface and then effectively transferred along the quasi-one-dimensional structures in CIGS. Moreover, we can expect multiplication of generated carriers due to the multi-exciton effects in nano-structures [3].

[1] H. Akai, <http://sham.phys.sci.osaka-u.ac.jp/kkr/>

[2] A. Filippetti and N. A. Spaldin, Phys. Rev. B 67 (2003) 125109.

[3] Y. Tani et al., Appl. Phys. Express 3 (2010) 101201.

1:03PM B7.00010 Computational Nano-materials Design of Self-Organized Cd(Te,S) and Cd(Te,Se) Type II Nanowire (Konbu-Phase) by Spinodal Nano-Decomposition for High-Efficiency Photovoltaic Solar-Cells, HIROSHI KATAYAMA-YOSHIDA, MASAMUNE OSHITANI, Graduate School of Engineering Science, Osaka University, KAZUNORI SATO, Graduate School of Engineering Science, Osaka University and PRESTO-JST — Based on multi-scale simulations combined ab initio electronic structure calculation (KKR-CPA) and Monte Carlo simulation (MCS) of the two-dimensional layer-by-layer crystal growth, we have designed the self-organized quasi-one-dimensional nano-structures (Konbu-Phase) fabricated by two-dimensional spinodal nano-decomposition for high-efficiency photovoltaic solar cells (PVSCs) in Cd(Te_{1-x}S_x), and Cd(Te_{1-x}Se_x). The Konbu-Phase enhances the nano-scale electron-hole separation in PVSCs due to their Type II band alignment. The Konbu-Phase also increases the efficiency of PVSCs by multi-exciton formation using the inverse Auger effect in the self-organized quasi-one-dimensional nanostructures. We also discuss how to fabricate Konbu-Phase starting from the uniform nano-particles made by the photo-chemical reactions. Reference: M. Oshitani, K. Sato, H. Katayama-Yoshida, Applied Physics Express 4 (2011) 022302.

1:15PM B7.00011 Half-Heusler semiconductors as piezoelectrics, ANINDYA ROY, UC Santa Barbara, JOSEPH W. BENNETT, KARIN M. RABE, DAVID VANDERBILT, Rutgers University — We use a first-principles rational-design approach to demonstrate the potential of semiconducting half-Heusler compounds as a previously-unrecognized class of piezoelectric materials. We scan a large number of compounds, testing for insulating character and calculating structural, dielectric, and piezoelectric properties. Of the 792 compounds considered, 234 are found to be nonmetallic, of which 189 are further found to be elastically stable. We compare the computed structural parameters to available experimental values for the half-Heusler compounds considered that have been experimentally studied, as reported in the Inorganic Crystal Structure Database. Calculated piezoelectric coefficients (d_{14}) and electromechanical coupling factors (k_{14}) are often high enough to compare favorably with those of piezoelectrics currently in use. We analyze how factors such as electronegativity and ionic radius influence the piezoelectricity of the compound. Moreover, we show that even if toxic or expensive elements are excluded, we are still left with many combinations having reasonably high piezoelectric response. Our results provide guidance for the experimental realization and characterization of high-performance materials of this class that may find practical applications.

1:27PM B7.00012 Oxygen transport in ceria: a first-principles study¹, SIMAK SERGEI, Linköping University, Linköping, Sweden — Ceria (CeO₂) is an important material for environmentally benign applications, ranging from solid-oxide fuel cells (SOFC) to oxygen storage [1-2]. The key characteristic needed to be improved is the mobility of oxygen ions. Optimization of ionic transport in ceria has been the topic of many studies. In particular, it has been discovered how the ionic conductivity in ceria might be improved by choosing the proper kind and concentration of dopants [3]. In this presentation we will approach the problem from a different direction by adjusting structural parameters of ceria via the change of external conditions. A systematic first-principles study of the energy landscape and kinetics of reduced ceria as a function of external parameters reveals a physically transparent way to improve oxygen transport in ceria.

[1] N. Skorodumova, S. Simak, B. Lundqvist, I. Abrikosov, and B. Johansson, Physical Review Letters 89, 14 (2002).

[2] A. Trovarelli, in Catalysis by Ceria and related materials (Imperial College Press, London, 2002).

[3] D. A. Andersson, S. I. Simak, N. V. Skorodumova, I. A. Abrikosov, and B. Johansson, Proceedings of the National Academy of Sciences of the United States of America 103, 3518 (2006).

¹We would like to thank the Swedish Research Council, (VR) for financial support and the Swedish National Infrastructure for Computing (SNIC) for computational resources. Thanks to the Swedish Government Strategic Research Area Grant in Materials Science

1:39PM B7.00013 First Principles Optical Absorption Spectra of Organic Molecules Adsorbed on Titania Nanoparticles, KOPINJOL BAISHYA, SERDAR OGUT¹, University of Illinois at Chicago, ERSEN METE, Balikesir University, OGUZ GULSEREN, Bilkent University, SINASI ELLIALTIÖGLU, Middle East Technical University, Turkey — We present results from first principles computations on passivated rutile TiO₂ nanoparticles in both free-standing and dye-sensitized configurations to investigate the size dependence of their optical absorption spectra. The computations are performed using time-dependent density functional theory (TDDFT) as well as GW-Bethe-Salpeter-Equation (GWBSE) methods and compared with each other. We interpret the first principles spectra for free-standing TiO₂ nanoparticles within the framework of the classical Mie-Gans theory using the bulk dielectric function of TiO₂. We investigate the effects of the titania support on the absorption spectra of a particular set of perylene-diimide (PDI) derived dye molecules, namely brominated PDI (Br₂C₂₄H₈N₂O₄) and its glycine and aspartine derivatives.

¹Supported by DOE Grant No. DE-FG02-03ER15488

1:51PM B7.00014 Stoichiometric anti-phase boundaries in monolayer boron-nitride¹, SIMONE S. ALEXANDRE, LIDIA C. GOMES, HELIO CHACHAM, RICARDO W. NUNES, U. F. Minas Gerais - Brazil — We propose a stoichiometric structure for domain boundaries in monolayer boron nitride, on the basis of the seeds of extended topological defect lines that have been observed in graphene under electronic irradiation [1]. The structure consists of a periodic extended line defect with an atomic structure consisting of alternating fourfold and eightfold BN rings. The structure is shown to be lower in energy than non-stoichiometric counterparts, and to lead to the formation of shallow electron and hole bands inside the band gap of the BN bulk matrix. We suggest that the existence of such defect bands may be experimentally observed in optical experiments.

[1] J. Kotakoski, A. V. Krashennnikov, and J. C. Mayer, Physical Review Letters, 106, 105505 (2011).

¹Authors acknowledge support from Brazilian Agencies Fapemig, CNPq, CAPES, and INCT - Carbon Materials

2:03PM B7.00015 Understanding Heat Dissipation in Carbon Nanotube Resonators: New Insights from Molecular Dynamics Simulation, RAJAMANI RAGHUNATHAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, P. ALEX GREANEY, School of Mechanical, Industrial and Manufacturing Engineering Oregon State University, Corvallis, OR 97331, JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139 — Dissipation in carbon nanotube (CNT) resonators under conditions of steady state continuous driving has been simulated within classical molecular dynamics (MD) making use of a newly developed “Phonostat” algorithm. A previous study on heat flow in CNT resonators using MD simulation showed an anomalous heat dissipation and gateway kind of behavior was proposed. Here, we focus on characterizing the “gateway” modes and identify the pathways of heat dissipation by clamping such modes using our phonostat algorithm. In this present study we see three or four different sets of heat flow behavior when different sets of gateway modes are clamped as against a single heat flow behavior presented in the previous study. Our new results are explained in terms of filling of different subsets of phonon modes and the magnitude of friction between them. Our simulation results show that controlling these gateway modes is the key to improve the quality factor (Q) of CNT resonators for sensing applications, which has been a major challenge till now.

Monday, February 27, 2012 11:15AM - 2:15PM –
Session B8 DMP GMAG: Focus Session: Frustrated magnetism - Spin ice 208

11:15AM B8.00001 Spin dynamics in the frozen state of the dipolar spin ice material $\text{Dy}_2\text{Ti}_2\text{O}_7$, H.M. REVELL, L.R. YARASKAVITCH, S. MENG, University of Waterloo, K.A. ROSS, H.M.L. NOAD, McMaster University, H.A. DABKOWSKA, Brockhouse Institute for Materials Research, B.D. GAULIN, McMaster University, J.B. KYCIA, University of Waterloo — Low temperature magnetic ac susceptibility measurements of single crystal dipolar spin ice $\text{Dy}_2\text{Ti}_2\text{O}_7$ are presented. The measured dynamics qualitatively agree with simulations based on current magnetic monopole theory, but not with thermal relaxation measurements, whose dynamics freeze out at a slower rate. The relaxation is found to exhibit thermally activated Arrhenius behavior with an activation energy of 9.79 K. A comparison between the measurement results of $\text{Ho}_2\text{Ti}_2\text{O}_7$ and $\text{Dy}_2\text{Ti}_2\text{O}_7$ will also be made.

11:27AM B8.00002 Anderson-Higgs transition in quantum spin ice $\text{Yb}_2\text{Ti}_2\text{O}_7$, L.J. CHANG, Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan, S. ONODA, Condensed Matter Theory Laboratory, RIKEN, Wako, Saitama 351-0198, Japan, Y. SU, Juelich Centre for Neutron Science JCNS-FRM II, Forschungszentrum Juelich GmbH, Outstation at FRM-II, Lichtenbergstrasse 1, D-85747 Garching, Germany, Y.-J. KAO, Department of Physics, and Center of Quantum Science and Engineering, National Taiwan University, Taipei 10607, Taiwan, K.D. TSUEI, National Synchrotron Radiation Research Center, HsinChu 30076, Taiwan, Y. YASUI, Department of Physics, Division of Material Science, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8602, Japan, K. KAKURAI, Quantum Beam Science Directorate, Japan Atomic Energy Agency, Tokai, Ibaraki 319-1195, Japan, M.R. LEES, Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom — We have carried out polarized elastic neutron-scattering experiments on single crystals $\text{Yb}_2\text{Ti}_2\text{O}_7$ from 1 K to 0.04 K. The results reveal that the diffuse [111]-rod scattering [1] is suppressed below $T_c \sim 0.21$ K, where magnetic Bragg peaks and a full depolarization of neutron spins are observed with the thermal hysteresis, indicating a first-order ferromagnetic transition. Theoretically, a quantum spin ice state [2] above T_c has been realized from an effective classical model where $\langle 111 \rangle$ Ising moments, i.e., pseudospin-1/2 interact mainly through a magnetic dipolar interaction [3], and a transition from magnetic Coulomb phase to Higgs phase has emerged at T_c in $\text{Yb}_2\text{Ti}_2\text{O}_7$. [1] K. A. Ross *et al.*, Phys. Rev. Lett. **103**, 227202 (2009). [2] S. Onoda *et al.*, J. Phys.: Conf. Series, in press. [3] S. T. Bramwell and M. J. P. Gingras, Science **294**, 1495 (2001).

11:39AM B8.00003 Schwinger-boson approach to spin-liquid and Higgs phases in quantum spin ice: $\text{Yb}_2\text{Ti}_2\text{O}_7$ and $\text{Pr}_2\text{Zr}_2\text{O}_7$, SHIGEKI ONODA, Condensed Matter Theory Laboratory, RIKEN — The most generic pseudospin-1/2 quantum spin ice model for rare-earth magnetic pyrochlore oxides, that include $\text{Yb}_2\text{Ti}_2\text{O}_7$ and $\text{Pr}_2\text{TM}_2\text{O}_7$ (TM=Sn, Zr, Hf, and Ir), is studied by means of a Schwinger-boson approach. From a projective symmetry group and a mean-field analysis on this magnetically anisotropic model, we classify and analyze quantum spin liquid phases in the space of four coupling constants, including both $U(1)$ and Z_2 spin liquids that are characterized by power-law decaying and exponentially decaying spin correlations, respectively, as well as Higgs phases showing long-range orders. We apply the analysis to cases of the model parameters extracted from both microscopic arguments and the fitting to neutron-scattering experiments of some of the above materials and clarify the dynamical magnetic excitation spectra that take the continuum form due to the deconfined monopolar spinons. The relevance to recent experimental results is discussed.

11:51AM B8.00004 Dynamical strings in quantum spin ice, YUAN WAN, OLEG TCHERNYSHYOV, Johns Hopkins University — Spin ice is a highly frustrated ferromagnet displaying rich emergent phenomena. Recently, new spin ice materials such as $\text{Yb}_2\text{Ti}_2\text{O}_7$ and $\text{Pr}_2\text{Zr}_2\text{O}_7$ have stood out as possible candidates for quantum spin ice, in which quantum fluctuations could play a major role. In this talk, we discuss new emergent phenomena in quantum spin ice in an external magnetic field applied along the (100) lattice direction. When quantum monopoles are confined by the external field, the open string binding a monopole pair (Dirac string) becomes a dynamical object with a field-dependent tension. The motion of an open string includes longitudinal expansion and contraction and transverse fluctuations. The emergent quantum string theory in this context allows for simple analytical solution and straightforward numerical simulation. Moreover, vibrational modes of the string can be detected by experimental techniques such as neutron scattering and THz spectroscopy.

12:03PM B8.00005 Higgs transitions of spin ice, STEPHEN POWELL, University of Maryland, College Park — Spin ice is a frustrated magnetic material displaying a variety of interesting phenomena. At low temperature, it exhibits a “Coulomb phase”, in which there is no magnetic order and correlations have power-law forms at long distances. In this talk, I will describe the effects of applying perturbations that favor ordered states and show that the resulting phase transitions cannot be described by the standard Landau paradigm. They are instead naturally viewed as Higgs transitions of an emergent gauge theory; this perspective leads to long-wavelength theories for the critical properties. I will present specific examples of transitions described by this approach that result from perturbations such as an applied magnetic field or additional spin-spin interactions.

12:15PM B8.00006 Loop statistics in the Coulomb phase, LUDOVIC JAUBERT, OIST, Okinawa, Japan, MASUD HAQUE, RODERICH MOESSNER, MPI-PkS, Dresden, Germany — The Coulomb phase is a classical gauge field theory arising in frustrated systems with “divergence free” constraints, such as spin ice [1]. In this talk, we show how this phase can be understood as a loop model, and characterized by their loop length distribution and fractal dimensions [2]. Comparing similar models in 2- and 3-dimensions allows us to extract insights from connections to Stochastic-Loewner Evolution (SLE) processes, percolation and polymer physics. We mention implications of these results for related models and experiments (Heisenberg magnets, itinerant electrons [3]).

[1] Henley, Annual Review of Condensed Matter Physics **1**, 179 (2010).

[2] Jaubert, Haque, Moessner, Phys. Rev. Lett. **107**, 177202 (2011)

[3] Jaubert, Pitaevski, Haque & Moessner, in preparation (2012).

12:27PM B8.00007 Similarities and differences between spin and water ice models, IVAN RYZHKIN, Institute of Solid State Physics RAS — In the present contribution we provide a brief survey of the amazing analogy between spin and water ice basically from the water ice physics point of view. Special attention is paid to the following question: which of the theoretical concepts developed in ice physics could be applied to the study of spin ice and other frustrated systems. We show that the analogy between ground states of these systems can be extended other properties. In Section 1 we outline the history and present state of the analogy, and thoroughly investigate the similarity between quasi-particle excitations in ordinary ice (point defects in the ice proton system) and in spin ice (magnetic monopoles). The magnetic monopole concentration is shown to have a break in its temperature dependence arising due the magnetic Coulomb interaction (melting of the Coulomb phase). In Section 2 we develop a theory of magnetic charge transport, study the magnetic relaxation as well as the screening of magnetic field in spin ice. The transport analogy between spin and water ice is shown to be of limited nature: it is impossible to produce a stationary magnetic current in the commonly accepted model of spin ice. An extended spin ice model is suggested which is free from this disadvantage. In Section 3 we discuss the problem of how the magnetic ordering is modified near the free surface of spin ice or near its interface with other magnets. The study is based on the concepts previously used in water ice physics. In concluding Section 4 we discuss the differences between water and spin ice models (differences in numerical relations between appropriate constants, limited nature of transport analogy) and indicate some other problems which are not considered in this contribution (thermal effects of charge currents, quantum properties of the models, effect of frustrations on electron energy spectrum).

1:03PM B8.00008 Spin Ice correlations in a macroscopic system¹, PAULA MELLADO, ANDRES CONCHA, L. MAHADEVAN, School of Engineering and Applied Sciences, Harvard University — We report the realization of spin ice like correlations in a macroscopic array of ferromagnetic rods arranged in a honeycomb lattice. We found that this system has a rich dynamics that can be rationalized as the result of the interplay between the viscous rotation of each rod and Coulomb like interactions between magnetic charges located at the ends of the magnets. The dynamical response of this system has also been explored by using an external magnetic dipole moving at a distance h from the lattice. A clear separation between the interaction strengths permitted us to observe localized as well as a collective dynamics depending on the value of two dimensionless numbers; one associated with the two relevant time scales of the system and the other related with the strength of internal and external magnetic forces. This new spin-ice realization will allow the manipulation of parameters almost impossible to control on its microscopic relatives, such as inertia, vacancies, and quenched geometrical disorder between others.

¹This work was supported by the Kavli Institute and the MacArthur Foundation.

1:15PM B8.00009 Internal field distribution in spin ice materials, CLAUDIO CASTELNOVO, GABRIELE SALA, Royal Holloway University, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems, SHIVAJI SONDHI, Princeton University — At low temperatures, spin ice is populated by a finite density of magnetic monopoles — point like topological defects with a mutual magnetic Coulomb interaction. Here we study the distribution of magnetic fields inside spin ice. This is of conceptual importance as it reflects the monopolar fields set up by defects in a spin ice configuration. We discuss its manifestations in experiments involving local field probes, such as NMR or muon spin rotation. Averaged over the bulk of the sample, this distribution resembles one set up by a random spin arrangement. However, somewhat counter intuitively, the density of low-field locations decreases as the local ferromagnetic correlations imposed by the ice rules develop. The $1/r^2$ Coulomb field of a single monopole is visible in (magnetic) voids of the lattice where lattice-scale effects due to the immediate proximity of other spins are suppressed.

1:27PM B8.00010 Probing the spin ice state in the cubic pyrochlore $\text{Ho}_2\text{Ge}_2\text{O}_7$, ALANNAH HALLAS, University of Manitoba, HAIDONG ZHOU, National High Magnetic Field Laboratory, STEVEN BRAMWELL, University College London, CHRIS WIEBE, University of Winnipeg, JASON GARDNER, National Institute of Standards and Technology — Spin ices are a remarkable magnetic ground state that can arise in geometrically frustrated pyrochlores, $\text{A}_2\text{B}_2\text{O}_7$, when magnetic rare earth ions are situated on the vertices of a lattice of corner sharing tetrahedra. Competing nearest-neighbor and long-range dipolar interactions result in a short-range ordered ground state for each tetrahedron in which two spins point in and two spins point out [1]. The excitations in spin ices are equally remarkable; spin ices are the only known hosts of magnetic monopoles, emergent quasiparticles with a net magnetic charge. The cubic pyrochlore $\text{Ho}_2\text{Ge}_2\text{O}_7$ was prepared with a high temperature and high pressure technique. Preliminary DC susceptibility, heat capacity and X-ray diffraction experiments confirmed that $\text{Ho}_2\text{Ge}_2\text{O}_7$ has the bulk properties of a spin ice including residual entropy equal to the Pauling value for water ice [2]. The results of a polarized neutron scattering experiment performed at ILL as well as AC susceptibility and heat capacity measurements will be presented, and compared to the canonical spin ices.

[1] S. T. Bramwell *et al.*, Phys. Rev. Lett. **87**, 047205 (2001).

[2] H. Zhou *et al.*, Nature Communications **2**, 478 (2011).

1:39PM B8.00011 Far infrared time domain terahertz spectroscopic study of $\text{Ho}_2\text{Ti}_2\text{O}_7$, LIDONG PAN, R. VALDES AGUILAR, Department of Physics & Astronomy, Johns Hopkins University, R.J. CAVA, Department of Chemistry, Princeton University, S.M. KOOHPAYEH, Institute for Quantum Matter, Department of Physics & Astronomy, Johns Hopkins University, N. PETER ARMITAGE, Department of Physics & Astronomy, Johns Hopkins University — We report a far infrared time domain terahertz spectroscopic study of the spin ice material holmium titanate. The complex dielectric constant was obtained in the terahertz frequency range. Several low energy excitations were identified from the optical spectra. We will discuss the possible nature of those excitations and their relevance to the spin ice physics.

1:51PM B8.00012 Calorimetric Study of Diluted Spin Ice Materials, TAORAN LIN, University of Waterloo, XIANGLIN KE, Pennsylvania State University, MISCHA THESBERG, McMaster University, PETER SCHIFFER, Pennsylvania State University, ROGER MELKO, MICHEL GINGRAS, University of Waterloo — Spin ice materials $\text{Dy}_2\text{Ti}_2\text{O}_7$ and $\text{Ho}_2\text{Ti}_2\text{O}_7$ have been the subject of ongoing interest for over ten years. The cooperative magnetic ground state can be mapped onto the proton disordered ground state in water ice, and its residual entropy follows the same Pauling's estimate. Interestingly it was found in a previous study that, upon dilution of the magnetic rare earth ions Dy^{3+} and Ho^{3+} by non-magnetic substitutes Y^{3+} , the residual entropy depends non-monotonically on the dilution level. In this work we investigate through Monte Carlo simulations microscopic models to account quantitatively for the calorimetric experimental measurements, and thus also the residual entropies as a function of dilution. Features of the dilution physics in the specific heat are captured quantitatively by the microscopic models and the interplay between dilution and frustration is understood on the basis of a Bethe lattice calculation. The effect of the dipolar interactions between magnetic spins are exposed numerically for various dilution concentrations. Our work explains the previous discrepancy of the residual entropy between different species of rare earth ions and the generalized Pauling's estimate.

2:03PM B8.00013 Spin Ice: Magnetic Excitations without Monopole Signatures using Muon Spin Rotation, SARAH DUNSIGER, Physik Department, Technische Universität München, D-85748 Garching, Germany, MICHEL GINGRAS, Department of Physics and Astronomy, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada, GRAEME LUKE, Department of Physics and Astronomy, McMaster University, Hamilton, Ontario L8S 4M1, Canada, YASUTOMO UEMURA, Department of Physics, Columbia University, New York, New York 10027, USA — Theory predicts the low-temperature magnetic excitations in spin ices consist of deconfined magnetic charges, or monopoles. A recent transverse-field (TF) muon spin rotation (μSR) experiment [S. T. Bramwell *et al.*, Nature **461**, 956 (2009)] reports results claiming to be consistent with the temperature and magnetic field dependence anticipated for monopole nucleation — the so-called second Wien effect. We demonstrate via a new series of μSR experiments in $\text{Dy}_2\text{Ti}_2\text{O}_7$ that such an effect is not observable in TF μSR . Rather, as found in many highly frustrated magnetic materials, we observe spin fluctuations which become temperature independent at low temperatures, behavior which dominates over any possible signature of thermally nucleated monopole excitations.

Monday, February 27, 2012 11:15AM - 2:15PM —
Session B9 DMP GMAG: Focus session: Complex Bulk Oxides: Iridates 209

11:15AM B9.00001 Dipoles on monopoles in spin ice, DANIEL KHOMSKII, Koeln University — Close connection of electricity and magnetism is one of the cornerstones of modern physics. This connection plays crucial role both from the fundamental point of view and in practical applications, including recent advance in spintronics and in the study and development of multiferroic materials. A new breakthrough was the recent proposal of Castelnovo, Moessner and Sondhi that in spin ice systems, e.g. in some pyrochlores, one can model the magnetic monopoles – the objects displaying the properties of isolated magnetic charges. Such monopoles are a hot topic nowadays. Usually one discuss mainly their thermodynamic and magnetic properties. I will show that every *magnetic monopole* in spin ice should have an *electric dipole* attached to it. This can be seen from the results obtained for frustrated Hubbard system [1]. Both the electronic mechanism discussed in [1] and the lattice effects (magnetostriction) lead to the conclusion that for 3in/1out and 3out/1in tetrahedra there should appear an electric dipole directed from the center of tetrahedron to the “special” spin. This will lead to electric activity of monopoles, and to possibility to address and influence them not only by magnetic, but also by an electric field. Several consequences of this effect will be discussed. In general, the analogy between electricity and magnetism goes even further than usually assumed: whereas electrons have *electric charge* and spin, i.e. *magnetic dipole*, magnetic monopoles in spin ice have both *magnetic charge* and *electric dipole*.

[1] L.N.Bulaevskii, C.D.Batista, M.V.Mostovoy and D.I.Khomsii, Phys.Rev. B78, 028402 (2008)

11:51AM B9.00002 Raman scattering study of the pressure- and field-dependent phases of Sr_2IrO_4 ¹, Y. GIM, M. KIM, S.L. COOPER, Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, 104 South Goodwin Avenue, Urbana, Illinois 61801-2902, G. CAO, Department of Physics and Astronomy, University of Kentucky, Lexington Kentucky 40506 USA — Transition metal oxides (TMOs) with a perovskite structure are of interest due to the many fascinating phenomena they exhibit. Among TMOs, iridates with 5d orbitals exhibit an unexpected insulating state due to large spin-orbit coupling. With the extended nature of the 5d orbital giving rise to a strong crystal field, the competition between the onsite Coulomb interaction and spin-orbit coupling—which have comparable energy scales—opens up the possibility for studying novel phases that develop when tuning this competition with using an external perturbation with magnetic field or pressure. In this talk we present temperature, magnetic field and pressure dependent Raman study of Sr_2IrO_4 , which provides an opportunity Pressure- and field-tuned Raman spectroscopy provides an opportunity to explore the novel phases of this material under extreme conditions.

¹Work is supported by the National Science Foundation under Grant NSF DMR 08-56321.

12:03PM B9.00003 Quantum Hall effects in a Weyl semimetal: Possible application in pyrochlore iridates, KAI-YU YANG, Boston College, YUAN-MING LU, Boston College/UC Berkeley, YING RAN, Boston College — There has been much interest in pyrochlore iridates $\text{A}_2\text{Ir}_2\text{O}_7$ where both strong spin-orbital coupling and strong correlation are present. A recent local density approximation calculation [X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Phys. Rev. B 83, 205101 (2011)] suggests that the system is likely in a three-dimensional topological semimetallic phase: a Weyl semimetal. Such a system has zero carrier density and arrives at the quantum limit even in a weak magnetic field. In this talk, I will discuss two quantum effects of this system in a magnetic field: a pressure-induced anomalous Hall effect and a magnetic-field-induced charge density wave at the pinned wave vector connecting Weyl nodes with opposite chiralities. A general formula of the anomalous Hall coefficients in a Weyl semimetal is also given. Both proposed effects can be probed by experiments in the near future and can be used to detect the Weyl semimetal phase.

12:15PM B9.00004 Electronic ground state properties of Iridate oxides from x-ray absorption spectroscopy¹, DANIEL HASKEL, M.A. LAGUNA MARCO, N.M. SOUZA-NETO, J.C. LANG, Argonne National Laboratory, G. FABBRIS, Washington University in St. Louis and Argonne National Laboratory, G. CAO, University of Kentucky, M. VAN VEENENDAAL, Northern Illinois University and Argonne National Laboratory — Element (Ir)- and orbital (5d)-specific $L_{2,3}$ edge x-ray absorption and magnetic circular dichroism measurements are used to probe the nature of the electronic ground state in magnetic insulators BaIrO_3 [1] and Sr_2IrO_4 [2,3]. A spin-only description of the magnetic ground state is directly ruled out by the measurements. Instead, the measurements show spin-orbit entanglement in 5d states resulting in a larger orbital (L_z) than spin (S_z) contribution to the magnetic moment, even in the presence of strong crystal field and band effects. Measured x-ray absorption cross sections at spin-orbit split $L_{2,3}$ edges impose constraints on the nature of the ground state [3]. Experiments under chemical- (doping) and applied-pressure conditions provide evidence for a delicate interplay between electronic bandwidth and Coulomb interactions leading to the gapped, spin-orbit coupled ground state of these complex oxides.

[1] M. A. Laguna Marco et al., Phys. Rev. Lett. 105, 216407 (2010).

[2] B. J. Kim et al., Phys. Rev. Lett. 101, 076402 (2008).

[3] L. C. Chapon and S. W. Lovesey, J. Phys. Condens. Matter 23, 252201 (2011).

¹Work at Argonne is supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC-02-06CH11357.

12:27PM B9.00005 Lattice-driven magnetoresistivity and metal-insulator transition in single-layered iridates¹, O.B. KORNETA, T.F. QI, L.E. DE LONG, G. CAO, Department of Physics and Astronomy and Center for Advanced Materials, University of Kentucky, M. GE, China High Magnetic Field Lab and University of Science and Technology of China, S. PARKIN, Department of Chemistry, University of Kentucky, P. SCHLOTTMANN, Department of Physics, Florida State University — Sr_2IrO_4 exhibits a novel insulating state driven by spin-orbit interactions. Here we report two novel phenomena, namely a large magnetoresistivity that is extremely sensitive to the orientation of magnetic field but exhibits no apparent correlation with the magnetization, and a robust metallic state that is induced by dilute electron (La^{3+}) or hole (K^{+}) doping on Sr^{2+} ions in Sr_2IrO_4 . This study reveals that a strong spin-orbit interaction alters the balance between the competing energies so profoundly that (1) the spin degree of freedom alone is no longer a dominant force; (2) underlying transport properties delicately hinge on the Ir-O-Ir bond angle via a strong magnetoelastic coupling; and (3) a highly insulating state in Sr_2IrO_4 is proximate to a metallic state, and the transition is governed by lattice distortions that can be controlled via either magnetic field or chemical doping.

¹This work was supported by NSF through grants DMR-0856234 (GC) and EPS-0814194(GC, LED), and by DoE through grants DE-FG02-97ER45653 (LED) and DE-FG02-98ER45707 (PS)

12:39PM B9.00006 Time-resolved optical study of magnetism in Sr_2IrO_4 , DAVID HSIEH, DARIUS TORCHINSKY, FAHAD MAHMOOD, MIT, GANG CAO, University of Kentucky, NUH GEDIK, MIT — We report a time-resolved optical pump-probe study of the Jeff=1/2 Mott insulator Sr_2IrO_4 . The temperature dependence of the electronic relaxation rate exhibits clear anomalies at magnetic ordering temperatures of 240K and 100K, which are consistent with the development of bulk decay channels via emission of magnetic excitations. We will then discuss time-resolved second harmonic generation studies and contrast the magnetic properties of the surface and the bulk.

12:51PM B9.00007 Unusual ferromagnetism and strong spin-orbit coupling in Post-Perovskite CaIrO_3 ¹, LUKE MARSHALL, JINGUANG CHENG, JIANSI ZHOU, JOHN B. GOODENOUGH, Texas Materials Institute, The University of Texas at Austin, DANIEL HASKEL, Advanced Photon Source, Argonne National Laboratory, MICHEL VAN VEENENDAAL, Advanced Photon Source, Argonne National Laboratory and Department of Physics, Northern Illinois University — Strong spin-orbit coupling (SOC) and strong correlations have been considered essential in understanding the unusual physical properties of the 4d and 5d transition-metal oxides, such as the SOC driven Mott insulating state in Sr_2IrO_4 . Recently, an unusual atomic-like orbital moment and strong SOC have been confirmed experimentally in $9R - \text{BaIrO}_3$ through analysis of the branching ratio at the Ir $L_{2,3}$ absorption edges as obtained from x-ray absorption and x-ray magnetic circular dichroism (XMCD) measurements. We have applied the same techniques to probe unusual ferromagnetism and SOC in the post-perovskite (pPv) CaIrO_3 , which is an insulator and exhibits weak ferromagnetism below $T_C \approx 110\text{K}$. The branching ratio at the Ir $L_{2,3}$ absorption edges, which is close to unity in pPv CaIrO_3 , appears to indicate an even stronger spin-orbit interaction in the pPv CaIrO_3 than in $9R - \text{BaIrO}_3$. However, it has been challenging to model the Ir 5d orbital moment, as probed by the XMCD measurements, due to the understood local octahedral-site distortions.

¹This work was supported by the NSF (Grant No: DMR 1122603 (MIRT), DMR 0904282)

1:03PM B9.00008 Exploring Magnetic Ordering in $\text{Sr}_3\text{Ir}_2\text{O}_7$ ¹, SOVIT KHADKA, CHETAN DHITAL, Physics Department, Boston College, WEI TIAN, Oak Ridge National Laboratory, TN, USA, STEPHEN WILSON, Physics Department, Boston College — Iridium oxide members of the Ruddlesden-Popper series have generated a great deal of interest recently due to their novel Mott insulating phases within these 5d-electron systems. These surprising Mott phases have been proposed to form due to a delicate interplay between spin orbit coupling effects and electronic correlation [1]. Here we present measurements probing the nature of the spin correlations and charge behavior in the bilayer variant of the Ruddlesden-Popper series, $\text{Sr}_3\text{Ir}_2\text{O}_7$. Our neutron scattering results reveal an antiferromagnetic spin structure and will be discussed in parallel with transport and bulk magnetization measurements detailing the electronic behavior in this material.

[1] B. J. Kim et al., Phys. Rev. Lett. 101, 076402 (2008).

¹This work was supported by NSF-CAREER Award DMR-1056625.

1:15PM B9.00009 Doping a Spin-Orbit Mott Insulator: Topological Superconductivity from the Kitaev-Heisenberg Model and Possible Application to $(\text{Na}_2/\text{Li}_2)\text{IrO}_3$, YI-ZHUANG YOU, Institute for Advanced Study, Tsinghua University, Beijing, China, ITAMAR KIMCHI, ASHVIN VISHWANATH, Department of Physics, University of California, Berkeley, CA, USA — We study the effects of doping a Mott insulator on the honeycomb lattice where spins interact via direction dependent Kitaev couplings J_K , and weak antiferromagnetic Heisenberg couplings J . This model is known to have a spin liquid ground state and may potentially be realized in correlated insulators with strong spin orbit coupling. The effect of hole doping is studied within a t - J - J_K model, treated using the SU(2) slave boson formulation, which correctly captures the parent spin liquid. We find superconductor ground states with spin triplet pairing that spontaneously break time reversal symmetry. Interestingly, the pairing is qualitatively different at low and high dopings, and undergoes a first order transition with doping. At high dopings, it is smoothly connected to a paired state of electrons propagating with the underlying free particle dispersion. However, at low dopings the dispersion is strongly influenced by the magnetic exchange, and is entirely different from the free particle band structure. Here the superconductivity is fully gapped and topological, analogous to spin polarized electrons with $p_x + ip_y$ pairing. These results may be relevant to honeycomb lattice iridates such as A_2IrO_3 ($\text{A} = \text{Li}$ or Na) on doping.

1:27PM B9.00010 Correlated Itinerant Electrons in Pyrochlore $\text{Bi}_2\text{Ir}_2\text{O}_7$ ¹, G. CAO, O.B. KORNETA, T.F. QI, Department of Physics and Astronomy and Center for Advanced Materials, University of Kentucky, XIANGANG WAN, Department of Physics, Nanjing University, Nanjing, China — Strong spin-orbit coupling in the 5d-based iridates rigorously competes with other relevant energies, and motivates novel insulating states. Therefore, a metallic state does not commonly occur in the iridates, but the unusual balance between different degrees of freedom in the iridates almost guarantee that it will exhibit extraordinary properties when it does occur. Here we report anomalous transport and thermodynamic properties including Hall effect of single-crystal $\text{Bi}_2\text{Ir}_2\text{O}_7$ along with our electronic structure calculations utilizing a LSDA+U scheme. The results will be discussed along with comparisons drawn with other pyrochlore iridates and related materials.

¹This work was supported by NSF through grants DMR-0856234 and EPS-0814194.

1:39PM B9.00011 Measurement of the Mott insulating gap of Sr_2IrO_4 with a scanning tunneling microscope¹, J. NICHOLS, University of Kentucky, G. CAO, K.-W. NG, john.nichols@uky.edu — Recently the 5d transition metal oxide Sr_2IrO_4 has become a material of interest. This is due to comparable interaction strengths between crystal field splitting, the Coulomb interaction, and spin-orbit coupling, resulting in a Mott insulating ground state that has a finite resistance even at cryogenic temperatures. In order to fully understand this material it is important to measure the Mott insulating gap. A scanning tunneling microscope is an excellent tool for studying this material for its ability to directly measure this gap. Our preliminary results show this gap measured on single crystals to be ~ 50 meV which is comparable to the activation energy of this sample. We will discuss our current STM results and compare our results with other optical conductivity data obtained from this material.

¹This research was supported by NSF grants DMR-0800367 and EPS- 0814194.

1:51PM B9.00012 Mapping the fluctuating Ir^{4+} dimers across the phase diagram of $\text{Cu}(\text{Ir}_{1-x}\text{Cr}_x)_2\text{S}_4$ ($0 \leq x \leq 0.6$)¹, E.S. BOZIN, Brookhaven National Laboratory, Y.S. HOR, J.F. MITCHELL, Argonne National Laboratory, S.J.L. BILLINGE, P. JUHAS, Brookhaven National Laboratory, Columbia University — Elucidating the role of fluctuations in systems with competing interactions, such as $\text{Cu}(\text{Ir}_{1-x}\text{Cr}_x)_2\text{S}_4$, enables comprehensive understanding of their physical properties. While CuIr_2S_4 exhibits complex behavior with metal-insulator transition accompanied by charge ordering and Ir^{4+} -spin-dimerization at 226 K, CuCr_2S_4 displays ferromagnetic metallic behavior ($T_C \sim 377$ K) understood within the double exchange model. Intermediate composition range sees suppression of end-member properties, with broad features observed in susceptibility around 180 K attributed to Cr^{3+} low spin to high-spin crossover [1]. Robust fluctuating Ir^{4+} dimers are detected and their evolution examined across the phase diagram by the X-ray atomic pair distribution function method. Although their long range order is destroyed already by $x \approx 0.05$, Ir^{4+} dimers exist locally at low temperature at all compositions studied. We provide detailed account of the Cr-doping and temperature dependence of the local dimers, and estimate characteristic length-scale on which they are observable. Fluctuating dimers disappear on heating, for intermediate compositions at temperatures above 180 K.

[1] R. Endoh et al., Phys. Rev. B 68, 115106 (2003).

¹Work at BNL and ANL is supported by DOE-OS contracts DE-AC02-98CH10886 and DE-AC02-06CH11357 respectively.

2:03PM B9.00013 Coupling of Orbital and Magnetic Orders to Colossal Negative Thermal Expansion in Novel Mott Insulators¹, T.F. QI, O.B. KORNETA, S. PARKIN, L.E. DE LONG, G. CAO, Center for Advanced Materials, University of Kentucky, P. SCHLOTTMANN, Department of Physics, Florida State University — Ca_2RuO_4 is intimately associated with both **negative volume thermal expansion (NVTE)** and **negative linear thermal expansion (NLTE)** when doped by a 3d transition metal ion M for Ru. The NVTE and NLTE observed in this system constitutes a compelling and extraordinary example in that (1) the coefficient of NVTE and NLTE reaches $-213 \times 10^{-6} \text{ K}^{-1}$ and $-148 \times 10^{-6} \text{ K}^{-1}$, respectively, constituting **colossal negative thermal expansion (NTE)**; (2) the NTE anomalies closely track the onset temperatures of orbital and magnetic orders, in sharp contrast to classic NTE that shows no relevance to physical properties; (3) the NTE and physical properties can be effectively tuned via varying M and x in $\text{Ca}_2\text{Ru}_{1-x}\text{M}_x\text{O}_4$; (4) the NTE occurs near room temperature and extends over a wide temperature interval ranging from 100 K to 350 K. Moreover, NTE and Invar effect commonly exist in these 4d-based ruthenates and 5d-based iridates, e.g. $\text{Sr}_{n+1}\text{Ir}_n\text{O}_{3n+1}$ and BaIrO_3 . These novel NTE materials provide a much-needed paradigm for functional materials with anomalous thermal expansion and electronic characteristics.

¹This work was supported by NSF through grants DMR-0856234 (GC) and EPS-0814194 (GC, LED), and by DoE through grants DE-FG02-97ER45653 (LED) and DE-FG02-98ER45707 (PS).

Monday, February 27, 2012 11:15AM - 2:15PM –
Session B10 DCMP DAMOP: Invited Session: Equilibration and Relaxation in Cold Atoms 210A

11:15AM B10.00001 Timescales for equilibration and adiabaticity in optical lattices¹, STEFAN NATU, Cornell University — What are the timescales governing local and global dynamics in strongly correlated systems? How do we probe this dynamics in an isolated quantum system without coupling the system to leads? High in-situ resolved experiments on bosons in optical lattices are answering precisely these questions by imaging the gas following a sudden change of the lattice potential. The results are striking. Experiments have revealed a disparity as large as two orders of magnitude between fast equilibration of local number fluctuations and slow global mass redistribution. In this talk, I will provide a simple model which captures all the relevant physics. Additionally, I will show that the fast timescales for local dynamics challenge the accepted notions of adiabaticity times, invalidating routinely used techniques such as band-mapping as useful probes of quantum many body systems. References: S. S. Natu, K. R. A. Hazzard and E. J. Mueller, Phys. Rev. Lett. 106 125301 (2011).

¹This work was supported by a grant from the Army Research Office with funding from the DARPA OLE program.

11:51AM B10.00002 Pomeranchuk effect and spin-gradient cooling of Bose-Bose mixtures in an optical lattice, WALTER HOFSTETTER, Goethe-University Frankfurt — We theoretically investigate finite-temperature thermodynamics and demagnetization cooling of two-component Bose-Bose mixtures in a cubic optical lattice, by using bosonic dynamical mean-field theory (BDMFT). We calculate the finite-temperature phase diagram, and remarkably find that the system can be heated from the superfluid into the Mott insulator at low temperature, analogous to the Pomeranchuk effect in ^3He . This provides a promising many-body cooling technique. We examine the entropy distribution in the trapped system and discuss its dependence on temperature and an applied magnetic field gradient. Our numerical simulations quantitatively validate the spin-gradient demagnetization cooling scheme proposed in recent experiments.

12:27PM B10.00003 The amplitude mode at the superfluid-mott insulator transition, DAVID PEKKER, Caltech — We study a two dimensional gas of repulsively interacting bosons in the presence of both an optical lattice and a trap using optical lattice modulation spectroscopy. The strongly interacting superfluid supports two types of low energy modes associated with the symmetry breaking at the phase transition: gapless phase (Goldstone) modes and gapped amplitude (Anderson-Higgs) modes. Both experimentally and in theoretical simulations lattice modulation spectroscopy shows an onset of absorption at a frequency associated with the amplitude mode gap, followed by a broad absorption peak at higher frequencies. From the simulations, we learn that energy is being absorbed by various amplitude modes, which inside a trap resemble the modes of a (gapped) drum. Our main results are: (1) despite coupling to the phase modes, modulation spectroscopy shows a sharp absorption onset at the frequency associated with the amplitude mode gap; (2) as we approach the Mott transition the gap softens and finally disappears at the transition point; (3) in the weak coupling regime, deep in the superfluid phase, the amplitude mode disappears.

1:03PM B10.00004 Two-dimensional Fermi gases, MICHAEL KOEHL, University of Cambridge — Pairing of fermions is ubiquitous in nature and it is responsible for a large variety of fascinating phenomena like superconductivity, superfluidity of ^3He , the anomalous rotation of neutron stars, and the BEC-BCS crossover in strongly interacting Fermi gases. When confined to two dimensions, interacting many-body systems bear even more subtle effects, many of which lack understanding at a fundamental level. Most striking is the, yet unexplained, effect of high-temperature superconductivity in cuprates, which is intimately related to the two-dimensional geometry of the crystal structure. In particular, the question how many-body pairing is established at high temperature and whether it precedes superconductivity are crucial questions to be answered. We will report on recent experiments of pairing in a two-dimensional atomic Fermi gas in the regime of strong coupling. We perform angle-resolved photoemission spectroscopy to measure the spectral function of the gas and we observe a many-body pairing gap even above the predicted superfluid transition temperature.

1:39PM B10.00005 Relaxation Dynamics and Pre-thermalization in an isolated Quantum System¹, JÖRG SCHMIEDMAYER, Vienna Center for Quantum Science and Technology (VCQ), Atominstitut, TU-Wien — Understanding non-equilibrium dynamics of many-body quantum systems is crucial for understanding many fundamental and applied physics problems ranging from decoherence and equilibration to the development of future quantum technologies such as quantum computers which are inherently non-equilibrium quantum systems. One of the biggest challenges is that there is no general approach to characterize the resulting quantum states. In this talk I will present how to use the full distribution functions of a quantum observable to study the relaxation dynamics in one-dimensional quantum systems and to characterize the underlying many body states. Interfering two 1 dimensional quantum gases allows to study how the coherence created between the two many body systems by the splitting process [1] slowly dies by coupling to the many internal degrees of freedom available [2]. To reveal the nature of the quantum states behind this de-coherence we analyze the interference of the two evolving quantum systems. The full distribution function of the shot to shot variations of the interference patterns [3,4], especially its higher moments, allows characterizing the underlying physical processes [5]. Two distinct regimes are clearly visible in the experiment: for short length scales the system is characterized by spin diffusion, for long length scales by spin decay [6]. After a rapid evolution the distributions approach a steady state which can be characterized by thermal distribution functions. Interestingly, its (effective) temperature is over five times lower than the kinetic temperature of the initial system. Our system, being a weakly-interacting Bosons in one dimension, is nearly integrable and the dynamics is constrained by constants of motion which leads to the establishment of a generalized Gibbs ensemble and pre-thermalization. We therefore interpret our observations as an illustration of the fast relaxation of a nearly integrable many-body system to a quasi-steady state through de-phasing. The observation of an effective temperature significant different from the expected kinetic temperature supports the observation of the generalized Gibbs state [6].

[1] T. Schumm *et al.* Nature Physics, **1**, 57 (2005).

[2] S. Hofferberth *et al.* Nature **449**, 324 (2007).

[3] A. Polkovnikov, *et al.* Proc. Natl. Acad. Sci. **103**, 6125 (2006); V. Gritsev, *et al.*, Nature Phys. **2**, 705 (2006);

[4] S. Hofferberth *et al.* Nature Physics **4**, 489 (2008);

[5] T. Kitagawa, *et al.*, Phys. Rev. Lett. **104**, 255302 (2010); New Journal of Physics, **13** 073018 (2011)

[6] Gring *et al.*, to be published

¹The experiments in Vienna were supported by the European Union integrated project AQUITE, the FWF and the Wittgenstein Prize. Understanding the theory came through our collaboration with T. Kitagawa and E. Demler.

Monday, February 27, 2012 11:15AM - 2:15PM – Session B11 DMP: Focus Session: Graphene/BN 210B

11:15AM B11.00001 Tunneling spectroscopy of graphene boron nitride heterostructures¹, DAVID GOLDHABER-GORDON, Stanford University — We report on the fabrication and measurement of a graphene tunnel junction using hexagonal boron nitride as a tunnel barrier between graphene and a metal gate. The tunneling behavior into graphene is altered by the interactions with phonons and the presence of disorder. We extract properties of graphene and observe multiple phonon-enhanced tunneling thresholds. Finally, differences in the measured properties of two devices are used to shed light on mutually-contrasting previous results of scanning tunneling microscopy in graphene.

¹This work can be found on arXiv:1108.2686v1 and was done in collaboration with F. Amet, J. R. Williams, A. G. F. Garcia, M. Yankowitz, K. Watanabe and T. Taniguchi

11:51AM B11.00002 Spin and valley quantum Hall ferromagnetism in graphene on hexa-Boron nitride substrates, ANDREA YOUNG, CORY DEAN, LEI WANG, HECHEN REN, PAUL CADDEN-ZIMANSKY, Columbia University, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS, JIM HONE, KEN SHEPARD, PHILIP KIM, Columbia University — In graphene subjected to a quantizing magnetic field, the strong Coulomb interactions and fourfold combined spin/valley degeneracy lead to an approximate SU(4) isospin symmetry within individual Landau levels). At partial filling, exchange interactions can drive the ground state to polarize ferromagnetically within this expanded isospin space, manifesting experimentally as additional integer quantum Hall plateaus outside the normal sequence. Here we report the observation of a wide number of these quantum Hall isospin ferromagnetic states. Using tilted field magnetotransport, we classify the states appearing at different Landau Level filling factors by their real spin structure. We find evidence for real spin polarized states supporting Skyrmionic excitations, charge- or spin- density order, and valley textured excitations at different filling factors. We also observe unexpected reentrant behavior in tilted field in the higher Landau levels. Our results confirm graphene as a highly isotropic SU(4) ferromagnet, in which symmetry breaking is dictated by the interplay between the Zeeman effect, lattice scale interactions, and disorder.

12:03PM B11.00003 Atomic Scale Observation of Electron-Electron Interactions in Single-Layer Graphene Devices on Boron Nitride Dielectrics, SUYONG JUNG, JUNGSEOK CHAE, NIKOLAI ZHITENEV, JOSEPH STROSCIO, National Institute of Standards and Technology, ANDREA YOUNG, CORY DEAN, LEI WANG, JAMES HONE, KEN SHEPARD, PHILIP KIM, Columbia University, NIST COLLABORATION, COLUMBIA UNIVERSITY COLLABORATION — We have performed scanning tunneling spectroscopy measurements on gated-graphene devices in the quantum Hall regime under varying disorder potential landscapes. Relatively thin hexagonal boron-nitride (h-BN) crystals are mechanically exfoliated on SiO₂/Si substrates and single-layer graphene films are later transferred on pre-located h-BN crystals. In this device scheme, we can investigate the interactions of Dirac particles with local impurities ranging from strongly disordered to weakly perturbed environments by adjusting the thickness of h-BN crystals, while varying both the Fermi-energy with respect to a Dirac point and magnetic field. In the h-BN devices, we have observed that the electron-hole puddles are larger in lateral size than those observed on SiO₂ devices, and resonance scatterings are significantly reduced due to weakened disorder potentials. Accordingly, we start observing well-defined Landau levels (LLs) as early as 0.5 T and the width of individual LLs, broadened by the scattering of charged carriers, is much narrower than those from graphene on SiO₂. In high magnetic fields, we observe the electronic structure of graphene devices is significantly altered by the electron-electron interactions and the formation of large interaction energy gaps. We will discuss the spatial, orbital quantum number, and magnetic field dependence of the observed interaction gaps.

12:15PM B11.00004 Landau Level Lifetimes and Residual Disorder in Single Layer Graphene on Boron-Nitride Substrates, JUNGSEOK CHAE, SUYONG JUNG, NIKOLAI B. ZHITENEV, JOSEPH A. STROSCIO, National Institute of Science and Technology, ANDREA YOUNG, CORY DEAN, LEI WANG, JAMES C. HONE, KEN L. SHEPARD, PHILIP KIM, Columbia University, NIST COLLABORATION, COLUMBIA UNIVERSITY COLLABORATION — Realization of the intrinsic electronic properties of graphene devices has been limited by charge scattering and surface roughness found when graphene is placed on SiO₂ substrates. Recently, graphene devices fabricated on hexagonal boron-nitride (h-BN) dielectrics have shown superior device performance compared with graphene placed directly on SiO₂ substrates. We have performed scanning tunneling microscopy / spectroscopy (STM / STS) measurements to investigate the local electronic structure of graphene devices on h-BN substrates as a function of charge density and magnetic field. The disorder potential is significantly reduced compared with graphene in direct contact with SiO₂. Correspondingly, the widths of Landau levels (LLs) are much narrower becoming comparable to those measured in epitaxial graphene on SiC. The energy and the spatial dispersion of LLs is used to analyze the Fermi velocity of the Dirac particles at different charge densities, an electron-hole asymmetry, and discrete splittings of LLs due to residual spatially varying disorder potential.

12:27PM B11.00005 STM of graphene on boron nitride, BRIAN LEROY, University of Arizona — Graphene on hexagonal boron nitride (hBN) has been shown to have significantly improved mobility and charge inhomogeneity based on electrical transport measurements. Using scanning tunneling microscopy, we have observed that the surface roughness is reduced by one order of magnitude as compared to graphene on SiO₂ devices. Near the Dirac point, graphene breaks up into a series of electron and hole puddles due to potential fluctuations. Using scanning tunneling spectroscopy, we have shown that the potential fluctuations are also reduced by an order of magnitude on hBN. The ultraflat and clean nature of graphene on hBN devices allows for the observation of scattering from buried step edges. The energy and spatial dependence of the scattering gives information about the dispersion relation of graphene and the chiral nature of the quasiparticles. In this talk, I will also discuss our recent spectroscopy measurements on hBN.

1:03PM B11.00006 Thickness Dependence of Electrical Breakdown in h-BN dielectric using C-AFM microscopy, AVINASH NAYAK, DONGHYI KOH, DEJI AKINWANDE, UT Austin — For nano-scale graphene transistor applications, hexagonal boron nitride (h-BN) is a highly desirable dielectric material that is being investigated not only because of its intrinsic properties but also because of its low lattice mismatch with hexagonal graphene. Currently, SiO₂ limits the carrier mobility of graphene due to substrate phonon coupling. Therefore, h-BN can be employed for mobility enhancement beyond the values achievable on standard dielectric. Decreasing the device dimensionality however, requires a more detailed understanding of electrical breakdown at the nanoscale. We will present on the intrinsic breakdown electric field (E_{BF}) of h-BN thin films in a metal-insulator-metal (MIM) configuration. This nanoscaled MIM structure is measured using conductive-atomic-force microscopy (C-AFM). Here, C-AFM is used to extract breakdown voltage for various thicknesses of mechanically exfoliated h-BN flakes. We measure the dielectric properties of h-BN flakes that vary from 2nm to 25nm and determine the ultimate scalability of hBN dielectrics.

1:15PM B11.00007 Transport in graphene-boron nitride heterostructures, FRANCOIS AMET, ANDREI GARCIA, JAMES WILLIAMS, DAVID GOLDBABER-GORDON, Stanford University — Transferring graphene on hexagonal boron nitride permits the fabrication of high mobility graphene devices. We report on in-plane transport measurements on dual gated graphene systems using boron nitride as a substrate. The low amount of disorder allows for ballistic effects to be probed, as we can gate-define regions narrower than the mean free path. This work is supported by the Center on Functional Engineered Nano-Architectonics.

1:27PM B11.00008 Tunable and Sizable Band Gap of Single Layer Graphene Sandwiched between Hexagonal Boron Nitride, JIAXIN ZHENG, HERUGE QU, QIHANG LIU, RUI QIN, JING ZHOU, DAPENG YU, ZHENGXIANG GAO, JING LU, State Key Laboratory of Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, P. R. China, GUANGFU LUO, SHIGERU NAGASE, Department of Theoretical and Computational Molecular Science, Institute for Molecular Science, Okazaki 444-8585, Japan, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182-0266, USA — It is a big challenge to open a tunable and sizable band gap of single layer graphene without big loss in structural integrity and carrier mobility. By using density functional theory calculations, we show that the band gap of single layer graphene can be opened to 0.16 (without electrical field) and 0.34 eV (with a strong electrical field) when sandwiched between two hexagonal boron nitride single layers in a proper way. The zero-field band gaps are increased by about 50% when many-body effects are included. Ab initio quantum transport simulation of a dual-gated FET out of such a sandwich structure further confirms an electrical field-enhanced transport gap. The tunable and sizeable band gap and structural integrity render this sandwich structure a promising candidate for high-performance single layer graphene field effect transistors.

1:39PM B11.00009 ABSTRACT WITHDRAWN —

1:51PM B11.00010 High quality charge- and spin transport in graphene on commercially available boron nitride¹, PAUL ZOMER, MARCOS GUIMARAES, SAROJ DASH, NIKOLAOS TOMBROS, BART VAN WEES, Zernike Institute for Advanced Materials, University of Groningen — In order to overcome the limitations that a silicon oxide substrate imposes on the electronic transport properties of graphene, hexagonal boron nitride (h-BN) has proven to be an excellent alternative. We present a fast, simple and accurate transfer technique of graphene, which yields atomically flat graphene flakes on h-BN that are almost completely free of bubbles or wrinkles. Using this transfer technique we prepared single- and bilayer graphene electronic devices on commercially available hexagonal boron nitride and extract mobilities as high as 125 000 cm²/Vs at room temperature and 275 000 cm²/Vs at 4.2 K. The high electronic quality is further confirmed by magnetotransport measurements, which show the development of the 1e²/h Landau level already at 5T (P. J. Zomer et al. arXiv:1110.1045v1). Finally, we present very recent results of spin transport in high mobility h-BN supported graphene flakes (P. J. Zomer et al. in preparation). In conclusion, the potential of commercially available boron nitride combined with our transfer technique makes high mobility graphene devices more accessible.

¹This work is financially supported by the Dutch Foundation for Fundamental Research on Matter (FOM) and NWO and is realized using NanoLab NL facilities.

2:03PM B11.00011 Examining CVD graphene quality using hexagonal boron nitride substrates¹, WILL GANNETT, WILLIAM REGAN, Dept of Physics, University of California, Berkeley and Materials Sciences Division, LBNL, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Material Laboratory, National Institute for Materials Science, Tsukuba, Japan, MICHAEL CROMMIE, ALEX ZETTL, Dept of Physics, University of California, Berkeley and Materials Sciences Division, LBNL — Chemical vapor deposition (CVD) of graphene has proven to be the most inexpensive and scalable synthesis technique for continuous graphene monolayers. However, CVD graphene typically has a lower mobility than that from exfoliation. This is likely due to a combination of intrinsic (defect and grain boundary) and extrinsic (substrate and contamination) effects. By fabricating CVD graphene transistors on hexagonal boron nitride (h-BN) substrates, we are able to reduce the extrinsic substrate interactions that otherwise occur with silicon dioxide layers. This greatly improves the mobility in our devices (up to 29000 cm²/Vs). While such improvements from h-BN have been previously observed in exfoliated graphene devices, its success with CVD graphene is particularly notable because it shows that the low mobilities observed in CVD graphene are not from intrinsic effects, and that current synthesis techniques are more than sufficient to consistently produce graphene with >10000 cm²/Vs. Furthermore, our research reveals that characterization of CVD growth recipes by measuring mobilities on silicon dioxide is insufficient, as scattering from the oxide will dominate, revealing little information about intrinsic graphene quality.

¹This research was supported in part by the U.S. Department of Energy, the National Science Foundation, and the Office of Naval Research.

Monday, February 27, 2012 11:15AM - 2:15PM —
Session B12 DCMP: Graphene: Electronic Structure and Interactions - Bilayer Graphene 210C

11:15AM B12.00001 Berry phase and pseudospin winding number in bilayer graphene¹, CHEOL-HWAN PARK, MIT and University of Oxford, NICOLA MARZARI, EPFL and University of Oxford — In 2006, two seminal studies on the novel quantum Hall effect of bilayer graphene [K. S. Novoselov et al., Nat. Phys. **2**, 177 (2006); E. McCann and V. I. Fal'ko, Phys. Rev. Lett. **96**, 086805 (2006)] appeared. Those papers claim that a non-trivial Berry phase of 2π in bilayer graphene is responsible for the novel quantum Hall effect described. Since then, it has become widely accepted by people working on the novel physics of graphene nanostructures that bilayer graphene has a non-trivial Berry phase of 2π (different from 0, as for conventional two-dimensional electron gas). In this talk, we show that (i) the relevant Berry phase for bilayer graphene is the same as that for a conventional two-dimensional electron gas and especially that (ii) what is actually obtained in the quantum Hall measurements is not the absolute value of the Berry phase of graphene multilayers but the pseudospin winding number. The results of our study ask for a re-interpretation of the numerous works related to the Berry phase in graphene multilayers.

¹We thank Steven G. Louie, Alessandra Lanzara, Choonkyu Hwang, and Davide Ceresoli for fruitful discussions, and Intel Corporation for support (CHP).

11:27AM B12.00002 Electron-hole asymmetry and band mass renormalization in bilayer graphene: elucidating the role of electron-electron interactions with first-principles GW calculations, LIANG Z. TAN, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — The electron-hole asymmetry and the band masses of bilayer graphene are fundamental quantities in various phenomena and in the applications of this material. *A priori*, both of these quantities can depend on a number of microscopic mechanisms, including single-particle effects such as next-nearest neighbor hopping amplitude, as well as many-body effects such as the electron-electron interaction. We calculate the low energy electronic structure of bilayer graphene from first-principles, within the GW approximation. Our results indicate that both the electron-hole asymmetry and the band mass are strongly renormalized by electron-electron interactions. Our results are in good agreement with recent Shubnikov-de Haas experiments on bilayer graphene.

11:39AM B12.00003 Spontaneous broken time reversal symmetry and persistent current states in bilayer graphene, JEIL JUNG, Department of Physics, University of Texas at Austin, USA, MARCO POLINI, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56126 Pisa, Italy, ALLAN MACDONALD, Department of Physics, University of Texas at Austin, USA — We report on the possibility of electron interaction driven spontaneously broken time reversal symmetry states in bilayer graphene through Fermi surface instability (aka Pomeranchuk instability) in both $\ell = 0$ and $\ell = 1$ channels. The conditions for spontaneous current carrying equilibrium states are most favorable in the regime of high interlayer potential difference and finite doping. These states are accompanied by valley polarization, which leads to a finite Hall conductivity that is approximately proportional to carrier density. Ref. cond-mat arXiv:1111.1765

11:51AM B12.00004 Time-reversal symmetry breaking states in bilayer graphene, LIJUN ZHU, VIVEK AJI, CHANDRA VARMA, University of California, Riverside — The time-reversal symmetry breaking states in bilayer graphene which do not break translational symmetry can be classified by the spatial symmetry of the spontaneous current patterns. Among the four possible states, only one has anomalous Hall effect. In a simple model with near-neighbor interactions, we compare their energies in the mean-field approximation. We also compare which of the states is compatible with the observed gapped state in bilayer graphene.

12:03PM B12.00005 Spontaneous symmetry breaking in bilayer graphene¹, MAXIM KHARITONOV, Center for Materials Theory, Rutgers University — Recent experiments [1-4] provided compelling evidence for the correlated electron behavior in undoped bilayer graphene at both zero and finite magnetic field. The key question concerns the nature of the broken-symmetry phases realized experimentally. I will present the phase diagram for the zero-density state in the quantum Hall regime ($\nu = 0$ state) obtained within the framework of quantum Hall ferromagnetism. Comparing these results with the experimental data of Refs. [1,4], I will argue that the $\nu = 0$ insulating state realized in bilayer graphene is the canted antiferromagnetic phase. I will also show that the (canted) antiferromagnetic phase can persist at all magnetic fields down to zero and argue that this is the most likely scenario for the insulating state observed in Ref. [4].

[1] R. T. Weitz et al., Science 330, 812 (2010).

[2] F. Freitag et al., arXiv:1104.3816 (2011).

[3] A. S. Mayorov, et al., Science 333, 860 (2011).

[4] J. Velasco Jr. et al., arXiv:1108.1609 (2011).

[5] M. Kharitonov, arXiv:1103.6285, arXiv:1105.5386, arXiv:1109.1553 (2011).

¹This work was supported by the U.S. DOE under contracts DE-FG02-99ER45790 and DE-AC02-06CH11357

12:15PM B12.00006 Transport Spectroscopy of Symmetry-Broken Insulating States in Bilayer Graphene, JAIRO VELASCO JR., LEI JING, WENZHONG BAO, YONGJIN LEE, University of California Riverside, PHILIP KRATZ, Stanford University, VIVEK AJI, MARC BOCKRATH, JEANIE LAU, CHANDRA VARMA, University of California Riverside, RYAN STILLWELL, DMITRY SMIRNOV, Florida State University, FAN ZHANG, JEIL JUNG, ALLAN MACDONALD, University of Texas Austin — The flat bands in bilayer graphene (BLG) are sensitive to electric fields E directed between the layers, and magnify the electron-electron interaction effects, thus making BLG an attractive platform for new two-dimensional (2D) electron physics. Theories have suggested the possibility of a variety of interesting broken symmetry states, some characterized by spontaneous mass gaps, when the electron-density is at the carrier neutrality point (CNP). The theoretically proposed gaps in bilayer graphene are analogous to the masses generated by broken symmetries in particle physics and give rise to large momentum-space Berry curvatures accompanied by spontaneous quantum Hall effects. Though recent experiments have provided convincing evidence of strong electronic correlations near the CNP in BLG, the presence of gaps is controversial. Here we present transport measurements in ultra-clean double-gated BLG, using source-drain bias as a spectroscopic tool to resolve a gap of ~ 2 meV at the CNP. The gap can be closed by an electric field $E \sim 15$ mV/nm but increases monotonically with a magnetic field B , with an apparent particle-hole asymmetry above the gap, thus providing a spectroscopic mapping of the ground states in BLG.

12:27PM B12.00007 Transport in Bilayer Graphene at the Charge Neutrality Point, WENZHONG BAO, University of Maryland at College Park, JAIRO VELASCO, University of California, Riverside, FAN ZHANG, University of Texas at Austin, Austin, LEI JING, University of California, Riverside, BRIAN STANDLEY, California Institute of Technology, DMITRY SMIRNOV, National High Magnetic Field Laboratory, Tallahassee, ALLAN MACDONALD, University of Texas at Austin, Austin, MARC BOCKRATH, CHUNNING LAU, University of California, Riverside, DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF CALIFORNIA, RIVERSIDE TEAM — Bilayer graphene (BLG) at the charge neutrality point is strongly susceptible to electronic interactions, and expected to undergo a phase transition into a state with spontaneous broken symmetries. We experimentally investigate transport properties of a large number ultra-clean BLG devices as functions of temperature, disorder, out-of-plane electric field, and charge density. We will discuss the results in terms of various theoretical models and possible phase transitions arising from the rich many body physics in this 2D system.

12:39PM B12.00008 Unconventional Landau levels in biased bilayer graphene, YEN-HUNG HO, WU-PEI SU, Physics Dept. and Texas Center for Superconductivity, University of Houston, Texas, USA, SING-JYUN TSAI, MING-FA LIN, Physics Dept., National Cheng Kung University, Taiwan — We utilize a generalized tight-binding model to study how the bias electric field impacts the magneto-electronic properties of graphene bilayer. With the availability of Landau wave function, the distribution among its sublattices enables the detailed observation of the Landau levels. The external electric field induces different electric potential on respective layers, which in turn lifts the inter-valley degeneracy. In addition, in a certain field range, Landau levels are coupled with each other and reveal the anomalous behavior: despite the serious hybridization of wave functions, these states in energy are still well-behaved Landau levels. These significant changes are directly reflected in the magneto-optical spectra, including the splitting of absorption peaks as well as the enhancement or quenching in response to field strength.

12:51PM B12.00009 Interaction-Enhanced Coherence in Graphene and Topological Insulator Bilayers¹, INTI SODEMANN, DMYTRO PESIN, ALLAN MACDONALD, University of Texas at Austin — We analyze the interlayer coherence properties of graphene and topological insulator electron-hole bilayers by solving imaginary-axis Dirac-model gap equations in the random phase approximation. By accounting self-consistently for the dynamical screening of Coulomb interactions in the gapped phase, we find that the gap can rise to values of the order of the Fermi energy in the strong interactions regime. For graphene, we comment on the supportive role of remote bands not included in our two-band Dirac model.

¹Work supported by the Nano-electronics Research Initiative (NRI) through the Southwest Academy for Nano-electronics (SWAN)

1:03PM B12.00010 Analysis of fermions on a honeycomb bilayer lattice with finite-range interactions in the weak-coupling limit¹, ROBERT THROCKMORTON, OSKAR VAFEK, Florida State University, National High Magnetic Field Laboratory — We extend previous analyses of fermions on a honeycomb bilayer lattice via weak-coupling renormalization group (RG) methods with extremely short-range and extremely long-range interactions to the case of finite-range interactions. In particular, we consider different types of interactions including screened Coulomb interactions, much like those produced by a point charge placed either above a single infinite conducting plate or exactly halfway between two parallel infinite conducting plates. We map out the phases that the system enters as a function of the range of the interaction. For spin- $\frac{1}{2}$ fermions, we discover that the system enters an antiferromagnetic phase for short ranges of the interaction and a nematic phase at long ranges, in agreement with the previous work. Our results can help reconcile the recent results of two seemingly contradictory experiments. We also consider the effects of an applied magnetic field on the system in the antiferromagnetic phase via variational mean field theory, obtaining results in qualitative agreement with the experimental data. We find that the antiferromagnetic order parameter increases with field, at first quadratically at low fields, then as $B/\ln(B/B_0)$ at higher fields.

¹Robert E. Throckmorton, Oskar Vafek, arXiv:1111.2076. Supported in part by the NSF CAREER Award under Grant no. DMR-0955561.

1:15PM B12.00011 Wave-packet dynamics in twisted bilayer graphene, LEDE XIAN, School of physics, Georgia Tech, ZHENGFEI WANG, School of physics, Georgia Tech; Department of Materials Science and Engineering, University of Utah, MEI-YIN CHOU, School of physics, Georgia Tech — It has been shown recently that high-quality epitaxial graphene (EPG) can be grown on the SiC substrate that exhibits interesting physical properties. In particular, the multilayer graphene films grown on the C-face show rotational disorder. It is expected that the twisted layers exhibit unique new physics that is distinct from that of either single layer graphene or graphite. In this work, the time-dependent wave-packet propagation in twisted bilayer graphene (TBG) is studied based on a tight-binding model with parameters derived from density functional theory. Our results demonstrate intriguing dynamical behavior of electrons in TBG, which is related to the specific interlayer coupling. By varying the twist angle and the initial wave packet, we can effectively control the propagation of electrons in TBG.

1:27PM B12.00012 Fermi-velocity reduction in twisted bilayer graphene: large-scale density-functional calculations, KAZUYUKI UCHIDA, JUN-ICHI IWATA, SHINNOSUKE FURUYA, ATSUSHI OSHIYAMA, University of Tokyo — Twisted bilayer graphene (BLG) in which two graphene layers are rotated with a certain angle has been observed experimentally and its electronic structure has been studied using mainly tight-binding models [1]. We here report large-scale electronic-structure calculations with local-density approximation in the density-functional theory that clarify salient nature of the twisted BLG with the small rotation angles. The calculations have been done using the real-space density-functional theory (RSDFT) scheme which we have developed for the next-generation massively parallel computers. Implementation of the ultrasoft pseudopotential scheme in RSDFT allows us to treat thousands -of-carbon-atom systems in moderate-size computers. We have found that the Fermi velocity of the Dirac electron in the twisted BLG is substantially reduced compared with that in single layer graphene when the twist angle is small enough. This corroborates the observed reduction in the tight-binding models. We have also found that the wave functions at the Fermi level is strongly localized at AA-stacked region in the BLGs, opening a possibility of new magnetic functions.

[1] A. Luican et al., PRL 106, 126802 (2011); G. Trambly et al., Nano letters 10, 804 (2010); S. Shallcross et al., PRB 81, 165105 (2010).

1:39PM B12.00013 A Full electric-field tuning of thermoelectric power in a dual-gated Bi-layer graphene device¹, WEI-LI LEE, CHANG-RAN WANG, WEN-SEN LU, LEI HAO, TING-KUO LEE, Institute of Physics, Academia Sinica, Taipei, Taiwan, FENG LIN, I-CHUN CHENG, Department of Electrical Engineering and Graduate Institute of Photonics and Optoelectronics, National Taiwan University, Taipei, Taiwan, JIANG-ZHANG CHEN, Institute of Applied Mechanics, National Taiwan University, Taipei, Taiwan — By using high quality microcrystals of hexagonal boron nitride as top gate dielectric, we fabricated dual-gated bilayer graphene devices. We demonstrate a full electric field tuning of thermoelectric power resulting from the opening of a band-gap by applying a perpendicular electric field on bilayer graphene. We uncover a large enhancement in thermoelectric power at low temperature. At 15 K, the thermoelectric power can be amplified by more than four-fold attaining a value of $\sim 50\mu\text{V/K}$ at a displacement field of 0.8 V/nm . Our result may open up a new possibility in thermoelectric application using graphene-based device.

¹This work is supported by NSC Taiwan NSC99-2112-M-001-032-MY3

1:51PM B12.00014 Phase diagram of the honeycomb bilayer from functional renormalization, MICHAEL SCHERER, STEFAN UEBELACKER, CARSTEN HONERKAMP, Institute for Theoretical Solid State Physics, RWTH Aachen University — The phase diagram for interacting electrons on the honeycomb bilayer with Bernal stacking is explored by means of the functional renormalization group. For half-filling and including a range of repulsive onsite, nearest-neighbor and next-to-nearest neighbor interactions we analyze the emergent instabilities and find antiferromagnetic, two types of charge-density-waves and quantum spin Hall order. The presented phase diagram covers the relevant region for the bilayer graphene parameters which overlaps with the phase boundary between the antiferromagnetic state and the quantum spin Hall state. We comment on the effect of small dopings.

2:03PM B12.00015 The Hubbard model on the bilayer honeycomb lattice with Bernal stacking

, THOMAS C. LANG, STEFAN ÜBELACKER, Institute for Theoretical Solid State Physics, RWTH Aachen University, ZI YANG MENG, Center for Computation and Technology, Louisiana State University, MICHAEL SCHERER, CARSTEN HONERKAMP, Institute for Theoretical Solid State Physics, RWTH Aachen University, ALEJANDRO MURAMATSU, Institute for Theoretical Physics III, University of Stuttgart, FAKHER F. ASSAAD, Institute for Theoretical Physics and Astrophysics, University of Würzburg, STEFAN WESSEL, Institute for Theoretical Solid State Physics, RWTH Aachen University — Using a combination of quantum Monte Carlo, the functional renormalization group and mean-field theory we study the Hubbard model on the bilayer honeycomb as a model for interacting electrons on bilayer graphene. The free bands consisting of two Fermi points with quadratic dispersions lead to a finite density of states, which triggers the antiferromagnetic instability and spontaneously breaks sublattice and spin rotational symmetry once a local Coulomb repulsion is introduced. We show that the antiferromagnetic instability is insensitive to the inclusion of extended Coulomb interactions and discuss effects on the sublattice magnetization and of finite size systems in numerical approaches.

Monday, February 27, 2012 11:15AM - 2:15PM –

Session B13 DMP GMAG: Focus Session: Low-Dimensional and Molecular Magnetism - 1D Magnetism/single-chain magnets - Theory 211

11:15AM B13.00001 Ferromagnetic versus helical order in edge sharing CuO₂ chains - a computational study, HELGE ROSNER, Max Planck Institute for Chemical Physics of Solids Dresden, Germany, ULRIKE NITZSCHE, Leibniz Institute for Solid State and Materials Research Dresden, ALEXANDER TSIRLIN, Max Planck Institute for Chemical Physics of Solids Dresden, Germany, ROMAN KUZIAN, STEFAN-LUDWIG DRECHSLER, Leibniz Institute for Solid State and Materials Research Dresden — The magnetic ground state of edge sharing CuO₂ spin 1/2 Heisenberg chains with nearest neighbor exchange J_1 and second neighbor exchange J_2 depends delicately on structural details of the crystal structure, like Cu-O-Cu bond angles, Cu-O distances and the position of the cations. Without taking into account a renormalization by the interchain coupling, a critical ratio $\alpha = -J_2/J_1$ separates a ferromagnetic from a helical ground state (FM for $\alpha < 1/4$, helical for $\alpha > 1/4$). Here, we present a density functional based band structure study that investigates the different influences of various structural parameters for Li₂ CuO₂ as example compound. We find that the ferromagnetic and antiferromagnetic contributions develop rather differently for the same structural changes. Therefore, the key parameter α for the ground state is especially sensitive for small structural changes that might be induced by temperature or pressure variation.

11:27AM B13.00002 Quantum criticality of dipolar spin chains, ALDO ISIDORI, ANNIKA RUPPEL, ANDREAS KREISEL, PETER KOPIETZ, Institute for Theoretical Physics, University of Frankfurt, 60438 Frankfurt, Germany, ALEXANDER MAI, REINHARD M. NOACK, Physics Department, University of Marburg, 35032 Marburg, Germany — We show that a one-dimensional chain of Heisenberg spins, interacting with long-range dipolar forces in a magnetic field perpendicular to the chain, exhibits a quantum critical point belonging to the two-dimensional Ising universality class. Within linear spin-wave theory (corresponding to the so-called Gaussian approximation) the long-wavelength magnon dispersion is characterized by a logarithmic singularity in the magnon velocity for vanishing momenta, due to the long range nature of dipolar interactions in one-dimension. However, in the vicinity of the critical point this logarithmic correction is renormalized to zero by the effects of quantum fluctuations, signaling the reemergence of scale invariance, in accordance with the Ising critical scenario. The quantum critical regime where linear spin-wave theory breaks down is studied using two independent non-perturbative methods, namely the density-matrix renormalization group (DMRG) and the functional renormalization group (FRG). The Ginzburg regime where non-Gaussian fluctuations are important is found to be rather narrow on the ordered side of the transition, and very broad on the disordered side.

11:39AM B13.00003 Spin transport in spin chains: Possible applications for spintronics, KEVIN VAN HOOGDALAM, DANIEL LOSS, University of Basel — One of the main issues in modern electronics is that as devices get ever smaller the removal of waste energy generated by Joule heating becomes problematic. A possible solution to this problem is offered by spintronics in non-itinerant systems. Here, we theoretically propose the spin-equivalent in such systems of several different components that are used in traditional electronics: the resistance, the diode, and the capacitance. The system we consider here consists of an antiferromagnetic spin chain with anisotropic exchange interaction, connected to two three-dimensional spin reservoirs. We use inhomogeneous Luttinger liquid theory to describe the system, and non-equilibrium methods to calculate the relevant transport properties.

References

- [1] K. A. van Hoogdalem and D. Loss, Phys. Rev. B **84**, 024402 (2011).
- [2] K. A. van Hoogdalem and D. Loss, in preparation.

11:51AM B13.00004 Fractionalization of electron's spin and orbital degrees of freedom in 1D¹, KRZYSZTOF WOHLFELD, MARIA DAGHOFFER, SATOSHI NISHIMOTO, IFW Dresden, Germany, GINIYAT KHALIULLIN, FKF-MPG Stuttgart, Germany, JEROEN VAN DEN BRINK, IFW Dresden, Germany — We show that electron's spin and orbital degrees of freedom can fractionalize in 1D antiferromagnets: although the orbital excitations are inherently coupled to spinons in antiferromagnetic Mott insulators, in 1D they separate into a *pure* orbiton and a single spinon. This is similar to the spin-charge separation in 1D but corresponds to an exotic regime where spinons are faster than holons [1]. The resulting large dispersion of the pure orbiton can be detected in e.g. quasi-1D cuprates [2]. [1] K. Wohlfeld, M. Daghofer, S. Nishimoto, G. Khaliullin, and J. van den Brink, Phys. Rev. Lett. **107**, 147201 (2011). [2] J. Schlappa *et al.*, to be published (2011).

¹We acknowledge support by Alexander von Humboldt Foundation and the Emmy-Noether Program.

12:03PM B13.00005 Accurate determination of the Gaussian transition in spin-1 chains with single-ion anisotropy, BRUCE NORMAND, SHIJIE HU, XIAOQUN WANG, Department of Physics, Renmin University of China, Beijing 100872, China, LU YU, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — The Gaussian transition in the spin-one Heisenberg chain with single-ion anisotropy is extremely difficult to treat, both analytically and numerically. We introduce an improved DMRG procedure with strict error control, which we use to access very large systems. By considering the bulk entropy, we determine the Gaussian transition point to 4-digit accuracy, $D_c/J = 0.96845(8)$, resolving a long-standing debate in quantum magnetism. With this value, we obtain high-precision data for the critical behavior of quantities including the ground-state energy, gap, and transverse string-order parameter, and for the critical exponent, $\nu = 1.472(2)$. Applying our improved technique at $J_z = 0.5$ highlights essential differences in critical behavior along the Gaussian transition line.

12:15PM B13.00006 Generalized Fidelity Susceptibilities as Applied to the $J_1 - J_2$ Heisenberg Chain, MISCHA THESBERG, ERIK S. SORENSEN, McMaster University — In this talk slightly generalized quantum fidelity susceptibilities for the antiferromagnetic Heisenberg $J_1 - J_2$ chain will be introduced. The differential change in these fidelities differ from the typical fidelity in that they are measured with respect to a term other than the one used for driving the system towards a quantum phase transition. We study three fidelity susceptibilities; χ_ρ , χ_D and χ_{AF} , which are related to the spin stiffness, the dimer order and antiferromagnetic order, respectively. I will discuss how these quantities can accurately identify the quantum critical point at $J_2=0.241167J_1$ in this model. This phase transition, being in the Berezinskii-Kosterlitz-Thouless universality class, is controlled by a marginal operator and is therefore particularly difficult to observe. In addition more recent work on the anisotropic Heisenberg triangular model will be discussed.

12:27PM B13.00007 Excitation structure of frustrated spin chains with dimerization and the description by the effective field theory¹, SHINTARO TAKAYOSHI, MASAKI OSHIKAWA, Institute for Solid State Physics, University of Tokyo — Heisenberg antiferromagnetic chain with alternating exchange interaction is an important model, which describes magnetic properties of real materials. Field theoretical approach is a powerful tool to investigate such kind of one-dimensional quantum magnets, and it is known that this lattice model is related with corresponding sine-Gordon effective field theory through the bosonization technique. We investigate the excitation spectrum and the correspondence between $S = \frac{1}{2}$ and 1 frustrated chain with dimerization and their effective field theories by both analytical and numerical methods, focusing on the mass ratio r of second breather to soliton. In the result, the $S = \frac{1}{2}$ and 1 cases are understood in a unified way. r becomes $\sqrt{3}$, the value predicted from sine-Gordon model by the introduction of next-nearest neighbor coupling $J_2 = J_{2c}$ where the marginal term in effective field theory vanishes. The universality class of transition is Tomonaga-Luttinger liquid and first order for $J_2 < J_{2c}$ and $J_2 > J_{2c}$, respectively. We also consider the effect of the marginal term on r quantitatively by using form factor perturbation theory and renormalization analysis.

¹Supported by Grants-in-Aid for JSPS Fellows (Grant No. 09J08714)

12:39PM B13.00008 Statistically interacting particles with shapes, DAN LIU, Physics Department, University of Rhode Island — Ising spin $s = \frac{1}{2}, 1, \frac{3}{2}$ chains with nearest and next-nearest neighbor coupling are interpreted as systems of floating particles. The particles are classified into species according to structure and into categories according to function. Species are distinguished by motifs consisting of several consecutive spins that interlink by sharing one or two sites. The four categories include compacts, hosts, tags, and hybrids. All particles from one set are excited from a selected Ising product state serving as pseudo-vacuum. Compacts and hosts float in segments of pseudo-vacuum. Tags are located inside hosts. Hybrids are tags with hosting capability. All particles are free of binding energies but subject to a generalized Pauli principle. In the Ising context, all particle energies are functions of the Hamiltonian parameters. However, the exact statistical mechanical analysis can be performed for particles with arbitrary energies. The entropy is a function of the particle populations from each species. Applications to jamming of granular matter in narrow channels and to DNA overstretching are in the works.

12:51PM B13.00009 Fisher zeros and correlation functions in Ising models, FELICITAS BEICHERT, CHRIS HOOLEY, University of St Andrews, VADIM OGANESYAN, City University of New York, RODERICH MOESSNER, Max-Planck-Institute for the Physics of Complex Systems — Phase transitions take place at singular points of the free energy. These correspond to zeros of the partition function when one tuning parameter is extended into the complex plane (so called Lee-Yang or Fisher zeros). It has been known since the 1960s that transition temperatures and critical exponents can be calculated from the distributions of these partition function zeros. We use this technique to calculate the spin-spin correlation function for the 1d Ising model and notice that it forms a spiral with a wavevector dependent on the position of the complex temperature on the contour of zeros. To extend this we will look at results from the 2d Ising model as well as the Ising model in a transverse field.

1:03PM B13.00010 Integrability in anyonic quantum spin chains via a composite height model, PAATA KAKASHVILI, Rutgers University, EDDY ARDONNE, NORDITA — Recently, properties of collective states of interacting non-abelian anyons have attracted a considerable attention. We study an extension of the ‘golden chain model’, a model of interacting Fibonacci anyons, where two- and three-body interactions are competing. Upon fine-tuning the interaction, the model is integrable. This provides an additional integrable point of the model, on top of the integrable point, when the three-body interaction is absent. To solve the model, we construct a new, integrable height model, in the spirit of the restricted solid-on-solid model solved by Andrews, Baxter and Forrester. The model is solved by means of the corner transfer matrix method. We find a connection between local height probabilities and characters of a conformal field theory governing the critical properties at the integrable point. In the antiferromagnetic regime, the criticality is described by the Z_k parafermion conformal field theory, while the $su(2)_1 \times su(2)_1 \times su(2)_{k-2}/su(2)_k$ coset conformal field theory describes the ferromagnetic regime.

1:15PM B13.00011 Out of equilibrium energy dynamics in low dimensional quantum magnets, STEPHAN LANGER, MARKUS HEYL, LMU Munich, IAN MCCULLOCH, U Queensland, Brisbane, Australia, FABIAN HEIDRICH-MEISNER, LMU Munich — We investigate the real-time dynamics of the energy density in spin-1/2 XXZ chains using two types of quenches resulting in initial states which feature an inhomogeneous distribution of local energies [1]. The first involves quenching bonds in the center of the chain from antiferromagnetic to ferromagnetic exchange interactions. The second quench involves an inhomogeneous magnetic field, inducing both, an inhomogeneous magnetization profile [2] and local energy density. The simulations are carried out using the adaptive time-dependent density matrix renormalization group algorithm. We analyze the time-dependence of the spatial variance of the bond energies and the local energy currents which both yield necessary criteria for ballistic or diffusive energy dynamics. For both setups, our results are consistent with ballistic behavior, both in the massless and the massive phase. For the massless regime, we compare our numerical results to bosonization and the non-interacting limit finding very good agreement. The velocity of the energy wave-packets can be understood as the average velocity of excitations induced by the quench.

[1] Langer et al. Phys. Rev. B in press; arXiv:1107.4136

[2] Langer et al. Phys. Rev. B 79, 214409 (2009)

1:27PM B13.00012 Dissipative phases in the one-dimensional Kondo-Heisenberg model¹, ALEJANDRO LOBOS, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742, USA, MIGUEL A. CAZALILLA, Centro de Física de Materiales CSIC-UPV/EHU and Donostia International Physics Center, E-20018, San Sebastian, Spain, PIOTR CHUDZINSKI, DPMC-MaNEP, University of Geneva, 24 Quai Ernest-Ansermet CH-1211 Geneva, Switzerland — Atomic-sized magnetic structures built on clean metallic surfaces are currently under intense investigation [1]. Besides their potential uses in quantum information storage and processing, these systems allow to ask fundamental questions in condensed matter physics. In particular, the interplay between the Kondo effect (i.e., the screening of the atomic magnetic moment by conduction electrons) and Heisenberg exchange interactions between magnetic impurities has been recently investigated with scanning tunneling microscopy (STM) [2]. Inspired by the above developments, we study an one-dimensional chain of $S=1/2$ Kondo impurities coupled by anisotropic Heisenberg-Ising exchange and embedded in a two-dimensional metallic substrate. Remarkably, in the case of easy-plane exchange, we find a novel quantum phase exhibiting long-range order at zero temperature. We discuss implications of the existence of this phase for possible experiments. References: [1] R. Wiesendanger, RMP 81, 1495 (2009). [2] P. Wahl et al, PRL 98, 056601 (2007) and references therein.

¹We acknowledge support from the Swiss National Foundation under MaNEP and division II, and the Joint Quantum Institute, University of Maryland, College Park, USA

1:39PM B13.00013 String solutions and Mott physics in quasi-one-dimensional antiferromagnets, MASANORI KOHNO, WPI Center for Materials Nanoarchitectonics, NIMS, Japan — Mott insulators are caused by repulsive interactions between electrons, whereas band insulators are due to full filling of a single-particle band. In the one-dimension (1D) Hubbard model, the upper Hubbard band (UHB) has been identified with k - Λ string solutions [1]. Similarly, in the 1D spin-1/2 antiferromagnetic Heisenberg model, the high-energy magnetic excitations in a magnetic field have been identified primarily with 2-string solutions [2]. We can intuitively understand the correspondence between the high-energy states and the UHB, by mapping the Heisenberg model to the hard-core boson model with repulsive interactions. Furthermore, noting that the high-energy states persist in anisotropic triangular antiferromagnets [3], we can interpret the high-energy magnetic excitations observed in quasi-1D antiferromagnets such as Cs_2CuCl_4 and $\text{CuCl}_2 \cdot 2\text{N}(\text{C}_5\text{D}_5)$ in a magnetic field in the context of the Mott physics: the high-energy magnetic excitations, whose origin can be traced back to the string solutions, are due to repulsive interactions between hard-core bosons (down-spins) mapped from the Heisenberg model. [1] M.K., Phys. Rev. Lett. 105, 106402 (2010). [2] M.K., Phys. Rev. Lett. 102, 037203 (2009). [3] M.K., Phys. Rev. Lett. 103, 197203 (2009).

1:51PM B13.00014 A family of spin- S chain representations of $\text{SU}(2)$ level k Wess-Zumino-Witten models, MARTIN GREITER, Institut fuer Festkoerperphysik, KIT, Postfach 3640, 76021 Karlsruhe, Germany, RONNY THOMALE, Department of Physics, Stanford University, Stanford, CA 94305, USA, STEPHAN RACHEL, Department of Physics, Yale University, New Haven, CT 06520, USA, PETER SCHMITTECKERT, Institute fuer Nanotechnologie, KIT, 76344 Eggenstein-Leopoldshafen, Germany — We investigate a family of spin- S chain Hamiltonians recently introduced by one of us [M. Greiter, Mapping of Parent Hamiltonians, Springer Tracts in Modern Physics, Vol 244 (Springer, Berlin, 2011)]. For $S = 1/2$, it corresponds to the Haldane-Shastry model. For general spin S , we numerically show that the low-energy theory of these spin chains is described by the $\text{SU}(2)_k$ Wess-Zumino-Witten model with coupling $k = 2S$. In particular, we investigate the $S = 1$ model whose ground state is given by a Pfaffian for even number of sites N . We reconcile aspects of the spectrum of the Hamiltonian for arbitrary N with trial states obtained by Schwinger projection of two Haldane-Shastry chains.

2:03PM B13.00015 Inhomogeneous Spin Chains and Luttinger Liquids, NICHOLAS SEDLMAYR, JAN OHST, JESKO SIRKER, SEBASTIAN EGGERT, University of Kaiserslautern — We consider a one-dimensional spin chain with inhomogeneous coupling, which can also be modeled as an inhomogeneous Luttinger liquid. The Luttinger liquid paradigm has proved a very successful theoretical tool for investigating one-dimensional wires. However, there remain open questions about what happens when such a system becomes inhomogeneous. The mapping between the spin chain and the Luttinger liquid allows us to use both numerics and field theory to analyze the problem. Of particular interest is the case where the Luttinger liquid is attached to external leads, as is necessary for example when measuring the conductance of the wire. In this paper we use an abrupt shift in the parameters of the Luttinger liquid to model these connections and see how this affects its behavior. In particular we analyze the relevant back-scattering perturbations at the connections, and identify a case where this relevant operator can be tuned to zero within an otherwise still inhomogeneous system. This of course has consequences not only for transport in the Luttinger liquid system but also for the magnetic susceptibility of the spin chain.

Monday, February 27, 2012 11:15AM - 2:15PM –
Session B14 GMAG DMP FIAP: Focus Session: Spins in Semiconductors - Spin Relaxation in Semiconductors and Diamond 212

11:15AM B14.00001 3D Electron Spin Relaxation Control by Electric Field in Quantum Wells, XAVIER MARIE¹, Université de Toulouse — We have measured the electron spin relaxation time in (111)-oriented GaAs quantum wells by time-resolved photoluminescence. By embedding the QWs in a PIN or NIP structure we demonstrate the tuning of the conduction band spin splitting and hence the spin relaxation time with an applied external electric field applied along the growth z direction. The application of an external electric field of 50 kV/cm yields a two-order of magnitude increase of the spin relaxation time which can reach values larger than 30 ns; this is a consequence of the electric field tuning of the spin-orbit conduction band splitting which can almost vanish when the Rashba term compensates exactly the Dresselhaus one [1]. The spin quantum beats measurements under transverse magnetic field prove that the D'Yakonov-Perel (DP) spin relaxation time is not only increased for the S_z electron spin component but also for both S_x and S_y . These results contrast drastically with the (001) and (110) quantum wells. The role of the cubic Dresselhaus terms on the spin relaxation anisotropy will finally be discussed. The tuning or suppression of the DP electron spin relaxation demonstrated here for GaAs/AlGaAs quantum wells grown on (111) substrates is also possible in many other III-V and II-VI zinc-blende nanostructures since the principle relies only on symmetry considerations. [1] A. Balocchi, Q. H. Duong, P. Renucci, B. L. Liu, C. Fontaine, T. Amand, D. Lagarde, and X. Marie, Phys. Rev. Lett 107, 136604(2011)

¹INSA-CNRS-UPS, LPCNO, 135 avenue de Rangueil, 31077 Toulouse, France

11:51AM B14.00002 Rotating Frame Spin dynamics of a Single Nitrogen Vacancy Center in Diamond Nanocrystal¹, ABDELGHANI LARAQUI, CARLOS MERILES, Department of Physics, City College of New York - CUNY — We investigate the spin dynamics of a nitrogen-vacancy (NV) center contained in individual diamond nanocrystals with an average diameter of 70 ± 20 nm in the presence of continuous microwave excitation. Upon periodic reversal of the microwave phase, we observe a train of rotary (Solomon) echoes that effectively extends the system coherence lifetime to reach several tens of microseconds, depending on the microwave power and phase inversion rate [1]. Starting from a model where the NV center interacts with a bath of paramagnetic defects on the nanocrystal surface, we use average Hamiltonian theory to compute the signal envelope from its amplitude at the echo maxima. A comparison between the effective Rabi and Solomon propagators shows that the observed response can be understood as a form of higher-order decoupling from the spin bath. The observed rotary echoes can be thought of as the rotating frame analog of Hahn's spin echoes, implying that the present scheme may find use for nanodiamond-based magnetic sensing. [1] A. Laraoui, C. A. Meriles, Phys. Rev. B **84**, 161403(R) (2011).

¹We acknowledge support from Research Corporation and from the National Science Foundation.

12:03PM B14.00003 Persistence of single spin coherence above room temperature in diamond¹, D.M. TOYLI, D.J. CHRISTLE, B.B. BUCKLEY, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA, A. ALKAUSKAS, C.G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, California, CA — The nitrogen vacancy (NV) center in diamond is unique among single spin systems because of its robust optical spin initialization, optical spin readout, and room temperature spin coherence. However, there is not yet an understanding of what processes limit the NV center's spin properties at higher temperatures. We address this question by performing pulsed electron spin resonance and spin-resolved optical lifetime measurements on single defects at elevated temperatures [1]. The measurements demonstrate that the NV center's spin coherence remains robust at high temperatures while its spin-dependent photoluminescence diminishes above 600 K due to nonradiative relaxation. These results provide an enhanced understanding of the NV center orbital structure and also suggest the possibility of using single spins in diamond for nanoscale thermometry with sensitivities on the order of $100 \text{ mK Hz}^{-1/2}$ over a broad temperature range.

[1] D. M. Toyli*, D. J. Christle*, A. Alkauskas, B. B. Buckley, C. G. Van De Walle, D. D. Awschalom, (*submitted*).

¹This work is funded by AFOSR, ARO, and DARPA.

12:15PM B14.00004 Optically trapped fluorescent nanodiamonds¹, VIVA R. HOROWITZ, BENJAMIN J. ALEMÁN, DAVID CHRISTLE, ANDREW N. CLELAND, DAVID D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — The electronic spin state of the nitrogen-vacancy (NV) center in diamond has gained considerable interest because it can be optically initialized, coherently manipulated, and optically read out at room temperature. In addition, nanoparticle diamonds containing NV centers can be integrated with biological and microfluidic systems. We have constructed and characterized an optical tweezers apparatus to trap fluorescent nanodiamonds in a fluid and measure their fluorescence. Particles are held and moved in three dimensions using an infrared trapping laser. Fluorescent detection of these optically trapped nanodiamonds enables us to observe nanoparticle dynamics and to measure electron spin resonance of NV centers. We will discuss applications using the electron spin resonance of trapped NV centers in nanodiamonds for magnetic field imaging in fluidic environments.

¹This work is funded by AFOSR and DARPA.

12:27PM B14.00005 Nuclear Polarization of Nanodiamond, EWA REJ, DAVID REILLY, School of Physics, The University of Sydney, NSW, 2006 — Nanoparticles with long nuclear spin relaxation times are candidates for use in the context of targeted therapeutic delivery [1] and magnetic resonance imaging [1,2]. We report progress towards the development of contrast agents [3] based on ¹³C in nanodiamond. Nuclear relaxation and electron spin resonance data is presented for particles produced using detonation and the high-pressure high temperature technique. We describe the development of a milli-Kelvin nuclear polarization setup that makes use of a dilution refrigerator and X-band microwave resonator with fast sample exchange. [1] Huang H., Pierstorff E., Osawa E., Ho D., "Active Nanodiamond Hydrogels for Chemotherapeutic Delivery", Nano Lett, 7, 3305-3314 (2007). [2] Aptekar J.W., Cassidy M. C., Johnson A. C., Barton R. A., Lee M. Y., Ogier A. C., Vo C., Anahtar M. N., Ren Y., Bhatia S. N., Ramanathan C., Cory D. G., Hill A. L., Mair R. W., Rosen M. S., Walsworth R. L., Marcus C. M., "Silicon nanoparticles as hyperpolarized magnetic resonance imaging agents", ACS Nano, 3, 4003-4008 (2009). [3] Manus L. M., Mastarone D. J., Waters E. A., Zhang X., Schultz-Sikma E. A., MacRenaris K. W., Ho D., Meade T. J., "Gd(III)-nanodiamond conjugates for MRI contrast enhancement", Nano Lett, 10, 484-489 (2010).

12:39PM B14.00006 Spin Lifetime Measurements of GaAsBi Films¹, BRENNAN PURSLEY, Department of Applied Physics, University of Michigan, G. VARDAR, Department of Materials Science and Engineering, University of Michigan, R.S. GOLDMAN, Department of Materials Science and Engineering and Department of Physics, University of Michigan, V. SIH, Department of Physics, University of Michigan — Substituting a small amount of As with Bi, the largest non-radioactive group V element, leads to a large reduction in the GaAs band gap and expected large spin-orbit effects ². Both properties are advantageous with potential applications ranging from infrared detectors to spin valves. Compressively strained GaAsBi films with varying bismuth compositions were grown on GaAs using molecular-beam epitaxy. Spin lifetimes were measured using the Hanle effect, a magneto-optical technique where an out-of-plane spin polarization is generated by circularly polarized light and then made to precess about an in-plane magnetic field. A Lorentzian lineshape can be fit to the field-dependent photoluminescence polarization to extract gT_s , where g is the Lande g-factor and T_s is a function of the carrier recombination time and spin dephasing time and provides a lower bound for both. Temperature and power dependent measurements were conducted and our extracted values for gT_s vary from 100ps to 1ns.

¹We would like to acknowledge NSF Grants DMR-1006835 and ECCS-0844908 and the Fulbright Foreign Student Fellowship.

²B. Fluegel et al., **Giant Spin-Orbit Bowing in GaAs_{1-x}Bi_x**, Phys. Rev. Lett. **97**, 067205 (2006).

12:51PM B14.00007 Carrier and Spin Dynamics in Narrow Gap Multi Quantum Well Structures¹, MITHUN BHOWMICK, KELLY MCCUTCHEON, GITI A. KHODAPARAST, Virginia Tech, TETSUYA D. MISHIMA, MICHAEL B. SANTOS, University of Oklahoma, DIPTA SAHA, GARY D. SANDERS, CHRISTOPHER J. STANTON, University of Florida — We studied carrier/spin dynamics in several $InSb/Al_xIn_{1-x}Sb$ multiple-quantum well structures using several time resolved differential transmission schemes in the mid-infrared. Our results demonstrate the unique and complex dynamics in InSb heterostructures that can be important for electronic and optoelectronic devices. We present experimental observations and compare them with theoretical calculations. Calculations are based on the 8-band Pidgeon-Brown model generalized to include confinement potential as well as pseudomorphic strain. Optical properties are calculated within the golden rule approximation and compared with one and two color, time-resolved pump-probe differential transmission.

¹Supported by: NSF-Career Award DMR-0846834, NSF- DMR-0706313, and NSF DMR-1105437

1:03PM B14.00008 Electric field-driven coherent spin reorientation and spin rephasing of optically generated electron spin packets in InGaAs¹, SEBASTIAN KUHNEN, KLAUS SCHMALBUCH, MARKUS HAGEDORN, PAUL SCHLAMMES, MARTEN PATT, II. Physikalisches Institut, RWTH Aachen University, Germany, MIHAIL LEPSA, Peter Gruenberg Institut (PGI-9), Forschungszentrum Juelich GmbH, Germany, GERNOT GUENTHERODT, BERND BESCHOTEN, II. Physikalisches Institut, RWTH Aachen University, Germany — Full electric-field control of spin orientations is one of the key tasks in semiconductor spintronics. We demonstrate that electric field pulses can be utilized for phase-coherent 2π spin rotation of optically generated electron spin packets in InGaAs epilayers using time-resolved Faraday rotation. Through spin-orbit interaction, the electric-field pulses act as local magnetic field pulses (LMFP). By the temporal control of the LMFP, we can turn on and off electron spin precession and thereby rotate the spin direction into arbitrary orientations in a 2-dimensional plane [1]. Moreover, using two subsequent pulses of opposite polarity allows us to perform spin echo measurements by reversing the spin precession direction. Although our spin transport experiment is in the diffusive regime, we unexpectedly observe that electric field-induced spin dephasing is reversible to a large extent.
[1] S. Kuhnlen *et al.* arXiv 1107.4307

¹This work has been supported by DFG through FOR912.

1:15PM B14.00009 Using spin fluctuations to reveal long hole spin lifetimes and hole-nuclear coupling in (In,Ga)As quantum dots¹, YAN LI, S.A. CROOKER, National High Magnetic Field Lab, Los Alamos National Lab, D. REUTER, A.D. WIECK, Ruhr-Universität Bochum, D.R. YAKOVLEV, M. BAYER, Technische Universität Dortmund — “Spin noise spectroscopy” is a recently-developed technique for passively measuring the spin dynamics of electrons and holes via their intrinsic random spin fluctuations. In accord with the fluctuation-dissipation theorem, the frequency spectra of this spin noise alone reveals spin dephasing times and Landé g -factors. Using these methods we measure hole spins confined in self-assembled (In,Ga)As/GaAs quantum dots (QDs). Owing to their p -type wavefunctions, holes experience much less hyperfine interaction with lattice nuclei as compared with confined electrons, leading in principle to long spin decoherence times which are favorable for potential qubit applications. We observe very long hole spin correlation times (~ 400 ns) in zero magnetic field, ultimately limited by dephasing from hole-nuclear hyperfine interactions. Suppressing this dephasing with small longitudinal fields (< 100 G) directly reveals the hyperfine coupling strength, and unveils intrinsic hole spin relaxation times up to $\sim 5 \mu\text{s}$. Importantly, the lineshape of the noise evolves from a Lorentzian to a power-law as the hole-nuclear dephasing is suppressed.

¹We acknowledge support from LANL LDRD program.

1:27PM B14.00010 Spin lifetimes in InGaAs quantum wells¹, YU-TSUNG TSAI, ANDREAS RUSS, THOMAS SCRACE, ATHOS PETROU, SUNY at Buffalo, Buffalo, NY, PINGYUE SONG, HANAN DERY, University of Rochester, Rochester, NY, GEORGE KIOSEOGLOU, University of Crete, Heraklion, Greece, CONNIE LI, BEREND JONKER, Naval Research Laboratory, Washington DC — We have carried out Hanle spin relaxation time measurements in InGaAs quantum well structures as well as in Fe-based spin-LEDs that incorporate InGaAs QWs. In the InGaAs QW structures the spin lifetime T_S at $T = 5$ K is equal to 2 ns while in spin LEDs T_S is only 0.17 ns. For the undoped QWs, T_S increases from 2 ns at 5 K to 4.5 ns at 15 K and then decreases monotonically. On the other hand, T_S in the LEDs increases monotonically with temperature. The origin for the difference in the spin lifetimes between undoped QWs and that within a LED structure can be understood by considering the corresponding differences in the band structure between the symmetric quantum well and the spin-LED. In the latter, the Rashba spin-orbit interaction due to the built-in asymmetry brings about a significant enhancement in spin relaxation. In addition, bias conditions in the spin-LED play a crucial role in determining the temperature trend of the spin relaxation. The bias voltage tunes the electron density and accordingly the spin dephasing could be either suppressed or enhanced by electron-electron scattering.

¹Work at SUNY is supported by NSF and ONR. Work at Rochester is supported by AFOSR and NSF

1:39PM B14.00011 T_1 spin lifetimes in n-doped quantum wells and dots, JOHN COLTON, KEN CLARK, DANIEL CRAFT, JANE CUTLER, DAVID MEYER, TYLER PARK, Brigham Young University — We have used a pump probe technique to measure T_1 spin lifetimes in n -type GaAs quantum wells and InAs self-assembled quantum dots. The circularly polarized pump laser pulse aligns the spins; the linearly polarized probe laser pulse probes the spin states of the selected well (or dots) via the Kerr (or Faraday) effect at some later time. Results for the quantum well sample include a spin-filling effect that depends on the direction from which the probe laser wavelength approaches that of the well, and spin lifetimes ranging from 50 to 2000 ns (depending on temperature and field conditions). The InAs quantum dots, doped such that each dot has approximately one extra electron, display T_1 lifetimes longer than 5 ms at 1 T and 1.5 K.

1:51PM B14.00012 Frequency-domain optical probing of coherent spins in semiconductors, JESSE BEREZOVSKY, JOHNATHON FREY, Case Western Reserve University — We have demonstrated a technique for measuring GHz-scale coherent spin dynamics in semiconductors using narrow-linewidth modulated lasers. This scheme, based on the Faraday effect, is carried out by adding a sinusoidal modulation at frequency Ω to continuous-wave pump and probe lasers. The result is to effectively shift the Fourier component of the Faraday rotation signal at Ω to zero frequency, where it can be measured by a low-bandwidth detector. By producing the Fourier transform of the time-domain spin dynamics, this method yields the same information as pulsed pump-probe measurements without the need for complex pulsed lasers, and with minimal spectral bandwidth, allowing for high-resolution spectroscopic measurements. The ability to perform Faraday rotation measurements with narrow-linewidth lasers is essential for observing spins in individual quantum dots, or for avoiding unintentional carrier excitation. We have employed this technique to observe coherent spin dynamics in CdSe nanocrystals using standard diode lasers. By fitting these results to the expected model, we can extract electron g -factors, and spin coherence and dephasing times in agreement with time-domain measurements.

2:03PM B14.00013 Quadratic magnetic field dependence of magnetoelectric photocurrent, JUNFENG DAI, HAI-ZHOU LU, SHUN-QING SHEN, FU-CHUN ZHANG, XIAODONG CUI, The University of Hong Kong, DEPARTMENT OF PHYSICS, THE UNIVERSITY OF HONG KONG TEAM, CENTRE OF THEORETICAL AND COMPUTATIONAL PHYSICS, THE UNIVERSITY OF HONG KONG TEAM — We experimentally study the spin and electric photocurrents excited by a linearly polarized light via direct interband transitions in an InGaAs/InAlAs quantum well. In the absence of a magnetic field, the linearly polarized light induces a pure spin current due to the spin-orbit coupling, which may be transformed into a measurable electric current by applying an in-plane magnetic field. The induced electric photocurrent is linear with the in-plane magnetic field. Here, we report a quadratic magnetic field dependence of the photocurrent in the presence of an additional perpendicular component of the magnetic field. We attribute the observation to the Hall effect of magnetoelectric photocurrent.

Monday, February 27, 2012 11:15AM - 2:15PM —

Session B15 DMP FIAP GMAG: Focus Session: Spins in Metals: Spin Torque Switching and Magnetic Anisotropy Control 213

11:15AM B15.00001 Switching Energy Barrier and Current Reduction in MTJs with Composite Free Layer¹, VIKTOR SVERDLOV, ALEXANDER MAKAROV, SIEGFRIED SELBERHERR, Institute for Microelectronics, TU Wien — We investigate the properties of a penta-layer magnetic tunnel junction (MTJ) with a composite soft layer by exhaustive micromagnetic simulations. The structure CoFe/spacer (1nm)/Py (4nm)/spacer (1nm)/ CoFe (Py is Ni₈₁Fe₁₉) with an elliptical cross-section (major axes 90nm and 35nm, correspondingly) is considered. The system with the composite soft layer is obtained by removing a central stripe of 5nm width from the monolithic free layer. The MTJ with a composite free layer switches two to three times faster than the one with a monolithic layer [1]. We have found that in the MTJ structure with the composite layer the switching energy barrier is decreased and becomes equal to the shape anisotropy energy barrier responsible for thermal stability. This results in a switching current density reduction. The physical reasons for the switching energy barrier reduction are discussed.

[1] A. Makarov *et al.*, *Phys. Status Solidi RRL* **5**, No. 12, 420-422 (2011).

¹This work is supported by the European Research Council through the grant #247056 MOSILSPIN.

11:27AM B15.00002 Switching Distributions in all perpendicular spin-valve nanopillars under thermal activation and spin-transfer torques, DANIEL GOPMAN, DANIEL BEDAU, Department of Physics, New York University, STEPHANE MANGIN, C. LAMBERT, Institute Jean Lamour, UMR CNRS 7198, Nancy University, ERIC FULLERTON, CMRR, University of California at San Diego, JORDAN KATINE, San Jose Research Center, Hitachi-GST, ANDREW KENT, Department of Physics, New York University — The free layer switching field distributions of spin-valve nanopillars with perpendicular magnetization have been studied. The distributions are consistent with expectations of a model based on thermal activation over a single field dependent energy barrier. However, at zero applied current there is a strong asymmetry between the P and AP states and the reverse, with energy barriers more than 50% higher for P to AP transitions. The inhomogeneous dipolar field from the polarizer is demonstrated to be at the origin of this symmetry breaking¹. I will show results on the effects of varying lateral geometry on this symmetry breaking. Also, I will introduce a low-cost method for studying the switching current distributions that applies a continuous waveform to sweep the dc current and simultaneously probe the magnetoresistance. This method permits the acquisition of over 10⁶ switching events in six hours, which presents the possibility to obtain deep statistics on the reversal process. The effect of the magnitude and direction of applied dc currents on the thermal stability of a nanomagnet has been investigated and the results will be examined within the acquired statistics. Supported by NSF Grant DMR-1006575.

¹D. B. Gopman *et al.*, arXiv:1111.1342v1 [cond-mat.mes-hall]

11:39AM B15.00003 Landau-Lifshitz Bloch Macrospin Simulations of Magnetization Switching Dynamics in Perpendicular Anisotropy CoNi/Pd Magnetic Multilayer Thin Films, UFUK KILIC, Bogazici University, Department of Physics, GIOVANNI FINOCCHIO, Dipartimento di Fisica della Materia e Ingegneria Elettronica, University of Messina, ISMAIL VOLKAN INLEK, IBRAHIM CINAR, GULEN AKTAS, OZHAN OZATAY, Bogazici University, Department of Physics — Heating magnetic multilayer thin films close to their Curie temperature (T_c) for brief periods of time, in the presence of a magnetic field, will potentially enable ultra-high density magnetic recording while maintaining thermal stability of perpendicular anisotropy magnetic media. This idea is to be exploited in thermally assisted magnetic recording (TAR) technology, which is currently being pursued by many academic and industrial research labs. In our study, we have performed macrospin simulations of the magnetization switching based on the numerical solution of Landau-Lifshitz-Bloch equation at such elevated temperatures (close to T_c) for a strongly exchange coupled and high perpendicular anisotropy CoNi/Pd magnetic multilayer thin film structure (T_c=448 K). We will discuss the results of a comprehensive model for this material system taking into account temperature dependencies of anisotropy, saturation magnetization and transverse and longitudinal susceptibilities and their effects on the switching process.

11:51AM B15.00004 Statistical and Time Resolved Studies of Switching in Magnetic Tunnel Junction based Orthogonal Spin Transfer Devices, HUANLONG LIU, DANIEL BEDAU, DIRK BACKES, New York University, JURGEN LANGER, Singulus Technologies AG, PRADEEP MANANDHAR, Spin Transfer Technologies, ANDREW KENT, New York University, Spin Transfer Technologies, NEW YORK UNIVERSITY TEAM, SINGULUS TECHNOLOGIES AG TEAM, SPIN TRANSFER TECHNOLOGIES TEAM — We report statistical and single-shot time-resolved studies of spin transfer switching in OST-MRAM devices. These devices consist of a perpendicular polarizer integrated into a layer stack with an in-plane magnetized free and reference layer, which form the electrodes of a magnetic tunnel junction [1]. The perpendicular polarizer provides an initial torque – designed to reduce the incubation delay in switching. The demagnetization field created during the switching can further accelerate the reversal process [2]. The devices switch reliably at 0.7 V and 500 ps duration for both voltage polarities. We record the change of the device resistance in real time during the pulse to obtain the time needed to initiate the switching τ_{start} and the time between the initiation and the end of the switching τ_{switch} for every single switching event. τ_{switch} is determined to be less than a few hundreds of picoseconds, on the order of the precession time due to the demagnetization field and we find evidence for precession reversal under certain conditions. We further present results on the effects of pulse amplitude and applied field on τ_{start} and τ_{switch} . This work was supported by Spin Transfer Technologies. [1] H. Liu *et al.*, APL 97, 242510 (2010). [2] A. D. Kent *et al.*, APL 84, 3897 (2004).

12:03PM B15.00005 Magnon contribution to the spin torque and magnetoresistance properties of FeCoB/MgO/FeCoB magnetic tunnel junctions, YUN LI, HSIN-WEI TSENG, Cornell University, Ithaca, NY 14853, JOHN READ, JORDAN KATINE, HGST, San Jose, California, 95135, DANIEL RALPH, ROBERT BUHRMAN, Cornell University, Ithaca, NY 14853 — We have studied the spin-torque excited ferromagnetic resonance (ST-FMR) and the tunneling magnetoresistance (TMR) properties of FeCoB/MgO/FeCoB magnetic tunnel junctions as a function of temperature from 300K to 10K. We find that while the TMR increases by ~ 50% upon cooling to 10 K, the in-plane spin torque and the perpendicular or field-like torque both decrease substantially. The results demonstrate that while magnon-assisted tunneling degrades TMR, it acts to significantly enhance ST in MTJs, in accord with theoretical prediction. Moreover, the bias-dependent structure in both the asymmetry of the in-plane ST and the parallel conductance of the MTJ is more pronounced at low temperature, indicative of this asymmetry being due substantially to the interfacial electronic structure of the electrodes.

12:15PM B15.00006 Magnetic field dependence of spin torque switching in nanoscale magnetic tunnel junctions, LIU YANG, GRAHAM ROWLANDS, Department of Physics and Astronomy, University of California, Irvine, CA, JORDAN KATINE, Hitachi Global Storage Technologies, San Jose, CA 95135, JURGEN LANGER, Singulus Technologies AG, 63796 Kahl/Main, Germany, ILYA KRIVOROTOV, Department of Physics and Astronomy, University of California, Irvine, CA — Magnetic random access memory based on spin transfer torque effect in nanoscale magnetic tunnel junctions (STT-RAM) is emerging as a promising candidate for embedded and stand-alone computer memory. An important performance parameter of STT-RAM is stability of its free magnetic layer against thermal fluctuations. Measurements of the free layer switching probability as a function of sub-critical voltage at zero effective magnetic field (read disturb rate or RDR measurements) have been proposed as a method for quantitative evaluation of the free layer thermal stability at zero voltage. In this presentation, we report RDR measurement as a function of external magnetic field, which provide a test of the RDR method self-consistency and reliability.

12:27PM B15.00007 Shot noise in double barrier epitaxial magnetic tunnel junctions, FARKHAD ALIEV, JUAN PEDRO CASCALES, DAVID HERRANZ, ANDRES GOMEZ-IBARLUCEA, Universidad Autonoma de Madrid Spain, CORIOLAN TIUSAN, MICHEL HEHN, AMANDINE DULLUARD, CHRISTINE BELLOUARD, Nancy-Universite France, TOMASZ SZCZEPANSKI, VITALII DUGAEV, Rzeszow University of Technology Poland, JOZEF BARNAS, Adam Mickiewicz University Poznan Poland — Shot noise has been shown to be an effective tool to study statistics of electron tunnelling in single barrier magnetic tunnel junctions [1-2]. Here we report on shot noise and tunnelling magnetoresistance measurements in fully epitaxial Fe/MgO/Fe/MgO/Fe double barrier magnetic tunnel junctions. We observed that the shot noise is essentially determined by the barriers' symmetry and relative magnetic configuration. Enhanced barrier asymmetry effectively suppresses electron correlations, and the noise approaches the Poissonian limit. The proposed model of sequential tunnelling (with spin relaxation) through the magnetic layer inside the tunnel barrier satisfactory explains the experimental observations. [1] R.Guerrero, et al., Phys. Rev. Lett. 97, 0266602 (2006). [2] R.Guerrero, et al, Appl. Phys. Lett. 91, 132504 (2007).

12:39PM B15.00008 Planar approximation for spin-transfer devices with tilted polarizer¹, YA. B. BAZALIY, University of South Carolina — Planar spin-transfer devices with dominating easy-plane anisotropy can be described by an effective one-dimensional equation for the in-plane angle [1-3]. Such a description provides an intuitive qualitative understanding of the magnetic dynamics. We apply the effective planar equation to describe magnetic switching and precession states in devices with a tilted polarizer [4]. The approach allows one to understand the dynamic regimes and sketch the switching diagram without performing the detailed calculations.

[1] Ya. B. Bazaliy, Appl. Phys. Lett. 91, 262510 (2007).

[2] Ya. B. Bazaliy, Phys. Rev. B 76, 140402(R) (2007).

[3] Ya. B. Bazaliy and F. Arammash, Phys. Rev. B 84, 132404 (2011).

[4] Ya. B. Bazaliy, arXiv:1109.1331 (2011).

¹Supported by the NSF grant DMR-0847159

12:51PM B15.00009 Modification of the Stoner-Wohlfarth Astroid by a Spin-Polarized Current¹, SHU YAN, ZHELIN SUN², YA. B. BAZALIY, Department of Physics and Astronomy, University of South Carolina, Columbia, SC 29208 — Conventional Stoner-Wohlfarth astroid describes the field-induced switching of a nanomagnet with a uniaxial anisotropy. Both theory and experiments show that the spin-transfer torque can change the switching behavior of nanomagnets and therefore modify the astroid. Such a modification was recently analyzed in the limit of small currents [1]. To explore the modification of the astroid by a current of arbitrary magnitude we propose an exact method capable of finding the switching boundaries for a magnet described by an LLG equation with the Slonczewski's spin-torque term. Our approach takes into account both the local destabilization of equilibria and the equilibrium collisions. The self-crossing nature of the modified astroid is explained and a novel region with three stable equilibria is predicted in our result.

[1] Y. Henry, S. Mangin and J. Cucchiara, J. A. Katine, and E. E. Fullerton, Phys. Rev. B 79, 214422(2009).

¹This work was supported by the NSF grant DMR- 0847159.

²Current affiliation: Department of electrical and computer engineering, UCSD, La Jolla, CA

1:03PM B15.00010 Origin of perpendicular magnetic anisotropy in Co/Ni multilayers on Ti layer, SEE-HUN YANG, IBM Almaden Research Center, KUEI-HUNG THOMS, Industrial Technology Research Institute, LUC THOMAS, STUART PARKIN, IBM Almaden Research Center — Magnetic materials in which their magnetic moment direction is oriented perpendicular to the plane of the magnetic layers in thin film heterostructures have been much studied for their potential application to spintronic devices. In particular, theories of current induced excitation, via the phenomenon of spin torque transfer, show that perpendicularly magnetized layers can be more easily excited or their magnetization direction switched than in-plane magnetized layers. In particular, Co/Ni multilayers are promising due to high spin polarization and small Gilbert damping compared to Co/Pt or Fe/Pt. However, their perpendicular magnetic anisotropy (PMA) is highly sensitive to the underlayer that is critical in device performance because, for instance, the current shunting can substantially reduce the spin transfer torque in magnetic racetrack memory. We observed an excellent PMA in annealed Co/Ni on Ti underlayer whose resistance is significantly greater than those of Co/Ni, thereby minimizing the current shunting. It is found that the PMA does not simply originate from magneto-crystalline effect (spin-orbit interaction) but mainly from magnetoelastic effect caused by compressive strain along (111) direction. We will present systematic results and quantitative analyses.

1:15PM B15.00011 Perpendicular magnetization of CoFeGe alloy films induced by MgO interface¹, MANLI DING, University of Virginia, SEBASTIAN SCHAFER, University of Alabama, XIAOPU LI, University of Virginia, TIM MEWES, University of Alabama, JOSEPH POON, University of Virginia — The perpendicular magnetization of CoFeGe alloy films was achieved in the structures of CoFeGe/MgO with the perpendicular magnetic anisotropy energy density (K_u) of $\sim 1 \times 10^6 \text{ erg/cm}^3$. The CoFeGe thickness dependence of K_u was investigated, indicating that the perpendicular anisotropy of CoFeGe is contributed by the interfacial anisotropy between CoFeGe and MgO. High-resolution transmission electron microscope images clearly show formation of bcc crystalline structure of CoFeGe well lattice matched with the (100)-oriented MgO barrier. Gilbert damping constant for the films was evaluated by using ferromagnetic resonance measurement.

¹Acknowledge for the financial support from Defense Advanced Research Projects Agency (DARPA).

1:27PM B15.00012 Voltage-Induced Ferromagnetic Resonance in Magnetic Tunnel Junctions, JIAN ZHU, University of California, Irvine, JORDAN KATINE, Hitachi Global Storage Technologies, GRAHAM ROWLANDS, YU-JIN CHEN, ZHENG DUAN, University of California, Irvine, JUAN ALZATE, PRAMEY UPADHYAYA, University of California, Los Angeles, JUERGEN LANGER, Singulus Technologies, PEDRAM KHALILI AMIRI, KANG WANG, University of California, Los Angeles, ILYA KRIVOROTOV, University of California, Irvine — We demonstrate excitation of ferromagnetic resonance in CoFeB/MgO/CoFeB magnetic tunnel junctions (MTJs) by the combined action of voltage-controlled magnetic anisotropy (VCMA) and spin transfer torque (ST). Our measurements reveal that GHz-frequency VCMA torque and ST in low-resistance MTJs have similar magnitudes, and thus that both torques are equally important for understanding high-frequency voltage-driven magnetization dynamics in MTJs. As an example, we show that VCMA can increase the sensitivity of an MTJ-based microwave signal detector to the sensitivity level of semiconductor Schottky diodes.

1:39PM B15.00013 Spin Torque in Asymmetric CoFeB/MgO/FeB Magnetic Tunnel Junctions

, HSIN-WEI TSENG, Cornell University, YUN LI, Cornell Univ., JOHN READ, Hitachi Global Storage Technology, San Jose, CA, DANIEL RALPH, ROBERT BUHRMAN, Cornell Univ., CORNELL UNIV. TEAM, HITACH GLOBAL STORAGE TECHNOLOGY COLLABORATION — Recent studies have shown that the use of asymmetric electrodes in MTJs can significantly affect spin torque (ST) behavior. We will report on the measurement via spin torque ferromagnetic resonance (ST-FMR) and switching phase diagram (SPD) studies of the in-plane and field-like (out-of-plane) torque of low resistance, asymmetric IrMn/FeB/MgO/FeCoB) and IrMn/FeCoB/MgO/FeB MTJ nanopillars in the as-grown state (TMR~22%) and the annealed state (TMR~90%), and in comparison to that of symmetric counterparts; IrMn/FeB/MgO/FeB) and Ir/Mn/FeCoB/MgO/FeCoB MTJs. For the asymmetric MTJs only, the ST-FMR data show a strong field-like torque for low voltage bias V that reverses sign when the free and pinned layers are reversed. At the higher V regime explored by the SPD the equivalent linear term in the field-like torque can dominate over the in-plane torque, resulting in either the parallel or antiparallel alignment being favored for both bias polarities, depending on the composition of the free layer.

1:51PM B15.00014 Influence of growth parameters on the spin-filtering properties of epitaxial ferrite tunnel barriers¹

¹, J.-B. MOUSSY², S. MATZEN³, CEA-Saclay, R. MATTANA⁴, F. PETROFF⁵, UMR CNRS/Thales, G.-X. MIAO⁶, J.S. MOODERA⁷, Francis Bitter Magnet Lab., CEA TEAM, UMR CNRS/THALES TEAM, MIT TEAM — In spintronics, spin-filtering is a physical phenomenon which has the potential to produce highly spin-polarized currents by the spin-selective transport of electrons across a ferromagnetic tunnel barrier. The insulating ferrites MnFe_2O_4 , CoFe_2O_4 and NiFe_2O_4 , whose Curie temperatures are above 300K, are promising candidates for spin-filtering at room temperature. In this work, we report on the in-depth study of structural, chemical and physical properties of epitaxial ferrite ultra-thin films and associated spin-filtering measurements as a function of different growth parameters. We analyze the effect of oxidation on the physical properties and the resultant spin-polarization. The influence of structural defects on the spin-filter efficiency is also put on view by tunneling magnetoresistance. Finally, we show the impact of the $\text{MgAl}_2\text{O}_4(001)$ substrates on the magnetic behavior of cobalt ferrite tunnel barriers revealing the important role played by strains in the spin-filter properties.

¹This work is supported by the Partner University Fund

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2:03PM B15.00015 Magnetoelectric Control of Magnetic Anisotropy in Ultrathin Fe Films¹

UWE BAUER, Massachusetts Institute of Technology, Cambridge, USA, MAREK PRZYBYLSKI, JURGEN KIRSCHNER, Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany, GEOFFREY S. D. BEACH, Massachusetts Institute of Technology, Cambridge, USA — Magnetoelectric switching of the magnetization vector could enable new low-power logic devices and non-volatile memory cells. Magnetoelectric switching typically requires complex multiferroic oxides or strain coupled magnetostrictive/piezoelectric composites. However, recently it has been demonstrated that surface magnetic anisotropy in ultrathin ferromagnetic metal films can be directly controlled by application of a strong electric field [1]. In this work we apply an electric field across a high- k oxide stack of MgO and ZrO_2 to induce charge at the surface of an ultrathin Fe film. By using high- k dielectric materials more charge can be induced at the surface of the ferromagnetic film and the efficiency of the magnetoelectric effect can be enhanced. Under application of just a few volts across the oxide stack we observe a strong magnetoelectric effect which results in a shift of the spin reorientation thickness by 0.5 atomic layers and a change in perpendicular surface anisotropy of $\sim 120 \mu\text{J}/\text{m}^2$. Moreover, by engineering the high- k oxide stack we realize a novel charge pumping mechanism that permits optical imprinting of the magnetic state in the continuous Fe film. [1] T. Maruyama *et al.* Nature Nanotechnology 4, 158 - 161 (2009)

¹Research at MIT is supported by the National Science Foundation through grant ECCS-1128439.

Monday, February 27, 2012 11:15AM - 2:15PM – Session B16 DCMP: Hubbard Model 251

11:15AM B16.00001 Charge and magnetic order in the triangular lattice Hubbard model at one-third filling¹

, MATTHEW ENJALRAN, Southern CT State University — Experimental work over the last decade on layered triangular lattice materials with itinerant electrons has increased the motivation to study these systems theoretically. As in insulating magnets, frustration in itinerant systems enriches the phase diagram of the material. In a class of organic charge transfer salts and sodium cobalt oxide spin liquid, superconducting, charged ordered, and magnetically ordered phases have been observed. With the kinetic energy of electrons, a Hubbard type model on a triangular lattice is an appropriate starting point to study much of the correlated physics of these systems. We consider a single band Hubbard model on a triangular lattice with variable electron filling and anisotropic hopping. Within mean-field theory we observe a transition at one-third filling on the isotropic lattice to a charge ordered antiferromagnet on a honeycomb sublattice at a critical interaction $U_c/t = 5.0$. We will also present preliminary results for other regions of the phase diagram.

¹CSU Research Grant

11:27AM B16.00002 Electronic reconstruction of doped Mott insulator heterojunctions¹

, M. CHARLEBOIS, Université de Sherbrooke, S.R. HASSAN, R. KARAN, IMSc Chennai, India, M. DION, D. SENECHAL, A.-M.S. TREMBLAY, Université de Sherbrooke — Correlated electron heterostructures became a possible alternative when thin-film deposition techniques achieved structures with a sharp interface transition [1]. Soon thereafter, Okamoto & Millis introduced the concept of “electronic reconstruction” [2]. We study here the electronic reconstruction of doped Mott insulator heterostructures based on a Cluster Dynamical Mean Field Theory (CDMFT) calculations of the Hubbard model in the limit where electrostatic energy dominates over the kinetic energy associated with transport across layers. The grand potential of individual layers is first computed within CDMFT and then the electrostatic potential energy is taken into account in the Hartree approximation. The charge reconstruction in an ensemble of stacked planes of different nature can lead to a distribution of electron charge and to transport properties that are unique to doped-Mott insulators.

[1] J. Mannhart, D. G. Schlom, Science 327, 1607 (2010).

[2] S. Okamoto and A. J. Millis, Nature 428, 630 (2004).

¹Vanier fellowship, NSERC, CRC, CIFAR, CFI, MDEIE, MIT-Harvard CUA

11:39AM B16.00003 Solving the Parquet Equations for the Hubbard Model beyond Weak Coupling, KA-MING TAM, Louisiana State University, HERBERT FOTSO, Georgetown University, SHUXIANG YANG, TAE-WOO LEE, J. RAMANUJAM, JUANA MORENO, MARK JARRELL, Louisiana State University — We find that imposing the crossing symmetry in the iteration process considerably extends the range of convergence for solutions of the parquet equations for the Hubbard model. When the crossing symmetry is not imposed, the convergence of both simple iteration and more complicated continuous loading (homotopy) methods are limited to high temperatures and weak interactions. We modify the algorithm to impose the crossing symmetry without increasing the computational complexity. We also imposed time reversal and a subset of the point group symmetries, but they did not further improve the convergence. We elaborate the details of the latency hiding scheme which can significantly improve the performance in the computational implementation. With these modifications, stable solutions for the parquet equations can be obtained by iteration more quickly even for values of the interaction that are a significant fraction of the bandwidth and for temperatures that are much smaller than the bandwidth. This may represent a crucial step towards the solution of two-particle field theories for correlated electron models.

11:51AM B16.00004 Correlation effects of one band hubbard model beyond the Gutzwiller Approximation, JUN LIU, YONGXIN YAO, CAI-ZHUANG WANG, KAI-MING HO, Iowa State University and Ames Lab — A novel scheme is introduced to go beyond the Gutzwiller approximation (GA). Starting from the scheme, we can see how the standard GA is recovered by relaxing physical constraints step by step. This not only adds to validity of the current scheme, but provides new insights into understanding the GA. Performance of the scheme on several testing cases is superior to the standard GA. We studied the one band Hubbard model in one, two and three dimensions to revisit relevant conclusions made under the GA as well as the slave boson formalism.

12:03PM B16.00005 Local electronic nematicity in the 2-dimensional Hubbard model¹, KUN FANG, GAYANATH FERNANDO, University of Connecticut, ARMEN KOCHARIAN, California State University — Recent measurements on magnetic and transport properties of some strongly correlated materials show a local electronic nematic phase which locally breaks the C_4 symmetry but keeps translational symmetry. We studied the 2-dimensional Hubbard model using the variational cluster approach and found a similar phase. The results showed this local nematicity is a property of the electron liquid and would appear even if there is no lattice distortion. Calculations of spin correlation were performed and compared to results from magnetic neutron scattering of real materials, which showed a distinct asymmetry along x and y directions.

¹The authors acknowledge the computing facilities provided by the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH1088

12:15PM B16.00006 Evolution of insulator-metal-insulator transitions under staggered lattice potentials, AARAM JOO KIM, MOO YOUNG CHOI, Department of Physics and Astronomy and Center for Theoretical Physics, Seoul National University, Seoul 151-747, Korea, GUN SANG JEON, Department of Physics, Ewha Womans University, Seoul 120-750, Korea — It is known that in the ionic Hubbard model metallic phases exist between band and Mott insulators in the presence of staggered lattice potentials. We investigate how the phase diagram depends on the strength of the staggered lattice potential, by means of the dynamical mean-field theory combined with the continuous-time quantum Monte Carlo method. Observed at finite temperatures is the crossover between metallic and band insulating phases while a first-order transition ending up with a critical point shows up between the metallic and Mott insulating phases. It is discussed how such transition behaviors evolve as the lattice potential grows at low temperatures.

12:27PM B16.00007 Mott transition and ferrimagnetism in the Hubbard model on the anisotropic kagome lattice, ATSUSHI YAMADA, KAZUHIKO SEKI, Department of Physics, Chiba University, ROBERT EDER, Karlsruhe Institute of Technology, YUKINORI OHTA, Department of Physics, Chiba University — Mott transition and ferrimagnetism are studied in the Hubbard model on the anisotropic kagome lattice using the variational cluster approximation and the phase diagram at zero temperature and half-filling is analyzed. The ferrimagnetic phase rapidly grows as the geometric frustration is relaxed, and the Mott insulator phase disappears in moderately frustrated region, showing that the ferrimagnetic fluctuations stemming from the relaxation of the geometric frustration is enhanced by the electron correlations. In metallic phase, heavy fermion behavior is observed and mass enhancement factor is computed. Enhancement of effective spatial anisotropy by the electron correlations is also confirmed in moderately frustrated region, and its effect on heavy fermion behavior is examined.

12:39PM B16.00008 Graphene two-leg ladder. A system with conducting, insulating and superconductive properties, GEORGE KARAKONSTANTAKIS, STEVEN KIVELSON, Stanford University — We use DMRG to study the ground-state phases of the Hubbard model defined on a one dimensional ladder of edge-sharing hexagons - a model which may be relevant to the electronic structure of polyacenes or graphene strips. At half filling we find a robust insulating phase with a large spin-gap, even at small U/t which, as a function of the strength of the third-neighbor hopping, exhibits a non-trivial cross-over from a band -insulator to a Mott insulator. The doped system exhibits a variety of conducting phases. Possible relevance of our results to the recently discovered high temperature superconductivity in K doped dibenzopentacene will be discussed, as well.

12:51PM B16.00009 Dominant superconducting fluctuations in the 1D extended Holstein-extended Hubbard model, SHAN-WEN TSAI, University of California, Riverside, KA-MING TAM, Louisiana State University, DAVID K. CAMPBELL, Boston University — The search for realistic 1D models that exhibit dominant superconducting (SC) fluctuations has a long history. In these 1D systems, the effects of commensurate band fillings - strongest at half-filling - and electronic repulsions typically lead to a finite charge gap and the favoring of insulating density wave ordering over superconductivity. We study a model - the extended Hubbard-extended Holstein (EHEH) model - with non-local electron-phonon interactions, in addition to electron-electron interactions. The EHEH model unambiguously possesses dominant superconducting fluctuations at half filling in a large region of parameter space. Using multi-scale functional renormalization group for the full model and a renormalization group for a bosonized form of the model, we prove the existence of dominant SC fluctuations in this model. Dominant SC fluctuations arise because the spin-charge coupling at high energy is weakened by the non-local electron-phonon interaction and the charge gap is destroyed by the suppression of the Umklapp process. The existence of the dominant SC pairing instability in this half-filled 1D system suggests that non-local boson-mediated interactions may be important in the superconductivity observed in high T_c cuprate and organic superconductors.

1:03PM B16.00010 Ground state and finite temperature behavior of $1/4$ -filled zigzag ladders¹

, R. TORSTEN CLAY, JEONG-PIL SONG, SAURABH DAYAL, Mississippi State University, SUMIT MAZUMDAR, University of Arizona — We consider the simplest example of lattice frustration in the $1/4$ -filled band, a one-dimensional chain with next-nearest neighbor interactions. For this zigzag ladder with electron-electron as well as electron-phonon interactions we present numerical results for ground state as well as thermodynamic properties. In this system the ground state bond distortion pattern is independent of electron-electron interaction strength. The spin gap from the ground state of the zigzag ladder increases with the degree of frustration. Unlike in one-dimension, where the spin-gap and charge ordering transitions can be distinct, we show that in the ladder they occur simultaneously. We discuss spin gap and charge ordering transitions in $1/4$ -filled materials with one, two, or three dimensional crystal structures. We show empirically that regardless of dimensionality the occurrence of simultaneous or distinct charge and magnetic transitions can be correlated with the ground state bond distortion pattern.

¹This work was supported by DOE grant DE-FG02-06ER46315.

1:15PM B16.00011 Phases of the two-leg Hubbard ladder in the large U limit

, LI LIU, HONG YAO, STEVEN KIVELSON, Stanford University, STEVEN WHITE, University of California, Irvine, DUNG-HAI LEE, University of California, Berkeley — We study the phase diagram of the two-leg Hubbard ladder in the large U limit using the density matrix renormalization group (DMRG). Already in the limit of infinite on-site repulsion U , we find a rich phase diagram in which commensurability effects are unexpectedly prominent: A fully spin-polarized “Nagaoka” metallic phase occurs for electron density, n , in the range $1 > n > n_1$, where $n_1 \approx 0.8$ is not obviously locked by any commensurability. There is an insulating, anti-ferromagnetic commensurate plaquette phase at $n=3/4$, and two-phase coexistence for $n_1 > n > 3/4$. For $3/4 > n > n_2 \approx 0.6$, there is a partially spin-polarized metallic state with a magnetization peak centered at $n=2/3$. For the most part, the ground state is a paramagnetic Luttinger liquid for $n_2 \geq n$, although an antiferromagnetic phase with a substantial charge gap (and which may or may not have a small spin-gap) arises at $n=1/2$. Interesting soliton excitations with fractional charge are found for the plaquette phase at $n=3/4$. We have also explored the evolution of these phases as a function of decreasing (but still large) U , both by studying the t - J model and of the underlying Hubbard model.

1:27PM B16.00012 Quantum Phase Transitions in an Ionic Hubbard Model in One Dimension

, JI-WOO LEE, SUNG MOON KIM, KYO YEON CHO, Myongji University — We study quantum phase transitions in an ionic Hubbard model in one dimension. This model accounts for electrons in alternating potentials with a lattice period of 2. For a specified alternating potential of strength Δ , we change the local repulsion between spin-up and spin-down electrons, U , for the model to exhibit a quantum phase transition from a band insulator to a Mott insulator. Via exact diagonalization with a modified Lanczos method, we find that, as we tune U , the ground-state energy shows a level crossing at half-filling. We obtain a phase diagram of the model by using a finite-size scaling method. Also, we find an interesting feature of double occupancy around the phase transitions.

1:39PM B16.00013 Ground state properties of the ionic Hubbard model on a two-leg triangular ladder at $3/4$ filling

, IVÁN GONZÁLEZ, Centro de Supercomputación de Galicia — We study numerically the ionic Hubbard model on a two-leg triangular ladder at $3/4$ filling. This model is believed to be the minimal microscopic model describing the physics of Na_xCoO_2 at $x = 0.5$, and shows a rich phase diagram that depends on a delicate balance between the Coulomb interaction U , the hopping amplitude t , and the ionic potential Δ . Motivated by experiments analyzing the dopant distribution on $\text{Na}_{0.5}\text{CoO}_2$, we focus in the case of a stripe-type ionic potential. In the correlated limit where the Coulomb interaction is large, the ground state of the model is a charge-transfer insulator for large ionic potential and turns metallic for zero ionic potential. Electronic structure calculations point to the regime $\Delta \sim |t|, t < 0$ as the one relevant for $\text{Na}_{0.5}\text{CoO}_2$, but previous calculations [1] have not fully clarify the nature of ground state of the model in such regime. The aim of this work is to study the metal-insulator transition that occurs in the region $U \gg \Delta \sim |t|$ of the phase diagram as well as the magnetic and charge structures of the associated ground states.

[1] J. Merino et al. Phys. Rev. B 80, 045116 (2009).

1:51PM B16.00014 Quantum Monte Carlo Studies on Attractive Hubbard Model with Anisotropic Spin-dependent Hopping on Two-leg Ladder Lattice¹

, HO KIN TANG, The Chinese University of Hong Kong, ZHONG BING HUANG, HuBei University, JIN HUA SUN, HAI QING LIN, The Chinese University of Hong Kong — Using spin-dependent hopping, it is possible to have a fully paired state with a gap for single fermion excitation and gapless Cooper pair excitation, called ‘Cooper-pair Bose-metal’ phase. Recently, the existence of this phase was suggested by a density matrix renormalization group studies² on the attractive Hubbard Model with two-leg ladder geometry and anisotropic spin-dependent hopping. We here present a detailed Quantum Monte Carlo (QMC) studies on this model to investigate its finite temperature properties, including correlation function, s-wave and d-wave pairing function, and finally to deduce the existence and behavior of ‘Cooper-pair Bose-metal’ phase.

¹Supported by the General Research Fund of the HKSAR Government

² Feiguin, A.E. and M.P.A. Fisher, *Exotic paired phases in ladders with spin-dependent hopping*. Physical Review B, 2011. **83**(11): p. 115104.

2:03PM B16.00015 An Exotic Spin Mode in a Non-Polarized Fermi Liquid With Net Spin-Current

, YI ZHANG, KEVIN BEDELL, Boston College, Department of Physics — We find an exotic spin excitation in an ordered magnetic system with an order parameter with a net spin current but no net magnetization. Starting from a Fermi liquid theory, similar to that for a weak ferromagnet, this excitation emerges from a state that is protected by a Pomeranchuk instability. We derive the propagating mode using Landau kinetic equation, using two different approaches and find that the dispersion of the mode is the same for both approaches in leading order.

Monday, February 27, 2012 11:15AM - 2:03PM –

Session B17 DMP GERA FIAP: Focus Session: Thermoelectrics - Nanowires and Other Nanostructures 252A

11:15AM B17.00001 Thermoelectric Transport in Bismuth Telluride Nanoplates, Semiconductor Nanowires, and Silicide Nanocomposites: Effects of Low Dimensionality, Surface States, Interface Structures, and Crystal Complexity , LI SHI, The University of Texas at Austin — This presentation will review recent measurement results of thermoelectric properties of individual bismuth telluride nanoplates, semiconductor nanowires, and silicide nanocomposites. In experiments with these realistic nanostructured materials, a number of factors influence the transport properties. For example, unintentional doping, interface roughness and impurities can often obscure the predicted effects of the low-dimensional electronic density of states and the protected surface states, the latter of which have been suggested for bismuth telluride and other thermoelectric materials, now also referred as topological insulators. Similarly, impurities and defects as well as contact thermal resistance can play an important role in phonon transport in nanostructures, making it nontrivial to quantify the actual effects of phonon-surface scattering and other intriguing low-dimensional phonon transport phenomena. Because of these experimental complications, diverse theoretical interpretations of experimental results have appeared in the literature, and will be discussed. Moreover, the effects of twin defects and crystal complexity on thermoelectric transport in nanostructures will be examined based on measurement results of III-V and silicide nanostructures.

11:51AM B17.00002 Universal Scaling Relations for the Thermoelectric Power Factor of Semiconducting Nanostructures , JANE CORNETT, ODED RABIN, University of Maryland — We present a model for the power factor (PF) of wires and thin films which bridges between strongly confined and bulk behavior. Relevant scattering mechanisms are considered in the framework of the relaxation time approximation. Previous models for the transport properties of nanostructured thermoelectric materials predicted vast improvements in the PF values over bulk due to discretization of the electron density-of-states function as the result of confinement. Using this model, we find that the PF of nanowires and thin films in fact falls below the bulk value for most of the experimentally-accessible size range. We find a non-monotonic relationship between PF and system size in all systems studied—regardless of the particular materials parameters and dominant scattering mechanisms. The effects of the size, dimensionality, temperature, carrier concentration and dominant scattering mechanism in single-carrier semiconductors will be discussed. In the framework of the *constant* relaxation time approximation, universal scaling relations for the power factor of all single-carrier semiconductors are obtained.

12:03PM B17.00003 Thermal conductivity of silicon nanowires: interplay between core defects and surface roughness , YUPING HE, GIULIA GALLI, UC Davis — Recent experiments [1] suggested that the thermal conductivity (κ) of Si nanowires may be reduced by about two orders of magnitude compared to that of bulk Si (κ_{bulk}), making them attractive materials for thermoelectric applications. Size reduction plays an important role [2] in determining such reduction but it does not fully account for recent measurements [1]. We investigated κ in wires with 15 nm diameter (comparable to experimental sizes) using large scale molecular dynamics simulations. We show that, unlike the case of thin [3] (2-3 nm diameter) rods, the presence of an amorphous layer at the surface accounts only for a decrease by a factor of 4 in κ with respect to that of wires with smooth surfaces. It is the combined effect of defects in the core and rippled surfaces that enables a decrease up to a factor of 90 with respect to κ_{bulk} . Work supported by DOE/SciDAC-e.

[1] A.I. Hochbaum et al., Nature 451, 163 (2008); A. I. Boukai et al., Nature, 451, 168 (2008).

[2] D.Li et al. APL 2003.

[3] D. Donadio and G. Galli, Phys. Rev. Lett. 102, 195901 (2009).

12:15PM B17.00004 Electric-Field Guided Synthesis of Standalone Nanowire Arrays for Thermoelectric Applications¹ , YEW SAN HOR, Department of Physics, Missouri University of Science and Technology — Theoretical studies have suggested that figure of merits of thermoelectric materials can be improved through fabrications of nanoscaled thermoelectric materials. Thin films are expected to result in up to a seven fold improvement in efficiency over bulk materials; even greater enhancement, up to 15 times in efficiency, is expected for very thin wires. Researchers have already succeeded in increasing the efficiency by making thin-layered materials and nanowires of a non-thermoelectric material, i.e. silicone. For practical applications, however, arrays of standalone nanowires or isolated thermoelectric nanowire devices without any template will be required. Here I present an electromagnetic field guided nanostructured synthesis of an array of standalone thermoelectric nanowires. This technique utilizing electric field as a guide in building highly ordered nanostructures will be an elegant, “bottom-up” method for nanofabrication without the need of a template. An array of quasi-one dimensional chalcogenide nanowires has been successfully grown in between two conducting plates. Thermoelectric transport measurements including thermalconductivity, thermoelectric power and figure of merit can be easily performed in the device, without any need of complicated electron beam lithography technique.

¹Supported by University of Missouri Research Board.

12:27PM B17.00005 Thermoelectric Property Characterization of Suspended Silicon Nanowires , ANNIE WEATHERS, Department of Mechanical Engineering, The University of Texas at Austin, Austin, TX 78712, USA, FENG ZHOU, Materials Science and Engineering Program, The University of Texas at Austin, Austin, TX 78712, USA, INSUN JO, Department of Physics, The University of Texas at Austin, Austin, TX 78712, USA, MICHAEL T. PETTES, JAEHYUN KIM, LI SHI, Department of Mechanical Engineering, The University of Texas at Austin, Austin, TX 78712, USA — A key challenge in the measurement of thermal and electrical properties of suspended nanowires (NWs) is the ability to obtain clean, reliable electrical and thermal contact between the nanowire and device. We report on a technique for aligning NWs to sub-micron accuracy on a suspended device made of two SiNx membranes with the assistance of a polymethyl methacrylate (PMMA) carrier layer. Electrical and thermal contact is made by using electron beam lithography to pattern a window in the PMMA over the device electrodes, followed by oxide etching and surface passivation in wet etchant, metal deposition through a shadowmask, and lift-off. We demonstrate this technique on rough Si nanowires grown by metal-assisted chemical etching. The whole assembly is clean and without contamination. Thermoelectric properties and their correlation with crystal structure will be discussed

12:39PM B17.00006 Thermoelectric Properties of Low-Dimensional Si and Ge Based Nanostructures , NEOPHYTOS NEOPHYTOU, HANS KOSINA, Technical University of Vienna — Low-dimensional thermoelectric nanostructures based on Si and Ge are promising candidates for high performance energy conversion and generation applications. 1D nanowires (NWs) and 2D superlattices of Si, Ge and Si/SiGe have experimentally demonstrated excellent performance. In these confined systems the electrical conductivity, the thermal conductivity, and the Seebeck coefficient can be designed to some degree independently so as to achieve enhanced ZT values as compared to the related bulk material values. In this work, we calculate the thermoelectric coefficients of scaled Si and Ge NWs and thin-layers. We use the sp3d5s* tight-binding model for the electronic structure and linearized Boltzmann transport theory. Our calculations include structures of feature sizes up to 12nm containing over 5500 atoms. This study indicates that the confinement length scale can be exploited as a degree of freedom in designing the material properties. We examine n-type and p-type materials of different cross section sizes and confinement/transport orientations and provide optimization directions for power factor improvement. Finally, using measured values for the lattice thermal conductivity, the ZT is estimated.

12:51PM B17.00007 Gate Controlled Tuning of Seebeck Coefficient in InAs Nanowires, JOHANNES GOOTH, PHILLIP WU, SOFIA SVENSSON, HEINER LINKE, Lund University — Here we present measurements of the Seebeck Coefficient in InAs nanowires grown by Chemical beam epitaxy. Nanowires were mechanically transferred onto a SiO₂ substrate with a global metallic backgate, and Ohmic contacts to a single nanowire were made by standard electron beam lithography techniques. We were able to tune the measured thermovoltage in the nanowire by field effect gating and correlate this behavior with the conductance through the nanowire. Interestingly, large enhancements in the thermoelectric power factor were seen at low temperature for certain gate voltages. Such controllability allows for optimizing the thermoelectric response of the nanowire at different substrate temperatures.

1:03PM B17.00008 Phonon transmission and thermal transport in GaAs-AlAs superlattices from first-principles, KEIVAN ESFARJANI, ZHITING TIAN, MARIA LUCKYANOVA, TENGFEI LUO, GANG CHEN, MIT, NANO-ENGINEERING TEAM — Using the Green's function method and Landauer's formula, we formulate phonon transport in a 3D superlattice. The theory is harmonic and describes coherent (elastic) transport of heat through a periodic structure which may also have disorder present at its interfaces. We compute the force constants from first-principles density functional calculations and use them to compute the transmission, and the thermal conductance of a GaAs-AlAs superlattice versus length and temperature. We also investigate the effect of mass disorder at the interface and anharmonicity, to locate the transition from coherent to incoherent transport. Results are finally compared with experimental measurements.

1:15PM B17.00009 Phonon density of states in nanocrystalline Si_{1-x}Gex explored by inelastic neutron scattering, STEPHEN WILSON, CHETAN DHITAL, ZHIFENG REN, Department of Physics, Boston College, Chestnut Hill MA, DOUG ABERNATHY, Spallation Neutron Source, Oak Ridge National Lab, Oak Ridge Tennessee — Recently there have been significant advances in the efficiencies of traditional thermoelectric compounds gained via the creation of thermoelectric nanocomposites possessing substantially reduced thermal conductivity relative to their bulk counterparts [1,2]. The dramatic reduction in the heat transport of these nanocomposites is often attributed to the increased interface scattering of phonons or induced surface/boundary modes; however notably little work has been put into exploring the detailed changes in the phonon density of states in many of these functional nanocomposite samples. Here we present inelastic neutron scattering measurements exploring the phonon density of states in a series of Si_{1-x}Gex thermoelectric nanocomposites. The evolution of the phonon spectral weight distribution and linewidths as a function of Ge-doping will be discussed and compared to the known bulk phonon density of states in this system.

[1] Giri Joshi et al., Nano Letters 8, 4670 (2008).

[2] X. Wang et al., App. Phys. Lett. 93, 193121 (2008).

1:27PM B17.00010 Ab-initio investigation of thermal transport in alloyed and nanostructured materials¹, DMITRI VOLJA, Massachusetts Institute of Technology, Department of Materials Science and Engineering, Cambridge, MA, BORIS KOZINSKY, Robert BOSCH LLC Research and Technology Center, Cambridge MA, JIVTESH GARG, Massachusetts Institute of Technology, Department of Materials Science and Engineering, Cambridge, MA, MARCO FORNARI, Central Michigan University, Department of Physics, Mount Pleasant, MI, NICOLA MARZARI, Ecole Polytechnique Federale de Lausanne — A whole spectra of intriguing physical properties appears in conventional materials when structural features reach nanoscale. Since thermal conductivity is controlled by the heat carriers' mean free paths, it becomes of paramount importance to understand and engineer the role of alloying and nanostructuring on transport coefficients. First-principles calculations often provide accurate microscopic parameters, but at significant computational cost even for ideal, perfect systems. We present a hybrid classical-quantum method to compute thermal conductivity from both harmonic and anharmonic terms using Boltzmann transport formalism. We combine first-principles calculations of harmonic terms and force-field calculations of third-order and fourth-order force constant. Results for SiGe will be discussed to show the validity of approach. We also discuss the effects of nanostructuring by introducing boundary scattering contributions, as well as mechanisms of filler rattling in thermoelectric skutterudites.

¹Support from Robert Bosch LLC as part of the MIT Energy Initiative

1:39PM B17.00011 ZT enhancement using nanocomposite materials, PAUL HANEY, National Institute of Standards and Technology — The effect of interface scattering on the performance of disordered, nanocomposite thermoelectric materials is studied theoretically (within a linear response formalism), using effective medium theory, and direct numerics. The general relation between interfacial and bulk transport properties which results in an enhanced ZT is determined. Given these requirements of interfacial transport properties, a series of microscopic calculations of interface scattering are presented to assess the feasibility of using nanocomposites for ZT enhancement.

1:51PM B17.00012 Anderson Localization of Phonons in Random Multilayer Thin Film Thermoelectrics, ANTHONY FRACHIONI, BRUCE WHITE, Binghamton University — Anderson localization of phonons in random multilayer thin films has been explored as a means for reducing lattice thermal conductivity in thermoelectric materials. Silicon based systems have been explored due to silicon's high crust abundance and Seebeck coefficient. Reverse non-equilibrium molecular dynamics simulations have been used to determine the thermal conductivity of silicon in which randomly selected atomic planes (20% of lattice planes) are subject to mass increase. The simulation results indicate that the lattice thermal conductivity of silicon can be decreased by a factor of over ten thousand (to 15 mW/m·K). Based on models in which the charge carrier mean free path is limited by scattering from the planes with mass disorder, the mobility of silicon is expected to reach values of 10 cm²/V·s. At this mobility the thermoelectric figure of merit, ZT, is found to be greater than ten when the mass ratio of the disordered planes to that of silicon approaches 10. These results indicate that the pursuit of nanostructured silicon thermoelectric materials in the form of random multilayers may provide a path to efficient and sustainable thermoelectric materials.

Monday, February 27, 2012 11:15AM - 2:15PM –

Session B18 DMP: Focus Session: Nanostructures and Metamaterials, Growth, Structure, and Characterization – Metamaterials with Gain and Active 252B

11:15AM B18.00001 Metamaterials with Gain¹, ORTWIN HESS, Imperial College London — Nanoplasmonic metamaterials are the key to an extreme control of light and allow us to conceive materials with negative or vanishing refractive index. Indeed, metamaterials enable a multitude of exciting and useful applications, such as subwavelength focusing, invisibility cloaking, and “trapped rainbow” stopping of light. The realization of these materials has recently advanced from the microwave to the optical regime. However, at optical wavelengths, metamaterials may suffer from high dissipative losses owing to the metallic nature of their constituent nanoplasmonic meta-molecules. It is therefore not surprising that overcoming loss restrictions by gain is currently one of the most important topics in metamaterials’ research. At the same time, providing gain on the nanoplasmonic (metamolecular) level opens up exciting new possibilities such as a whole new type of metamaterial nano-laser with a cavity length of about a tenth of the wavelength. The talk gives an overview of the state of the art of gain-enhanced metamaterials. Particular focus will be placed on nano-plasmonic metamaterials (such as double-fishnet metamaterials) with integrated laser dyes as gain medium. The successful compensation of loss by gain is demonstrated on the meta-molecular level. On the basis of a comprehensive, microscopic Maxwell-Bloch Langevin approach of spatio-temporal light amplification and lasing in gain-enhanced nanoplasmonic (negative-index) metamaterials a methodology based on the discrete Poynting’s theorem is introduced that allows dynamic tracing of the flow of electromagnetic energy into and out of “microscopic” channels (light field, plasmons, gain medium). It is shown that steady-state amplification can be achieved in nanoplasmonic metamaterials. Finally, a complex spatio-temporal interplay of light-field and coherent absorption dynamics is revealed in the lasing dynamics of a nanoplasmonic gain-enhanced double-fishnet metamaterial.

¹Support by the Leverhulme Trust is gratefully acknowledged.

11:51AM B18.00002 Metamaterials with gain and interpretation of transmission in pump-probe experiments¹, THOMAS KOSCHNY, Ames Laboratory and Dept. of Phys. and Astronomy, Iowa State University, Ames, Iowa 50011, U.S.A., ZHIXIANG HUANG, Ames Lab and Dept. of Phys., Iowa State Univ., Ames, Iowa 50011, U.S.A. and Anhui Univ., China, COSTAS M. SOUKOULIS, Ames Lab and Dept. of Phys., Iowa State Univ., Ames, Iowa 50011, U.S.A. and IESL, FORTH, Heraklion, Greece — We establish a new approach for pump-probe simulations of metallic metamaterials coupled to the gain materials. It is of vital importance to understand the mechanism of the coupling of metamaterials with the gain medium. Using a four-level gain system, we have studied light amplification of arrays of metallic split-ring resonators (SRRs) with a gain layer underneath. We find that the differential transmittance $\Delta T/T$ can be negative for SRRs on the top of the gain substrate, which is not expected, and $\Delta T/T$ is positive for the gain substrate alone. These simulations agree with pump-probe experiments and can help to design new experiments to compensate the losses of metamaterials. We numerically investigate loss compensation and transmission in pump-probe experiments in resonant metamaterials with gain using an FDTD algorithm coupled to semiclassical rate equations. We explain experimentally observed negative differential transmission by gain-dependent impedance.

¹Work at Ames Laboratory was supported by the Department of Energy (Basic Energy Science) under Contract No. DE-ACD2-07CH11358. This work was partially supported by the European Community FET project PHOME (No. 213390)

12:03PM B18.00003 Spontaneous emission enhancement in a plasmonic nanocavity¹, KASEY RUSSELL, TSUNG-LI LIU, SHANYING CUI, EVELYN HU, Harvard University School of Engineering and Applied Sciences — Recently, metallic optical cavities containing coupled emitters have been fabricated that operate at visible frequencies. These cavities are capable of tightly confining light, greatly modifying the electromagnetic density of states in the location of the optical emitters. Here, we present measurements from a metal-based optical cavity that greatly modifies both the spectral and temporal characteristics of the coupled emitters. Our design is based on plasmonic coupling between a silver nanowire and a planar silver substrate, with a layer of optical emitters within the gap between the two silver components. The field confinement of the structure results in a 1000-fold enhancement of the spontaneous emission rate of the coupled emitters. These results suggest that metal-based optical cavities can allow quantum cavity electrodynamics of emitters such as colloidal quantum dots and organic dyes.

¹Supported by NSF/NSEC under NSF/PHY-06-46094

12:15PM B18.00004 Directionally emitting plasmon laser and circuits, RENMIN MA, XIAOBO YIN, RUPERT OULTON, VOLKER SORGER, XIANG ZHANG, UC Berkeley — Scaling down of the laser promises unprecedented ultra-dense and ultra-fast integrated photonics. The research of nanoscale lasers is rapidly advancing and a variety of approaches have been explored including whispering gallery lasers, photonic crystal lasers, metallic lasers. However, a major obstacle of integrating nanolasers with other components is the strong divergence of emission from a sub-wavelength laser cavity due to the diffraction of light. Here, we demonstrate a deep sub-wavelength plasmon laser that directs more than 70% of its radiation into an embedded semiconductor waveguide. The laser naturally integrates photonic and electronic functionality allowing both efficient electrical modulation and wavelength multiplexing. A maximum modulation depth of 11 dB for a small 1 V of bias sweep is achieved. We demonstrate an ultra-compact plasmonic circuit integrating five independently modulated multi-colored laser sources multiplexed onto a single semiconductor waveguide, illustrating the potential of plasmon lasers for large scale, ultra-dense photonic integration.

12:27PM B18.00005 Electromagnetically induced transparency and absorption in metamaterials: self-consistent theory and experiments¹, PHILIPPE TASSIN, Ames Lab/Iowa State Univ. and Vrije Univ. Brussel, LEI ZHANG, ADITYA JAIN, RONGKUO ZHAO, THOMAS KOSCHNY, Ames Lab/Iowa State Univ., COSTAS SOUKOULIS, Ames Lab/Iowa State Univ. and FORTH — There has recently been a lot of interest in slow-light metamaterials that provide transparency windows combining low absorption with high group delay. This phenomenon was explained by a two-resonator model involving a radiative resonator that couples directly to the incident field and a dark resonator that can only be excited through coupling with the radiative resonator. However, in our most recent experiments on wire/SRR metamaterials, we have observed a much richer behavior—we measure not only transparency windows with incisions in the absorption spectrum (electromagnetically induced transparency), but also narrow spectral features with absorption larger than the background absorption of the radiative element (electromagnetically induced absorption). We have developed a model in which the coupling of the electromagnetic waves to the radiative resonator is treated explicitly. An important attribute of this model, which is in excellent agreement with our experiments and full-wave simulations, is the self-consistent treatment of the spectral broadening of the bright resonator originating from the dipole radiation as opposed to the bare linewidth due to dissipation. We discuss the conditions under which electromagnetically induced transparency/absorption can be observed.

¹This work was supported by Ames Laboratory (U.S. DOE) and the U.S. Office of Naval Research (Award No. N000141010925).

12:39PM B18.00006 Lighting up dark plasmon modes with electron beam, KIN HUNG FUNG, Massachusetts Institute of Technology, ANIL KUMAR, University of Illinois at Urbana-Champaign, NICHOLAS X. FANG, Massachusetts Institute of Technology — Dark plasmon modes couple weakly with free-space photons. It is, therefore, generally believed that far-field detection of dark plasmon modes is difficult. In this talk, we discuss how an electron beam can light up dark plasmon modes and show theoretically and experimentally that bright and dark modes in a single metal bowtie nanoantenna can be studied at the far field using cathodoluminescence spectroscopy.

12:51PM B18.00007 Direct modulation of lanthanide emission at sub-lifetime scales using electric and magnetic dipole transition, SINAN KARAVELI, AARON J. WEINSTEIN, RASHID ZIA, Brown University — Lanthanide ions, such as trivalent Europium (Eu³⁺) and Erbium (Er³⁺) are technologically important, high quantum yield light emitters that exhibit both magnetic dipole (MD) and electric dipole (ED) transitions. It is well known that the transition rate of an emitter in an inhomogeneous optical environment, e.g. an emitter near a mirror, is modified due to self-interference effects, leading to either enhancement or inhibition of spontaneous emission. However, due to the opposite symmetry of their emitted fields, ED and MD transitions exhibit differing self-interference. Here, we leverage this difference to show large spectral tuning and sub-lifetime dynamic modulation of Eu³⁺ emission. Specifically, we use a moving gold mirror to selectively enhance the ED and MD transitions in Eu³⁺ doped Y₂O₃. Controlling the emitter-mirror distance allows us to tune the emission spectra from 580 nm to 715 nm. Modulating the mirror position with a piezoelectric crystal allows us to dynamically tune the Eu³⁺ emission at speeds faster than the excited state lifetime.

1:03PM B18.00008 Strong Coupling of Molecular Absorption and Mid-Infrared Metamaterial Resonances, JOSHUA MASON, University of Massachusetts, Lowell, GRAHAM ALLEN, Connecticut College, VICTOR PODOLSKIY, University of Massachusetts, Lowell, DANIEL WASSERMAN, University of Illinois, Urbana Champaign — Here we present numerical, analytical, and experimental evidence for strong optical coupling between a mid-infrared perfect absorber thin-film metamaterial and a molecular absorption resonance within a dielectric medium. Clear anti-crossing behavior is exhibited numerically and experimentally when the metamaterial resonance is scanned through the dielectric molecular resonance; a coupled oscillator model is used to present a further analytical description. The anti-crossing is used to demonstrate and quantify the strength of the optical coupling within the thin film. Such a device can potentially be developed for mid-infrared sensing applications and actively tunable metamaterial optical components.

1:15PM B18.00009 Magnetic Dipole Emission Lines in Trivalent Lanthanide Ions, CHRISTOPHER DODSON, RASHID ZIA, Brown University — Magnetic dipole (MD) transitions offer a unique opportunity to study light-matter interactions beyond the electric dipole approximation. Modified spontaneous emission from MD transitions can serve as an ideal way to study optical magnetic fields in metamaterials and related nanostructures. While many MD absorption lines have been identified, only a few MD emission lines in solid state systems are widely known. Here we seek to expand the known MD emission lines by calculating all such transitions in the trivalent lanthanide ions. We use intermediate coupling to construct a detailed free-ion Hamiltonian including electrostatic, spin-orbit, two- and three-body, spin-spin, spin-other-orbit, and electrostatically correlated spin-orbit interactions. Determining the free-ion energy levels allows the calculation of ground-state MD absorption lines, and their respective oscillator strengths, as well as spontaneous emission rates for all MD mediated transitions. Many strong MD emission lines are predicted throughout the visible and near infrared spectrum. Corresponding electric quadrupole transitions were also calculated and found to have negligible contribution. If time permits, we will also present direct experimental measurements characterizing these new MD emission lines.

1:27PM B18.00010 Self-assembled quantum dots as active emitters for silicon photonic crystal nanocavities, THOMAS ZABEL, NORMAN HAUKE, STEFAN LICHTMANNECKER, FABRICE LAUSSY, RICHARD GEIGER, JONATHAN FINLEY, Walter Schottky Institut, Technical University Munich, Germany, GERHARD ABSTREITER, Walter Schottky Institut, Technical University Munich, Institute for Advanced Study, Technical University Munich, Germany, DOMINIQUE BOUGEARD, Institut fuer Experimentelle und Angewandte Physik, University Regensburg, Germany, YASUHIKO ARAKAWA, University of Tokyo, Inst. for Nano Quant. Inform. Electr., Inst. of Ind. Sci., Tokyo, Japan, Institute for Advanced Study — We present a study of the properties of active (Si)Ge self-assembled quantum dot (QD) emitters coupled to Si photonic crystal (PC) nanocavities up to room temperature and evaluate the potential of such nanostructures for the realization of efficient silicon based light sources in the near-infrared regime. The Si-Ge system allows the formation of type I and type II band alignment QD, depending on the epitaxy conditions. We first discuss the emission properties of different types of QD. In particular we present type I SiGe islands designed to produce a strong emission due to a large wave function overlap of confined electrons and holes. We then investigate the coupling properties of (Si)Ge QD emitters to 2D Si PC cavities. We interpret the experimentally observed correlation between the photoluminescence intensity of the QDs and the quality factor of the PC cavity using simulations based on a dissipative master-equation approach [1]. As a further step towards efficient light sources, we currently study the coupling of electrically pumped (Si)Ge QDs to 2D PC in contacted diode structures. [1] N. Hauke, et al. Phys. Rev. B 84, 085320 (2011)

1:39PM B18.00011 Broadband Transparency of Graded Anisotropic Metamaterial¹, KA SHING HUI, HON PING LEE, LEI SUN, KIN WAH YU, The Chinese University of Hong Kong — We have investigated the scattering of electromagnetic waves from a graded anisotropic sphere whose dielectric permittivity is radially anisotropic, with different radial and tangential components described by the graded Drude model. The Rayleigh scattering cross section (RSCS) has been calculated analytically and numerically by the Rayleigh scattering theory. The electric polarization and the electromagnetic field distribution are also examined in a quasi-static condition. Due to the scattering cancellation mechanism, the results reveal that the RSCS can be rather smaller over a wider frequency range, indicating the so called broadband transparency. Furthermore, compared with the non-graded and graded isotropic structure, the anisotropic structure leads a better broadband transparency.

¹Supported by the General Research Fund of the HKSAR Government

1:51PM B18.00012 Reconfigurable Gradient Index using VO₂ Memory Metamaterials, MICHAEL GOLDFLAM, University of California San Diego, TOM DRISCOLL, UCSD and Duke University, BRIAN CHAPLER, OMAR KHATIB, University of California San Diego, NAN JOKERST, SABARNI PALIT, DAVID SMITH, Duke University, BONG-JUN KIM, ETRI, GIWAN SEO, University of Science and Technology, HYUN-TAK KIM, ETRI and UST in Korea, MASSIMILIANO DI VENTRA, DIMITRI BASOV, University of California San Diego — We have demonstrated tuning of a metamaterial device that incorporates a form of spatial gradient control. Electrical tuning of the metamaterial was achieved through a vanadium dioxide layer which interacts with an array of split ring resonators. Through design of the device and contact geometry, we achieved a spatial gradient in the magnitude of permittivity, writeable using a single transient electrical pulse. This induced gradient in our device was observed on spatial scales on the order of one wavelength at 1 THz. Thus we have demonstrated the viability of elements for use in future devices with potential applications in beamforming and communications.¹ Various contact geometries are currently being investigated with the goal of implementing finer control over gradients and expanding on the possible applications of such devices.

¹M. D. Goldflam, et. al., Appl. Phys. Lett. 99, 044103 (2011).

2:03PM B18.00013 Waves and rays in meta-microcavities: from positive “n” to negative “n” and from order to chaos¹, NATALIA M. LITCHINITSER, SUNY at Buffalo, JORGE V. JOSE, Indiana University — The emergence of metamaterials and, in particular, negative index metamaterials (NIMs) triggers reconsideration of many fundamental physical phenomena. Importantly, the majority of unique properties of NIMs stand out when NIMs are combined with conventional positive index materials (PIMs). In this talk, we consider the wave and ray properties of electromagnetic wave interaction in two-dimensional microcavities that contain a combination of PIM and NIM with negative dielectric permittivity and magnetic permeability. We consider closed and open cavities and total and partial reflection and refraction at the boundaries between the media with different indices of refraction. By using a combination of analytic and numerical methods we are able to classify the different types of possible solutions in this type of mixed PIM-NIM regions. In particular, we derive the special properties of whispering gallery modes as well as the constructive and destructive interference due to wave refraction/reflection across different refractive media boundaries. Finally, we discuss possible practical applications of this type of mixed refractive indices microcavities.

¹This work was partially supported by US Army Research Office Award # W911NF0910075.

Monday, February 27, 2012 11:15AM - 2:15PM —
Session B19 FHP: Invited Session: One Hundred Fifty Years of Maxwell's Equations (1862-2012) 253AB

11:15AM B19.00001 The discovery of Maxwell's equations, FRANCIS EVERITT, Stanford University — In January 1865, Maxwell at age 34 wrote a letter to his cousin Charles Cay describing various doings, including his work on the viscosity of gases and a visit from two of the world's leading oculists to inspect the eyes of his dog “Spice”. He added, “I have also a paper afloat, with an electromagnetic theory of light, which, till I am convinced to the contrary, I hold to be great guns.” That paper “A Dynamical Theory of the Electromagnetic Field” was his fourth on the subject. It was followed in 1868 by another, and then in 1873 by his massive two volume Treatise on Electricity and Magnetism. Even so, by the time of his death in 1879 as he was beginning a radically revised edition of the Treatise, much remained to be done. We celebrate here the 150th anniversary of Maxwell's first astonished realization in 1862 of the link between electromagnetism and light. So revolutionary was this that 15 or more years went by before Lorentz, Poynting, FitzGerald, and others came to address it, sometimes with improvements, sometimes not. Not until 1888 did Hertz make the essential experimental discovery of radio waves. What is so remarkable about Maxwell's five papers is that each presents a complete view of the subject radically different from the one before. I shall say something about each, emphasizing in particular Maxwell's most unexpected idea, the displacement current, so vastly more interesting than the accounts of it found in textbooks today. Beyond lie other surprises. The concept of gauge invariance, and the role the vector potential would play in defining the canonical momentum of the electron, both go back to Maxwell. In 1872 came a paper “On the Mathematical Classification of Physical Quantities”, which stands as an education in itself. Amid much else, there for the first time appears the distinction between axial and polar vectors and those new operational concepts related to quaternion theory: *curl*, *divergence*, and *gradient*.

11:51AM B19.00002 Maxwellians and the Remaking of Maxwell's Equations, BRUCE HUNT, University of Texas — Although James Clerk Maxwell first formulated his theory of the electromagnetic field in the early 1860s, it went through important changes before it gained general acceptance in the 1890s. Those changes were largely the work of a group of younger physicists, the Maxwellians, led by G. F. FitzGerald in Ireland, Oliver Lodge and Oliver Heaviside in England, and Heinrich Hertz in Germany. Together, they extended, refined, tested, and confirmed Maxwell's theory, and recast it into the set of four vector equations known ever since as “Maxwell's equations.” By tracing how the Maxwellians remade and disseminated Maxwell's theory between the late 1870s and the mid-1890s, we can gain a clearer understanding not just of how the electromagnetic field was understood at the end of the 19th century, but of the collaborative nature of work at the frontiers of physics.

12:27PM B19.00003 Using Maxwell's Equations in the late 1800s, JED BUCHWALD, Caltech — Between the publication of Maxwell's *Treatise on Electricity and Magnetism* in 1873 and the early 1900s his field equations were not considered to be fundamental by many Cambridge-trained physicists. Instead, they were thought to derive from Hamilton's principle given an appropriate energy expression. Such an expression usually assigned a velocity or a position function to field quantities, though this was not invariably done. Precisely because the Hamiltonian, and not the derivative field equations, was taken to be basic, new effects could be generated by adding terms to the energy expression. This was how the Faraday and Kerr magneto-optic effects were handled. The program however never did generate a method for incorporating dissipative phenomena, as Oliver Heaviside (who disliked the use of Hamilton's principle) demonstrated. The procedure was in the end decisively abandoned when J. G. Leathem, a student of Joseph Larmor a Cambridge, demonstrated that it could not handle a particularly subtle magneto-optic process.

1:03PM B19.00004 Maxwell and quantum optics, ROY GLAUBER, Harvard Univ — No abstract available.

1:39PM B19.00005 Taking Off From Maxwell's Equations, FRANK WILCZEK, Massachusetts Institute of Technology — I will discuss how we are still discovering new continents in the conceptual world opened up by Maxwell's equations. I will very briefly sketch, in particular, how very natural extensions of those equations describe superconductivity and the deep structure of fundamental particle interactions. Then I'll show how a newer cluster of extensions connects ideas about (perhaps no longer all that) exotic quantum particles and materials.

Monday, February 27, 2012 11:15AM - 2:15PM —
Session B20 FEd FIAP: Invited Session: Astronomy's Detectors and Physics Education 253C

11:15AM B20.00001 The basic physics of astronomical detectors, our eyes on the Universe, JAMES BELETIC, Teledyne Imaging Sensors — The universe is an amazingly huge place. While humankind has directly explored Earth's sister planets with space probes, we don't have the means to venture beyond the solar system, and so almost all information about the universe comes from sensing light that happens our way. Astronomy is constantly striving to find better ways to sense the feeble amount of energy from distant stars and galaxies. This quest has led to a new generation of large telescopes on the ground and in space. Possibly more important than the development of bigger telescopes is the rapid advancement in solid state detector technology. In the x-ray, visible and infrared wavelengths, the most advanced detectors are based on two fundamental technologies: (1) nearly perfect detector materials that efficiently convert photon energy to electrical charge, and (2) very sensitive transistors that convert a few electrons into a measurable voltage. This talk presents the basic physics of astronomical detectors and provides an introduction to the more specialized talks that follow in this session of presentations. Since detectors of light are critical to nearly every aspect of scientific research and involve a wide range of physical phenomena, this session of talks will provide the audience with physics lessons that can be readily incorporated in an undergraduate physics curriculum.

11:51AM B20.00002 Advanced CCD and CMOS image sensor technology at MIT Lincoln Laboratory, VYSHNAVI SUNTHARALINGAM, Advanced Imaging Technology, MIT Lincoln Laboratory, 244 Wood Street Lexington, MA 02420-9108 — The Advanced Imaging Technology (AIT) program area at Lincoln Laboratory addresses a broad range of complex imaging problems by using a wide variety of silicon-based imager technologies, including charge-coupled devices (CCDs), active-pixel sensors (APSs), photodiode arrays, and Geiger-mode avalanche-photodiode (GMAPD) arrays that are single-photon sensitive. Many of these devices, including some very large imaging devices that require low defect levels, are fabricated by us from silicon wafers in our class-10 Microelectronics Laboratory. We also operate a fully equipped packaging facility that is capable of developing and performing innovative device packaging of imaging (and other) devices. In this talk, we present an overview of Lincoln Laboratory's image sensor technologies, describe how they work and how they are built. We discuss several imaging device parameters that can be optimized for high sensitivity. These include quantum efficiency (including fill-factor), charge-transfer efficiency (moving the charge from the pixel to the output port without loss or added spurious charge), and the noise to read this charge out. The overall goal is to convert most or all of the photons that impinge on the device to photoelectrons and then to read out these photoelectrons without losing any and without adding read noise. Further, we will describe design elements or methods that can help with different specific applications: the orthogonal-transfer CCD (OTCCD), an electronic shutter for back illuminated imagers, the Geiger-mode avalanche photodiode (GMAPD) circuit element, and three-dimensionally integrated CMOS focal planes. Several examples of application to high-sensitivity, high-speed, and broad-wavelength range problems will be presented.

12:27PM B20.00003 Gamma-ray Bursts, Black Holes, and Exoplanets: How CCD Detectors have Revolutionized Astronomy, GEORGE RICKER, Massachusetts Institute of Technology — I will tell the story of my research group's role in the development of astronomical charge-coupled detectors (CCDs) by relating the contributions of four MIT research students to projects which we have undertaken together over the past three decades. These projects have empowered observations extending over four decades of the electromagnetic spectrum, enabling discoveries ranging from gamma-ray burst emitting collapsars at cosmological distances, to accretion-driven black holes in the Galaxy, and to exoplanets in the solar neighborhood. This story will illustrate the key contributions which student researchers can make when a novel detector technology arrives on the scene. Finally, I will also describe some of the ways in which their early education in these possibilities has impacted my students' future careers as astronomers and experimental physicists.

1:03PM B20.00004 Coupling physics to understanding the performance of detector arrays, ZORAN NINKOV, Rochester Institute of Technology — Over the last few decades developments in microelectronics have led to the development of arrays of detectors that can be used to measure unprecedentedly small levels of signal. Such arrays have been used over to detect electromagnetic radiation ranging in energy from the X-ray through sub-millimeter wavelengths and also particles. Perhaps nowhere have the improvements been more astonishing than in devices available for the visible part of the spectrum (400 – 1000 nm). The most successful detector array in this spectral region is the Charge Coupled Detector (CCD) whose inventors were recognized with the Nobel Prize in Physics in 2009. In this talk I will review some of the detectors and technologies that are used in low light level imaging. I will also describe a full year sequence of classes (i.e. a theory class, a CCD camera building class and a CCD camera performance measurement class) that students at the Rochester Institute of Technology can take to make them knowledgeable as to the physics underlying the operation and performance of such detector arrays. Finally I will discuss the associated laboratory classes that students must take to measure the performance of the camera they have built and what aspects of fundamental physics are integrated into their understanding. These classes have been taken by both calculus and non-calculus trained students. The classes appeal to students with both types of backgrounds as it couples an understanding of Physics to something that they have built and use.

1:39PM B20.00005 Detecting the Cosmic Microwave Background at the Frontier of Cosmology and in the Classroom, JOHN KOVAC, Harvard University, Departments of Astronomy and of Physics — The 3K blackbody Cosmic Microwave Background (CMB), while exceedingly faint, is the most abundant light in the Universe, permeating all of space as a relic of the hot, dense, primordial fireball. Its detection in 1965 established the Big Bang as the standard model of cosmology and earned its co-discoverers Penzias and Wilson a Nobel Prize. Over the past two decades, advances in detector technology driven by CMB research have produced telescopes with ever-increasing numbers of photon background-limited microwave detectors, capable of mapping fine structure of the CMB to micro-Kelvin precision. These have had enormous impact, determining the geometry of the universe, quantifying the dark matter and dark energy that dominate it, and detecting the faint polarization arising from the primordial seeds of structure. The current frontier is defined by new arrays of thousands of superconducting, polarized detectors producing maps approaching nano-Kelvin precision. In this decade, these measurements will answer questions about the physics driving the earliest moments of the Big Bang and will survey the large-scale structure of the universe, determining neutrino masses and constraining the nature of dark energy. The advanced detector technology fueling this frontier provides superb device-physics training for graduate students and postdocs working on current-generation CMB telescopes. At the same time, careful experimental techniques developed for CMB observations can now be combined with inexpensive high-quality satellite TV detectors to allow even undergraduates to detect the CMB, reproducing Penzias and Wilson's famous discovery. I describe one such undergraduate class at Harvard, which builds CMB telescopes from scratch in a few weeks with a modest budget, teaching students about microwave techniques and detectors and allowing them to find their own evidence for the Big Bang.

Monday, February 27, 2012 11:15AM - 2:15PM –
Session B21 DMP: Focus Session: Search for New Superconductors: Methodologies and New Materials 254A

11:15AM B21.00001 An Enlightened Combinatorial Search for New Superconductors¹, IVAN SCHULLER, Center for Advanced Nanoscience, UCSD — I describe a methodology for the fast search for new superconducting materials. This method consists of a parallel synthesis of a highly inhomogeneous alloy covering large areas of the metallurgical phase diagram combined with a very sensitive, fast, microwave-based method, which allows large non-superconducting portions of the sample to be discarded. Once an inhomogeneous sample containing a minority phase superconductor is identified, we revert to well-known, thorough identification methods, which include standard physical and structural methods. We show how a systematic structural study helps in avoiding miss-identification of new superconducting materials when there are indications from other methods of new discoveries. The application of these ideas to the La-Si-C system, which exhibits promising normal state properties, sometimes correlated with superconductivity, will be discussed. Although this system shows indications of a new superconducting compound, the careful analysis described here shows that the superconductivity in this system can be attributed to intermediate binary and single phases. Searches in other Rare Earth-Si based systems will also be described. Work done in collaboration with J. de la Venta, Ali C. Basaran, J. G. Ramirez, T. Grant, A. J. S. Machado, M. R. Suchomel, R. T. Weber, Z. Fisk, P. Gupta, O. Shpyrko and D. Basov.

¹Work supported by an AFOSR MURI grant.

11:51AM B21.00002 Search for New Superconductors in RE-Si and Al-B Systems: a High Pressure High Temperature Approach¹, MIGUEL ANGEL ALARIO-FRANCO, Universidad Complutense de Madrid, JOSE DE LA VENTA, ALI BASARAN, IVAN K. SCHULLER, University of California - San Diego, TED GRANT, ZACHARY FISK, University of California - Irvine — We have searched for the presence of superconductivity in the RE-Si and Al-B systems using HP-HT synthesis. The RE-Si system has some of the common features that are present in high TC superconducting materials. We have synthesized Ce, Pr, Nd and Gd silicides undoped and doped with C and B. On the other hand, AlB₂ has some similarities with the superconducting MgB₂. We have tried to synthesize AlB₂ way off stoichiometry using HP-HT and thin films Phase Spread Alloy. The Al_{0.67}B₂ would be the MgB₂ equivalent and good reason to expect superconductivity. We discuss the results for both systems after a careful analysis of several physical properties (SQUID, Modulated Microwave Absorption) and x-ray powder diffraction.

¹This study was supported by an AFOSR MURI “Search For New Superconductors For Energy And Power Applications.”

12:03PM B21.00003 Search for new materials: phase spread alloy thin film fabrication and characterization, MOSES MARSH, ALI BASARAN, JOSE DE LA VENTA, OMAR KHATIB, OLEG SHPYRKO, DMITRI BASOV, IVAN SCHULLER, University of California, San Diego — We use the phase spread alloy (PSA) method of fabricating compositionally heterogeneous thin films as an efficient way to produce and screen new, interesting materials (e.g. superconductors, magnetoresistive compounds, etc.). This method uses co-sputtering to deposit material with smoothly varying element concentration across a substrate. Both local and non-local probes are used to verify the composition of the sample. Using the La-Si-C system as an example, we perform x-ray fluorescence from a synchrotron source, x-ray diffraction from a lab source, atomic force microscopy, and infrared spectroscopy on one sample to verify the presence of different phases and their properties.

12:15PM B21.00004 Search for new superconductors in rare-earth silicide systems¹, ALI BASARAN, JOSE DE LA VENTA, IVAN K. SCHULLER, University of California, San Diego, TED GRANT, ZACHARY FISK, University of California, Irvine — We have searched for the presence of superconductivity in the RE₅Si₃ system doped with C or B as a light element (RE: La, Ce, Pr, and Eu). High temperature superconductors and RE₅Si₃ systems have some common properties. Both systems have a layered tetragonal crystal structure. They are multi-element compounds and are also doped with a light element to introduce the superconductivity. In this study, multiphase bulk samples were made using arc-melting. Phase spread alloy thin films were also prepared in a sputtering system. We used magnetic field modulated microwave absorption spectroscopy (MFMMMS), which is a very sensitive contactless technique to detect superconductivity, as the first screening for the existence of superconductivity in an inhomogeneous sample. We will present some of our results from MFMMMS and SQUID measurements and compare them with structural refinement from X-Ray data.

¹This study was made possible by the generous support of AFOSR MURI “Search for New Superconductors for Energy and Power Applications.”

12:27PM B21.00005 Superconductivity in the K-Mo-O system¹, L.M.S. ALVES, C.A.M. DOS SANTOS, Escola de Engenharia de Lorena, Universidade de Sao Paulo, N. DILLEY, Quantum Design, Inc., M.D.R. MARQUES, J.A. AGUIAR, Universidade Federal de Pernambuco, Recife, PE — The rutile-type structure belongs to space group $P4_2/mnm$. Some transition metals form dioxides with variants rutile structure are known as pseudorutiles. These dioxides have interesting physical properties but they are still poorly understood. MoO₂ is one of them. Polycrystalline samples of MoO₂ can be easily prepared using stoichiometric amounts of Mo and MoO₃ through solid state reaction at temperatures near 700 °C. This material is a highly conductive oxide and exhibits Mo-Mo metallic bonds along *c*-axis. On the other hand, previous results show that the physical properties of the MoO₂ are substantially changed with potassium doping [1]. This work unambiguously demonstrates that the K_xMoO₂ system exhibits superconductivity. Electrical resistivity and magnetization measurements were carried out from 2 to 300 K. The electrical and magnetic measurements show that the superconducting critical temperature ranges from 3 to 10 K. The phase composition responsible for the superconductivity is still under investigation.

[1] L. M. S. Alves et al., Phys. Rev. B **81**, 174532 (2010).

¹This material is based upon support by FAPESP (2009/14524-6, 2009/54001-2 e 2010/06637-2), FACEPE (0589/1.05-08), and CNPq/NSF (490182/2009-7).

12:39PM B21.00006 High spin-low spin transition in insulating CaMn₂Sb₂¹, J.W. SIMONSON, G. SMITH, M.C. ARONSON, Department of Physics and Astronomy, Stony Brook University — Layered manganese pnictides are often interesting compounds to compare with the iron pnictide superconductors. To this end, we have synthesized high quality flux-grown single crystals of CaMn₂Sb₂, which forms in a trigonal CaAl₂Si₂-type structure characterized by corrugated triangular Mn layers. Previously reported as a bad metal, we observe instead that this compound exhibits a distinct insulating trend in temperature-dependent resistivity measurements, including an enhancement of up to two orders of magnitude between 200 K and T_N = 85 K. Measurements of ac susceptibility exhibit an orientation- and highly field-dependent plateau across the same temperature range, while heat capacity measurements reveal a sharp feature at 85 K as well as a broad anomaly centered near 195 K. Curie-Weiss behavior above 300 K indicates the presence fluctuating moments with prevailing ferromagnetic interactions, corresponding to less than half the static moment reported for the antiferromagnetic ordered state. These results imply a temperature-induced high spin-low spin insulator-insulator transition.

¹Research supported by a DOD National Security Science and Engineering Fellowship via the AFOSR.

12:51PM B21.00007 An infrared study of electron delocalization in Mn-based relatives of the pnictides, KIRK POST, University of California, San Diego, JACK SIMONSON, CARLOS MARQUES, GREG SMITH, Department of Physics and Astronomy, Stony Brook University, OMAR KHATIB, University of California, San Diego, ZHIPING YIN, MARIA PEZZOLI, Department of Physics, Rutgers and Stony Brook University, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University, DIMITRI BASOV, University of California, San Diego, MEIGAN ARONSON, Department of Physics and Astronomy, Stony Brook University — Current data suggest that the viability of parent compounds to become superconducting is intimately tied to electron correlations.^{1,2} Further comparisons between the ground states of the cuprate and pnictide parent compounds indicate that doping across an electron delocalization transition (EDT) may be key to obtaining a higher critical temperature.³ These insights lead us to study the Mn-based compounds that are isostructural with pnictides and are antiferromagnetic insulators like the cuprates. Specifically, we have explored the effects of doping on LaMnPO_{1-x}F_x and Ca_{1-x}La_xMn₂Sb₂ via optical spectroscopy, transport, and magnetic measurements in parallel to theoretical band structure calculations. Our studies show that LaMnPO is highly resistant to electron delocalization. Likewise, in CaMn₂Sb₂, full delocalization was not attained even though a shift in the band edge was observed.

¹M. Quazilbash *et. al.* Nature Physics 5, 647 (July 2009)

²P.A. Lee *et. al.* Reviews of Modern Physics 78, 17 (January 2006)

³J. Simonson *et. al.* ArXiv:11105938

1:03PM B21.00008 Strong Electronic Correlations in YMn_2Ge_2 , DANIEL MCNALLY, JACK SIMONSON, GREG SMITH, MEIGAN ARONSON, Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY 11794, USA — Exotic phases, like superconductivity, often emerge near electron delocalization transitions in strongly interacting systems. Magnetization, heat capacity and resistivity measurements were performed on single crystals of the antiferromagnetic metal YMn_2Ge_2 , which is isostructural to the ThCr_2Si_2 -type iron pnictides. Above the antiferromagnetic ordering temperature $T_N=425$ K, the magnetic susceptibility displays Curie-Weiss like behaviour with a fluctuating moment $\mu = 3.3 \mu_B/\text{Mn atom}$, larger than the ordered moment of $2.2 \mu_B/\text{Mn atom}$. Heat capacity measurements yield a Sommerfeld coefficient $\gamma = \frac{C}{T} = 8.5 \text{ mJ/mol Mn K}^2$, nearly three times larger than $\gamma_{Ru} = 3.3 \text{ mJ/mol Mn K}^2$ for its non-magnetic isostructural analog YRu_2Ge_2 , indicating strong electronic correlations in YMn_2Ge_2 . The quasiparticle mass enhancement $\frac{m^*}{m_{Ru}} = \frac{\gamma}{\gamma_{Ru}} = 2.6$ is similar to the value observed in the 122-type iron pnictides. Fermi-liquid behaviour of the resistivity $\rho = \rho_0 + AT^2$ is observed over a very broad range of temperatures between 0.5 K and 300 K, with the resistivity at low temperature $\rho(0.5 \text{ K}) = 8 \mu\Omega \text{ cm}$ indicating high sample quality

1:15PM B21.00009 Magnetic, Thermal and Transport Properties of $\text{LaNi}_2(\text{Ge}_{1-x}\text{P}_x)_2$ ¹, R.J. GOETSCH, V.K. ANAND, ABHISHEK PANDEY, D.C. JOHNSTON, Ames Lab. and Dept. Phys. Astron., Iowa State Univ., Ames, IA 50011 — Polycrystalline samples of $\text{LaNi}_2(\text{Ge}_{1-x}\text{P}_x)_2$ ($x = 0, 0.25, 0.50, 0.75, 1$) with the tetragonal ThCr_2Si_2 structure were investigated by heat capacity C_p , magnetic susceptibility χ , and electrical resistivity ρ measurements for temperatures $1.8 \text{ K} \leq T \leq 300 \text{ K}$. The $\rho(T)$ data for each sample reveal metallic behavior that follows the Bloch-Grüniesen theory. The low- T $C_p(T)$ data for the series yielded Sommerfeld coefficients $\gamma = 6\text{--}12 \text{ mJ/mol K}^2$ and Debye temperatures $\Theta_D = 300\text{--}480 \text{ K}$. The $\chi(T)$ data showed nearly T -independent paramagnetism except for LaNi_2Ge_2 , where data up to 1000 K exhibit a broad peak at $\approx 300 \text{ K}$. A possible onset of superconductivity is seen for LaNi_2P_2 at 2.1 K. Analytic functions accurately representing the Bloch-Grüniesen and Debye functions are presented that are very useful for fitting $\rho(T)$ and lattice $C_p(T)$ data, respectively.

¹Research supported by the USDOE under Contract No. DE-AC02-07CH11358.

1:27PM B21.00010 Superconductivity in $\text{WO}_{2.6}\text{F}_{0.4}$ synthesized by reaction of WO_3 with Teflon¹, DAIGOROU HIRAI, ESTEBAN CLIMENT-PASCUAL², ROBERT CAVA, Princeton University — $\text{WO}_{3-x}\text{F}_x$ ($x < 0.45$) perovskite-like oxyfluorides were prepared by a chemically reducing fluorination route using the polymer polytetrafluoroethylene (Teflon). The symmetry of the crystal structures of $\text{WO}_{3-x}\text{F}_x$ changes from monoclinic to tetragonal to cubic as the fluorine content increases. Fluorine doping changes insulating WO_3 to a metallic conductor, and superconductivity ($T_c = 0.4 \text{ K}$) was discovered in the samples with fluorine contents of $0.41 < x < 0.45$. This easy fluorination method may be applicable to other systems and presents an opportunity for finding new oxyfluoride superconductors.

¹This work was supported by the AFOSR MURI on superconductivity.

²present affiliation: Universidad Carlos III de Madrid

1:39PM B21.00011 Type-I Superconductivity in Ytterbium Diantimonide, LIANG L. ZHAO, Rice University, STEFAN LAUSBERG, MANUEL BRANDO, Max Planck Institute for Chemical Physics of Solids, H. KIM, M.A. TANATAR, R. PROZOROV, Ames Laboratory, E. MOROSAN, Rice University — The layered antimonide compound YbSb_2 crystallizes with a ZrSi_2 -type orthorhombic structure, different from other rare earth diantimonides. Unusual for a binary compound, Type-I superconductivity has been observed in YbSb_2 . In this talk, we present the results from anisotropic magnetization, resistivity, heat capacity and magneto-optical Faraday effect measurements on YbSb_2 single crystals, showing a clear superconducting transition at $T_c = 1.25 \text{ K}$. The estimated electron-phonon coupling $\lambda = 0.51$, together with the jump in electronic specific heat $\Delta C_{es}/\gamma T_c = 1.36$, indicate the system to be a weak-coupling BCS superconductor. Magnetization, as well as heat capacity measured under field, clearly suggest a Type-I behavior, which is confirmed by the estimated Ginzburg-Landau parameter $\kappa = 0.13$. According to the H - T phase diagram, the critical field H_c is around 60 Oe.

1:51PM B21.00012 $\text{Cu}_{1-x}\text{BiSO}$: the first Fe-pnictide-structured compound without Fe or Pnictogen¹, LUCIANO ORTENZI, Max Planck Institute for Solid State Research, Stuttgart, SILKE BIERMANN, Centre de Physique Théorique, Ecole Polytechnique, France, OLE KROGH ANDERSEN, Max Planck Institute for Solid State Research, Stuttgart, Germany, IGOR I. MAZIN, Naval Research Laboratory, Washington, DC 20375, USA, LILIA BOERI, Max Planck Institute for Solid State Research, Stuttgart, Germany — The electronic structure of 1111 transition metal pnictides offers a large variety of low-energy phenomena depending on the electronic filling explored. Based on first principles calculations I study the electronic filling d^{10-x} represented by $\text{Cu}_{1-x}\text{BiSO}$: a band insulator that becomes metallic upon hole doping. I argue that the electron-phonon coupling is very strong in this material, and probably drives superconductivity. The critical temperature is however strongly depressed by the proximity to ferromagnetism. The competition between these two different order parameters brings about a high tunability of the system that can go from conventional to unconventional superconductivity by varying such parameters as doping or pressure.

¹This research was supported by the Deutsche Forschungsgemeinschaft under Priority Program 1458

2:03PM B21.00013 Possible Evidence for Novel Superconductivity in LaRu_3Si_2 , HAI-HU WEN, SHENG LI, BIN ZENG, XIANGANG WAN, JIAN TAO, FEI HAN, HUAN YANG, ZHIHE WANG, Physics Department, Nanjing University, China, CENTER FOR SUPERCONDUCTING PHYSICS AND MATERIALS TEAM — Superconductivity in LaRu_3Si_2 with the honeycomb structure of Ru has been investigated. It is found that the normal state specific heat C/T exhibits a deviation from the Debye model down to the lowest temperature. A relation $C/T = \gamma_n + \beta T^2 \cdot \text{AtIn}T$ which concerns the electron correlations can fit the data very well. The suppression to the superconductivity by the magnetic field is not the mean-field like, which is associated well with the observation of strong superconducting fluctuations. The field dependence of the induced quasiparticle density of states measured by the low temperature specific heat shows a non-linear feature, indicating the significant contributions given by the delocalized quasiparticles. The Wilson ratio estimated here is about 3.3, indicating also a strong correlation effect. Interestingly, the Fe-doping can suppress the superconductivity very easily, while Co-doping kills the superconductivity very slowly. The possible reasons are discussed. All these results suggest that the electronic correlation effect exists in LaRu_3Si_2 and superconductivity may be novel.

Monday, February 27, 2012 11:15AM - 2:15PM –
Session B22 DMP DCOMP: Focus Session: Fe-based Superconductors- ARPES and Fermi Surfaces 254B

11:15AM B22.00001 Distinct Fermi Surface Topology in $A_x\text{Fe}_{2-y}\text{Se}_2$ Revealed by ARPES

DAIXIANG MOU, National Lab for Superconductivity, Institute of Physics, Chinese Academy of Sciences — The discovery of superconductivity with a transition temperature above 30 K in $A_x\text{Fe}_{2-y}\text{Se}_2$ (A =alkali metal or Thallium) triggered a new wave of research on the iron-based superconductors. The new $A_x\text{Fe}_{2-y}\text{Se}_2$ superconductor exhibits many unique characteristics which make it a new platform to uncover the pairing mechanism of the iron-based superconductors. In this talk, we will show the electronic structures of $A_x\text{Fe}_{2-y}\text{Se}_2$ by means of ARPES, including Fermi Surface topology, superconducting gap structure and electron dynamics. The observed Fermi surface topology with only electron-like pockets is distinct from other iron-based superconductors and challenges the pairing mechanism based on scattering between electron-like and hole-like Fermi surface sheets. Nearly isotropic superconducting gap without nodes is revealed for all Fermi surface sheets which favors s-wave pairing symmetry. Other related topics, such as Fe vacancy order and phase separation, will also be discussed from viewpoint of our ARPES results.

[1] D. Mou, S. Liu, J. He, et. al, Phys. Rev. Lett. 106, 107001 (2011).

[2] L. Zhao, D. Mou, S. Liu, et al., Phys. Rev. B 83, 140508(R) (2011).

11:51AM B22.00002 Role of Degeneracy, Hybridization, and Nesting in the Properties of Multi-Orbital Systems

ANDREW NICHOLSON, QINGLONG LUO, WEIHAO GE, University of Tennessee and Oak Ridge National Laboratory, JOSE RIERA, Universidad Nacional de Rosario, MARIA DAGHOFER, IFW Dresden, GEORGE MARTINS, Oakland University, ADRIANA MOREO, ELBIO DAGOTTO, University of Tennessee and Oak Ridge National Laboratory — To understand the role that degeneracy, hybridization, and nesting play in the magnetic and pairing properties of multiorbital Hubbard models we here study numerically two types of two-orbital models, both with hole-like and electron-like Fermi surfaces (FS's) that are related by nesting vectors $(\pi, 0)$ and $(0, \pi)$ [1]. In one case the bands that determine the FS's arise from strongly hybridized degenerate dxz and dyz orbitals, while in the other the two bands are determined by non-degenerate and non-hybridized s-like orbitals. In the weak coupling regime it is shown that only the model with hybridized bands develops metallic magnetic order, while the other model exhibits an ordered excitonic orbital-transverse spin state that is insulating and does not have a local magnetization. Thus this state would be observed by ARPES experiments, but not by neutron scattering. However, both models display similar insulating magnetic stripe ordering in the strong coupling limit when Coulomb interactions create strong hybridization of the orbitals.

[1] A. Nicholson, et al., Phys. Rev. B 84, 094519 (2011).

12:03PM B22.00003 Thermoelectric power of $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$, $0 \leq x \leq 0.025$: tracking changes in Fermi surface topology¹

H. HODOVANETS, E.D. MUN, A.N. THALER, S.L. BUD'KO, P.C. CANFIELD, Ames Laboratory/ Iowa State University, Ames, IA 50011, USA — Temperature-dependent, in-plane, thermoelectric power (TEP) data will be presented for single crystals of $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$, ($0 \leq x \leq 0.025$). Previously reported TEP data for this system showed a big jump in the TEP data from $x=0.02$ to $x=0.024$ suggesting a Lifshitz transition, a result which was later confirmed by ARPES measurement. Given that TEP and ARPES delineated a rather large region for the Lifshitz transition to occur, and the underdoped side of the phase diagram is poorly explored, newly careful measurements of TEP on tightly spaced concentrations of Co, $0 \leq x \leq 0.025$, were carried out. The data show clear evidence of a Lifshitz transition, but instead of a discontinuous jump in TEP between $0 \leq x \leq 0.025$, there is a more gradual evolution in the $S(T)$ plots as x is increased.

¹Work at the Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

12:15PM B22.00004 Angle-resolved photoemission spectroscopy study of $\text{Ba}(\text{Fe}_{1-x}\text{Ru}_x)_2\text{As}_2$

TIAN QIAN, NAN XU, PIERRE RICHARD, Institute of Physics, Chinese Academy of Sciences, GUANGHAN CAO, ZU'AN XU, Zhejiang University, HONG DING, Institute of Physics, Chinese Academy of Sciences — Ru-doped BaFe_2As_2 compounds were discovered to show superconductivity in a relatively wide doping range. We have performed angle-resolved photoemission spectroscopy measurements on a series of Ru-doped BaFe_2As_2 samples. We observed that band dispersions become more three-dimensional and Fermi velocities increase significantly with Ru doping. We will report these results and discuss implications to its superconductivity.

12:27PM B22.00005 What role does the Fermi surface play in tuning the properties of iron arsenic superconductors?¹

R.S. DHAKA, CHANG LIU, R.M. FERNANDES, RUI JIANG, T. KONDO, A. THALER, J. SCHMALIAN, S.L. BUD'KO, P.C. CANFIELD, ADAM KAMINSKI, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — External control parameters such as pressure or chemical substitution are the key to extend the phase space and achieve high temperature (T_c) superconductivity in the FeAs family. These materials show interesting properties where it is important to understand the role of Fermi surfaces (FS's) in the mechanism of yielding higher T_c . Here, we use angle-resolved photoemission to study the electronic structure of the $\text{Ba}(\text{Fe}_{1-x}\text{Ru}_x)_2\text{As}_2$ as a function of Ru concentration (x). We find that the substitution of Ru for Fe is isoelectronic, i. e., it does not change the value of the chemical potential. More interestingly, there are no measured significant changes in the shape of the FS or in the Fermi velocity over a wide range [1]. We contrast this unusual behavior with the Co substitution, where even small substitutions induce large changes not only in the size of the FS pockets but also in the FS topology [2]. Given that the suppression of the antiferromagnetic and structural phase has been associated with the emergence of the superconducting state, Ru substitution must achieve this via a mechanism that does not involve changes of the Fermi surface. We speculate that this mechanism relies on magnetic dilution that leads to the reduction of the effective Stoner enhancement.

[1] R. S. Dhaka, et al., PRL, (2011).

[2] Chang Liu, et al., Nature Physics, 6, 419 (2010).

¹The work was supported by US DOE (DE-AC02-07CH11358).

12:39PM B22.00006 Fermi surface in BaFe_2As_2 via SdH measurements on detwinned crystals¹

TAICHI TERASHIMA, NOBUYUKI KURITA, MEGUMI TOMITA, SHINYA UJI, Natl. Inst. Mat. Sci., KUNIHITO KIHOU, CHUL-HO LEE, YASUhide TOMIOKA, TOSHIMITSU ITO, AKIRA IYO, HIROSHI EISAKI, AIST, TIAN LIANG, MASAMICHI NAKAJIMA, SHIGEYUKI ISHIDA, SHIN-ICHI UCHIDA, Univ. Tokyo, HISATOMO HARIMA, Kobe Univ. — We have completely determined the Fermi surface in the antiferromagnetic orthorhombic phase of BaFe_2As_2 by measuring Shubnikov-de Haas oscillations in detwinned single crystals (T. Terashima et al., PRL 107, 176402 (2011)). The determined Fermi surface consists of one hole and two electron pockets, and the carrier compensation is satisfied, the carrier number being 0.024 holes and electrons per primitive unit cell. The Fermi surface can well be accounted for by an LSDA band-structure calculation using the experimental crystal structure. The mass enhancements m^*/m_{band} are found to be 2–3. The Sommerfeld coefficient estimated from the determined Fermi surface and effective masses agrees well with an experimental value. Previous ARPES reports are not very consistent with our determined Fermi surface.

¹This work was supported by JST, TRIP.

12:51PM B22.00007 Fermi surface topology and low-lying electronic structure of a new iron-based superconductor $\text{Ca}_{10}(\text{Pt}_3\text{As}_8)(\text{Fe}_2\text{As}_2)_5$, CHANG LIU, MADHAB NEUPANE, SU-YANG XU, Joseph Henry Laboratory and Dept. of Physics, Princeton University, Y.J. WANG, Department of Physics, Northeastern University, NI NI, J.M. ALLRED, Department of Chemistry, Princeton University, L.A. WRAY, Joseph Henry Laboratory and Dept. of Physics, Princeton University; Advanced Light Source, Lawrence Berkeley National Laboratory, HSIN LIN, R.S. MARKIEWICZ, ARUN BANSIL, Department of Physics, Northeastern University, ROBERT J. CAVA, Department of Chemistry, Princeton University, M. ZAHID HASAN, Joseph Henry Laboratory and Dept. of Physics, Princeton University — We report a first study of low energy electronic structure and Fermi surface topology for the recently discovered iron-based superconductor $\text{Ca}_{10}(\text{Pt}_3\text{As}_8)(\text{Fe}_2\text{As}_2)_5$ (the 10-3-8 phase, with $T_c \sim 8$ K), via angle resolved photoemission spectroscopy (ARPES). Despite its triclinic crystal structure, ARPES results reveal a fourfold symmetric band structure with the absence of Dirac-cone-like Fermi dots (related to magnetism) found around the Brillouin zone corners in other iron-based superconductors. Considering that the triclinic lattice and structural supercell arise from the Pt_3As_8 intermediary layers, these results indicate that those layers couple only weakly to the FeAs layers in this new superconductor at least near the surface, which has implications for the determination of its potentially novel pairing mechanism.

1:03PM B22.00008 Recent advance in ARPES data analysis of dispersive features in Fe-based superconductors, PENG ZHANG, PIERRE RICHARD, TIAN QIAN, XI DAI, HONG DING, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, YIMING XU, Materials Sciences Division, Lawrence Berkeley National Laboratory — Angle-resolved photoemission spectroscopy (ARPES) is a powerful tool to image the electronic band dispersion of materials, especially in multi-band systems such as the Fe-based superconductors. Here we present a new method to visualize ARPES data based on the mathematical concept of curvature, which improves the advantages and the reliability of the second derivative method in tracking the positions of extrema from the experimental data. We apply it to the Fe-based superconductors. We reveal clear kink features and FS contours, making it easier to capture the essential physics from the data.

[1] P. Zhang, P. Richard, T. Qian, Y.-M. Xu, X. Dai and H. Ding, *A precise method for visualizing dispersive features in image plots*, Rev. Sci. Instrum. **82**, 043712 (2011).

1:15PM B22.00009 Fermi Surfaces of Iron-Pnictide High- T_c Superconductors from the Limit of Local Magnetic Moments¹, MIGUEL ARAUJO, Universidade de Evora, Portugal, PEDRO SACRAMENTO, Instituto Superior Tecnico, Lisbon, JOSE RODRIGUEZ, California State University at Los Angeles — We study a 2-orbital t-J model for an isolated square lattice of iron atoms, which stack up to form an iron-pnictide high- T_c superconductor. The two orbitals in question are the degenerate $d_{\pm} = 3d_{(x \pm iy)z}$ ones, which maximize the Hund's Rule coupling. First-neighbor and second-neighbor hopping (t) and Heisenberg exchange (J) are included. A Schwinger-boson-slave-fermion mean-field analysis yields a hidden half metal state in which holes hop through a $\backslash_{d+} \backslash_{d-}$ spin background without much hopping across orbitals. This state is characterized by an inner and an outer Fermi surface pocket centered at the Γ point. The Fermi surface pockets resemble those predicted by band structure calculations that include all five 3d orbitals. By sweeping the Hund's coupling, we also identify a quantum-critical point (QCP) where zero-energy spin-wave excitations exist at the momenta associated with commensurate spin-density-wave (cSDW) order. These low-energy spin-waves result in nested Fermi-surface pockets centered at cSDW momenta. Exact diagonalization of one hole in the 2-orbital t-J model over a 4×4 square lattice yields low-energy spectra that are consistent with the nested Fermi surfaces that are predicted to exist at the QCP.

¹Research supported in part by the AFOSR under grant FA9550-09-1-0660 and by the FCT under grant PTDC/FIS/101126/2008.

1:27PM B22.00010 dHvA measurements of the Fermi surface of LiFeP and its relation to the nodal gap structure, A. CARRINGTON, C. PUTZKE, I. GUILLAMON, University of Bristol, A.I. COLDEA, M.D. WATSON, University of Oxford, D. VIGNOLLES, D. LEOEUF, LNCMI-Toulouse, A. MCCOLLAM, HMFL-Nijmegen, I.I. MAZIN, NRL-Washington, S. KASAHARA, T. TERASHIMA, T. SHIBAUCHI, Y. MATSUDA, Kyoto University — The iron-pnictides are highly unusual in that there appears to be considerable variation in the structure of the superconducting gap across the different materials. The 111 compounds, LiFeX ($X=\text{As}, \text{P}$) superconduct at ambient pressure in their undoped stoichiometric form. LiFeP ($T_c=5\text{K}$) was found to have superconducting gap nodes whereas LiFeAs ($T_c=17\text{K}$) does not. Linking these differences in gap structure to Fermi surface features could provide a key test of microscopic theories which seek to explain superconductivity in iron pnictides. Here we report de Haas-van Alphen effect data which determine, almost completely, the *bulk* Fermi surface of LiFeP . The topology of the Fermi surface, which consists of quasi nested electron and hole sheets, is in good agreement with DFT band structure calculations when allowance for small band energy shifts is made. We find that one hole sheet has an anomalously small mass enhancement (compared to the others) which suggest it interacts weakly. This is probably because of its mixed orbital character rather than for any geometrical reason. We suggest that this could be the driver for node formation in this material.

1:39PM B22.00011 Evidence of Strong Coupling in Antiferromagnetic Ordered Iron Chalcogenide $\text{Fe}_{1.02}\text{Te}$ Observed by Photoemission, ZHONGKAI LIU, Stanford University, RUIHUA HE, Lawrence Berkeley National Laboratory, DONGHUI LU, SLAC National Accelerator Laboratory, MING YI, Stanford University, YULIN CHEN, MAKOTO HASHIMOTO, ROB MOORE, SLAC National Accelerator Laboratory, SUNGKWAN MO, Lawrence Berkeley National Laboratory, JIN HU, TIJIANG LIU, ZHIQIANG MAO, Tulane University, THOMAS DEVEREAUX, SLAC National Accelerator Laboratory, ZAHID HUSSAIN, Lawrence Berkeley National Laboratory, ZHI-XUN SHEN, Stanford University, STANFORD UNIVERSITY TEAM, SLAC NATIONAL ACCELERATOR LABORATORY TEAM, TULANE UNIVERSITY COLLABORATION, LAWRENCE BERKELEY NATIONAL LABORATORY COLLABORATION — The role of many-body effects is one of the central questions for unconventional superconductivity. For the recently discovered iron-based superconductors, the strength of electronic correlations is still an unsettled issue. For one of them, iron chalcogenides, a strong correlation scenario has both been proposed by theory and suggested by experiments. However, the metallic behavior in the antiferromagnetic ordered state in $\text{Fe}_{1.02}\text{Te}$ seems to deviate from such scenario. Our discovery of evidence of strong coupling in electronic bandstructure probed by angle resolved photoemission (ARPES) reconciles this contrast. Our finding also highlights the non-trivial enrichment of many-body effects when multiple ingredients of interactions reinforce each other.

1:51PM B22.00012 Three-dimensionality and orbital characters of Fermi surface in $\text{Tl}_{0.5}\text{Rb}_{0.3}\text{Fe}_{1.63}\text{Se}_2$ ¹, SHANCAI WANG, Renmin University of China, PIERRE RICHARD, NAN XU, GANG XU, Institute of Physics, Chinese Academy of Sciences Beijing 100190, China, YU LI, GENFU CHEN, Renmin University of China, TIAN QIAN, HONG DING, Institute of Physics, Chinese Academy of Sciences Beijing 100190, China — We report a comprehensive study of the tridimensional electronic bands in the recently discovered Iron-selenide superconductor $\text{Tl}_{0.5}\text{Rb}_{0.3}\text{Fe}_{1.63}\text{Se}_2$ ($T_c \sim 32$ K) with angle-resolved photoemission spectroscopy (ARPES). We determined the orbital characters and the k_z dependence of the low-energy electronic structure by tuning the polarization and the photon energy of the incident photons. We observed a small 3D electron pocket near the Brillouin Zone (BZ) center and a 2D like electron pocket near the zone boundary. The photon energy dependence, the polarization analysis and the LDA calculations suggest a significant contribution from the Se $4p_z$, Fe $3d_{xy}$ and the Fe $3d_{z^2}$ orbitals. Comparing with iron-pnictide superconductors, the emergence of Se $4p_z$ states may be the cause of the different magnetic properties between iron-chalcogenides and iron-pnictides.

¹Chinese National Science Foundation and Ministry of Science and Technology of China

2:03PM B22.00013 ARPES measurements of superconducting gaps in iron-chalcogenide superconductors, PIERRE RICHARD, H. MIAO, T. QIAN, Y.-B. SHI, N. XU, X.-P. WANG, P. ZHANG, H. DING, X. DAI, Institute of Physics, Chinese Academy of Sciences, J.-P. HU, Purdue University, Y.-M. XU, Lawrence Berkeley National Laboratory, Y. TANAKA, K. NAKAYAMA, K. UMEZAWA, T. SATO, T. TAKAHASHI, Tohoku University, H.-B. YANG, Z.-J. XU, J.-S. WEN, G.-D. GU, Brookhaven National Laboratory — The size and momentum dependence of the superconducting gap are crucial to the determination of the mechanism leading to Cooper pairing. Previous ARPES results on iron-pnictides superconductors reveal nearly-isotropic superconducting gaps with size varying from one Fermi surface to another. Here we show that this scheme is also valid in the iron-chalcogenide superconductors. We demonstrate that the superconducting gaps can be fitted by a single function derived from local pairing scenarios. Our finding of an apparent universality in iron-based superconductivity is a serious challenge to weak coupling approaches and rather favors pairing from local antiferromagnetic exchange interactions.

Monday, February 27, 2012 11:15AM - 2:15PM –
Session B23 DCMP: Superconductivity Theory I: Cluster DMFT, t-J model, renormalization group 255

11:15AM B23.00001 Pair Structure and the Pairing Interaction in a Bilayer Hubbard model, THOMAS MAIER, Oak Ridge National Laboratory, DOUGLAS SCALAPINO, University of California, Santa Barbara — The bilayer Hubbard model with an intra-layer hopping t and an inter-layer hopping $t_{\perp}$ provides an interesting testing ground for several aspects of what has been called unconventional superconductivity. One can study the type of pair structures which arise when there are multiple Fermi surfaces. One can also examine the pairing for a system in which the structure of the spin-fluctuation spectral weight can be changed. Using a dynamic cluster quantum Monte Carlo approximation, we find that near half-filling, if the splitting between the bonding and anti-bonding bands $t_{\perp}/t$ is small, the gap has B_{1g} ($d_{x^2-y^2}$ -wave) symmetry but when the splitting becomes larger, A_{1g} ($s^{\pm}$ -wave) pairing is favored. We also find that in the $s^{\pm}$ pairing region, the pairing is driven by inter-layer spin fluctuations and that T_c is enhanced.

11:27AM B23.00002 Influence of the cluster-shape on the d-wave-transition temperature T_c in the dynamical cluster approximation: A case study for the 2D repulsive Hubbard model, PETER STAAR, ETH Zurich, THOMAS MAIER, Oak Ridge National Laboratory (ORNL), THOMAS SCHULTHESS, ETH Zurich, ITP ETH ZURICH - ORNL TEAM — The dynamical cluster approximation (DCA) is a systematic extension beyond the single site approximation of dynamical mean field theory to include non-local correlations. The method maps the infinite lattice self-consistently on a cluster with N_c sites, which is embedded into a mean field. Since the correlations within the cluster are treated exactly, it is ideal to investigate phase-transitions such as d-wave superconductivity. Since a Quantum Monte Carlo integration is used to obtain the DCA self-consistency, the sign-problem prevents us to solve large cluster problems ($N_c > 32$). Meanwhile, the transition temperatures T_c from smaller clusters fluctuate due to a large dependency on the cluster-shape. Here, we investigate whether this cluster-dependency originates from the quantum impurity problem, or from the mesh on which we solve the Bethe-Salpeter (BS) equation. By exploiting the localized nature of the self-energy Σ and the vertex function Γ in real space, we can reconstruct these functions on arbitrary fine meshes in momentum-space and investigate its impact on the solutions of the BS equation. We will show that the 8-site cluster has a finite T_c for small doping-levels and that the 16-site clusters have converged transition temperatures.

11:39AM B23.00003 Superconductivity and the Pseudogap in the 2d Hubbard model¹, EMANUEL GULL, Columbia University, OLIVIER PARCOLLET, Institut de Physique Théorique (IPhT), CEA, ANDREW J. MILLIS, Columbia University — Using a numerically exact continuous-time quantum Monte Carlo impurity solver and the DCA cluster dynamical mean field method with cluster sizes up to 16, we have been able to access the superconducting phase of the two dimensional Hubbard model for parameters believed to be relevant to high temperature copper oxide superconductivity. We present results for the phase diagram, the gap to transition temperature ratio, and the interplay of the pseudogap and the superconducting gap. The gap results are obtained by direct inference from imaginary frequency data and analytically continued spectral functions.

¹This work is supported by NSF-DMR-1006282. Calculations were supported by CEA Saclay and CNRS2011-211

11:51AM B23.00004 Strongly correlated superconductivity and Mott transition¹, A.-M.S. TREMBLAY, Université de Sherbrooke, SORDI GIOVANNI, ILL, Grenoble, France, PATRICK SEMON, Université de Sherbrooke, K. HAULE, Rutgers University — Whether the pseudogap temperature T^* intercepts or merges with the superconducting dome is one of the key questions in the field of high-temperature superconductors. We study the normal and the d-wave superconducting phases at finite temperature in the two-dimensional Hubbard model within cellular dynamical mean-field theory and continuous-time quantum Monte Carlo. Above the critical value for the Mott transition, the superconducting T_c has a dome-like shape as a function of doping. The pseudogap temperature T^* intercepts the superconducting dome. Removing superconductivity, one finds that in the normal state, T^* ends at a finite-doping first-order transition that occurs at temperatures below the superconducting dome. That first order transition between a pseudogap metal and a strongly correlated metal is linked to the Mott transition at half-filling. Refs: G. Sordi et al., PRL 104, 226402 (2010); G. Sordi et al., PRB 84, 075161 (2011); G. Sordi et al., arXiv:1110.1392 (2011).

¹Support: NSERC, CRC, CIFAR, CFI, MDEIE (Quebec), MIT-Harvard CUA

12:03PM B23.00005 Multi-band Hubbard Model Simulation for Unconventional Superconducting System¹, SHI-QUAN SU, MICHAEL S. SUMMERS, THOMAS A. MAIER, Oak Ridge National Lab — To simulate the new experiment findings on unconventional superconductor materials such as Cuprates and iron pnictides, it is inevitable to go beyond single-band model and capture the physics from multi-band effects. We carried out a novel Dynamical Cluster Quantum Monte Carlo study on multi-band Hubbard model, implementing the Continuous Time Quantum Monte Carlo algorithm as quantum solver. We studied various of single-particle properties aiming to observe the experiment concerned issues such as the spontaneous symmetry breaking to nematic order.

¹Shi-Quan Su works under contract number DE-AC05-00OR22750 between the U.S. Department of Energy and Oak Ridge Associated Universities. A portion of this research was conducted at the Center for Nanophase Materials Sciences.

12:15PM B23.00006 Scaling of the transition temperature of hole-doped cuprate superconductors with the charge-transfer energy, CHUCK-HOU YEE, Rutgers University, CEDRIC WEBER, University of Cambridge, KRISTJAN HAULE, GABRIEL KOTLIAR, Rutgers University — We use first-principles calculations to extract two essential microscopic parameters, the charge-transfer energy and the inter-cell oxygen-oxygen hopping, which correlate with the maximum superconducting transition temperature T_{cmax} across the cuprates. We explore the superconducting state in the three-band model of the copper-oxygen planes using cluster Dynamical Mean-Field Theory with an exact diagonalization impurity solver. We find that variations in the charge-transfer energy largely accounts for the trend in T_{cmax} across the cuprate families.

12:27PM B23.00007 A contractor-renormalization study of Hubbard plaquette clusters, DROR ORGAD, SHIRIT BARUCH, Hebrew University of Jerusalem — We implement the contractor-renormalization method to study the checkerboard Hubbard model on various finite-size clusters as function of the inter-plaquette hopping t' and the on-site repulsion U at low hole doping. We find that the pair-binding energy and the spin gap exhibit a pronounced maximum at intermediate values of t' and U , thus indicating that moderate inhomogeneity of the type considered here substantially enhances the formation of hole pairs. The rise of the pair-binding energy for $t' < t'_{\max}$ is kinetic-energy driven and reflects the strong resonating valence bond correlations in the ground state that facilitate the motion of bound pairs as compared to single holes. Conversely, as t' is increased beyond $t'_{\max}$ antiferromagnetic magnons proliferate and reduce the potential energy of unpaired holes and with it the pairing strength. For the periodic clusters that we study the estimated phase ordering temperature at $t' = t'_{\max}$ is a factor of 2–6 smaller than the pairing temperature.

12:39PM B23.00008 Effects of disorder in the Checkerboard Hubbard model, PETER SMITH, MALCOLM P. KENNETT, Simon Fraser University — The checkerboard Hubbard model (CHM) is an unusual example of a model for strongly correlated electrons that has a region in parameter space where a controlled perturbative solution is possible. The square lattice in two dimensions is divided into four-site plaquettes for which the intra-plaquette hopping (t) is stronger than the inter-plaquette hopping (t'). We study the ground state properties of the CHM in the presence of disorder using exact diagonalization on clusters of up to twelve sites as a function of t'/t , disorder strength and interaction strength. We consider both site and bond disorder and calculate the pair binding energy and the spin gap. We comment on the implications of our results for superconductivity in this model.

12:51PM B23.00009 Superconducting pair-pair correlations in the half-filled Hubbard model on the anisotropic triangular lattice: absence of long-range order¹, S. DAYAL, R. T. CLAY, Mississippi State University, MS, S. MAZUMDAR, University of Arizona, AZ — We report calculations of superconducting pair-pair correlations for the half-filled band Hubbard model on an anisotropic triangular lattice using the path-integral renormalization group (PIRG) method. Mean-field studies have suggested that $d_{x^2-y^2}$ superconductivity occurs near the boundary between metallic and antiferromagnetic phases in this model. We calculate bond orders, spin structure factors, and superconducting pair-pair correlations at zero temperature. Our results are consistent with previous studies of the metal-insulator transition and antiferromagnetism in this model. However, we do not find any parameter region where pair-pair correlations are enhanced by the Hubbard U , except for trivial enhancement of on-site correlations. The superconducting pair-pair correlations at larger distances decrease monotonically with increasing U , with a distance dependence approaching that of noninteracting fermions, indicating the absence of frustration-driven superconductivity within the model.

¹This work was supported by DOE grant DE-FG02-06ER46315.

1:03PM B23.00010 Two temperature scales in the d-wave pair correlation length of the 2D t-J model, WILLIAM PUTIKKA, Physics Department, Ohio State University — Two temperature scales are observed in the d-wave pair correlation length for doping $\delta \sim 0.25$. Both the s-wave and d-wave pair correlation lengths increase with decreasing temperature starting at very high temperatures. By $T \sim 3J$ both symmetries have grown to $\sim 1/3$ of a lattice spacing. For $T > 3J$ the s-wave correlation length is a few percent larger than d-wave. At $T \sim 3J$ both symmetries are saturating, with the growth in the correlation length flattening for both symmetries. The s-wave correlation length does not grow at lower temperatures. The d-wave correlation length does resume growing at $T \sim 0.8J$, with the growth at low temperatures much stronger than it was at high temperatures. The d-wave correlation length reaches a size of one lattice spacing at $T \sim 0.25J$ with no sign of saturating. Interestingly, both of these temperature scales also occur in the t-J model momentum distribution $n_{\mathbf{k}}$. The features that are found in the temperature dependence of the 2D $n_{\mathbf{k}}$ on the zone diagonal are very similar to the temperature dependence of the 1D t-J model $n_{\mathbf{k}}$. These observations can be understood by having spin-charge separated degrees of freedom.

1:15PM B23.00011 Two routes to disorder-induced magnetism and nematicity in the cuprates, BRIAN M. ANDERSEN, Niels Bohr Institute, University of Copenhagen, PETER J. HIRSCHFELD, University of Florida, RASMUS B. CHRISTENSEN, Niels Bohr Institute, University of Copenhagen, SIEGFRIED GRASER, Augsburg University — We study disorder-induced magnetism within the Gutzwiller approximation applied to the t-J model relevant for cuprate superconductors. We identify two distinct disorder-induced magnetic phases depending on the strength of the scatterers. For weak potential scatterers, charge reorganization may push local regions in-between the impurities across the magnetic phase boundary, whereas for strong scatterers a local static magnetic moment is formed around each impurity. We calculate the density of states and find a universal low-energy behavior independent of both disorder and magnetization. However, the magnetic regions are characterized by larger (reduced) superconducting gap (coherence peaks) [1]. Recent studies have highlighted the role of a electronic nematic liquid underdoped cuprates. We calculate the spin susceptibility with a small explicitly broken rotational symmetry to show how the induced spin response asymmetry is enhanced by correlations. In the disorder-induced stripe phase, impurities become spin nematogens with a C2 symmetric impurity resonance state, and the disorder-averaged spin susceptibility remains only C2 symmetric at low energies, similar to recent data from neutron scattering on underdoped YBCO [2].

[1] R. B. Christensen et al., accepted Phys. Rev. B (2011).

[2] B. M. Andersen et al., submitted to EPL (2011).

1:27PM B23.00012 Band structure effects on superconductivity in the weak-coupling Hubbard model, WEEJEE CHO, SRINIVAS RAGHU, STEVEN KIVELSON, Stanford University — The repulsive Hubbard model is the paradigmatic model for the study of unconventional superconductivity. In order to explore the influence of various features of the band structure on the magnitude and character of the pairing, we use a well-controlled perturbative renormalization group (RG) method to study the weak coupling limit of the model on the square lattice with various modifications: The first is the checkerboard model described by the strong hopping t and the weak hopping t' . The second is the bilayer model described by the intra-layer hopping t and the inter-layer hopping $t_{\perp}$. We obtain the pairing symmetry and strength as functions of the relevant band parameters. Large changes in the effective pairing strength are found and their origins explained.

1:39PM B23.00013 Effects of longer-range interactions on unconventional superconductivity¹, SRINIVAS RAGHU, Stanford University, EREZ BERG, Harvard University, ANDREY CHUBUKOV, University of Wisconsin, Madison, STEVEN KIVELSON, Stanford University — We analyze the effect of the non-vanishing range of electron-electron repulsion on the mechanism of unconventional superconductivity. We present asymptotically exact weak-coupling results for dilute electrons in the continuum and for the 2D extended Hubbard model, as well as density-matrix renormalization group results for the two-leg extended Hubbard model at intermediate couplings, and approximate results for the case of realistically screened Coulomb interactions. We show that T_c is generally suppressed in some pairing channels as longer range interactions increase in strength, but superconductivity is not destroyed. Our results confirm that electron-electron interaction can lead to unconventional superconductivity under physically realistic circumstances.

¹NSF-DMR-0906953 (AVC), DMR-0758356 (SAK), DMR-0757145, DMR-0705472 (EB)

1:51PM B23.00014 Three-particle interactions in effective one-band models for unconventional superconductivity, STEFAN MAIER, CARSTEN HONERKAMP, RWTH Aachen — We discuss different approximations for effective low-energy interactions in multiband models for weakly interacting correlated electrons. In the study of Fermi surface instabilities of the conduction band(s), the standard approximation consists in keeping just those terms in the bare interactions that couple only to the conduction band(s), while corrections due to virtual excitations into bands away from the Fermi surface are typically neglected. In order to include important aspects of these virtual interband excitations, we present an improved truncation of the functional renormalization group (fRG) that keeps track of the three-particle vertex in the conduction band. Within a simplified two-patch treatment of a two-band model, we demonstrate that these corrections can have a rather strong effect in parts of the phase diagram by changing the critical scale for *d*-wave pairing close to a phase boundary. The improved truncation scheme is applied as well to the Emery model within a multi-patch channel-decomposed fRG.

2:03PM B23.00015 Effective interactions in multi-band systems from constrained summations, CARSTEN HONERKAMP, RWTH Aachen University, Germany — The application of many-body techniques for the study of correlation effects and unconventional superconductivity requires the formulation of an effective low-energy model that contains only the relevant bands near the Fermi level. However the bands away from the Fermi level are known to renormalize the low-energy interactions substantially. Here we compare different schemes to derive low-energy effective theories for interacting electrons in solids. The frequently used constrained random phase approximation (cRPA) is identified as a particular resummation of higher-order interaction terms that includes important parts of the leading virtual corrections. We then propose an adapted renormalization group scheme that includes the cRPA, but also allows one to go beyond the cRPA approximation. We study a simple two-band model in order to demonstrate the differences between the different approximations.

Monday, February 27, 2012 11:15AM - 2:15PM — Session B24 FIAP: Electronic Structure: Theory and Spectra 256

11:15AM B24.00001 Valence band effective Hamiltonians in nitride semiconductors, ATCHARA PUNYA, NUCHARÉE SCHWERTFAGER, WALTER LAMBRECHT, Department of Physics, Case Western Reserve University, 10900 Euclid Avenue, Cleveland, OH 44106 — Valence band effective Hamiltonians are useful to determine the electronic states of shallow impurities, quantum wells, quantum wires and quantum dots within the effective mass approximation. Although significant experimental and theoretical work has been performed, basic parameters such as the Rashba Sheka Pikus (RSP) Hamiltonian parameters are still uncertain. In this work, the electronic band structures of AlN, GaN and InN, all in the wurtzite crystal structure, as well as the RSP Hamiltonian parameters are determined by using the QSGW approximation in a FP-LMTO implementation. The corrections offered by this approach beyond the LDA are important to obtain the splittings and effective masses accurately. The present GW implementation, which allows for a real space representation of the self-energy, enables us to interpolate exactly to a fine *k*-mesh and hence to obtain accurate effective masses. We find the crystal field splitting in GaN (12 meV) in much closer agreement with experiment than previous work and obtain a negative SO coupling for InN. Moreover, we have generalized the method of invariants to crystals with orthorhombic symmetry, such as ZnSiN₂, ZnGeN₂, ZnSnN₂ and CdGeN₂ and determined the corresponding Hamiltonian parameters.

11:27AM B24.00002 ABSTRACT WITHDRAWN —

11:39AM B24.00003 Hybrid Density Functional Study of (Hg,Cd)Te Systems, JEREMY W. NICKLAS, JOHN W. WILKINS, The Ohio State University — The HgCdTe alloy is used in high-performance infrared detection applications with a band gap range extending across the infrared spectrum. HgTe in particular has sparked interest for its topological insulating behavior in quantum well devices due to its band inverted nature. We test the quality of the newer hybrid screened functional, HSE, on the two contrasting materials: HgTe (semimetal) and CdTe (semiconductor) to see how well it performs under a range of computational setups [1]. A direct comparison of HSE with the standard DFT functional PBE to experiment for the HgCdTe alloy reveals HSE is able to reproduce the experimental crossover composition of 17% Cd concentration when the alloy goes from a semimetal to semiconductor, whereas PBE overestimates this composition at 67% Cd concentration. HSE also predicts a higher valence band offset of 0.53 eV in the HgTe/CdTe heterostructure than previous first-principle and early experimental results, but in good agreement with the more recent experimental results. Supported by DOE-Basic Energy Science DOE-BES-DMS (DEFG02-99ER45795). Computing resources are provided by NERSC and OSC.

[1] Jeremy W. Nicklas and John W. Wilkins, Phys. Rev. B 84, 121308(R) (2011)

11:51AM B24.00004 Ab-initio description of satellites in graphite, MATTEO GUZZO, LORENZO SPONZA, CHRISTINE GIORGETTI, FRANCESCO SOTTILE, Ecole Polytechnique, FR, DEBORA PIERUCCI, MATHIEU G. SILLY, FAUSTO SIROTTI, Synchrotron SOLEIL, FR, JOSHUA J. KAS, JOHN J. REHR, U. Washington, LUCIA REINING, Ecole Polytechnique, FR — The GW method from Many-Body Perturbation Theory has been very successful in describing photoemission spectra in a variety of systems. In particular, GW is known to give good quasiparticle properties like band-gaps, but it has shown some limitations in the description of complex correlation effects like satellites. Satellite peaks in photoemission come from higher-order excitations and are still poorly studied in the valence bands. In perturbative GW the spectral function can describe additional features beside the quasiparticle peaks, but these satellites are known to be too weak and too low in energy, as it appears from calculations on the Homogeneous Electron Gas and some real materials. We have recently shown that including additional diagrams in the Green's function (similarly to what has been done with the cumulant expansion) we obtain an excellent description of satellites series in the test case of bulk silicon, where GW is unable to cope. We now focus on a more complex system, i.e. graphite, with this same approach. Using our newly measured XPS valence data, we investigate the effects of anisotropies on satellites and give a prediction on the spectral changes following the transition towards a single graphene layer.

12:03PM B24.00005 Isotope dependence of band gap in semiconductors, TAKASHI KORETSUNE, SUSUMU SAITO, Tokyo Institute of Technology — Recently, carrier confinement was observed in diamond superlattice consisting of pure ¹²C and ¹³C layers. This interesting phenomenon comes from large isotope dependence of fundamental gap width in diamond. To understand this carrier confinement and design related nanodevices, we investigate the effect of electron-phonon couplings on quasiparticle energies in semiconductors composed of carbon and other light elements using first-principles methods based on the density functional theory. The calculated isotope dependence as well as temperature dependence of band gap in diamond is found to agree well with the experiment. We also discuss the isotope dependence in binary compounds such as boron nitride and silicon carbide.

12:15PM B24.00006 Clarification of the relations between stacking structures of sp^3 network materials and their band gaps, YU-ICHIRO MATSUSHITA, SHINNOSUKE FURUYA, ATSUSHI OSHIYAMA, The University of Tokyo — Silicon carbide (SiC) has been discovered in various polymorphs. Each polymorph is characterized by its stacking of atomic planes. The band gap varies substantially in each polymorph from 2.40 eV to 3.33 eV in spite that the local atomic structures are identical to each other [1]. The mechanism of this intriguing property have been poorly understood. To clarify the fundamental reasons for this band-gap variation, we have performed the electronic-structure calculations in the density functional theory. We have found that the Kohn-Sham orbital at the conduction-band bottom distributes broadly around the interstitial channel, thus floating in the matter. The way of the floating depends on the stacking of the atomic planes and determines the band gap in each polymorph. We also find that the floating state appears in other sp^3 -bonded materials, and the band-gap variation is common to the covalent materials. References [1] Properties of Silicon Carbide edited by G. L. Harris (INSPEC, London, 1995).

12:27PM B24.00007 Nonequilibrium “melting” of a charge density wave insulator via an ultrafast infrared laser pulse¹, WEN SHEN, YIZHI GE, AMY LIU, Georgetown University, H.R. KRISHNAMURTHY, India Institute of Science, TOM DEVEREAUX, Stanford University, JIM FREERICKS, Georgetown University — In equilibrium, electrons interacting with lattice vibrations have a transition either to a charge density wave phase (a static modulation of the electronic charge) or to a superconductor (electron pairs move without resistance). If the coupling is weak, the system orders in the Bardeen-Cooper-Schrieffer scenario, where the ordering occurs at some transition temperature T_c and a gap simultaneously forms in the density of states. In strong-coupling, preformed pairs bind at a high temperature (forming a gap in the density of states) and the ordering only occurs at a lower temperature. We employ an exact solution of a model for pump-probe time-resolved photoemission spectroscopy to show how, in nonequilibrium, a third scenario arises: the gap disappears in the presence of a nonzero order parameter, and then reforms well after the pulse has passed. This nonequilibrium “phase transition” scenario qualitatively describes all of the available experiments on the ultrafast melting of a charge density wave.

¹National Science Foundation, Department of Energy, National Energy Research Scientific Computing Center

12:39PM B24.00008 Engineering Electronic Band Structure for New Elpasolite Scintillators, MAO-HUA DU, Koushik Biswas, DAVID SINGH, Oak Ridge National Laboratory — The utilization of scintillator materials is one of the primary methods for radiation detection. Elpasolites are a large family of quaternary halides that have recently attracted considerable interest for their potential applications as γ -ray and neutron scintillators. A large number (on the order of 10^3) of different chemical compositions exist in the elpasolite family of compounds. This wide range of compositions offers numerous opportunities for fine-tuning the material chemistry to target specific scintillation properties, but they also pose significant challenges in identifying the most promising ones. Many elpasolite scintillator materials currently under development suffer from low light output and long scintillation decay time. The low light output is partially due to a large band gap while the long scintillation decay time is a result of the slow carrier transport to Ce impurities, where carriers recombine to emit photons. We suggest that these problems may be mitigated by optimizing the band gap and carrier mobility by selecting constituent elements of proper electronegativity. For example, cations with lower electronegativity may lower the conduction band and increase the conduction band dispersion simultaneously, resulting in higher light output and faster scintillation. We demonstrate by first-principles calculations that the strategy of manipulating electronegativity can lead to a number of new elpasolite compounds that are potentially brighter and faster scintillators.

12:51PM B24.00009 Origin of the variation of exciton binding energy in semiconductors, MARC DVORAK, ZHIGANG WU, Colorado School of Mines — Electron-hole interaction plays a crucial role in optical properties, and the exciton binding energy (E_b) in technologically important semiconductors varies from merely a few meV to around 100 meV, which is not well understood. In this work, we investigate the origin of the variation of E_b in semiconductors, employing first-principle calculations based on the density functional theory (DFT) and the many-body perturbation theory with Green's function (GW/BSE). Our results clearly show that E_b decreases as the spread of electron distribution, which measures the magnitude of electron delocalization, increases. This is due to the increased electronic screening when electrons tend to be more delocalized. Furthermore, the spread distribution of the top valence electrons is of central importance in determining excitonic screening, which leads to weakly bound electrons and holes in semiconductors. Thus, the variation of exciton binding energy in semiconductors can be understood from the computed magnitude of electron delocalization of top valence bands of these materials using DFT.

1:03PM B24.00010 Modeling Shallow Core-Level Transitions in the Reflectance Spectra of Gallium-Containing Semiconductors, NICHOLAS STOUTE, DAVID ASPNES, North Carolina State University, DE ASPNES GROUP TEAM — The electronic structure of covalent materials is typically approached by band theory. However, shallow core level transitions may be better modeled by an atomic-scale approach. We investigate shallow d-core level reflectance spectra in terms of a local atomic-multiplet theory, a novel application of a theory typically used for higher-energy transitions on more ionic type material systems. We examine specifically structure in reflectance spectra of GaP, GaAs, GaSb, GaSe, and $\text{GaAs}_{1-x}\text{P}_x$ due to transitions that originate from Ga3d core levels and occur in the 20 to 25 eV range. We model these spectra as a Ga^{+3} closed-shell ion whose transitions are influenced by perturbations on 3d hole-4p electron final states. These are specifically spin-orbit effects on the hole and electron, and a crystal-field effect on the hole, attributed to surrounding bond charges and positive ligand anions. Empirical radial-strength parameters were obtained by least-squares fitting. General trends with respect to anion electronegativity are consistent with expectations. In addition to the spin-orbit interaction, crystal-field effects play a significant role in breaking the degeneracy of the d levels, and consequently are necessary to understand shallow 3d core level spectra.

1:15PM B24.00011 Ab-initio study of dilute nitride substitutional and split-interstitial impurities in gallium antimonide (N-GaSb)¹, PRIYAMVADA JADAUN, HARI P. NAIR, SETH R. BANK, SANJAY K. BANERJEE, The University of Texas at Austin — We present an ab-initio density functional theory study of dilute-nitride GaSb. Adding dilute quantities of nitrogen causes rapid reduction in bandgap of GaSb (~ 300 meV for 2% N). Due to this rapid reduction in bandgap, dilute-nitrides provide a pathway for extending the emission of GaSb based type-I diode lasers into the mid-infrared wavelength region (3-5 micron). In this study we look at the effect of substitutional N impurity on the electronic properties of our system and compare it with the band-anticrossing model, a phenomenological model, which has been used to explain giant band bowing observed in dilute-nitride alloys. We also study the effect of Sb-N split interstitials which are known to be non-radiative recombination centers. Furthermore we also discuss the stability of the Sb-N split interstitial relative to substitutional nitrogen to determine if the split interstitials can be annihilated using post-growth annealing to improve the radiative lifetime of the material which essential for laser operation.

¹NSF Teragrid machine Ranger at Texas Advanced Computing Center.

1:27PM B24.00012 Electronic properties of InP in terms of an ab-initio LDA, YURIY MALOZOVSKY, LASHOUNDA FRANKLIN, Department of Physics, Southern University and A&M College, Baton Rouge, LA 70813, CHINEDU EKUMA, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, GUANG-LIN ZHAO, DIOLA BAGAYOKO, Department of Physics, Southern University and A&M College, Baton Rouge, LA 70813 — We present results from ab-initio local density approximation (LDA) calculations of electronic and related properties of zinc blende indium phosphide (InP). Our computations employed the Ceperley and Alder LDA potential and the linear combination of atomic orbital (LCAO) formalism. The implementation of the LCAO formalism followed the Bagayoko, Zhao, and Williams (BZW) method. Consequently, we solved self consistently both the Kohn Sham equation and the one giving the ground state charge density in terms of the wave functions of the occupied states. Self-consistency, for the latter equation, requires a search for the optimal basis set. This search entails increases of the size of the basis set and the related modifications of angular symmetry and of available radial functions. Our calculated, direct band gap of 1.398 eV (1.40 eV), at the Γ point, is in excellent agreement with experimental values. The calculated density of states (DOS) also agree with experimental finding. The calculated electron and hole effective masses differ by 10% from some corresponding experimental ones. We discuss the equilibrium lattice constant and optical properties.

1:39PM B24.00013 Self Consistent Calculations of Electronic Properties of Systems with an Energy or a Band Gap, DIOLA BAGAYOKO, LASHOUNDA FRANKLIN, Department of Physics Southern University and A&M College, Baton Rouge, LA 70813, CHINEDU EKUMA, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, YURIY MALOZOVSKY, Department of Physics Southern University and A&M College, Baton Rouge, LA 70813 — We re-examine the process of performing self consistent calculations of electronic and related properties of finite systems (with an energy gap) and of crystals with a band gap. This work applies to calculations utilizing density functional and $X\alpha$ potentials and to other approaches that entail solving a system of inherently coupled equations. In particular, the local density approximation (LDA) is defined by a system of equations that reduces to two equations upon the selection of V_{xc} . We show how the Bagayoko, Zhao, and Williams (BZW) method solves the relevant system of equations and leads to results in excellent agreement with experimental ones. We discuss such results for w-ZnO, rutile TiO₂, w-CdS, zb-CdS, zb-InP, Ge, Ca B₆, and other materials. Work funded by the National Science Foundation, through LASiGMA [NSF Award EPS-1003897 and No. NSF (2010-15)-RII-SUBR], LONI [Award No. 2-10915], and Ebonyi State, Federal Republic of Nigeria.

1:51PM B24.00014 Infrared Refractive Index of Silicon: Parity and Sum-Rule Tests¹, WILLIAM KARSTENS, Saint Michaels College, MITIO INOKUTI², Argonne National Laboratory, DAVID Y. SMITH, University of Vermont and Argonne National Laboratory — We have resolved conflicting reports for the IR refractive index of silicon using general considerations of linear response theory. We find that use of unphysical series expansions in the analysis of channel spectra has been a significant source of systematic error. Recognition that the index is an even function of photon energy is crucial for analysis of these measurements and clarifies data presentation. In the region of high IR transparency of elemental semiconductors, the index may be expanded in a rapidly convergent Taylor series. Coefficients of terms in the $(2n)^{th}$ power of energy are proportional to the $(2n+1)^{th}$ inverse moment of the electronic absorption spectrum. In the favorable case of intrinsic Si, the electronic absorption is sufficiently well known that independent values of the intercept, slope and curvature of plots of index vs. the square of photon energy may be calculated. Index data sets with parameters significantly different from these suffer from systematic errors or refer to impure samples. Using these parity and sum-rule tests we have prepared a composite index data set for intrinsic silicon that represents a best fit to reliable measurements from microwaves to the visible. Applications to germanium and diamond will be discussed.

¹Supported in part by the US Department of Energy, Office of Nuclear Physics under contract DE-AC02-06CH11357.

²Deceased

2:03PM B24.00015 Electronic Structure of NiFe₂O₄ using screened Hybrid Functionals, HUNTER SIMS, MINT Center and Dept. of Physics, University of Alabama, DIPANJAN MAZUMDAR, MINT Center, University of Alabama, SANJOY SARKER, MINT Center and Dept. of Physics, University of Alabama, ARUNAVA GUPTA, MINT Center, University of Alabama, QI SUN, JAN MUSFELDT, Department of Chemistry, University of Tennessee — As an insulating ferrimagnet with a high Curie temperature, NiFe₂O₄ (NFO) may be a promising candidate for future spin-based applications. Recent demonstration of spin-Seebeck effect in magnetic insulators indicates that important new phenomena may be discovered in such materials. Unfortunately, density functional theory cannot give a full account of its properties; most notably, LDA calculations find it to be metallic. LDA+U yields an insulator but underestimates the band gap. The recently-implemented screened hybrid functionals method (HSE06) represents only a moderate increase in computational effort compared to traditional DFT. This method allows one to modify the PBE-approximated exchange potential with a portion of the Hartree-Fock exchange. We present LDA, LDA+U, and HSE06 calculations of the density of states and band structure of NFO. We show that hybrid methods greatly improve agreement with the experimental band gap over LDA +U. We find that NFO is an indirect band gap system with the spin-down channel having the lower, indirect gap, whereas the majority channel possess a direct gap with over a 0.5eV difference with the minority gap. Comparison of our theoretical results with recent optical measurements on NFO thin films is also presented.

Monday, February 27, 2012 11:15AM - 2:15PM —
Session B25 DCOMP GSCCM DMP: Focus Session: Simulation of Matter at Extreme Conditions - Shock-Induced Chemistry 257A

11:15AM B25.00001 Extending DFT to Long Time-Scales: Using the Density Functional Tight Binding Approach for Materials Under Extreme Temperatures and Pressures¹, NIR GOLDMAN, Lawrence Livermore National Laboratory — We report here on density functional tight binding (DFTB) simulations of covalently bonded materials over a pressure range of 10 – 2,000 GPa and a temperature range of 300 – 30,000 K using both standard and new interaction potentials we have created for these conditions. Density Functional Theory (DFT) has been shown to accurately reproduce the high pressure-temperature chemistry, phase boundaries, and EOS of many materials. DFT-MD simulations, though, scale poorly with computational effort and thus are generally limited to nanometer system sizes and picosecond time-scales. In contrast, chemical kinetic effects and phase changes can span up to nanosecond timescales and significantly longer length scales. The DFTB method holds promise as a high throughput simulation capability by providing orders of magnitude increase in computational efficiency while retaining most of the accuracy of Kohn-Sham DFT. We show that DFTB interaction potentials can be created by (a) fitting the DFTB repulsive energy to measured and computed compression data, and (b) using an extended basis set that includes *d*-orbital interactions, as needed. Our new potential for carbon yields accurate material properties for diamond, graphite, the BC8 phase, and simple cubic carbon, as well as for the shock Hugoniot of diamond compressed up to the conducting liquid. We also discuss simulations of the long-time scale reactivity of H₂O₂ under detonation conditions, and shock compression of astrophysical ice mixtures and the subsequent synthesis of pre-biotic materials. Our results provide a straightforward method by which DFTB can be made to provide equation of state and long-time scale chemical kinetic data at a similar accuracy to standard quantum codes. Our approach could be extended to any number of materials related to geology and planetary science, including silicon, SiO₂, and hydrocarbon systems.

¹This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory (LLNL) under Contract DE-AC52-07NA27344.

11:51AM B25.00002 Pressure-induced Polymerization in Substituted Acetylenes, RAJA CHELLAPPA, DANA DATTELBAUM, STEPHEN SHEFFIELD, Los Alamos National Laboratory — A fundamental understanding of shock-induced chemical reactions in organics is still lacking and there are limited studies devoted to determining reaction mechanisms, evolution of bonding, and effect of functional group substitutions. The fast timescale of reactions occurring during shock compression create significant experimental challenges (diagnostics) to fully quantify the mechanisms involved. Static compression provides a complementary route to investigate the equilibrium phase space and metastable intermediates during high pressure chemistry, although at a much slower timescale. In this study, we present our results from our ongoing high pressure in situ synchrotron x-ray diffraction and vibrational spectroscopy experiments on substituted acetylenes: tert-butyl acetylene [TBA: $(\text{CH}_3)_3\text{C}\equiv\text{CH}$] and ethynyl trimethylsilane [ETMS: $(\text{CH}_3)_3\text{SiC}\equiv\text{CH}$]. We observed that the onset pressure of chemical reactions (at room temperature) in these compounds is significantly higher in static compression (TBA: 11 GPa and ETMS: 26 GPa) when compared to shock input pressures (TBA: 6.1 GPa and ETMS: 6.6 GPa). The products were polymeric in nature, recovered to ambient conditions with little degradation and fully characterized using spectroscopy, calorimetry, and other techniques to identify reaction mechanisms.

12:03PM B25.00003 Non-equilibrium Molecular Dynamics Studies of Interfacial Chemistry in Shocked Ni/Al Nanolaminates¹, JASON QUENNEVILLE, Spectral Sciences, Inc., NARESH THADHANI, Georgia Institute of Technology — The response of Ni/Al composite materials to shock loading has been studied using non-equilibrium molecular dynamics and an EAM force field. The simulation cells consist of layered Ni and Al laminates with at least 3 million particles in a 1:1 mole ratio. The main thrust of our research is to gain a better understanding of the chemistry that occurs at the Ni/Al interface when the real material is shocked. Initial geometries were chosen so as to identify the factors important to reaction in the complex macro-scale material. Specifically, we vary the orientation of the interface with respect to the shock wave and the geometry of the interface (*i.e.*, deviation from planarity) to study how mixing and reactivity of Ni and Al are affected. Our results show a clear dependence of pressure and temperature on interface orientation, in agreement with continuum-scale simulations.

¹Research funded by DTRA Grant No. HDTRA1-10-1-0038.

12:15PM B25.00004 Near-Equivalency of Inter and Intramolecular Hydrogen Bonding Under High-Pressure, M. RIAD MANAA, LAURENCE FRIED, Lawrence Livermore National Laboratory — Triamino-trinitro-benzene (TATB, $\text{C}_6\text{H}_6\text{N}_6\text{O}_6$) exhibits unusually strong intramolecular hydrogen bonding as evidenced by the high rotational energy barrier of the nitro and amino groups. In the condensed phase, the competing intermolecular hydrogen bonding becomes pronounced at high-pressure in its graphitic-like crystal structure. We report density functional theoretical calculations of the equation of state of TATB under hydrostatic compression of up to 250 GPa. Our results show increasing bond equivalency between the intramolecular and intermolecular hydrogen bonds of the amino and nitro groups in the region $30 < P < 70$ GPa, beyond which the difference between the two bond distances remains constant. This approximate bond equivalency is manifested by a rapid decrease of the intermolecular -NO—HN- distance along the b lattice direction from 2.6 Å at the zero pressure equilibrium geometry to 1.72 Å at 67 GPa, and by a decrease of the intramolecular -NO—HN- bond from 1.65 Å to 1.57 Å for the same pressure region. It is expected that vibrational motions involving the NO—HN modes are sensitive to the nearly equivalent hydrogen bonding, as recent spectroscopic IR analysis of the NH_2 stretches revealed.

12:27PM B25.00005 Modeling of electron-ion coupling in shocked materials, EVAN REED, Stanford University — This work describes and implements a quasi-statistical approach to electron-ion coupling in shocked matter. By combining this approach with the multi-scale shock technique (MSST) and a tight-binding model, the magnitude and role of electronic excitations in shocked energetic materials are studied theoretically using quantum molecular dynamics simulations. Focusing on the detonating primary explosive HN_3 (hydrazoic acid), this work finds that the material transiently exhibits a high level of electronic excitation characterized by carrier densities in excess of 10^{21} cm^{-3} , or one electronic excitation for every 8 molecules. Electronic excitations enhance the kinetics of chemical decomposition by about 30%. The electronic heat capacity has a minor impact on the temperatures exhibited, on the order of 100 K.

12:39PM B25.00006 Quantum-based Molecular Dynamics Simulations of Shock-induced Reactions with Time-resolved Raman Spectra, MARC CAWKWELL, EDWARD SANVILLE, JOSHUA COE, ANDERS NIKLASSON, Los Alamos National Laboratory — Shock-induced reactions in liquid hydrocarbons have been studied using quantum-based, self-consistent tight-binding (SC-TB) molecular dynamics simulations with an accurate and transferable model for interatomic bonding. Our SC-TB code LATTE enables explicit simulations of shock compression using the universal liquid Hugoniot. Furthermore, the effects of adiabatic shock heating are captured precisely using Niklasson's energy conserving extended Lagrangian Born-Oppenheimer Molecular Dynamics formalism. We have been able to perform relatively large-scale SC-TB simulations by either taking advantage of the sparsity of the density matrix to achieve $O(N)$ performance or by using graphics processing units to accelerate $O(N^3)$ algorithms. We have developed the capability for the on-the-fly computation of Raman spectra from the Fourier transform of the polarizability autocorrelation function via the density matrix perturbation theory of Niklasson and Challacombe. These time-resolved Raman spectra enable us compare the results of our simulations with identical diagnostics collected experimentally. We will illustrate these capabilities with a series of simulations of shock-induced reaction paths in a number of simple molecules.

12:51PM B25.00007 Molecular Simulation of Shock Hugoniot for Polymers, T. SIRK, T. CHANTAWANSRI, E. BYRD, B. RICE, J. ANDZELM, Army Research Laboratory — The behavior of polymers under extreme conditions (high pressure and temperature) is of interest for a variety of applications, such as polymer-bonded explosives, coatings, adhesives, and light-weight armor. Material properties and response at extreme conditions can be determined through shock experiments, which are often difficult to measure experimentally because of difficulties in traversing a large range of pressures (up to hundreds of gigapascals) and temperatures (thousands of kelvin) with available instrumentation. In addition, interesting behavior, such as observed behind a shock front, occurs at extremely short time- and length-scales (nanoscale), which poses problems in characterizing the material using current experimental capabilities. To further understand shocked systems, simulation methods such as molecular dynamics (MD) and quantum mechanics (QM) can be used to provide insight into atomic-level phenomena. Using classical MD and QM, we have calculated the principle shock Hugoniot curves for four polymers: poly[methyl methacrylate], poly[ethylene], poly[styrene], and hydroxyl-terminated poly[butadiene]. In the MD calculations, we considered both a non-reactive (*i.e.* PCFF) and reactive (*i.e.* ReaxFF) forcefield, respectively, where calculations were performed in LAMMPS. The QM calculations were performed with density functional theory (DFT) using dispersion corrections as implemented in CP2K. We have applied both atom centered pseudopotentials (DCACPs) and Grimme van der Waals corrections in our study. Overall, results obtained by QM show much better agreement with available experimental data for the range of up to 20 GPa than classical force fields. At pressures where reactions can occur the short simulation time available in MD modeling prevents us from fully exploring possible reaction pathways.

1:03PM B25.00008 Amorphous Polymeric Nitrogen from Dynamic Shock Simulation¹, TODD BEAUDET, WILLIAM MATTSON, BETSY RICE, U.S. Army Research Laboratory — In recent years there has been significant interest in polymeric phases of nitrogen at low pressure for potential application as an energetic material. This interest was bolstered by experimental evidence of metastable amorphous polymeric nitrogen at low pressure.^{2,3} While considerable theoretical work has been done on many crystal phases of nitrogen, simulating amorphous polymeric nitrogen has been more challenging. Starting from first principles dynamic shock simulation of cubic-gauche nitrogen⁴ we demonstrate a form of polymeric nitrogen at low pressure that may be directly related to amorphous polymeric nitrogen.

¹This research was supported in part by an appointment to the U.S. Army Research Laboratory Postdoctoral Fellowship Program administered by the Oak Ridge Associated Universities through a contract with the U.S. Army Research Laboratory.

²Goncharov, A. F. *et al.*, Phys. Rev. Lett. **85**, 1262 (2000)

³Eremets, M. I. *et al.*, Nature **411**, 170 (2001)

⁴Mattson, William D. and Balu, Radhakrishnan, Phys. Rev. B **83**, 174105 (2011)

1:15PM B25.00009 ABSTRACT WITHDRAWN —

1:27PM B25.00010 Ethane and Xenon mixing: density functional theory (DFT) simulations and experiments on Sandia's Z machine, RUDOLPH MAGYAR, SETH ROOT, THOMAS MATTSSON, KYLE COCHRANE, Sandia National Laboratories — The combination of ethane and xenon is one of the simplest binary mixtures in which bond breaking is expected to play a role under shock conditions. At cryogenic conditions, xenon is often understood to mix with alkanes such as Ethane as if it were also an alkane, but this model is expected to break down at higher temperatures and pressures. To investigate the breakdown, we have performed density functional theory (DFT) calculations on several xenon/ethane mixtures. Additionally, we have performed shock compression experiments on Xenon-Ethane using the Sandia Z - accelerator. The DFT and experimental results are compared to hydrodynamic simulations using different mixing models in the equation of state. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of the Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

1:39PM B25.00011 Dynamic Response of a Carbon Fiber – Epoxy Composite, SCOTT ALEXANDER¹, WILLIAM REINHART, Sandia National Laboratories — The dynamic response of carbon fiber reinforced epoxy composite materials was investigated under planar impact loading. The samples were unidirectional (all carbon fibers oriented in a single direction) with fiber fill volumes from 62 to 68%. Gun driven planar impact tests with impact velocities of 0.1-2.0 km/s were conducted allowing samples to be compressed up to about 15 GPa. Velocity interferometry was used to measure particle velocities from which the compressed state of the samples was determined. Wave speeds for shocks traveling along the carbon fibers are significantly higher than for those traveling transverse to the fibers or through the bulk epoxy. As a result, the dynamic material response is dependent on the relative shock - fiber orientation. Shocks traveling along the fiber direction exhibit both elastic and plastic characteristics over the stress range tested. Shocks traveling transverse to the fibers show only a single wave response similar to but slightly stiffer than the bulk response of the epoxy. Results will be presented detailing these findings which provide a basis for modeling this class of directional composite materials.

¹Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL8

1:51PM B25.00012 Calculation of Transport Coefficients in Binary Yukawa Mixtures¹, TOMORR HAXHIMALI, ROBERT RUDD, Lawrence Livermore National Laboratory — We employ classical molecular dynamics (MD) to estimate species diffusivity and viscosity in binary Yukawa Mixtures. The Yukawa potential is used to describe the screened Coulomb interaction between the ions, providing the basis for models of dense stellar materials, inertial confined plasmas, and colloidal particles in electrolytes. We calculate transport coefficients in equilibrium simulations using the Green-Kubo relation over a range of thermodynamic conditions including the viscosity and the self-diffusivity for each component of the mixture. The inter-diffusivity (or mutual diffusivity) can then be related to the self-diffusivities by using a generalization of the Darken equation. We have also employed non-equilibrium MD to estimate inter-diffusivity during the broadening of the interface between two regions each with a high concentration of either species. The main motivation in this work is to build a model that describes the transport coefficients in binary Yukawa mixtures over a broad range of thermodynamic conditions.

¹This work was performed under the auspices of the US Dept. of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344.

2:03PM B25.00013 Fracture of Constructional Materials with the Covering at Shock-Wave Loadings, PAVEL RADCHENKO, Institute of Strength Physics and Materials Science SB RAS, Russia, ANDREY RADCHENKO, Tomsk State University of Architecture and Building, Russia — The behavior of constructional materials with a covering subjected to shock load is numerically modeled. The covering on a material is applied by the method of high velocity oxygen fuel. The materials created by a similar method, are widely applied in aerospace branch, both for creation of engines and for creation of details of cases. Possibility of application of multilayered coverings essentially expands the spectrum of researches for the analysis of separate layer influence on behavior of a design as a whole. Features of behavior of this sort of materials is an actual problem as well as construction of authentic models of behavior of materials with coverings as a whole. Influence of a material of a covering, quantity of layers and their geometrical parameters on fracture and shock-wave processes in a material is investigated. The range of velocities of interaction from 50 to 2000m/sec is considered. As projectiles steel cylinders and spheres were used.

Monday, February 27, 2012 11:15AM - 2:15PM —

Session B26 DCOMP DMP: Focus Session: Physics of Energy Storage Materials - Advanced Materials 257B

11:15AM B26.00001 How can one tell if a lithium-ion battery will last for 10 years in experiments that only take a few weeks?¹, JEFF DAHN, Dalhousie University — Lithium-ion batteries are now being used in electric vehicles. There are four main factors which will determine the success of Li-ion batteries in this application: a) safety; b) cost; c) performance and d) lifetime. Each of the factors is presently the subject of much debate and much R+D. I will only speak about lifetime here. Testing the lifetime of Li-ion batteries for automotive applications under **realistic** conditions of temperature and number of cycles per day is very time consuming. In fact, such a test should take a decade or more, if the batteries are expected to last a decade in the field. Tests of such duration slow the product improvement cycle immensely. In this lecture, I will discuss how high precision measurements of the coulombic efficiency of Li-ion cells and batteries can be used to predict the relative lifetimes, on the decade-long scale, of these devices in measurements that only take a few weeks. The measurements enable the rapid comparison of technologies using new electrode materials, electrolyte additives and cell designs so that the product improvement cycle can be significantly shortened. I will describe the requirements of the instruments needed to make these measurements and point out that nothing suitable is, as yet, commercially available. There is a major need for such equipment and an associated business opportunity.

¹In collaboration with Chris Burns, Aaron Smith, Nupur Sinha, and Hannah Dahn, Dalhousie University.

11:51AM B26.00002 Organic electrodes for high rate capability Lithium-ion batteries, Y.Y. ZHANG, Y.Y. SUN, Rensselaer Polytechnic Institute, S.X. DU, H.J. GAO, Institute of Physics, Chinese Academy of Sciences, S.B. ZHANG, Rensselaer Polytechnic Institute — Lithium-ion batteries (LIBs) for power-intensive applications such as in electric vehicles require high discharge rate, i.e., high Li diffusion rate (or low Li diffusion barrier) in electrode and electrolyte materials. Based on first-principles calculations, we found that organic salt, di-lithium terephthalate (Li2TPA), a promising anode material recently tested in experiment, could have high rate capability. We further predict that di-potassium terephthalate (K2TPA) could exhibit even lower Li diffusion barrier. The calculated Li diffusion barrier in fully lithiated K2TPA is only 150 meV, which yields Li diffusion rate orders of magnitude higher than that in Li-intercalated graphite at room temperature. The calculated anode voltage vs metal lithium and specific energy density are 0.62 V and 209 mAh/g, respectively. In addition, the volume change of K2TPA in charging/discharging is only 5%, much smaller than that in Li-intercalated graphite. These unique advantages call for further investigation of the organic salts, both the TPA-based and beyond, for power-intensive LIB applications either as anode or cathode materials.

12:03PM B26.00003 First Principles Study for Lithium Intercalation and Diffusion Behavior in Orthorhombic Nb2O5 Electrochemical Supercapacitor, CHI-PING LIU, FEI ZHOU, VIDVUDS OZOLINS, University of California, Los Angeles — Unlike batteries, electrochemical supercapacitors require not only high energy density, but also very fast rates of electronic and ionic transport. Experimental results show that niobium oxide exhibits an outstanding power density and fast ionic charging rates. We investigate lithium intercalation and diffusion behavior in orthorhombic niobium oxide (T-Nb2O5) by using first-principles density-functional theory (DFT) calculations. We find that the Li ions can only intercalate in the 001 family of lattice planes with the lowest niobium occupancy due to electrostatic-repulsion between Li+ and Nb5+. Besides, since Li diffusion along the z direction is hindered by a high diffusion barrier (2.64 eV), the overall Li intercalation and diffusion can only occur within 001 planes. Furthermore, the diffusion barriers within the 001 planes are found to have a broad distribution of values from around 50 meV to 1000 meV; the diffusion barrier is determined by the neighboring oxygen-oxygen distance. The barrier remains low (around 60 meV) when the neighboring oxygen distance along the diffusion path is larger than 3.9 Å, thus leading to fast Li ion diffusion. These results explain the excellent performance of Nb2O5 as a cathode material for electrochemical supercapacitors.

12:15PM B26.00004 Multiscale Simulations of Energy Storage in Polymers, V. RANJAN, NC State University, Raleigh, A. VAN DUIN, Penn State University, State College, M. BUONGIORNO NARDELLI, J. BERNHOLC, NC State University, Raleigh and ORNL, Oak Ridge, TN — Polypropylene is the most used capacitor dielectric for high energy density storage. However, exotic materials such as copolymerized PVDF and, more recently, polythiourea, could potentially lead to an order of magnitude increase in the stored energy density [1,2]. In our previous investigations we demonstrated that PVDF-CTFE possesses non-linear dielectric properties under applied electric field. These are characterized by transitions from non-polar to polar phases that lead enhanced energy density. Recent experiments [3] have also suggested that polythiourea may be another potential system with high energy-density storage and low loss. However, the characteristics of this emerging material are not yet understood and even its preferred crystalline phases are not known. We have developed a multiscale approach to predicting polymer self-organization using the REAX force field and molecular dynamics simulations. We find that polythiourea chains tend to coalesce in nanoribbon-type structures and prefer an anti-polar interchain ordering similar to PVDF. These results suggest a possible role of topological phase transitions in shaping energy storage in this system.

[1] B. Chu et al, Science 313, 334 (2006).

[2] V. Ranjan et al., PRL 99, 047801 (2007).

[3] Q. Zhang, private communication

12:27PM B26.00005 Addressing the challenges of solar thermal fuels via atomic-scale computational design and experiment, ALEXIE KOLPAK, TIMOTHY KUCHARSKI, JEFFREY GROSSMAN, Massachusetts Institute of Technology — By reversibly storing solar energy in the conformations of photo-isomers, solar thermal fuels (STFs) provide a mechanism for emissions-free, renewable energy storage and conversion in a single system. Development of STFs as a large-scale energy technology has been hampered by technical challenges that beset the photo-isomers of interest: low energy density, storage lifetime, and quantum yield; UV absorption; and irreversible degradation upon repeated cycling. In this talk, we discuss our efforts to design new STFs that overcome these hurdles. We present computational results on various STFs based on our recently proposed photo-isomer/template STF concept [Kolpak and Grossman, Nano Letters 11, 3156 (2011)], as well as new experimental results on azobenzene-functionalized carbon nanotube STFs. Our approach yields significant improvements with respect to STFs studied in the past, with energy densities similar to Li-ion batteries, storage lifetimes > 1 year, and increased quantum yield and absorption efficiency. Our strategy also suggests mechanisms for inhibiting photo-isomer degradation. With a large phase space yet to be explored, there remain numerous possibilities for property enhancement, suggesting that STFs could become a competitive renewable energy technology.

12:39PM B26.00006 Photoswitchable Molecular Rings for Solar-Thermal Energy Storage, ENGİN DURGUN, ALEXIE M. KOLPAK, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology — Solar-thermal fuels reversibly store solar energy in the chemical bonds of molecules by photoconversion, and can release this stored energy in the form of heat upon activation. Many conventional photoswitchable molecules could be considered as solar thermal fuels, although they suffer from low energy density and short lifetime in the photo-excited state, rendering their practical use unfeasible. We present a new approach to design systems for solar thermal fuel applications, wherein well-known photoswitchable molecules are connected by different linker agents to form molecular rings. This approach allows for a significant increase in both the amount of stored energy per molecule and the stability of the fuels. Our results suggest a range of possibilities for tuning the energy density and thermal stability as a function of the type of the photoswitchable molecule, the ring size, and/or the type of linkers.

12:51PM B26.00007 Physics of Materials for Sodium-Ion Batteries, JAY WHITACRE, Carnegie Mellon University — Sodium is used as a functional ionic species in a variety of electrochemical energy storage devices. This talk will examine several manifestations of sodium ion use, and will focus deeply on a novel class of aqueous electrolyte sodium ion batteries that have been developed over the past 5 years. While these new systems are typically lower in energy density, they are very robust and low in cost, making them appealing for a number of stationary energy storage applications. Specific topics to be covered include: sodium ion intercalation compounds, sodium/carbon interaction at potentials below 0V vs NHE, the behavior of porous thick electrodes in different electrolyte solutions, and the future outlook for sodium ion battery research.

1:27PM B26.00008 Computational studies of carbon-onions for electrochemical capacitor applications, P. GANESH, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, P.R.C. KENT, Center for Nanophase Materials Sciences and Computer Science and Mathematics Division, V. MOCHALIN, Department of Materials Science and Engineering, Drexel University, LUKAS VLCEK, Chemical Sciences Division, Oak Ridge National Laboratory Oak Ridge, ADRI VAN DUIN, Department of Mechanical and Chemical Engineering, Penn State University — Supercapacitors bridge the gap between conventional batteries and electrolytic capacitors. Recently, onion-like carbon structures have [1] shown to have capacitances four orders of magnitude higher and energies an order of magnitude higher than conventional capacitors, making them the fastest growing competitors for energy storage. We study the formation of carbon-onions from nanodiamonds using reactive force-fields [2]. Our study suggests that the temperature and mechanical stability as well as the final-equilibrium structure are strongly dependent on the inclusion of long-range forces. We are currently developing reactive-force fields to allow mesoscopic modeling of reactions of carbon nanostructures with aqueous electrolytes. Progress along these lines will also be presented. This material is based upon work supported as part of the Fluid Interface Reactions, Structures and Transport (FIRST) Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

[1] D. Pech et. al, Nature Nanotechnology 5, 651 (2010)

[2] Adri C. T. van Duin et.al, J. Phys. Chem. A 105, 9396 (2001)

1:39PM B26.00009 Supercapacitor Electrodes with High-energy and power densities prepared from monolithic NiO/Ni Nanocomposite¹, QI LU, University of Delaware — Despite significant progresses in the development for high-performance supercapacitors, it lacks techniques to realize the full potential of electrode material by achieving simultaneously tailored pore structure, electrode conductivity, and crystallinity. Moreover, the problem of being difficult for industrial scale manufacture still exists. For an attempt to address all these issues, we recently developed a simple and cost-effective process, which is also scalable, for achieving supercapacitor electrodes with both high energy and power densities. We first produce nickel nanoparticles with a modified polyol method. A simple mechanical compaction of nanoparticles and a followed thermal treatment result in compact, stable, highly porous Ni/NiO electrodes that do not require a support. During the charging process, OH⁻ electrolytic ions are bound to the NiO, giving off electrons. The process is reversed when the stored electrical energy is drawn off as current. The high granularity NiO provides a large inner surface area, and the conductive network of the metal particles is maintained. High energy density of about 60 Wh kg⁻¹ and power density of 10 kW kg⁻¹ were simultaneous achieved with a slow charge/fast discharge process.

¹This work is supported the Office of Naval Research under the Grant Number N00014-08-1-0432

1:51PM B26.00010 An ab-initio approach to modeling high temperature thermodynamics of non stoichiometric ceria, CHIRANJEEVI BALAJI GOPAL, AXEL VAN DE WALLE, None — Ceria is a very promising material for fuel cell electrolytes because of its high oxygen ion diffusivity. Also, its ability to thermodynamically create oxygen vacancies in its structure at high temperatures and get oxidized at low temperatures has found use in thermochemical splitting of water to generate hydrogen. Although the experimental phase diagram for ceria is well established in the composition of interest, there have not been significant attempts at studying the oxygen vacancy thermodynamics at elevated temperatures from first principles. We performed GGA+*U* calculations ceria to study the electronic structure and ground state energies of various concentrations and configurations of oxygen vacancies in ceria. The energies are then fitted to a Cluster expansion Hamiltonian to efficiently model the interactions between the different species: Ce³⁺, Ce⁴⁺, O²⁻ and oxygen vacancies. Lattice Monte Carlo simulations are then performed to obtain the free energy as a function of temperature and oxygen chemical potential through thermodynamic integration. We are also investigating the effect of lattice vibrational contribution to the phase diagram by including a temperature dependent cluster expansion.

2:03PM B26.00011 Defect-Induced Segregation and Lattice Stability of BSCF Perovskites¹, MAIJA KUKLJA, ONISE SHARIA, Materials Science and Engineering Department, University of Maryland, College Park, MD, USA, YURI MASTRIKOV, Institute for Solid State Physics, University of Latvia, Kengaraga str. 8, Riga LV-1063, Latvia, EUGENE KOTOMIN, Max Planck Institute for Solid State Research, Heisenbergstr., 1, D-70569, Stuttgart, Germany — Among novel advanced materials for clean energy, Ba_xSr_{1-x}Co_{1-y}Fe_yO_{3-δ} (BSCF) are considered as promising materials for cathodes in solid oxide fuel cells (SOFC) and oxygen permeation membranes. BSCF exhibits a good oxygen exchange performance, mixed ionic and electronic conductivity, high oxygen vacancy concentration, and low diffusion activation barrier, which largely define the oxygen reduction chemistry. However, understanding the interplay between the structural disorder and crystalline stability in BSCF is extraordinarily complex and essentially unexplored. We present first principles calculations of an ideal BSCF crystal and the crystal containing point defects, Frenkel and Schottky disorders, cation and antisite exchanges, and a set of relevant solid-solid solutions. We discuss possible mechanisms of defect-induced (in)stability, solid-state decomposition reactions, and phase transitions of the BSCF lattice as a function of oxygen vacancy concentration for cubic and hexagonal BSCF in the context of available experiments. This research explains the observed SOFC performance reduction and provides insights on enhancing energy conversion.

¹Supported in part by FP7 NASA-OTM project and National Science Foundation.

Monday, February 27, 2012 11:15AM - 2:15PM –
Session B27 DCMP: Invited Session: Magneto-Electric and Magneto-Optical Properties of Topological Insulators 258AB

11:15AM B27.00001 Magneto-Optical Properties of Electrically Gated Topological Insulators¹

, DENNIS DREW, CNAM, Physics Department, University of Maryland — Topological insulators (TI) are a predicted new quantum state of matter in which spin-orbit coupling gives rise to topologically protected surface states with unpaired spin-helical Dirac cones. TIs are predicted to have exotic properties including Majorana fermions induced by the proximity effect from a superconducting film, an intrinsic magnetoelectric effect and hybridized spin-plasmon modes. The magneto-electric effect leads to Faraday and Kerr rotations quantized in units of the fine structure constant. This effect corresponds to $1/2$ integer quantum Hall step and is predicted both in field and in the absence of a magnetic field when magnetic order gaps the Dirac spectrum. A key difference between this half integer QHE in TIs and the usual integer QHE is that the former cannot be measured by a dc transport experiment. I will describe experiments designed to measure the Kerr rotation in Bi₂Se₃, one example of a topological insulator. Gating the surface isolates the surface response from the bulk signals due to unavoidable bulk carriers from defects and impurities. Preliminary results will be presented on the surface state Kerr rotation for Bi₂Se₃ doped with Mg (ungapped) and Bi₂Se₃ doped with Sm (magnetically gapped).

¹Work supported by DOE (Contract No.DE-SC0005436).

11:51AM B27.00002 Magneto-Electric Effect in Three-Dimensional Topological Insulators from Surface Magnetic Disorder and Ferromagnetic Thin Film

, KENTARO NOMURA, Institute for Materials Research, Tohoku Univdsity — Topologically nontrivial gapped phases can be characterized by the bulk topological indices and the surface gapless modes. The topological magneto-electric (ME) effect is a novel manifestation of the bulk-surface correspondence in which the bulk magnetization is generated by a circulating quantized Hall current flowing at the surface of topological insulators. To realize the topological ME effect, there are two difficulties: (a) one needs to attach an insulating ferromagnetic layer with the magnetization normal to the surface all pointing out or in. (b) The Fermi energy must be tuned accurately within the small gap of the surface Dirac spectrum opened by the exchange interaction. In this talk we discuss the anomalous quantized Hall current on the surface of a magnetically doped topological insulator, basing on the two-dimensional surface Dirac Hamiltonian with magnetic disorder. The scaling analysis indicates that, in sharp contrast to the time-reversal-invariant cases, the all surface states tend to be localized while the Hall conductivity is quantized no matter whether the Fermi level resides within or out of the surface gap. This resolves problem(b). Furthermore it is shown that this also resolves problem (a) with the simultaneous application of magnetic and electric fields parallel or antiparallel to each other. By this method, doped local spins can be controlled by the bulk energy which can overcome the magnetic anisotropy and Zeeman splitting at the surface. We also comment on the generalization of the topological responses to the case of topological superconductors and superfluids. This work was done in collaboration with Naoto Nagaosa, Shinsei Ryu, and Akira Furusaki. K. Nomura and N. Nagaosa, Phys. Rev. Lett. 106, 166802 (2011); K. Nomura, S. Ryu, A. Furusaki, N. Nagaosa, arXiv:1108.5054.

12:27PM B27.00003 Scotch Tape and Spectroscopy, Probing and Manipulating the surface of a Topological Insulator¹

, KENNETH BURCH, Department of Physics and Institute of Optical Sciences, U. of Toronto — Recently there has been a great deal of interest in studying the surfaces of materials with topologically non-trivial electronic states. In addition to probing the surfaces of topological insulators it is highly desirable to put them in proximity with other materials (ferromagnets and superconductors) to induce new particles such as Majoranna Fermions. I will discuss our groups efforts to study these materials using mechanical exfoliation and a variety of spectroscopic techniques (Raman, IR and tunneling). In addition I will detail a new method we have devised that enables us to produce high temperature superconductivity in a topological insulator via the proximity effect.

¹This work was supported by NSERC,CFI,NSF and ORF

1:03PM B27.00004 Giant terahertz Faraday rotation in graphene

, ALEXEY KUZMENKO, University of Geneva — The Faraday rotation of the polarization of light in a medium, where the time-reversal symmetry is broken due to external magnetic field, is an optical analogue of the Hall effect. We recently demonstrated that graphene, the thinnest existing material, can turn the polarization of terahertz radiation by several degrees in modest magnetic fields, which is a spectacular manifestation of the cyclotron resonance. In this talk I will review our Faraday rotation spectroscopy studies of single-layer and twisted multilayer epitaxial graphene with an emphasis on the physical information that one can extract from these measurements and potential applications.

[1] I. Crassee et al. Nature Physics **7**, 48 (2011).

[2] I. Crassee et al. Phys. Rev. B, **84**, 035103 (2011).

1:39PM B27.00005 Ultrafast Probing of Dynamical Spin-Charge Coupling in Topological Insulators¹

, NUH GEDIK, MIT — The three-dimensional topological insulator (TI) is a new quantum phase of matter that exhibits quantum-Hall-like properties, even in the absence of an external magnetic field. Charge carriers on the surface of a TI behave like a two-dimensional gas of massless helical Dirac fermions for which the spin is ideally locked perpendicular to the momentum. In this talk, I will discuss recent experiments in which we used the angular momentum of circularly polarized ultrafast laser pulses to directly visualize and manipulate the spin-charge coupling in TIs. By using laser pulses in the UV region, we performed novel time of flight based angle-resolved photoemission spectroscopy that enabled simultaneously mapping all three components of spin over the entire Dirac cone of a TI. We find that an idealized description of helical Dirac fermions only applies within a small energy window about the Dirac point, beyond which strong textural deformations occur. Utilizing the pump-probe technique, we selectively obtained time-resolved dynamics of surface and bulk excitations. By using circularly polarized laser pulses in the optical region, we achieved preferential excitation of spin species on one side of the surface Dirac cone, resulting in a charge imbalance in momentum space and thus causing a current flow with a direction dependent on photon helicity.

¹Supported by DOE BES Grant number DE-FG02-08ER46521

Monday, February 27, 2012 11:15AM - 2:15PM —

Session B28 DMP: Focus Session: Dopants and Defects in Semiconductors - Nitrides 258C

11:15AM B28.00001 Optical signatures of defects in nitride semiconductors

, ANDREW ARMSTRONG, Sandia National Laboratories — Despite successful commercialization of GaN-based light emitting diodes (LEDs) and high frequency transistors, crystal defects continue to have a strong and often undesired impact on the opto-electronic properties of the III-Nitride family of materials. Fully realizing the potential of this fascinating materials system requires a better understanding of the physical origin of defects, their dependence on both substrate quality and epitaxial growth conditions, and their influence on electrical and optical properties. This talk will discuss the use of deep level optical spectroscopy (DLOS) to quantitatively study defect states in GaN-based materials. As a photocapacitance technique, DLOS is able to probe defect levels that are otherwise inaccessible to thermally-stimulated defect spectroscopies in wide band gap materials, such as the III-Nitrides. DLOS quantifies both the energy level and density of defects and probes defect states with nanoscale depth resolution. Beyond the canonical application of DLOS to thin films, this talk will describe new developments of DLOS to quantitatively study defect states in a wide variety of structures with nanoscale dimensionality, including InGa_N/GaN multi-quantum wells and AlGa_N/GaN core-shell nanowires. The microscopic origin of observed defect states and their influence on the electrical and optical properties of GaN-based LEDs and nanowire devices will be discussed. The reported studies establish DLOS as a critical technique for nanoscale dimensional defect metrology that is able to advance the development of conventional and emerging opto-electronic devices.

11:51AM B28.00002 Shallow versus deep nature of Mg acceptors in nitride semiconductors¹, JOHN LYONS, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — Although Mg doping is the only known method for achieving p-type conductivity in nitride semiconductors, Mg is not a perfect acceptor. Hydrogen is known to passivate the Mg acceptor, necessitating a post-growth anneal for acceptor activation. Furthermore, the acceptor ionization energy of Mg is relatively large (200 meV) in GaN, thus only a few percent of Mg acceptors are ionized at room temperature. Surprisingly, despite the importance of this impurity, open questions remain regarding the nature of the acceptor. Optical and magnetic resonance measurements on Mg-doped GaN indicate intriguing and complex behavior that depends on the growth, doping level, and thermal treatment of the samples. Motivated by these studies, we have revisited this topic by performing first-principles calculations based on a hybrid functional. We investigate the electrical and optical properties of the isolated Mg acceptor and its complexes with hydrogen in GaN, InN, and AlN. With the help of these advanced techniques we explain the deep or shallow nature of the Mg acceptor and its relation to optical signals often seen in Mg-doped GaN. We also explore the properties of the Mg acceptor in InN and AlN, allowing predictions of the behavior of the Mg dopant in ternary nitride alloys.

¹This work was supported by NSF and by the Solid State Lighting and Energy Center at UCSB.

12:03PM B28.00003 Effect of Doping Profile and Concentration on the Near-Infrared Optical Properties of AlGaIn/GaN and AlInN/GaN Heterostructures, MAYRA CERVANTES, COLIN EDMUNDS, DONGHUI LI, LIANG TANG, JIAYI SHAO, GEOFF GARDNER, MICHAEL MANFRA, OANA MALIS, Purdue University — Intersubband (ISB) devices utilizing III-nitrides have recently attracted attention for near- and far- infrared optoelectronic applications. In order to achieve efficient ISB transitions, large doping densities are typically required ($>10^{18} \text{ cm}^{-3}$). The large impurity density has significant effects on the band structure and material quality, effects that are reflected in important device parameters such as transition energies and linewidths. To determine the optimal doping concentration and profile for III-N intersubband devices, we carried out a systematic study of optical and structural properties of strained AlGaIn/GaN and lattice-matched AlInN/GaN heterostructures grown by MBE on quasi-bulk GaN substrates. The lattice-matched AlInN/GaN system is targeted because it allows growth of thick strain-free materials. However, it also presents some considerable growth challenges due to the vastly different optimal growth conditions for Al and In containing nitrides. The transition energy and line profile were determined by direct and photoinduced absorption measurements, while the material quality was assessed using TEM and high resolution x-ray diffraction. The FWHM of the ISB transition at $1.9 \mu\text{m}$ was found to vary up to 60% with the position of delta doping in the quantum well.

12:15PM B28.00004 Field-enhanced vacancy diffusion in AlGaIn¹, KEITH H. WARNICK, YEVGENIY PUZYREV, Dept. of Physics and Astronomy, Vanderbilt University, TANIA ROY, Dept. of Electrical Engineering and Computer Science, Vanderbilt University, DANIEL M. FLEETWOOD, Dept. of Electrical Engineering and Computer Science, Dept. of Physics and Astronomy, Vanderbilt University, RONALD D. SCHRIMPF, Dept. of Electrical Engineering and Computer Science, Vanderbilt University, SOKRATES T. PANTELIDES, Dept. of Physics and Astronomy, Vanderbilt University; Materials Science and Technology Division, Oak Ridge National Laboratory — Room-temperature (RT) native defect diffusion does not generally occur in semiconductors because of high activation energies ($>1.5 \text{ eV}$). However, recent observations of plastic deformation in AlGaIn/GaN High Electron Mobility Transistors (HEMTs) have been attributed to diffusive processes. Here we report first-principles density-functional calculations of the formation and migration energies of vacancies, including the effect of strain and electric fields. We find that triply-negatively charged cation vacancies are the enablers of self-diffusion, as follows: though strain alone is insufficient, we find significant activation barrier lowering due to the applied electric field acting on charged vacancies, reducing cation vacancy barriers in AlGaIn to $\sim 1 \text{ eV}$ or lower where RT diffusion becomes significant. The described mechanism of electric field enhanced vacancy diffusion is relevant for other materials, including several oxides that also feature charged vacancies with low formation energy.

¹This work was supported in part by ONR MURI grant N-00014-08-1-0655 and by the McMinn Endowment at Vanderbilt University.

12:27PM B28.00005 Role of native defects and related complexes in absorption and luminescence of AlN¹, QIMIN YAN, ANDERSON JANOTTI, Materials Department, University of California at Santa Barbara, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, CHRIS G. VAN DE WALLE, Materials Department, University of California at Santa Barbara — AlN is a wide-band-gap material that has been considered as a substrate for GaN-based optoelectronic devices, or in its own right for deep ultraviolet light-emitting diodes and laser diodes. The band gap of 6.2 eV in principle allows transparency in the visible to UV range, but in practice AlN crystals exhibit several sub-band-gap absorption and emission bands, likely due to the presence of native defects and impurities (the most common being oxygen). Using first-principles calculations with the screened hybrid functional of Heyd, Scuseria, and Ernzerhof (HSE), we investigate the structural, electronic, and optical, properties of N and Al vacancies, and their complexes with O impurities in AlN. Defect charge transition levels and stable charge states are determined from the calculated formation energies, and absorption and emission energies are obtained by constructing configuration coordinate diagrams. Our results indicate that Al vacancies and O impurities are responsible for several absorption/emission lines observed experimentally, in particular for the absorption band around 2.85 eV (which gives AlN crystals a yellowish color) and the emission around 3.20 eV emission (375 nm), often observed in O-doped AlN. Mechanisms for each of these processes will be discussed in detail.

¹This work was supported by NSF and by the UCSB SSLEC.

12:39PM B28.00006 Effective mass calculations for shallow acceptors in nitrides¹, JACOB EMMERT-ARONSON, W.R.L. LAMBRECHT, CWRU — In the effective mass approximation for shallow acceptors in semiconductors, the defect eigenstates are written as a product of a slowly varying envelope function and the band extrema Bloch functions. The Kohn-Luttinger Hamiltonian describing the valence band manifold in zincblende, or its generalization for other crystals structures, then becomes a set of coupled differential equations for the envelope function. These can be solved by a variational approach with hydrogenic type basis functions. We have implemented this approach for the appropriate Hamiltonians for zincblende, wurtzite and an orthorhombic crystal structure occurring for II-IV-N₂ semiconductors. The Hamiltonian parameters used were extracted from first-principles GW calculations. The central cell correction to the Coulomb potential was added based on pseudopotential differences as proposed by Mireles and Ulloa (Phys. Rev. B 58, 3879 (1998)). Results are presented for various acceptors in GaN, AlN, InN, ZnGeN₂ and ZnSnS₂. The effects of varying the crystal field splitting parameter, and the type of pseudopotentials (including or not semicore d-states) were investigated.

¹Supported by SOURCE at CWRU

12:51PM B28.00007 Evidence for mobile electrons in p-type GaN:Mg¹, MARY ELLEN ZVANUT, WILLIAM WILLOUGHBY, University of Alabama at Birmingham — Although Mg-doping is the only successful means of achieving p-type conductivity in GaN, little is known about the local environment of the impurity. Our work focuses on a unique phenomena revealed in the electron paramagnetic resonance (EPR) spectrum attributed to Mg: an angular dependent line-shape suggesting the presence of free carriers. 10 GHz EPR measurements were made at 4 K with the magnetic field in the plane of the c-axis. Samples included 0.5 – 1.5 μm thick Mg-doped GaN films grown on sapphire by molecular beam epitaxy or chemical vapor deposition. As expected, the angular dependence of the g value reflects axial symmetry. Unexpected is the line shape change from pure Lorentzian with the magnetic field 30° from the c-axis to increasingly Dysonian upon rotation. The latter reflects the presence of mobile carriers due to, for instance, an interfacial conducting layer, polarization charge, or loosely bound electrons from Ga near neighbors. The new EPR analysis suggests local fields surround the Mg impurity which influence the acceptor's response.

¹Samples were grown at Ga Tech, Sandia National Lab, and Duke University. The work is supported by NSF.

1:03PM B28.00008 A Combined Excitation Experiment and the Emission Nature of Eu in GaN, JONATHAN POPLAWSKY, Physics Department, Lehigh University, ATSUSHI NISHIKAWA, YASUFUMI FUJIWARA, Division of Materials and Manufacturing Sciences, Osaka University, VOLKMAR DIEROLF, Physics Department, Lehigh University — We have developed a fiber based confocal optical microscope that operates inside of a commercial SEM instrument (JEOL 6400) enabling the excitation of a sample either by a laser or by electron beam, and hence combining the complimentary techniques of photoluminescence (PL) and cathodoluminescence (CL). The capabilities of the instrument are demonstrated by experiments involving the excitation of europium ions in-situ doped in Mg doped GaN thin films. The combination of the Eu and Mg defect create new optically active centers (Eu/Mg centers) that absorb energy from electron-hole pairs (EHP) more efficiently than the normal Eu centers in non co-doped GaN (Eu centers). However, the luminescence from these centers decrease as a function of EHP exposure time. The instrument used enables us to perform PL studies before and after electron beam exposure to investigate the nature of this effect. We use a below band gap PL excitation source tuned to resonantly excite the Eu centers using their ⁷F₀ to ⁵D₀ transitions. This allows us to determine their relative numbers and monitor changes of each of the relevant centers. Utilizing these data, the nature of the decrease in emission is investigated with our new and unique experimental apparatus.

1:15PM B28.00009 Magneto-Optical Studies of Rare Earth Doped III-V Nitrides, BRANDON MITCHELL, NATHANIEL WOODWARD, JONATHAN POPLAWSKY, VOLKMAR DIEROLF, Lehigh University, H.X. JIANG, Texas Tech Institute — We investigated the site selective optical and magneto-optical properties of Neodymium doped Gallium and Aluminum Nitride and Erbium doped Gallium Nitride. For our current study, we applied magnetic fields parallel and antiparallel to the C-axis of the crystals and observed the resulting Zeeman splitting both in excitation and emission transitions. On the basis of these measurements, we determined the effective g-factors of all the states involved in the Nd³⁺ transitions. For erbium doping, we observed the Zeeman splitting of the ⁴I_{13/2} and ⁴I_{15/2} levels. Due to small crystal field splitting and large Zeeman splitting, the assignment of levels and corresponding g-factors is very complex. In addition, we observed unexpected asymmetries in the emission intensities when we compared the spectra obtained for fields parallel and antiparallel to the growth direction. The degree of this asymmetry depends on the substrate material and is unambiguously related to the strain and resulting internal fields that are induced by lattice mismatch. The asymmetry behavior parallels the ferromagnetic behavior that is induced by the rare earth ions in GaN and hence our observation suggests that magnetization can be controlled by strain.

1:27PM B28.00010 Origins of Persistent Photoconductivity in Highly Mismatched Semiconductor Alloys, R.L. FIELD III, Department of Physics, University of Michigan, G. VARDAR, Department of Materials Science and Engineering, University of Michigan, Y. JIN, Department of Physics, University of Michigan, T. DANNECKER, Tyndall National Institute, University College Cork, Y.Q. WANG, Materials Science and Technology Division, Los Alamos National Laboratory, C. KURDAK, Department of Physics, University of Michigan, R.S. GOLDMAN, Department of Materials Science and Engineering, University of Michigan — Persistent photoconductivity (PPC) is a nonequilibrium phenomenon in which an illumination-induced increase in conductivity of a semiconductor persists following the termination of illumination. The PPC effect has been explained in terms of the large-lattice-relaxation (LLR) model, in which photoexcited carriers are unable to relax to equilibrium due to an energy barrier between shallow donor and deep donor complex (DX) center configurations. To date, an experimental identification of atomistic configurations in support of a model for the PPC effect has yet to be reported. Here, we examine the origins of the PPC effect in GaAsN alloy films, providing the first direct correlation between the concentration of interstitials and the strength of the PPC effect. Thus, the PPC effect in GaAsN is attributed to a change in the bond orientation or a shift in the center of mass of either N-N or N-As pairs. Similar investigations of GaAsBi alloy films will be discussed.

1:39PM B28.00011 Influence of excitation frequency on A₁(LO) and E₂ Raman modes in In rich In_{1-x}Ga_xN thin films, AMBESH DIXIT, Wayne State University (Current IIT Rajasthan, India), J.S. THAKUR, R. NAIK, Wayne State University, V.M. NAIK, University of Michigan-Dearborn — MBE grown In_{1-x}Ga_xN ($x = 0, 0.1, 0.3$ and 0.54) thin films with bandgap energies varying from 0.77 to 1.85 eV have been investigated using Raman spectroscopy with 1.58 and 2.41 eV excitation energies. The carrier mobility for InN film is 900 cm²/V-s and decreases with increasing x with its value being 20 cm²/V-s for In_{0.46}Ga_{0.54}N. We observe a one-mode behavior of the A₁(LO) and E₂ modes. An enhancement in intensity of A₁(LO) and 2A₁(LO) replica modes in In_{1-x}Ga_xN films with bandgap energies close to the excitation energy is observed. For samples with $x > 0$, the A₁(LO) mode shows a higher intensity relative to E₂ mode which indicates a resonant enhancement of the A₁(LO) mode due to Frölich interaction. We find that the energies of longitudinal optical modes (A₁(LO) and 2A₁(LO)) vary nonlinearly, unlike the E₂ mode, with increasing Ga fraction. The width and asymmetry of the A₁(LO) band is higher for the lower excitation energy (1.58 eV). This is perhaps due to the structural disorder in the deeper regions of the films or due to the distribution of regions with different indium fractions. This may explain the lower carrier mobilities observed in In_{1-x}Ga_xN films with higher values of x .

1:51PM B28.00012 Defect and Impurity Properties of Hexagonal Boron-nitride, BING HUANG, SU-HUAI WEI, National Renewable Energy Lab — By using both GGA and hybrid functional calculations, we have systematically calculated the properties of defects and impurity in hexagonal boron-nitride (*h*-BN). Our calculations show that the defect configurations and the local bond lengths around defects are sensitive to their charge states. The possible highest negative charge states of defects are largely determined by the nearly-free-electron state at the conduction band minimum. The in-gap defect levels got from hybrid functional calculations are much deeper than those got from GGA calculations. The formation energies of neutral defects calculated by hybrid functional and GGA are close to each other, but the defect transition energy level between charge states and neutral state respect to valence band maximum are quite different in GGA and hybrid functional calculations. Finally, we show that the charged defect configurations as well as the transition energy levels exhibit interesting layer effects.

2:03PM B28.00013 Non-linear piezoelectric polarization in III-V and nitride semiconductors, PIERRE-YVES PRODHOMME, ANNIE BEYA-WAKATA, GABRIEL BESTER, Max-Planck-Institut für Festkörperforschung — Piezoelectricity can have a large impact on the electronic and optical properties of quantum well and quantum dots based devices such as lasers, light emitting diodes, infrared photodetectors. In particular it has been shown to be important in III-V and nitride semiconductors. The piezoelectric effect in quantum Well or in Quantum Dots is usually taken into account by neglecting the non linear term in the piezoelectric tensor. We have calculated the second order piezoelectric tensor for all the III-V (including the nitrides) semiconductors in the Wurtzite and Zincblende structure. And we have derived a relation between the proper and the improper second order piezoelectric coefficients. This relation is used to calculate the proper coefficients which are the experimentally measurable ones. We have calculated the piezoelectric field in several Quantum wells and compare our values to experiment. We show that the second order can be so large for Zinc-Blende materials that it cancels the first order term, we demonstrate also that for Nitrides this effect is much lower. However we show that for severely strained structure such as quantum dots or thin films, the second order piezoelectric effect can even exceed the spontaneous polarization in the nitrides.

Monday, February 27, 2012 11:15AM - 1:51PM –
Session B29 GQI: Focus Session: Quantum Optics with Superconducting Circuits: Many-Body Physics, Phase Transitions, & Bistability 259A

11:15AM B29.00001 Cavity-Free Photon Blockade Induced by Many-Body Bound States¹, HUAIXIU ZHENG, DANIEL GAUTHIER, HAROLD BARANGER, Duke University — We show theoretically that a variety of strong quantum nonlinear phenomena occur in a completely open one-dimensional waveguide coupled to an N-type four-level system. This system could be realized, for example, in experiments using superconducting circuits. We focus on photon blockade, photon-induced tunneling, bunching or anti-bunching, and the creation of single-photon states, all in the absence of a cavity. Many-body bound states appear due to the strong photon-photon correlation mediated by the four-level system. These bound states cause photon blockade, generating a sub-Poissonian single-photon source [1]. Such a source is crucial for quantum cryptography and distributed quantum networking; our work thus supports the notion that open quantum systems can play a critical role in the manipulation of individual, mobile quanta, a key goal of quantum communication. [1] H. Zheng, D. J. Gauthier, and H. U. Baranger, Phys. Rev. Lett. in press (2011), arXiv:1107.0309.

¹Supported by the U.S. Office of Naval Research, the U.S. NSF (TAMOP program), and the Fitzpatrick Inst. for Photonics.

11:27AM B29.00002 Experimental investigation of a nonequilibrium delocalization-localization transition of photons in circuit quantum electrodynamics, JAMES RAFTERY, DEVIN UNDERWOOD, WILLIAM SHANKS, SRIKANTH SRINIVASAN, ANTHONY HOFFMAN, HAKAN TURECI, ANDREW HOUCK, Princeton University — Strong photon-qubit coupling in the circuit quantum electrodynamics architecture may lead to quantum phase transitions of light. Recent theoretical and experimental efforts have been made toward examining such quantum phase transitions in large systems; however, interesting crossovers may also exist in significantly smaller and more controllable systems. A sharp nonequilibrium self-trapping transition of light has been predicted in a system comprising two coupled resonators each containing a single qubit. A delocalized regime, where photons coherently oscillate between the two cavities, transitions via dissipation into a localized regime, where photons cannot tunnel. We realized this system experimentally using two capacitively coupled superconducting microwave coplanar waveguides each containing a single transmon qubit. We present our experimental investigation of the system using time and frequency domain measurements to probe its dynamics.

11:39AM B29.00003 Disorder in a Kagome Lattice of Superconducting Coplanar Waveguide Resonators¹, DEVIN UNDERWOOD, WILL SHANKS, ANTHONY HOFFMAN, Department of Electrical Engineering, Princeton University, JENS KOCH, Department of Physics and Astronomy, Northwestern University, ANDREW HOUCK, Department of Electrical Engineering, Princeton University — It has been proposed that arrays of electromagnetic cavities, coupled to two level quantum systems can be used to realize quantum phase transitions of polaritons. One possible experimental realization is a circuit quantum electrodynamics architecture, in which transmon qubits are coupled to superconducting coplanar waveguide resonators (CPWRs); however, for this to be successful, arrays of resonators must be fabricated with low disorder. Results will be reported on characterization of an array of 12 niobium resonators on a sapphire substrate in a honeycomb pattern with the photonic lattice sites forming a Kagome star. These arrays were characterized by measuring many devices of the same design, and using statistical methods for analysis. Furthermore we investigate the origins of disorder, and its dependence on fluctuations in the CPWR geometry.

¹NSF Graduate Fellowship

11:51AM B29.00004 Double symmetry breaking and 2D quantum phase diagram in spin-boson systems, PIERRE NATAF, Laboratoire Maeriaux et Phenomenes Quantiques, Universite Paris Diderot-Paris 7 et CNRS — When the collective coupling between a chain of spins (two-levels systems) and a bosonic mode becomes comparable with the two-level transition frequency, superradiant quantum phase transitions for the cavity vacuum can occur, for instance within the Dicke model [1]. Here, the quantum ground state properties of two independent chains of pseudo-spins interacting with the same bosonic field are investigated [2]. Each chain is coupled to a different quadrature of the field, leading to two independent symmetry breakings for increasing values of the two spin-boson interaction constants. A 2D phase diagram is provided with 4 different phases that can be characterized by the complex bosonic coherence of the ground states and can be manipulated via non-abelian Berry effects. Possible realizations of such model in circuit QED are discussed, generalizing the previous proposals to implement the standard Dicke model [3,4].

[1] C. Emary, and T. Brandes, Phys. Rev. Lett. 90, 044101 (2003).

[2] P. Nataf, A. Baksic and C. Ciuti, arXiv:1111.1617 (2011).

[3] P. Nataf and C. Ciuti, Nat. Commun. 1 :72 (2010).

[4] P. Nataf and C. Ciuti, Phys. Rev. Lett. 104, 023601 (2010).

12:03PM B29.00005 Quantum hysteresis in coupled qubit-radiation systems¹, O.L. ACEVEDO, F.J. RODRIGUEZ, L. QUIROGA, Universidad de los Andes, N.F. JOHNSON, University of Miami — We study theoretically the dynamical response of a set of solid-state qubits arbitrarily coupled to a radiation field which is confined in a cavity. Driving the coupling strength in round trips, between weak and strong values, we quantify the hysteresis or irreversible quantum dynamics. The matter-radiation system is modeled as a finite-size Dicke model which has previously been used to describe equilibrium (including quantum phase transition) properties of systems such as quantum dots in a microcavity, and superconducting circuit QED. Here we extend this model to address *non-equilibrium* situations. Analyzing the system's quantum fidelity, we find that the near-adiabatic regime exhibits the richest phenomena, with a strong asymmetry in the internal collective dynamics depending on which phase is chosen as the starting point. We identify significant deviations from the conventional Landau-Zener-Stuckelberg formulae, in particular from cycles starting in the superradiant phase. In the diabatic or impulsive regime, the system remains quenched and there is little hysteresis. By contrast, depending on the specifications of the cycle, the radiation subsystem can exhibit the emergence of non-classicality, complexity and sub-Planckian structures as evidenced by its Wigner function.

¹Facultad de Ciencias Research Funds, Universidad de los Andes.

12:15PM B29.00006 Coupled Qubit-Cavity Arrays: Evolution of resonance with hopping, FELIX NISSEN, University of Cambridge, JONATHAN KEELING, Scottish Universities Physics Alliance, University of St Andrews — Recent experiments on the light-matter interaction in superconducting qubits have sparked interest in the prospect of studying collective behaviour of coupled qubit-cavity arrays. Any such behaviour will necessarily be non-equilibrium, as the photon loss present in real cavities must be compensated by pumping. We study an array of coupled qubit-cavity systems, with the simplest pumping scheme, using a coherent field. Such pumping might be thought to destroy any interesting physics by imposing coherence on the system. Yet we show that the emerging phenomena are remarkably rich, focussing on the evolution from the antiresonance feature known in the Jaynes-Cummings model [1] as one increases hopping strength between the coupled cavities. We study both the coherent field (as can be measured by homodyne detection) and the fluorescence spectrum, comparing numerical simulations to analytic approximations valid in the limits of large and small hopping. The steady state coherent field depends non-monotonically on the hopping strength, as a crossover occurs from polariton blockade physics at small hopping to semiclassical behaviour at large hopping.

[1] Bishop et al., Nat. Phys. 5, 105 - 109 (2009)

12:27PM B29.00007 Superradiant Phase Transitions and the Standard Description of Circuit QED, OLIVER VIEHMANN, JAN VON DELFT, Physics Department, ASC, and CeNS, LMU Munich, FLORIAN MARQUARDT, Institute for Theoretical Physics, FAU Erlangen-Nuremberg — We investigate the equilibrium behavior of a superconducting circuit QED system containing a large number of artificial atoms. It is shown that the currently accepted standard description of circuit QED via an effective model fails in an important aspect: it predicts the possibility of a superradiant phase transition, even though a full microscopic treatment reveals that a no-go theorem for such phase transitions known from cavity QED applies to circuit QED systems as well. We generalize the no-go theorem to the case of (artificial) atoms with many energy levels and thus make it more applicable for realistic cavity or circuit QED systems.

12:39PM B29.00008 Photon thermalization and condensation in circuit QED by engineered dissipation, DAVID MARCOS, ANDREA TOMADIN, Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, SEBASTIAN DIEHL, Institute for Theoretical Physics, University of Innsbruck, PETER RABL, PETER ZOLLER, Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences — The ability to engineer the coupling between a quantum system and its environment opens the possibility to dissipatively prepare entangled and quantum many-body states. Of particular interest is the case in which the system undergoes a phase transition driven by the coupling to a reservoir. Here we show how to engineer dissipation in the context of coupled cavity arrays, and more specifically in circuit QED. We propose an implementation based on coupled LC resonators and superconducting qubits, which under asymmetric coherent driving, leads to thermalization of photons to the symmetric state between neighboring sites. Above a critical threshold of the driving intensity, a macroscopic occupation of this symmetric mode is found.

12:51PM B29.00009 Stabilizing manifolds of quantum states by reservoir engineering¹, ZAKI LEGHTAS, INRIA Paris-Rocquencourt, KURTIS GEERLINGS, SHYAM SHANKAR, Applied Physics Dept. Yale University, MAZYAR MIRRAHIMI, INRIA Paris-Rocquencourt, MICHEL DEVORET, Applied Physics Dept. Yale University, QLAB TEAM, SISYPHE TEAM — We consider the problem of stabilizing a manifold of states by reservoir engineering. Qubits are coupled to resonators in the strong dispersive limit for which the dispersive shift is much larger than the cavity decay rate. The resonators are driven by microwave fields. By adequately choosing the frequencies of these fields, we can transfer the entropy of the quantum system into its environment. This stabilization is autonomous and continuous in time, and does not rely on a precise control of the drive field amplitudes. The scheme does not require any knowledge of measurement outcomes thus simplifying its experimental realization. Experimental data on dynamical cooling of a transmon qubit coupled to a compact resonator will be shown. Finally, applications to quantum error correction will be discussed.

¹Work supported by ANR (French National Research Agency), IARPA, ARO and the NSF.

1:03PM B29.00010 Adiabatic state preparation of interacting two-level systems, RICHARD BRIERLEY, CELESTINO CREATORE, Cavendish Laboratory, JJ Thomson Avenue, Cambridge, CB3 0HE, UK, PETER LITTLEWOOD, Argonne National Laboratory, 9700 S Cass Ave., Argonne, IL 60439, USA, PAUL EASTHAM, School of Physics, Trinity College, Dublin 2, Ireland — We consider performing adiabatic rapid passage (ARP) using frequency-swept optical pulses to excite a collection of interacting two-level systems. Such a model arises in a wide range of many body quantum systems, such as circuit QED or interacting quantum dots, where a nonlinear component couples to light. We analyse the one-dimension case using the Jordan-Wigner transformation. In the mean field limit, the system can be described by a Lipkin-Meshkov-Glick Hamiltonian. Both approaches provide complementary insights into the behaviour of an interacting model under ARP, suggesting our results are generically applicable. We find ARP can still be used for state preparation in the presence of interactions but the parameters required to achieve full occupation depend on the strength of the interaction. In particular, for a fixed pulse time, stronger interactions require a larger pulse bandwidth, introducing new restrictions on the pulse form required.

1:15PM B29.00011 Collective quantum coherence in large superconducting circuits with approximate S_N symmetry, DAVID FERGUSON, Northwestern University, ANDREW HOUCK, Princeton University, JENS KOCH, Northwestern University — The vast majority of superconducting circuits consist of a minimum number of circuit elements, following an implicit conjecture that any increase in circuit complexity thwarts quantum coherence. Recent experiments have evidenced that this conjecture is not compelling and quantum coherence can persist for much larger circuits [1]. A tool for the design of future circuits, we present theory for the fluxonium qubit, a device which includes a large number, N , of array junctions. Taking into account the degrees of freedom of all junctions and the approximate S_N permutation symmetry, we identify the relevant collective mode and pinpoint an approximate decoupling of additional modes. This allows us to derive the effective models previously used. We also discuss corrections going beyond these models which include subspaces of states that transform as non-trivial representations of the permutation group.

[1] V. E. Manucharyan, J. Koch, L. I. Glazman, and M. H. Devoret, Science **326**, 113 (2009)

1:27PM B29.00012 Quantum crossover of the switching rate of a modulated oscillator, VITTORIO PEANO, Michigan State University, LINGZHEN GUO, MICHAEL MARTHALER, Karlsruhe Institute of Technology, MARK DYKMAN, Michigan State University, GERD SCHOEN, Karlsruhe Institute of Technology — Experiments with Josephson bifurcation amplifiers have reached the regime where switching between coexisting stable vibrational states is due to quantum fluctuations. In switching the oscillator goes over the effective dynamical barrier that separates the states. It was found earlier that, for small damping, the barrier height calculated for $T \rightarrow 0$ is smaller than for $T = 0$. Respectively, the switching rates calculated in these two limits are exponentially different, the effect of fragility. If other parameters are fixed, both barrier heights are proportional to the number of bound quantum states localized mostly in the basin of attraction of the corresponding stable state. Here we show that for large but finite values of the number of states the $T = 0$ solution is stabilized. For some temperature T_c there occurs a sharp crossover to the finite-temperature regime. Our analytical results are corroborated by numerical results.

[1] Vijay et al., Rev. Sci. Instr. (2009)

[2] M. Dykman et al., JETP (1988)

[3] M. Marthaler et al, PRA (2005)

1:39PM B29.00013 Observation of single artificial atom optical bi-stability and its application to single-shot readout in circuit quantum electrodynamics, LUYAN SUN, Department of Physics and Applied Physics, Yale University, ERAN GINOSSAR, Advanced Technology Institute and Department of Physics, University of Surrey, MIKHAEL GUY, MATTHEW REED, HANHEE PAIK, Department of Physics and Applied Physics, Yale University, LEV S. BISHOP, Joint Quantum Institute and Condensed Matter Theory Center, Department of Physics, University of Maryland, ADAM SEARS, ANDREI PETRENKO, TERESA BRECHT, LUIGI FRUNZIO, STEVEN GIRVIN, ROBERT SCHOELKOPF, Department of Physics and Applied Physics, Yale University — The high power transient behavior of superconducting qubit-cavity systems has recently been used to perform high fidelity readout of transmon qubits [1]. We show that in the steady state, the system exhibits a bi-stable behavior that can be observed on the single-shot level, with the cavity state switching stochastically between dim and bright states. The switching times are shown to be long compared to the cavity and qubit lifetimes. Some features of the bi-stability can be explained by mean field theory, while its switching dynamics is studied with large scale simulations. Understanding these dynamics will be crucial for studying the transient response, an essential aspect of the qubit readout. We will discuss progress on optimizing readout by shaping the measurement pulse.

[1] M. D. Reed, L. DiCarlo, B. R. Johnson, L. Sun, D. I. Schuster, L. Frunzio, and R. J. Schoelkopf, Phys. Rev. Lett. 105, 173601 (2010)

Monday, February 27, 2012 11:15AM - 2:15PM – Session B30 GQL: Quantum Error Correction and Quantum Control 259B

11:15AM B30.00001 Fault-tolerant quantum computation with asymmetric Bacon-Shor codes¹, PETER BROOKS, JOHN PRESKILL, California Institute of Technology — Bacon-Shor codes are quantum subsystem codes which are constructed by combining together two quantum repetition codes, one protecting against Z (phase) errors and the other protecting against X (bit flip) errors. In many situations, for example flux qubits, the noise is biased such that faults that produce Z errors are much more common than faults that produce X errors; in these cases it is natural to consider an asymmetric Bacon-Shor code where the code protecting against Z errors is longer than the code protecting against X errors. This work describes fault-tolerant constructions for gadgets that achieve universal fault-tolerant quantum computation using asymmetric Bacon-Shor codes. Gadgets take advantage of the Bacon-Shor structure by breaking up into parallel smaller gadgets that act on a single row or column, with majority voting of the separate results. For a bias of $\epsilon/\epsilon' = 10^4$, we prove a threshold around 2.5×10^{-3} . The effective error strength is shown to decrease rapidly (faster than polynomial) with decreasing ϵ . Therefore it may be practical to use Bacon-Shor codes directly with no additional concatenation. This could greatly reduce the resource overhead required for fault-tolerant computation with biased noise.

¹Supported in part by NSF under Grant No. PHY-0803371, by DOE under Grant No. DE-FG03-92-ER40701, and by NSA/ARO under Grant No. W911NF-09-1-0442.

11:27AM B30.00002 Quantum Error Correction: Optimal, Robust, or Adaptive? Or, Where is The Quantum Flyball Governor?¹, ROBERT KOSUT, SC Solutions, MATTHEW GRACE, Sandia National Laboratories — In *The Human Use of Human Beings: Cybernetics and Society* (1950), Norbert Wiener introduces feedback control in this way:

“This control of a machine on the basis of its actual performance rather than its expected performance is known as *feedback* ... It is the function of control ... to produce a temporary and local reversal of the normal direction of entropy.”

The classic classroom example of feedback control is the all-mechanical flyball governor used by James Watt in the 18th century to regulate the speed of rotating steam engines. What is it that is so compelling about this apparatus? First, it is easy to understand how it regulates the speed of a rotating steam engine. Secondly, and perhaps more importantly, *it is a part of the device itself*. A naive observer would not distinguish this mechanical piece from all the rest. So it is natural to ask, where is the *all-quantum* device which is self regulating, ie, the Quantum Flyball Governor? Is the goal of quantum error correction (QEC) to design such a device? Developing the computational and mathematical tools to design this device is the topic of this talk.

¹Support from ONR/MURI and IARPA QCS.

11:39AM B30.00003 Unified approach to approximate quantum error correction via the transpose channel, PRABHA MANDAYAM, The Institute of Mathematical Sciences, Taramani, Chennai - 600 113, India, HUI KHOON NG, DSO National Laboratories, and Centre for Quantum Technologies, NUS, Singapore — Much of the existing work on error correction focuses on the standard paradigm of perfect quantum error correction (QEC), where the recovery operation perfectly reverses the effects of a noise channel. Recent studies on approximate QEC(AQEC) have demonstrated possible advantages that arise from relaxing the requirement for perfect correction. However, while the recovery operation for perfectly correctable codes is well-known, finding the recovery for approximately correctable codes often requires difficult numerical procedures. We demonstrate an analytical, universal and near-optimal recovery map-the transpose channel- for AQEC codes, with optimality defined in terms of the worst-case fidelity. Using the transpose channel, we provide an alternative interpretation of the QEC conditions and generalize them to a set of conditions for AQEC codes. This forms the basis of a simple algorithm for finding AQEC codes. Our analytical approach is a departure from earlier work relying on exhaustive numerical search for the optimal recovery map, with optimality defined based on entanglement fidelity. Our results can also be extended to the general case of approximate operator quantum error correction, thus bringing us closer to a unified, analytical framework for AQEC.(Ref:PRA,81,062342(2010))

11:51AM B30.00004 Design of additive quantum codes via the codeword-stabilized framework¹, LEONID P. PRYADKO, ILYA DUMER, ALEXEY A. KOVALEV, UC, Riverside — Codeword stabilized (CWS) construction defines a quantum code by combining a classical binary code with some underlying graph state. In general, CWS codes are non-additive but become additive stabilizer codes if derived from a linear binary code. Generic CWS codes typically require complex error correction; however, we show that the CWS framework is an efficient tool for constructing good stabilizer codes with simple decoding. We start by proving the lower Gilbert-Varshamov bound on the parameters of an additive CWS code which can be obtained from a given graph. We also show that cyclic additive CWS codes belong to a previously overlooked family of single-generator cyclic stabilizer codes; these codes are derived from a circulant graph and a cyclic binary code. Finally, we present several families of simple stabilizer codes with relatively good parameters, including a family of the smallest toric-like cyclic CWS codes which have length, dimension, and distance as follows: $[[t^2 + (t+1)^2, 1, 2t+1]]$, $t = 1, 2, \dots$

[1] A. A. Kovalev, I. Dumer, and L. P. Pryadko, preprint arXiv:1108.5490 (2011).

¹Supported in part by the ARO grant W911NF-11-1-0027 (LP & ID), and by the NSF grant 1018935 (LP)

12:03PM B30.00005 Error-threshold for topological subsystem quantum error-correcting codes

, RUBEN S. ANDRIST, Department of Physics, ETH Zurich, HECTOR BOMBIN, Perimeter Institute for Theoretical Physics, MIGUEL ANGEL MARTIN-DELGADO, Departamento de Fisica, Universidad Complutense, HELMUT G. KATZGRABER, Department of Physics and Astronomy, Texas A&M University and ETH Zurich — In general, stability against noise in a quantum computer can be achieved by storing quantum information redundantly. For instance, topological quantum error correction averts decoherence effects by encoding qubits in non-local degrees of freedom, while actively correcting for local errors. The key merit of these topological stabilizer codes lies in the intrinsic locality of the operations for syndrome measurement and error correction. Topological subsystem codes further facilitate practical applications by requiring only measurements of adjacent qubit pairs. We numerically determine the error threshold of topological subsystem codes for the depolarizing channel by mapping the problem onto a classical statistical spin model with bond disorder, which is analyzed via large-scale Monte Carlo simulations. In this picture, faulty qubits correspond to antiferromagnetic interactions between classical spins and the point in the disorder–temperature phase diagram where ferromagnetic order is lost corresponds to the error threshold of the underlying quantum bit system.

12:15PM B30.00006 Correlated Errors in the Surface Code¹

, DANIEL LOPEZ, Universidade Federal do ABC - Brazil, E. R. MUCCILO, University of Central Florida, E. NOVAIS, Universidade Federal do ABC - Brazil — A milestone step into the development of quantum information technology would be the ability to design and operate a reliable quantum memory. The greatest obstacle to create such a device has been decoherence due to the unavoidable interaction between the quantum system and its environment. Quantum Error Correction is therefore an essential ingredient to any quantum computing information device. A great deal of attention has been given to surface codes, since it has very good scaling properties. In this seminar, we discuss the time evolution of a qubit encoded in the logical basis of a surface code. The system is interacting with a bosonic environment at zero temperature. Our results show how much spatial and time correlations can be detrimental to the efficiency of the code.

¹ Financial support by the ONR, by NSF CCF:1117241, and INCT-IQ (Brazil).

12:27PM B30.00007 Quantum Circuits for Measuring Levin-Wen Operators

, NICK BONESTEEL, Dept. of Physics and NHMFL, Florida State University, DAVID DIVINCENZO, Forschungszentrum Juelich & RWTH Aachen — We give explicit quantum circuits (expressed in terms of Toffoli gates, CNOTs and single qubit rotations) which can be used to perform quantum non-demolition measurements of the commuting set of vertex and plaquette operators that appear in the Levin-Wen model [1] for the case of doubled Fibonacci anyons. Such measurements can be viewed as syndrome measurements for the quantum error correcting code defined by the ground states of the Levin-Wen model — a scenario envisioned in [2]. A key component in our construction is a quantum circuit $\mathcal{F}$ that acts on 5 qubits at a time and carries out a so-called F -move, a unitary operation whose form is essentially fixed by a self-consistency condition known as the pentagon equation. In addition to our measurement circuits we also give an explicit 7 qubit circuit which can be used to verify that $\mathcal{F}$ satisfies the full pentagon equation as well as a simpler 2 qubit circuit which verifies the essential nontrivial content of this equation.

[1] M.A. Levin and X.-G. Wen, Phys. Rev. B **71** 045110 (2005).

[2] R. Koenig, G. Kuperberg, and B.W. Reichardt, Ann. Phys **325**, 2707 (2010).

12:39PM B30.00008 Exchange-Only Dynamical Decoupling in the 3-Qubit Decoherence Free Subsystem¹

, BRYAN FONG, JACOB WEST, HRL Laboratories, LLC — The Uhrig dynamical decoupling sequence achieves high-order decoupling of a single system qubit from its dephasing bath through the use of bang-bang Pauli pulses at appropriately timed intervals [1]. This high-order decoupling property of the Uhrig sequence has been extended to decouple general noise from single [2] and multiple [3] qubit systems, using single-qubit Pauli pulses. For the 3-qubit decoherence free subsystem (DFS) and related subsystem encodings, Pauli pulses are not naturally available operations; instead, exchange interactions provide all required encoded operations [4]. Here we demonstrate that exchange interactions alone can achieve high-order decoupling against general noise in the 3-qubit DFS. We present decoupling sequences for a 3-qubit DFS coupled to classical and quantum baths and evaluate the performance of the sequences through numerical simulations. References: [1] G. S. Uhrig, Phys. Rev. Lett. **98**, 100504 (2007). [2] J. R. West, B. H. Fong, and D. A. Lidar, Phys. Rev. Lett. **104**, 130501 (2010). [3] Z.-Y. Wang and R.-B. Liu, Phys. Rev. A **83**, 022306 (2011). [4] J. Kempe et al., Phys. Rev. A **63**, 042307 (2001).

¹Sponsored by the United States Department of Defense. Approved for public release, distribution unlimited.

12:51PM B30.00009 Upper bounds on coherence preservation in dynamical decoupling¹

, KAVEH KHODJASTEH, Dartmouth College, TAMÁS ERDÉLYI, Texas A&M University, LORENZA VIOLA, Dartmouth College — We explore the fundamental limits on coherence preservation by dynamical decoupling in terms of control time scales and the spectral bandwidth of the environment. Our main focus is a decohering qubit controlled by arbitrary sequences of π pulses. Using methods from mathematical analysis, we establish a non-perturbative lower bound for the coherence loss in terms of the minimum pulse separation and the cutoff frequency of the environment. We argue that similar bounds are applicable to a variety of open-loop unitary control methods while we find no explicit dependence of such lower bounds on the total control time. We use these findings to generate bandwidth adapted dynamical decoupling sequences that can preserve a qubit up to arbitrary long times within the best fidelities theoretically possible given the available control resources. Our analysis reinforces the impossibility of fault-tolerance accuracy thresholds under purely reversible error control.

¹Supported by NSF Grant No. PHY-090372

1:03PM B30.00010 Generalized Uhrig Dynamical Decoupling for Multi-Level Quantum Systems

, SUJEET SHUKLA, LIANG JIANG, JOHN PRESKILL, Institute for Quantum Information, Caltech, ADILET IMAMBEKOV, Department of Physics and Astronomy, Rice University — Dynamical decoupling can efficiently suppress decoherence induced by the system-environment interaction. Recently, Uhrig proposed an efficient dynamical decoupling scheme, which uses only N pulses to suppress dephasing noise to $O(T^{N+1})$ for a qubit system with total time evolution T . We generalize Uhrig's dynamical decoupling scheme from 2-level to L -level quantum systems. We find that $M = (L - 1)N$ pulses are sufficient to suppress dephasing noise to $O(T^{N+1})$. We observe interesting patterns in the timing of these pulses, which depend on both L and N with various asymptotic forms for large L or large N .

1:15PM B30.00011 Universal Dynamical Decoupling and Quantum Walks in Functional Spaces

, ADILET IMAMBEKOV, Department of Physics and Astronomy, Rice University, LIANG JIANG, Institute for Quantum Information, Caltech — We investigate the universal dynamical decoupling (DD) schemes, which can restore the coherence of quantum system independent of the details of system-environment interaction. We introduce a general mapping between DD sequences and quantum walks in functional spaces, and use it to prove the universality of various DD schemes such as quadratic DD, nested Uhrig DD, and Uhrig concatenated DD, as well as previously known universal schemes of concatenated DD, Uhrig DD and concatenated Uhrig DD.

1:27PM B30.00012 Protecting adiabatic quantum computation by dynamical decoupling, GREGORY QUIROZ, DANIEL LIDAR, University of Southern California — Adiabatic quantum computation (AQC) relies heavily on a system's ability to remain in its ground state with high probability throughout the entirety of the adiabatic evolution. System-environment interactions present during the evolution manifest decoherence, thereby increasing the probability of excitation. In this work, it is shown that the existence of such noise-producing terms can be dramatically reduced by Dynamical Decoupling (DD). In particular, we consider a multi-qubit system subjected to a classical bath modeled by random Gaussian-correlated noise. The performance of deterministic schemes such as Concatenated Dynamical Decoupling (CDD) and Nested Uhrig Dynamical Decoupling (NUDD) are analyzed for Grover's search algorithm and the two-qubit Satisfiability (2-SAT) problem. The CDD evolution substantially increases noise suppression with increasing concatenation level. In contrast, improvements in performance are only observed for specific sequence orders in the NUDD scheme. These results are verified for both adiabatic evolutions in terms of the total adiabatic run time and minimum pulse interval.

1:39PM B30.00013 ABSTRACT WITHDRAWN —

1:51PM B30.00014 Polar codes for achieving the classical capacity of a quantum channel, SAIKAT GUHA, Raytheon BBN Technologies, MARK WILDE, McGill University — We construct the first near-explicit, linear, polar codes that achieve the capacity for classical communication over quantum channels. The codes exploit the channel polarization phenomenon observed by Arikan for classical channels. Channel polarization is an effect in which one can synthesize a set of channels, by "channel combining" and "channel splitting," in which a fraction of the synthesized channels is perfect for data transmission while the other fraction is completely useless for data transmission, with the good fraction equal to the capacity of the channel. Our main technical contributions are threefold. First, we demonstrate that the channel polarization effect occurs for channels with classical inputs and quantum outputs. We then construct linear polar codes based on this effect, and the encoding complexity is $O(N \log N)$, where N is the blocklength of the code. We also demonstrate that a quantum successive cancellation decoder works well, i.e., the word error rate decays exponentially with the blocklength of the code. For a quantum channel with binary pure-state outputs, such as a binary-phase-shift-keyed coherent-state optical communication alphabet, the symmetric Holevo information rate is in fact the ultimate channel capacity, which is achieved by our polar code.

2:03PM B30.00015 Improved coded optical communication error rates using joint detection receivers¹, ZACHARY DUTTON, SAIKAT GUHA, JIAN CHEN, JONATHAN HABIF, RICHARD LAZARUS, Raytheon BBN Technologies — It is now known that coherent state (laser light) modulation is sufficient to reach the ultimate quantum limit (the Holevo bound) for classical communication capacity. However, all current optical communication systems are fundamentally limited in capacity because they perform measurements on single symbols at a time. To reach the Holevo bound, joint quantum measurements over long symbol blocks will be required. We recently proposed and demonstrated the "conditional pulse nulling" (CPN) receiver – which acts jointly on the time slots of a pulse-position-modulation (PPM) codeword by employing pulse nulling and quantum feedforward – and demonstrated a 2.3 dB improvement in error rate over direct detection (DD). In a communication system coded error rates are made arbitrary small by employing an outer code (such as Reed-Solomon (RS)). Here we analyze RS coding of PPM errors with both DD and CPN receivers and calculate the outer code length requirements. We find the improved PPM error rates with the CPN translates into >10 times improvement in the required outer code length at high rates. This advantage also translates increase the range for a given coding complexity. In addition, we present results for outer coded error rates of our recently proposed "Green Machine" which realizes a joint detection advantage for binary phase shift keyed (BPSK) modulation.

¹This work supported by the DARPA InPho program.

Monday, February 27, 2012 11:15AM - 2:15PM —
Session B31 DCMF: Topological Insulators: Semimetals and Interactions 260

11:15AM B31.00001 Adler-Bell-Jackiw anomaly in Weyl semi-metals: Application to Pyrochlore Iridates, VIVEK AJI, University of California at Riverside — Weyl semimetals are three dimensional analogs of graphene where the energy of the excitations are a linear function of their momentum. Pyrochlore Iridates are conjectured to be examples of such a system, with the low energy physics described by twenty four Weyl nodes. An intriguing possibility is that these materials provide a physical realization of the Adler-Bell-Jackiw anomaly. In this talk we report on the properties of pyrochlore iridates in an applied magnetic field. We find that the dispersion of the lowest Landau level depends on the direction of the applied magnetic field. As a consequence the magneto-conductivity in an electric field, applied parallel to the magnetic field is highly anisotropic, providing a detectable signature of the semi-metallic state.

11:27AM B31.00002 Dirac Semimetal in Three Dimensions, STEVE YOUNG, Makineni Laboratories, Department of Chemistry, University of Pennsylvania, SAAD ZAHEER, JEFFREY TEO¹, CHARLES KANE, EUGENE MELE, Department of Physics and Astronomy, University of Pennsylvania, ANDREW RAPPE, Makineni Laboratories, Department of Chemistry, University of Pennsylvania — In a Dirac semimetal the conduction and valence bands contact at discrete points in the Brillouin zone, dispersing linearly away from these critical points with the low energy physics described by a four band Dirac Hamiltonian. In 2D this situation is realized in graphene in the absence of spin-orbit coupling. 3D Dirac semimetals are predicted to exist at the phase transition between a topological insulator and an ordinary insulator when inversion symmetry is preserved. Here we show that 3D Dirac points can also be protected by crystallographic symmetries in particular space groups and enumerate the criteria necessary to identify these groups. As an example of a Dirac semimetal, we present calculations for β -Cristobalite BiO_2 which exhibits Dirac points at the three symmetry related X points of the FCC Brillouin zone. We find that β -Cristobalite BiO_2 is metastable, so it can be physically realized as a 3D analog to graphene. We provide a systematic approach that includes crystallographic symmetry arguments and physical and chemical considerations to identify other such materials and rule out possible alternatives such as HgTe . This would greatly expand the range of applications that take advantage of properties arising from Dirac points.

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11:39AM B31.00003 Semi-metal and Topological Insulator in Perovskite Iridates, VIJAY SHANKAR V, JEAN-MICHEL CARTER, Department of Physics, University of Toronto, M. AHSAN ZEB, Cavendish Laboratory, University of Cambridge, HAE-YOUNG KEE, Department of Physics, University of Toronto — The two-dimensional (2D) layered perovskite Sr_2IrO_4 was proposed to be a spin-orbit (SO) Mott insulator, where the effect of Hubbard interaction is amplified on a narrow $J_{eff} = \frac{1}{2}$ band due to strong spin-orbit coupling. On the other hand, the three-dimensional (3D) orthorhombic perovskite SrIrO_3 remains metallic. We construct a tight-binding model for SrIrO_3 to understand the physical origin of the metallic behaviour and study possible metal-insulator transitions. In particular, we identify possible perturbations that turn the material into a topological insulator.

11:51AM B31.00004 Topological Insulators and Semimetals with Point Group Symmetries¹, CHEN FANG, Princeton University, MATTHEW GILBERT, University of Illinois at Urbana Champaign, XI DAI, Chinese Academy of Sciences, ANDREI BERNEVIG, Princeton University — In this work, we study the theory of topological phases in systems with point group symmetries (PGSs) in one-, two- and three-dimension. The systems we study in general do not require time-reversal symmetry, and hence may be realized in both non-magnetic and magnetic materials. We show that a point group symmetry introduces new quantum numbers which reveal themselves in the entanglement spectrum as mid-gap states. PGSs also define a series of topological semimetals, in which the band touching points are protected by certain symmetries. We apply our theory to 3D ferromagnetic semimetal HgCr_2Se_4 which possesses a double-vortex band crossing protected by C_4 rotation symmetry.

¹ONR - N00014-11-1- 0635, Darpa - N66001-11-1-4110, AFOSR FA9550-10-1-0459, ONR N0014-11-1-0728 and a gift the Intel Corporation

12:03PM B31.00005 Diamagnetism of Weyl semimetals, SI WU, ALEXANDER ZYUZIN, ANTON BURKOV, University of Waterloo — We present a study of the diamagnetic orbital response in a Weyl semimetal, the recently discovered gapless topological phase of matter. Weyl semimetal is a three-dimensional (3D) material, characterized by the presence of isolated Dirac (Weyl) point nodes in its band structure. It can be thought of as the closest 3D analog of graphene. It is known from graphene studies that two-dimensional (2D) Dirac fermions have a highly nontrivial singular diamagnetic response to an applied perpendicular magnetic field, reflecting the quantum critical nature of the ground state of undoped graphene. Here we investigate the analogous orbital response of 3D Dirac fermions in a Weyl semimetal to an applied magnetic field. As in 2D graphene, we find strong signatures of quantum criticality in the diamagnetic response of 3D Weyl semimetal. In particular, we find that the orbital susceptibility has a characteristic logarithmic dependence on the applied field, deviation of the chemical potential from the charge-neutral position and temperature. This unusual diamagnetic response can be used for experimental characterization of Weyl semimetals.

12:15PM B31.00006 Weyl Semimetal in a Topological Insulator Multilayer, ANTON BURKOV, University of Waterloo, LEON BALENTS, Kavli Institute for Theoretical Physics, UCSB — We propose a simple realization of the three-dimensional (3D) Weyl semimetal phase, utilizing a multilayer structure, composed of identical thin films of a magnetically-doped 3D topological insulator (TI), separated by ordinary-insulator spacer layers. We show that the phase diagram of this system contains a Weyl semimetal phase of the simplest possible kind, with only two Dirac nodes of opposite chirality, separated in momentum space, in its bandstructure. This Weyl semimetal has a finite anomalous Hall conductivity, chiral edge states, and occurs as an intermediate phase between an ordinary insulator and a 3D quantum anomalous Hall insulator. We discuss unusual transport properties of the Weyl semimetal, and in particular point out quantum critical-like scaling of the DC and optical conductivity.

12:27PM B31.00007 3D Weyl Semimetal in a Honeycomb Array of Topological Nano-wires, MOHAMMAD VAZIFEH, MARCEL FRANZ, Department of Physics and Astronomy, University of British Columbia — The Weyl semimetal phase has been recently introduced and suggested to exist in strongly correlated pyrochlore iridates as well as in the non-interacting layered Normal/Topological band insulator systems. This unusual phase has a number of interesting properties in the bulk and at the surface arising from the appearance of isolated point-like hedge-hog topological defects (known as Weyl-Dirac points) in the Bloch-state manifold. Here we discuss the possible emergence of this phase in a honeycomb arrangement of the parallel topological insulator nano-rods each exposed to a half-integer multiple of magnetic flux quantum. We consider direct hopping between rods as well as the electron-electron interaction between them. We discuss how the initially degenerate Weyl points can be separated in the Brillouin zone by various perturbations breaking either inversion or time-reversal symmetry.

12:39PM B31.00008 Charge transport in Weyl semimetals, PAVAN HOSUR, SIDDHARTH PARAMESWARAN, U C Berkeley, USA, ASHVIN VISHWANATH, U C Berkeley, USA; Lawrence Berkeley National Lab, USA — Weyl semimetals are three-dimensional phases with band touchings, whose low-energy excitations are governed by the Weyl equation. They can be thought of as higher dimensional cousins of graphene. Recent theoretical work predicted certain pyrochlore iridates such as $\text{Y}_2\text{Ir}_2\text{O}_7$ to be in this phase. We study charge transport in Weyl semimetals in the presence of Coulomb interactions or disorder at temperature T and compare our results to existing data on $\text{Y}_2\text{Ir}_2\text{O}_7$ and $\text{Eu}_2\text{Ir}_2\text{O}_7$. In the interacting clean limit, we determine the conductivity by solving a quantum Boltzmann equation within a “leading log” approximation and find it to be proportional to T , upto logarithmic factors arising from the flow of couplings. In the noninteracting disordered case, we compute the finite-frequency Kubo conductivity and show that it exhibits distinct behaviors for low and high frequencies compared to T . The behavior of Weyl semimetals in a magnetic field will also be briefly discussed.

12:51PM B31.00009 Magnetic Instability on the Surface of Topological Insulators, ADY STERN, YUVAL BAUM, Weizmann Institute of Science — Gapless surface states that are protected by time reversal symmetry and charge conservation are among the manifestations of 3D topological insulators. In this work we study how electron-electron interaction may lead to spontaneous breaking of time reversal symmetry on surfaces of such insulators. We find that a critical interaction strength exists, above which the surface is unstable to spontaneous formation of magnetization, and study the dependence of this critical interaction strength on temperature and chemical potential.

1:03PM B31.00010 Plasmons in Topological Insulators, GODFRY GUMBS, Department of Physics and Astronomy, Hunter College, City University of New York, 695 Park Avenue, New York, NY 10065, USA, OLEKSIY ROSLYAK, Department of Physics and Astronomy, Hunter College, City University of New York, 695 Park Avenue, New York, NY 10065, USA, DANHONG HUANG, Air Force Research Laboratory, Space Vehicles Directorate, Kirtland Air Force Base, NM 87117, USA — A theory is presented for calculating the plasmon mode dispersion relation in three-dimensional topological insulators (TI). There are two-dimensional (2D) conducting surface states. The conducting states localized close to the surface of the semi-infinite slab have a well defined Dirac cone. The bulk energy gap is large and comparable with room temperature. We investigate plasmon excitations of those surface bound electrons in the long wavelength limit employing the random-phase approximation. Results from our calculations show that for a quasi-1DTI, the plasmon dispersion relation is given by $\omega_p \approx q(1 - \omega_0 \ln(q))$ where $\omega_0 = \frac{2e^2}{\pi\epsilon_0} \frac{3}{10}$. On the other hand, for the conventional 1DEG, the plasmon dispersion satisfies $\omega_p \approx q\sqrt{-\omega_0 \ln(q)}$, with $\omega_0 = 2n_{1D}e^2/\epsilon_0 m$ and n_{1D} denoting the linear electron density. The plasmons in 1DTI are density-independent as they are in metallic armchair graphene nanoribbons but obey different dispersion relation. The material parameters we chose correspond to Bi_2Te_3 crystals.

1:15PM B31.00011 Topological Insulators with electron-electron interactions, DAVID SCHMELTZER, City College of NY — We consider the effect of interaction for the 3 dimensional Topological insulators. We show that effectively the system is equivalent to non-interacting Topological Insulators in 4+1 dimensions.

1:27PM B31.00012 Actinide Topological Insulator Materials with Strong Interaction¹, XIAO ZHANG, HAIJUN ZHANG, Department of Physics, Stanford University, CLAUDIA FELSER, Johannes Gutenberg University of Mainz, SHOU-CHENG ZHANG, Department of Physics, Stanford University — Topological band insulators have recently been discovered in spin-orbit coupled two and three dimensional systems. In this work, we theoretically predict a class of topological Mott insulators where interaction effects play a dominant role. In actinide elements, simple rocksalt compounds formed by Pu and Am lie on the boundary of metal to insulator transition. We show that interaction drives a quantum phase transition to a topological Mott insulator phase with a single Dirac cone on the surface.

¹This work is supported by the ARO with grant number W911NF-09-1-0508.

1:39PM B31.00013 Fractional quantum Hall effect and plasmons in topological insulators¹, ASHLEY DASILVA, Pennsylvania State University — I will discuss theoretical studies of the effect of Coulomb interactions at the topological insulator surface in the presence of a magnetic field. Coulomb interaction can cause composite fermion formation and the fractional quantum Hall effect. We predict the stability of the fractional quantum Hall effect by considering the form of the effective interparticle interaction: if it is sufficiently short ranged, then there will be composite fermion formation. We will also study plasmons and magnetoplasmons of the surface states both for an ideal topological insulator and for a topological insulator with bulk conduction.

¹This work was supported by the PSU MRSEC under NSF grant number DMR-0820404

1:51PM B31.00014 Half quantum spin Hall effect on the surface of weak topological insulators¹, CHAOXING LIU, Institute for Theoretical Physics and Astrophysics, University of Wuerzburg, 97074 Wuerzburg, Germany, XIAOLIANG QI, SHOUCHENG ZHANG, Department of Physics, McCullough Building, Stanford University, Stanford, CA 94305-4045 — We investigate interaction effects in three dimensional weak topological insulators (TI) with an even number of Dirac cones on the surface. We find that the surface states can be gapped by a surface charge density wave (CDW) order without breaking the time-reversal symmetry. In this sense, timereversal symmetry alone can not robustly protect the weak TI state in the presence of interactions. If the translational symmetry is additionally imposed in the bulk, a topologically non-trivial weak TI state can be obtained with helical edge states on the CDW domain walls. In other words, a CDW domain wall on the surface is topologically equivalent to the edge of a two-dimensional quantum spin Hall insulator. Therefore, the surface state of a weak topological insulator with translation symmetry breaking on the surface has a “half quantum spin Hall effect,” in the same way that the surface state of a strong topological insulator with time-reversal symmetry breaking on the surface has a “half quantum Hall effect.” The on-site and nearest neighbor interactions are investigated in the mean field level and the phase diagram for the surface states of weak topological insulators is obtained.

¹CXL acknowledge financial support by the Alexander von Humboldt Foundation of Germany and is grateful for the hospitality of the Institute for Advanced Study in Tsinghua University.

2:03PM B31.00015 2D symmetry protected topological orders and their protected gapless edge excitations, XIE CHEN, Massachusetts Institute of Technology, ZHENG-XIN LIU, Tsinghua University, XIAO-GANG WEN, Massachusetts Institute of Technology — Topological insulators/superconductors with time reversal or particle-hole symmetry protected gapless edge excitations have been well characterized and classified in free fermion systems. However, it is not clear in general interacting boson or fermion systems, when such symmetry protected topological(SPT) orders exist with gapless edge excitations that are protected even against strong interactions. Here, we present a systematic construction of 2D interacting bosonic models with non-trivial SPT orders for any on-site symmetry of group G . We demonstrate the non-trivialness of the models by rigorously proving that the gapless edge excitations of the system is stable against any interaction as long as symmetry is not broken. We prove this result by developing the tool of matrix product unitary operator to study the nonlocal symmetry transformation on the edge degrees of freedom and revealing its relation to the non-trivial 3-cocycles of the symmetry group G . This relation between SPT orders and group cocycles has actually been established in 1D interacting systems and led to a complete classification of 1D SPT orders. We show here that this relation also extends to > 2 spatial dimensions and possibly provides a (partial) classification of SPT orders in all interacting systems.

Monday, February 27, 2012 11:15AM - 2:15PM —
Session B32 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides - Relaxors, Nanostructures, and Morphotropic Phase Boundary 261

11:15AM B32.00001 Symmetry determination of piezoelectric $(1-x)\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ - $x\text{PbTiO}_3$ single crystal near morphotropic phase boundary, KYOUHYUN KIM, DAVID PAYNE, JIAN-MIN ZUO, University of Illinois, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING COLLABORATION — The symmetry of $(1-x)\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ - $x\text{PbTiO}_3$ single crystal (PMN- x PT) is investigated at the morphotropic phase boundary with $x=31\%$. The XRD result indicates that the average symmetry of annealed PMN-31%PT single crystal is in close agreement with the monoclinic M_C (Pm) phase, but with strain. The local symmetry of PMN-31PT are then investigated at three different directions of $[001]_C$, $[010]_C$, $[011]_C$ and $[111]_C$ by using convergent electron diffraction (CBED) technique with a probe size of 2 nm. The dynamical theory is used to simulate the CBED patterns for the reported phases of PMN- x PT. The CBED results show that significant deviations of the experimental CBED patterns from the simulations. The deviations in the CBED results are considered as a result from a local distortion induced by the different B cations of Mg^{2+} , Nb^{5+} and Ti^{4+} . The local symmetry of PMN-31%PT is not defined by any reported phases and the symmetry of PMN-31%PT seen in X-ray diffraction is the average of local structures

11:27AM B32.00002 Phase diagram and skin effect of the relaxor ferroelectric $(1-x)\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3+x\text{PbTiO}_3$, PETER GEHRING, DANIEL PHELAN, EFRAIN RODRIGUEZ, National Institute of Standards and Technology, ZUO-GUANG YE, Simon Fraser University — We revisit the phase diagram of the relaxor ferroelectric PMN- x PT using neutron powder diffraction to test suggestions that defects in the oxygen stoichiometry and/or strain affect the ground state crystal structure. Two identical sets of PMN- x PT powders were prepared with $x = 0.10, 0.20, 0.30$, and 0.40 . One set was annealed in air at 873K for 2h. For a given composition and temperature the same structural phase is observed in each set, thus indicating that the effects of strain and oxygen vacancies are minimal. But the distortions measured in the annealed samples are consistently smaller than those in the as-grown samples. In addition, the average grain size of the annealed samples is approximately twice that of the as-grown samples (1.2 ± 0.6 microns vs 0.6 ± 0.3 microns). This result is consistent with a skin effect in which Ti-poor bulk crystals show significantly smaller distortions than do powders of the same composition. The diffraction patterns for both the as-grown and annealed samples with compositions $x = 0.10$ and $x = 0.20$ are best refined using the monoclinic Cm space group, which agrees with recent speculation by Singh et al., Phys. Rev. B **74**, 024101 (2006).

11:39AM B32.00003 Model for Relaxor Ferroelectrics¹, GIAN GUZMAN-VERRI, CHANDRA VARMA, Department of Physics and Astronomy, University of California at Riverside — We consider a model of a lattice made of polarizable unit cells with local and dipole interactions and disorder. Without disorder, it is well known that dipole interactions alone do not lead to ferroelectricity. We show by a cluster expansion in disorder and by a high temperature series expansion that in the presence of sufficient disorder, the model with both local and dipole interactions has locally correlated regions at low temperatures but has no long-range order. We compare our results with measurements of the static and dynamic structure factor by neutron scattering [1]. References: 1. S.N. Gvasaliya, B. Roessli, R.A. Cowley, P. Huber, S. Lushnikov, J. Phys.: Condens. Matter **17** 4343 (2005).

¹This research was partially funded by the UC Lab Fees Research Program 09-LR-01-118286-HELF.

11:51AM B32.00004 Molecular Dynamics Studies of Structure, Dynamics and Dielectric Response in a Relaxor Ferroelectric, ILYA GRINBERG, University of Pennsylvania — Since the first synthesis of the classic $\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3$ (PMN) material in 1961, relaxor ferroelectrics have been the subject of ongoing experimental and theoretical investigation due to their fundamental scientific interest and their importance in technological applications. We use atomistic molecular dynamics simulations to study relaxor behavior in the 0.75PMN-0.25PT material. Even for a fairly small simulation size of 1000 atoms, the system exhibits frequency dispersion and deviation from the Curie-Weiss law typical of relaxor materials. Analysis of the time autocorrelation functions for individual atoms allows us to identify the Nb atoms with a high concentration of neighboring Ti atoms as the nucleation sites for the relaxor behavior. This is due to the higher coupling between the cation displacements induced by the presence of overbonded oxygen atoms. We also analyze local structure and dynamics in PMN-PT using instantaneous, time-averaged and frequency resolved pair distribution functions (PDF). We find that dynamic Pb and Ti off-centering is present even in the paraelectric phase, below T_b the rate of growth of local Pb off-centering increases, followed by the freezing in of the local displacement direction at an intermediate temperature T_c and a transition to a ferroelectric-like phase at T_f . Thus there is a sequence of four phases, PE, dynamic relaxor, mixed dynamic and frozen phase, and the non-ergodic frozen relaxor phase. We identify the average instantaneous local cation off-centering as the order parameter for the dynamic relaxor phase, and the time-averaged local cation off-centering as the order parameter for the two lower-temperatures relaxor phases. Examination of the dynamic PDF data reveals the shape and the range of correlation between the cation displacements. We also show that the relaxor phase is characterized by the appearance of strong nearest-neighbor correlation between the off-center displacements along the Cartesian directions.

12:27PM B32.00005 First-principles calculations of finite temperature Sc and O NMR parameters in $\text{Pb}(\text{Sc}_{2/3}\text{W}_{1/3})\text{O}_3$ ¹, HENRY KRAKAUER, ERIC J. WALTER, JEREMY ELLDEN, GINA L. HOATSON, ROBERT L. VOLD, College of William and Mary — Understanding the dynamics of complex relaxor ferroelectrics is important to characterizing their large electromechanical coupling. Preliminary NMR measurements of Sc electric-field-gradients (EFG) in $\text{Pb}(\text{Sc}_{2/3}\text{W}_{1/3})\text{O}_3$ (PSW) show a strong temperature dependence in the range $T = 250 - 330$ K. To understand this behavior, we use the first-principles GIPAW² method within the Quantum Espresso (QE) package³ to calculate ⁴⁵Sc and ¹⁷O chemical-shifts and EFG tensors. To study finite temperature effects, we incorporate the thermal expansion of the lattice and sample thermal disorder, using the phonon degrees of freedom. As in our previous studies of perovskites,⁴ we show that the ¹⁷O chemical shifts in PSW also exhibit a linear correlation with the nearest-neighbor B-O bond length.

¹Supported by NSF, ONR.

²C. J. Pickard and F. Mauri, Phys. Rev. B **63**, 245101 (2001);

³P. Giannozzi et al., Journal of Physics: Condensed Matter **21**, 395502 (2009)

⁴D. L. Pechkis, E. J. Walter, and H. Krakauer. J. Chem. Phys. **135**, 114507 (2011); *ibid.* **131**, 184511 (2009)

12:39PM B32.00006 Critical Slowing Down in the Relaxor Ferroelectric $\text{K}_{1-x}\text{Li}_x\text{TaO}_3$ (KLT), LING CAI, JEAN TOULOUSE, Lehigh University, Physics Department — In this report, we illustrate an essential characteristic of mixed crystals such as KLT: the strong dependence of their macroscopic properties on the spatial distribution of the mixed ions in the crystal. As a prototypical relaxor ferroelectric, KLT exhibits a large dielectric constant, low frequency dispersion and a broad relaxation peak. Lithium randomly substitutes for potassium and, because of its smaller size, moves off-center in one of six possible $\langle 100 \rangle$ directions thus forming a local dipole. Correlations between these dipoles lead to the appearance of Polar Nanodomains (PNDs), the size and polarization of which depend on local density fluctuations or type of distribution of the Li ions (random homogeneous or locally clustered). The dielectric constant of two KLT crystals with almost identical average Li concentrations displays two radically different behaviors, which can be traced to two very different distributions of the lithium ions in the two crystals. This is particularly striking of the critical behaviors in the two separate crystals. A first order structural transition is observed in one crystal but critical slowing down is observed in the other. The type of spatial distribution present in each crystal can be inferred from the dielectric results.

12:51PM B32.00007 EIT-like effect due to hetero-phase oscillations near the phase transition of relaxor ferroelectrics, JEAN TOULOUSE, RADHA K. PATTNAIK¹, Lehigh University, LYNN A. BOATNER, Oak Ridge National Laboratory — We report the observation of a remarkable “transparency window” in the dielectric resonant absorption spectrum of the relaxor ferroelectric $\text{K}_{1-x}\text{Li}_x\text{TaO}_3$ (KLT) in the vicinity of its weakly first order transition. This phenomenon is shown to be conceptually similar to the electro-magnetically induced transparency (EIT) phenomenon observed in certain atomic vapors. In KLT however, it reveals the presence of hetero-phase (cubic-tetragonal) fluctuations and provides unique information on the nature and mechanism of the phase transition in relaxors.

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1:03PM B32.00008 Temperature evolution of the linear birefringence in striated single crystals of $\text{KTa}_{1-x}\text{Nb}_x\text{O}_3$ (KTN), DANIEL JACKSON, Dept. of Phys., Lehigh University, Bethlehem PA, 18015, USA, RADHA PATTNAIK, Phys. Dept., Lafayette College, Easton, PA 18042, USA, AHARON AGRANAT, Dept. of Appl. Phys., The Hebrew University of Jerusalem, Jerusalem 91904, Israel, JEAN TOULOUSE, Dept. of Phys., Lehigh University, Bethlehem PA, 18015, USA — We report the temperature evolution of a special linear birefringence in 3 crystals of $\text{KTa}_{1-x}\text{Nb}_x\text{O}_3$ (KTN), with $x=0.155$, 0.27 and 0.36 respectively, upon approaching the cubic-tetragonal phase transition. This birefringence, which is in violation of crystalline symmetry conditions, is caused by growth striations in the crystal that give rise to local strain and result in an average uniaxial behavior due to the photoelastic effect. Simultaneously, the set of parallel striations acts as a volume phase grating which can produce diffracted beams. Upon approaching the phase transition, the measured birefringence displays a rapid temperature dependence which is due to the formation of polar nano-domains (PND). These are incipient tetragonal uniaxial domains preferentially oriented with their c-axis perpendicular to the plane of the striations. As the birefringence increases, the diffraction efficiency unexpectedly decreases, indicating that the phase grating amplitude is occluded by the PND formation. The striation pattern is well defined in the 15.5% crystal, more diffuse in the 36% crystal, and there are no obvious striations in the 27% crystal. Experimental results are presented and a simple phenomenological model for the birefringence behavior is proposed and discussed.

1:15PM B32.00009 Strain effects on Coherent Epitaxial Ferroelectric $\text{Pb}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{O}_3$, ASIF KHAN, SAYEEF SALAHUDDIN, UC Berkeley — A comprehensive study of strain coupling to ferroelectricity in coherent epitaxial $\text{Pb}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{TiO}_3$ thin films is presented. The epitaxial strain variants are obtained by growing coherent PZT thin films on three different substrates, SrTiO_3 , DyScO_3 and GdScO_3 by pulsed laser deposition technique. The strain sensitivity of remnant polarization is found to be less in the epitaxial strain variants with larger tetragonality. Despite the fact that the tetragonality of PZT is more sensitive to the epitaxial strain than that of BaTiO_3 , the polarization-strain coupling is weaker in PZT than in BTO. These results underpins that the strong sensitivity of ferroelectricity to epitaxial strain is not a universal characteristic of complex oxide ferroelectrics and may depend on the intricate details of individual material systems.

1:27PM B32.00010 Structural and Ferroelectric Properties of Epitaxial ultrathin $\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3$ Films Prepared on $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3/(\text{LaAlO}_3)_{0.3}(\text{Sr}_2\text{AlTaO}_6)_{0.7}$ Substrates, NORA ORTEGA, DANILO BARRIONUEVO, Department of Physics and Institute of Functional Nanomaterials, University of Puerto Rico, ASHOK KUMAR, University of Puerto Rico, RAM KATIYAR, Department of Physics and Institute of Functional Nanomaterials, University of Puerto Rico — The existence of ferroelectricity in ultrathin films opens the possibility to further miniaturize devices based on FE materials, i.e. ferroelectric tunnel junctions take advantage of tunnel electroresistance effect. We have fabricated epitaxial $\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3$ thin and ultrathin films using pulsed laser deposition on (001) on $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3/(\text{LaAlO}_3)_{0.3}(\text{Sr}_2\text{AlTaO}_6)_{0.7}$ (LSMO/LSAT) substrates. The film thickness ranged between 3 to 100 nm. X-ray diffraction analysis revealed PZT and LSMO films are (001) oriented perovskite structure. Atomic force microscopy of the PZT/LSMO(40nm)/LSAT structures show the surface is smoothness, densely packed, and free of cracks. The surface roughness on a $3 \times 3 \mu\text{m}^2$ area of the 100 nm and 3 nm thick films is ~ 2 nm and ~ 0.3 nm respectively. Well defined ferroelectric loop was observed in Pt/PZT(100nm)/LSMO(40nm)/LSAT structure with a remanent polarization $\sim 38 \mu\text{C}/\text{cm}^2$ and a coercive field ~ 80 kV/cm. The ferroelectric nature of the PZT ultrathin films (7–3 nm) was characterized using piezo force microscopy, a clear contrast between up and down ferroelectric domains was observed after writing positive and negative polarized in $2 \times 2 \mu\text{m}^2$ and $1 \times 1 \mu\text{m}^2$ areas respectively.

1:39PM B32.00011 Ab Initio Investigation of Free Energy Landscape near Morphotropic Phase Boundary, DUCHAO LV, Department of Materials Science and Engineering, The Ohio State University, JU LI, Department of Nuclear Science and Engineering and Department of Materials Science and Engineering, Massachusetts Institute of Technology, YUNZHI WANG, Department of Materials Science and Engineering, The Ohio State University, XIAOBING REN, Ferroic Physics Group, National Institute for Materials Science, FRONTIER INSTITUTE OF SCIENCE AND TECHNOLOGY TEAM¹ — For pressure induced morphotropic phase boundary (MPB) in PbTiO_3 , although ground states have been investigated intensely, the overall free energy landscapes and so the transition paths are never systematically considered by ab initio method. Also there is little information about the oxygen octahedral tilts in monoclinic (M), orthorhombic (O) and triclinic (Tri) structures. In this work, in order to obtain the free energy landscapes, necessary oxygen octahedral tilts are considered not only in tetragonal (T) and rhombohedral (R) but also in M, O and Tri. According to the landscapes in the vicinity of MPB, firstly, the T-R transition path is not unique, since T-R and T-O-R paths have similar barriers; secondly, T-R barrier is ultra-low. Those explain the easy polarization rotation and so the ultra-high piezoelectric constant. Also, ground states are obtained by considering the oxygen octahedral tilts in T, R, M and O, and our results consist with the conclusion by J. Frantti, et.al in 2007. The fully relaxed M is actually T or R, which is indicated by the free energy landscapes. The ground state goes directly from T to R through MPB.

¹in Xi'an Jiaotong University, China

1:51PM B32.00012 ABSTRACT WITHDRAWN —

2:03PM B32.00013 Measuring the curves of dispersion for dielectrics using a low-energy laser and a thermal source of radiation, ROBERT LANNING, CRISTIAN BAHRIM, DON DUPLAN, Lamar University, WEI-TAI HSU, National Central University, Taiwan — We propose a simple and accurate method for finding curves of dispersion for solid and liquid dielectrics using polarized light reflected by their surface near the Brewster angle. A precision of 0.0001 for indices of refraction can be achieved from running a parabolic fit through the experimental data for the parallel component of the reflectance normalized to the total reflectance in a region only 15 degrees wide around the Brewster angle [1]. This precision allows accurate measurements of small changes in the indices of refraction that cannot be measured with other existing methods. For example, such changes can be produced by the temperature variation on the dielectric surface. In this paper we show that using a low-energy laser beam (such as the inexpensive red diode laser of 650 nm) and a thermal (blackbody) source of radiation one can easily generate precise curves of dispersion in the visible and ultraviolet spectrum for any dielectric transparent to this radiation. Our interpretation is based on the Lorentz model for the interaction between dipoles on the dielectric surface and the incident optical field. The average thermal energy of the blackbody source can be associated to an effective frequency. This thermal energy contributes to a higher frequency of oscillation of these dipoles and can be measured as a slight increase in the value of the refractive index. The project was partially supported by the McNair Scholars Program and STAIRSTEP-NSF-DUE grant# 0757057. [1] Bahrim C and Hsu W-T, 2009 *Am. J. Phys.* **77** (4) 337-343.

Monday, February 27, 2012 11:15AM - 1:27PM —

Session B34 DCP: Focus Session: Impact of Ultrafast Lasers II: Multidimensional Methods

107A

11:15AM B34.00001 Control over coherent light fields enables multidimensional coherent spectroscopy and multispectral coherent control, KEITH A. NELSON, Department of Chemistry, MIT — Using a combination of spatial and temporal shaping of optical laser fields, fully coherent spectroscopy and coherent control can be carried out to high order from optical to THz spectral ranges. A single beam with a single femtosecond pulse can be transformed into multiple beams and multiple pulses, reconfigurably under computer control with no human alignment needed, retaining full phase coherence among all the noncollinear fields. This enables multiple-quantum 2D and 3D Fourier transform optical spectroscopy of excitons and exciton-polaritons in inorganic quantum wells and microcavities, in organic J-aggregate films, and in inorganic/organic hybrid structures, the results of which will be discussed. Spatiotemporal shaping also enables coherent control over THz phonon-polariton waves in ferroelectric crystals. The THz waves can be coherently superposed to reach extremely large field amplitudes both in the host crystals and in free space, and the fields can be further enhanced in dipolar antenna and metamaterial structures, enabling highly nonlinear coherent spectroscopy and coherent control in the THz regime. Results from solid, liquid, and gas phases, including multiple-quantum rotational coherences in molecular gases and THz-induced phase transitions in crystalline solids, will be presented. Prospects for further generalization of the approach all the way to the hard x-ray regime will be discussed.

11:51AM B34.00002 Solvent Influenced Fluxionality Studied by Ultrafast Chemical Exchange Spectroscopy, MATTHEW ROSS, Program in Applied Physics, University of Michigan, KEVIN KUBARYCH, Department of Chemistry, University of Michigan — Two-dimensional infrared spectroscopy (2DIR) allows unprecedentedly detailed understanding of the dynamics of chemical systems in the condensed phase. Carbonyl vibrations of small transition metal complexes report intramolecular dynamics and solvent-solute interactions due to their strong oscillator strengths and moderate environmental sensitivity. We studied the fluxional dynamics of iron pentacarbonyl ($\text{Fe}(\text{CO})_5$), which is unique in that it contains nearly perfectly uncoupled vibrational modes. We seek to probe the “molecularity” of condensed phase activated barrier crossings beyond the continuum Kramers theory picture. Using 2DIR chemical exchange spectroscopy, we show how the dynamics of Berry pseudorotation, the only significant mechanism for vibrational mode mixing on our experimental timescale, is sensitive to interactions with the environment. In a wide range of solvents, we have investigated the effects of hydrogen bonding with alcohols and friction from high viscosity alkanes. In addition, we have monitored vibrational energy redistribution as a solvation shell probe. Moreover, recently implemented mid-infrared pulse shaper based methods allow increased flexibility in experimental design, enabling experimental techniques that are not possible using passive optics.

12:03PM B34.00003 Constant-Speed Vibrational Signaling along Polyethyleneglycol Chain up to 60Å Distance, ZHIWEI LIN, IGOR RUBTSOV, Tulane University — A series of azido-PEG-succinimide ester oligomers with a number of repeating PEG units of 0, 4, 8, and 12 (azPEG0, 4, 8, and 12) was investigated using a relaxation-assisted two-dimensional infrared (RA 2DIR) spectroscopy method. The RA 2DIR method relies on the energy transport in molecules and is capable of correlating the frequencies of vibrational modes separated by large through-bond distances. Excitation of the azido group in the compounds at ca. 2100 cm⁻¹ generates an excess energy which propagates in the molecule as well as dissipates into the solvent. We discovered that a part of the excess energy propagates ballistically via the covalent backbone of the molecules with a constant speed of ca. 550 m/s. The transport is described as a propagation of a vibrational wavepacket having a mean-free-path length of ca. 11Å. The discovery has the potential for developing new efficient signal transduction strategies for molecular electronics and biochemistry. It also permits extending the distances accessible in RA 2DIR structural measurements up to ca. 60Å.

12:15PM B34.00004 Two dimensional electronic spectroscopy of coherent energy transfer processes., GREG ENGEL, University of Chicago — No abstract available.

12:51PM B34.00005 Effects of Symmetry on Intense-field Ionization of Heterocyclic Organic Molecules¹, TIMOTHY SCARBOROUGH, DAVID FOOTE, CORNELIS UITERWAAL, University of Nebraska - Lincoln — We report on the ultrafast photoionization of pyridine, pyridazine, pyrimidine and pyrazine. These four molecules represent a systematic series of perturbations into the structure of a benzene ring which explores the substitution of a C-H entity with a nitrogen atom, creating a heterocyclic structure which remains isoelectronic with benzene. Other than pyridine, each molecule has the same molecular formula, with the only difference being the placement of the perturbing nitrogen atoms (ortho-, meta- or para-substitutions). Differences in the intense-field behavior of these molecules are caused by the symmetry of the perturbation to the benzene system, primarily influenced through the interactions of lone-pair states surrounding the nitrogen atoms. Data is recorded under intense-field, single-molecule conditions. 50 fs, 800 nm pulses are focused into the molecular vapor, and ion mass spectra are recorded for intensities of $\sim 10^{13}$ W/cm² to $\sim 10^{15}$ W/cm². We measure ion yields in the absence of the focal volume effect without the need for deconvolution of the data. For all targets, stable singly- and doubly-charged parent ions (C_{6-n}H_{6-n}N_n⁺⁽⁺⁾) are observed with features suggesting resonance enhancement (REMPI).

¹This material is based upon work supported by the National Science Foundation under Grant Nos. PHY-0855675 and PHY-1005071.

1:03PM B34.00006 Experimental determination of Hamiltonian via 3D Fourier-transform spectroscopy¹, HEBIN LI, ALAN BRISTOW, MARK SIEMENS, GALAN MOODY, STEVEN CUNDIFF, JILA, University of Colorado and National Institute of Standards and Technology, Boulder, CO 80309 — Prediction and control of quantum mechanical processes requires knowledge about the system Hamiltonian. For coherent control, information about interfering quantum pathways or the underlying Hamiltonian is essential for achieving deterministic control. Even in cases of closed-loop control, a priori knowledge about the system Hamiltonian provides guidance for designing an efficient learning algorithm and a good initial guess for faster convergence. The complete Hamiltonian of a complicated system, especially the effects of inter-particle interactions and coupling to the environments, can only be determined experimentally. Here we demonstrate an experimental determination of the Hamiltonian of an atomic vapor, achieved by using 3-dimensional Fourier transform (3DFT) spectroscopy. The 3DFT spectra provide complete information about the third-order coherent response of the vapor. The contributions from different quantum pathways are unambiguously isolated such that the components of the Hamiltonian, including energy levels, dipole moments and relaxation rates, can be determined. The 3DFT spectroscopy opens an avenue towards identifying the Hamiltonian of complex molecular systems, which can be useful for designing coherent control strategies and for studying the molecular dynamics.

¹The work was supported by the NSF Physics Frontier Center program through the JILA AMO Physics Center.

1:15PM B34.00007 Nonradiative-decay mechanisms in CdSe nanoparticles: MUPPETS (multiple population-period transient spectroscopy) in excitonic systems¹, MARK BERG, KALYANASIS SAHU, SEAN KERN, Dept of Chemistry and Biochemistry, University of South Carolina — Nonradiative decay in semiconductor nanoparticles on the picosecond to nanosecond time scale is complex and poorly understood. Here, two-dimensional (2D) incoherent spectroscopy (MUPPETS) is applied to these processes in CdSe nanoparticles. For the first time, MUPPETS is extended to multilevel, excitonic systems to yield an analog of 2D coherent correlation spectroscopies. In core-only CdSe particles, the transfer of an excited electron from the core to the surface follows a highly dispersed, power-law decay in 1D measurements. 2D-MUPPETS measurements show that the rate dispersion is not due to relaxation nor due to multi-step kinetics, but results solely from particle-to-particle heterogeneity in the barrier to the surface. A model in which surface defects are distributed within the dipolar electric field of the particle accounts for the power-law decay. A second study of CdSe:ZnS core-shell particles uses correlation MUPPETS to distinguish biexcitons from photoproducts with a fast relaxing single exciton. Even when both species have similar lifetimes, they are distinguishable by having opposite signs and different symmetries in the two time intervals of a 2D experiment. Potential correlations between biexciton and exciton rates are sought, but are not found.

¹Based upon work supported by the National Science Foundation under CHE-0809306 and CHE-1111530

Monday, February 27, 2012 11:15AM - 1:51PM —
Session B35 DCP: General Theory 107B

11:15AM B35.00001 The evolution of dielectric properties of sodium, silicon and argon clusters¹, KOBLAR JACKSON, Department of Physics, Central Michigan University, Mt. Pleasant, MI 48859, MINGLI YANG, Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China, LI MA, Department of Physics, Northwest University, Xi'an 710069, China, JULIUS JELLINEK, Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439, USA — We used a computational scheme based on site-specific polarizabilities to study the evolution of the dielectric properties of sodium, silicon and argon clusters. In this approach, the total cluster polarizability is decomposed into local dipole (LD) and charge-transfer (CT) parts. The local dipole part measures the redistribution of charge within an atomic volume, while the CT part describes the movement of charge between volumes. We find distinct differences in the relative contributions of the LD and CT components to the total polarizability as a function of cluster size for the different cluster types and relate this to the development of metallic behavior. The method also directly probes the extent of electrostatic screening of the cluster interior to an applied electric field.

¹This work was supported by the Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences, U.S. Department of Energy under Contracts No. DE-AC02-06CH11357 (JJ) and DE-SC0001330 (KAJ).

11:27AM B35.00002 Topological Solitons between Two Magic Number In-clusters on a Si(100) Surface Break the Even/Odd Symmetry in the Self-Selection of Their Distance, YUH-LIN WANG, M.Y. LAI, J.P. CHOU, C.M. WEI, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan, O.A. UTAS, N.V. DENISOV, V.G. KOTLYAR, D. GRUZNEV, A. MATETSKY, A.V. ZOTOV, A.A. SARANIN, Institute of Automation and Control Processes, Vladivostok, Russia — Depositing particles randomly on a 1D lattice is expected to result in an equal number of particle pairs separated by even or odd lattice units. Unexpectedly, the even-odd symmetry is broken in the self-selection of distances between indium magic-number clusters on a Si(100)-2x1 reconstructed surface. Cluster pairs separated by even units are less abundant because they are linked by silicon atomic chains carrying topological solitons, which induce local strain and create localized electronic states with higher energy. Our findings reveal a unique particle-particle interaction mediated by the presence or absence of topological solitons on alternate lattices.

11:39AM B35.00003 Determination of ground state structures of selected medium-sized clusters via first-principles global search, JIJUN ZHAO, Dalian University of Technology — Due to the existence of numerous local isomers on the potential energy surface, determining the most stable structures of medium-sized clusters is one of the most challenging tasks in cluster physics. Recent years, we have explored the potential energy surface of medium-sized clusters using first-principles calculations combined with global search methods like genetic algorithm and simulate annealing. The examples on a few selected examples such as B_{80}/B_{101} , $Na_{1-3}Si_{1-11}$, and $(WO_3)_{2-12}$ clusters will be briefly illustrated. The size-dependent electronic properties of these clusters will also be discussed and compared with available experimental data.

11:51AM B35.00004 Novel building blocks for materials by design: Janus particles and other patchy colloids¹, RIGOBERTO HERNANDEZ, MATTHEW C. HAGY, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332-0400 — The emergent assembly of nonisotropically structured colloidal particles can lead to novel materials with requisite optical or mechanical properties. We have developed two models—one that includes detailed interactions between particles and another that coarse-grains the interactions—so as to explore the equilibrium and dynamics effected by varying interaction heterogeneities. In particular, we have performed a series of simulations of systems consisting of Janus particles—in which each of two hemispheres can be characterized by a single interaction type such as charge or degree of hydrophobicity. The equilibrium structure of Janus clusters has been the subject of experimental and theoretical studies by Grannick and coworkers. We find that the bulk Janus systems give rise to surprising equilibrium structure and dynamics which can be tuned through both the volume fraction and the interactions. The coarse-grained model provides surprisingly good agreement with the more detailed particle-model for the equilibrium structure while overestimating the relaxation rates.

¹This research partially supported by NSF CHE 1112067 utilizing HPC resources provided through NSF CHE 0946869 and XSEDE No. CTS090079.

12:03PM B35.00005 Structure and Diffusion of Nanoparticles at the Liquid-Vapor Interface, SHENGFENG CHENG, GARY GREST, Sandia National Laboratories — Large-scale molecular dynamics has been used to simulate a layer of nanoparticles diffusing on the surface of a liquid. Both a low viscosity liquid, represented by Lennard-Jones monomers, and a high viscosity liquid, represented by linear homopolymers, are studied. The organization and diffusion of the nanoparticles are studied as the coverage and the contact angle between the nanoparticles and liquid are varied. Results are compared to simulations of identical nanoparticles in two-dimensions. We show that when the interaction between the nanoparticles and liquid is reduced the contact angle increases and the nanoparticles ride higher on the liquid surface, which enables them to diffuse faster. In this case the short range order is also reduced as seen in the pair correlation function. For low contact angles, nanoparticles diffuse into the liquid for high coverages.

12:15PM B35.00006 Supersymmetric Quantum Mechanics For Atomic Electronic Systems¹, THOMAS MARKOVICH, MASON BIAMONTE, DON KOURI, University of Houston — We employ our new approach to non-relativistic supersymmetric quantum mechanics (SUSY-QM), (J. Phys. Chem. A 114, 8202(2010)) for any number of dimensions and distinguishable particles, to treat the hydrogen atom in full three-dimensional detail. In contrast to the standard one-dimensional radial equation SUSY-QM treatment of the hydrogen atom, where the superpotential is a scalar, in a full three-dimensional treatment, it is a vector which is independent of the angular momentum quantum number. The original scalar Schrödinger Hamiltonian operator is factored into vector “charge” operators: $\vec{Q}$ and $\vec{Q}^\dagger$. Using these operators, the first sector Hamiltonian is written as $H_1 = \vec{Q}^\dagger \cdot \vec{Q} + E_0^1$. The second sector Hamiltonian is a tensor given by $H_2 = \vec{Q}\vec{Q}^\dagger + E_0^1$ and is isospectral with H_1 . The second sector ground state, $\vec{\psi}_0^{(2)}$, can be used to obtain the excited state wave functions of the first sector by application of the adjoint charge operator. We then adapt the aufbau principle to show this approach can be applied to treat the helium atom.

¹Supported by R.A. Welch Foundation Grant E-0608

12:27PM B35.00007 Ion correlations in the electrical double layer near liquid/liquid interfaces, GUILLERMO IVAN GUERRERO GARCIA, MONICA OLVERA DE LA CRUZ, Department of Chemistry and Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, USA — Equilibrium properties of the electrical double layer of monovalent salts near the interface between two immiscible electrolyte solutions are studied via Monte Carlo simulations, for several electrolyte concentrations. The corresponding results are collated with experimental data and the classical Verwey-Niessen theory of point ions. The observed differences between the simulation data and the mean field approach of “back-to-back” electrical double layers stresses the importance of including properly ionic correlations near dielectric discontinuities.

12:39PM B35.00008 Molecular Dynamics Simulation of Adsorption of Methane and Chloromethane on Molybdenum via Hybrid EAM/OPLS Interactions¹, GARY LEUTY, MESFIN TSIGE, Department of Polymer Science, The University of Akron — The question of liquid adsorption on the surface of a solid substrate has been of major interest to computational science even from its inception. Accurate depictions of adsorption phenomena require accurate modeling of both phases of the simulated system. In cases in which accuracy of the models leads to the adoption of potentially inconvenient or incompatible force fields, questions arise as to whether joint systems can perform as well as needed to gather optimal data. The current investigation uses molecular dynamics (MD) tools to focus, in part, on how well-developed models for liquid simulation (OPLS, built on a Lennard-Jones foundation) can combine with tested models for metals (based on functionals of electron density) to describe the adsorption of methane and chloromethane on the surface of molybdenum. Comparisons have been made between the differences in effect of a hybrid EAM/OPLS system and systems focusing solely on Lennard-Jones-based interactions, as well as the effect of large asymmetry and polarity differences in adsorbate species, on the structure and dynamics of layers adsorbed directly at the surface of the metal substrate. Preliminary results suggest that the surface landscape and corrugation play a significant role in choice of surface binding sites.

¹Authors gratefully acknowledge support from the ACS Petroleum Research Fund and the National Science Foundation.

12:51PM B35.00009 First Principles Study of Adsorption of O_2 on Al Surface with Hybrid Functionals, HENGRUI LIU, HONGJUN XIANG, XIN GAO GONG, Key Laboratory for Computational Physical Sciences (MOE) and Surface Physics Laboratory, Fudan University — Adsorption of O_2 molecule on Al surface has been a long standing puzzle for the first principles calculation. We have studied the adsorption of O_2 molecule on the Al(111) surface using hybrid functionals. In contrast to the previous LDA/GGA, the present calculations with hybrid functionals successfully predict that O_2 molecule can be absorbed on the Al(111) surface with a barrier around 0.2~0.4 eV, which is in good agreement with experiments. Our calculations predict that the LUMO of O_2 molecule is higher than the Fermi level of the Al(111) surface, which is responsible for the barrier of the O_2 adsorption.

1:03PM B35.00010 Octaselenododecane ($C_4H_8Se_8$): a novel polyselenoether crown macrocycle¹, STEVEN RICHARDSON, Howard University, MICHAEL MEHL, MARK PEDERSON, Naval Research Laboratory — In this work we have used density-functional theory (DFT/GGA-PBE) to calculate the structural, electronic, and vibrational properties of octaselenododecane ($C_4H_8Se_8$), a novel twelve-membered crown-shaped heterocycle which contains four diselenide groups.² Our all-electron DFT calculations have yielded results that are in excellent agreement with the observed experimental x-ray diffraction data and infrared and Raman vibrational spectra for the solid state phase of octaselenododecane. In addition to obtaining good general agreement with the selected IR and Raman frequencies reported to lie within the range of 282-2925 cm^{-1} , we have obtained other vibrational modes which have not been reported in the literature. In particular, we have computed a Raman active mode at 267 cm^{-1} which is in good agreement with the experimental band at 282 cm^{-1} and have determined that it represents significant asynchronous stretches of diselenide groups within the heterocycle. Our gas phase calculations also show the presence of strong low frequency distortions that are suppressed in the crystal due to close Se-Se intramolecular interactions.

¹We are grateful to the Office of Naval Research for financial support of this work.

²G. Hua, J. M. Griffin, S. E. Ashbrook, A. M. Z. Slawin, and J. D. Wollins, *Angew. Chem. Int. Ed.* **2011**, 50, 4123-4126.

1:15PM B35.00011 Bias Dependent Switching Behavior of STM-Induced Melamine/Cu(001) Switch, TATSUHIKO OHTO, KOICHI YAMASHITA, Department of Chemical System Engineering, The University of Tokyo, HISAO NAKAMURA, Nanosystem Research Institute (NRI), RICS, AIST, IVAN RUNGGER, STEFANO SANVITO, School of Physics and CRANN, Trinity College Dublin — The manipulation or stimulation of molecules using Scanning Tunneling Microscopy (STM) is a technique that recently has deserved deep attention for its potential applications in molecular electronics. The melamine/Cu(001) system was found to show switching behavior in very wide range of applied bias. Although its mechanism was analyzed by a statistic model, the relationship between the switching rate and bias is still far to be fully clarified. In this context, we performed a campaign of exhaustive first-principles calculations to obtain most of the parameters for resonance model; such model is able to predict the switching rate as functions of bias and current. The energy barrier was calculated using the nudged elastic band method, with the aid of recent implementation of current-induced forces into SMEAGOL code, which is based on the nonequilibrium Green's function method with Density Functional Theory. The electron-phonon coupling and then the Inelastic Tunneling Spectroscopy signal are calculated to validate the one-phonon approximation. The spatial distribution of molecular orbitals and their coupling with vibrational modes are very useful to understand the switching behavior.

1:27PM B35.00012 ABSTRACT WITHDRAWN —

1:39PM B35.00013 Kirkwood-Buff analysis of liquid mixtures in AdResS: Towards an open boundary simulation scheme, DEBASHISH MUKHERJI, Max-Planck Institute for Polymer Research, NICO VAN DER VEGT, Center for Smart Interfaces, TU Darmstadt, KURT KREMER, Max-Planck Institute for Polymer Research, LUIGI DELLE SITE, Department of Mathematics, FU Berlin — Many biophysical processes in water are determined by interactions of cosolvents with the hydration shells of dissolved (bio)molecules. Computational approaches to study these systems are mostly limited to the closed boundary simulations. While closed boundaries are perfectly suitable in many cases, problems arise when concentration fluctuations are large, or intimately linked to the physical phenomenon. For example, in non-ideal mixtures of water/cosolvent and a biomolecule, the excess of water/cosolvent, close to a protein surface, leads to water/cosolvent depletion elsewhere. This complicates a comparison with experiments that are conducted under osmotic conditions. Therefore, we use Adaptive Resolution Simulation (AdResS) scheme, which describes a small sub-volume of a much larger system in atomistic detail, maintaining thermodynamic equilibrium with a surrounding coarse grained reservoir. We show that the Kirkwood-Buff integrals (KBI), which directly connect thermodynamic properties to the molecular distributions, can be efficiently calculated within the small open boundary all atom region and the coarse-grained reservoir maintains the correct particle fluctuations. Results will be presented for the methanol/water mixture and solvation of amino acids in urea/water mixture.

Monday, February 27, 2012 11:15AM - 2:15PM —
Session B36 DCP: Focus Session: New Energy II 107C

11:15AM B36.00001 Theories of plasmon enhanced optical processes important in solar energy, GEORGE SCHATZ, Northwestern University — This talk will focus on the development of electronic structure methods that can be combined with electrodynamics calculations to describe enhancement in chemical reaction rates that arise from plasmon excitation of noble metal nanoparticles. Two types of enhancement are described: passive and active. In the passive case, the nanoparticle produces an enhanced electromagnetic field that acts externally to the nanoparticle to enhance a photochemical process, while in the active case, plasmon excitation leads to electron transfer to or from the noble metal nanoparticle. Examples and applications of each type will be described.

11:51AM B36.00002 Porphyrin Molecular Multilayer Thin-Films on Gold (111) Electrodes for Electro-optical Applications, ALEXANDRA KRAWICZ, Chemistry Department, RPI, GUOQUANG QIAN, KIM LEWIS*, Physics Department, RPI, PETER DINOLFO*, Chemistry Department, RPI — We have developed a Layer-by-Layer (LbL) method for the fabrication of thin-film molecular multilayers on gold (111) electrodes. Copper(I) catalyzed azide-alkyne cycloaddition (CuAAC) coupling reactions were used for surface attachment and subsequent LbL deposition of porphyrin building blocks. The electrochemical and photophysical properties of the thin-films can be tuned through synthetic modification of the individual components, resulting in new porphyrin multilayers for applications in light harvesting and molecular electronics. Herein, we demonstrate the reproducible growth trends and optical properties of these films. Multilayer growth was followed by UV-Vis absorption and reflectance spectroscopy. Film thickness (FT) and optical constants were obtained from spectroscopic ellipsometry. Topology and surface roughness was examined by TM-AFM, while the copper content was quantified by XPS. The redox characteristics were studied by electrochemical methods, whereas the conductance of individual porphyrin constructs was examined by STM using the molecular break junction method. The multilayers show consistent linear growth in absorbance and FT over tens of layers and continuity in their molecular structure.

12:03PM B36.00003 Nonadiabatic Excited-State Molecular Dynamics (NA-ESMD): Numerical tests of convergence and parameters, TAMMIE NELSON, Los Alamos National Laboratory, SEBASTIAN FERNANDEZ-ALBERTI, Universidad Nacional de Quilmes, VLADIMIR CHERNYAK, Wayne State University, ADRIAN ROITBERG, University of Florida, Gainesville, SERGEI TRETIKOV, Los Alamos National Laboratory — Nonadiabatic molecular dynamics simulations, involving multiple coupled potential energy surfaces, often requires a large number of independent trajectories in order to achieve the desired convergence of the results, and simulation relies on different parameters that should be tested and compared. In addition to influencing the speed of the simulation, the chosen parameters combined with frequently implemented approximations can lead to unanticipated changes in the accuracy of the simulated dynamics. We have previously developed a nonadiabatic excited state molecular dynamics (NA-ESMD) methodology employing Tully's fewest switches surface hopping (FSSH) algorithm. In this study, we seek to investigate the impact of the number of trajectories and the various parameters on the simulation of the photoinduced dynamics of distyrylbenzene (a small oligomer of polyphenylene vinylene) within our developed framework. Various user-defined parameters are analyzed: classical and quantum integration time steps, and the number of trajectories used for statistical averaging. Common approximations such as reduced number of nonadiabatic coupling terms and the classical path approximation (CPA) are also investigated.

12:15PM B36.00004 Probing Nanointerfaces of Nanoparticle-Based Solar Energy Conversion: Molecular Dynamics on the Angstrom Scale¹, RICHARD OSGOOD², Columbia University, Laboratory for Light-Surface Interactions, Center for Integrated Science and Engineering — Charge-induced surface chemistry following solar-illumination of nanometer-scale semiconductor particles is one possible route to low-cost solar energy conversion. Because of their high surface to volume ratio interfaces play a major role in the performance of this technology and thus the physics of charges interacting with adsorbed molecules is of central interest. In this talk, after a brief review of related work, we will focus on our advances in understanding molecular-dissociation-dynamics at the interface of nanometer-scale TiO₂ crystals and large organic molecules. Clearly the standard probes of beam-based molecule dynamics are not easily adaptable to small nanointerfaces. Instead our work uses STM imaging to examine dynamics of fragments following tip-induced electron injection into organic molecules on TiO₂ (110) and on ~10nm nanocrystals (110). Our experiments have used halogenated anthracene to probe the efficiency and fragment trajectory following dissociative electron capture. Our work has examined nanoparticle synthesis, adsorbate-molecule orientation, thermal and injected-electron chemistry, and adsorbate charge-mediated fragmentation trajectories.

¹DOE Grant NO. DE-FG02-90ER14104

²Second author: Denis Potapenko

12:51PM B36.00005 Band gap engineering iron pyrite for sustainable solar energy conversion, ALISON HATT, Lawrence Berkeley National Lab, ALEXANDER SEBENIUS, Harvard University, JEFFREY NEATON, Lawrence Berkeley National Lab — In the quest to develop sustainable materials for solar energy conversion, iron pyrite (FeS₂) holds great promise as a solar absorber. The electronic band gap of FeS₂, however, is not well matched to the solar spectrum. Here we explore chemical doping as a strategy to engineer the band gap of FeS₂, as has been successfully demonstrated with other semiconducting materials. Using first-principles calculations, we first establish the relationship between pressure, lattice distortions, and the electronic structure of FeS₂, and rationalize the results in terms of distortions in the crystal-field splitting of Fe. We then investigate the effects of doping FeS₂ with transition metal elements, wherein our strategy is guided by the knowledge of band gap dependence on local distortions.

1:03PM B36.00006 Photochemistry of chemisorbed and physisorbed O₂ on reduced rutile TiO₂(110), GREG KIMMEL, Pacific Northwest National Laboratory — The ultraviolet (UV) photon-stimulated reactions of oxygen on TiO₂(110) are studied. For chemisorbed O₂, the photochemistry depends on the O₂ coverage. For small coverages, only ~14% desorbs while the rest either dissociates during UV irradiation, or remains molecularly adsorbed on the surface. For the maximum coverage of chemisorbed oxygen, the fraction of O₂ that photodesorbs is ~40%. However when physisorbed O₂ is also present, ~70% of the initially chemisorbed O₂ photodesorbs. Experiments using O₂ isotopologues show that UV irradiation results in exchange of atoms between the chemisorbed and physisorbed oxygen. Annealing chemisorbed oxygen to 350 K maximizes these exchange reactions. The exchange products photodesorb in the plane perpendicular to the bridge-bonded oxygen rows at an angle of 45°. Remarkably, the chemisorbed species is stable under multiple cycles of UV irradiation with physisorbed O₂, and the atoms in the chemisorbed species can be changed from ¹⁸O to ¹⁶O and then back to ¹⁸O via the exchange reactions. The results show that annealing oxygen adsorbed on TiO₂(110) to ~350 K produces a stable chemical species with interesting photochemical properties. Possible forms for the photoactive species include O₂ adsorbed in a bridging oxygen vacancy or tetraoxygen.

1:39PM B36.00007 Energy Materials in Extreme Environments, RUSSELL J. HEMLEY, Director, Geophysical Laboratory, Carnegie Institution of Washington — The critical shortage of abundant, affordable, and clean energy calls upon novel materials with extreme properties for energy production, storage, conversion, and transfer that are superior to materials that now exist or are in use today. Twenty-first century energy technology also demands enhanced performance from existing materials under extreme environments of pressure, temperature, chemistry, radiation, and electromagnetic fields. Investigating the behavior of materials in extreme pressures and temperatures, in particular, provides the fundamental knowledge needed to address these problems. These studies are leading to the discovery of both new materials with enhanced performance as well as new physical and chemical phenomena, and take advantage of advances at national x-ray, infrared, neutron, and laser facilities. An important example is the continued study of hydrogen-rich materials, from investigations of transformations in pure hydrogen, which has now been pressurized well above 300 GPa, to the discovery of new hydrogen storage materials and hydriding reactions induced by extreme conditions. Other examples include studies of carbon-based materials, which are also deepening our understanding of carbon sources and cycling within the planet.

Monday, February 27, 2012 11:15AM - 2:15PM –
Session B37 SPS: SPS Undergraduate Research I 108

11:15AM B37.00001 BREAK –

11:27AM B37.00002 Committee Work or How I Learned to Stop Complaining and Love the Process, CABOT ZABRISKIE, Old Dominion University — Over the course of their career, most American scientists, be it at an independent university, government lab, or in the private sector, will at some point receive public funding to perform their research. Yet most of these individuals have only a vague sense of how their money was originally allocated. Most may be familiar with the intricacies of NSF, NIST, or any one of the agencies that compose the alphabet soup of the Federal Government, but what about before that, when the money and subsequent directives are being allocated to these agencies? In other words, what about congress? In an effort to better understand this process and to contribute to the reciprocal understanding by congress I embarked on a 10 week internship with the House Committee on Science, Space, and Technology, funded by the John and Jane Mather Foundation as part of the SPS Summer Internship Program. In my time with the committee I was able to attend multiple hearings and seminars on the Hill and see how policies with regard to science are created. In this talk I will discuss my experience and observations, for example that no one wished to be viewed as anti-science and that even those who are looked upon as very critical are often more critical of the opposing side of the aisle than of the actual science itself. In fact, I saw that the biggest hindrance to science in the political setting is the lack of understanding of just what it is. This the same problem faced by the general public and the steps toward fixing this issue may very well be the same.

11:39AM B37.00003 Wetting in Color: Designing a colorimetric indicator for wettability, KEVIN RAYMOND, IAN B. BURGESS, NATALIE KOAY, MATHIAS KOLLE, MARKO LONCAR, JOANNA AIZENBERG, Harvard University — Colorimetric litmus tests such as pH paper have enjoyed wide commercial success due to their inexpensive production and exceptional ease of use. While such indicators commonly rely on a specific photochemical response to an analyte, we exploit structural color, derived from coherent scattering from wavelength-scale porosity rather than molecular absorption or luminescence, to create a Wetting-in-Color-Kit (WICK). This inexpensive and highly selective colorimetric indicator for organic liquids employs chemically encoded inverse-opal photonic crystals to translate minute differences in liquids' wettability to macroscopically distinct, easy-to-visualize color patterns. The highly symmetric re-entrant inter-pore geometry imparts a highly specific wetting threshold for liquids. We developed surface modification techniques to generate built-in chemistry gradients within the porous network. These let us tailor the wettability threshold to specific liquids across a continuous range. As wetting is a generic fluidic phenomenon, we envision that WICK could be suitable for applications in authentication or identification of unknown liquids across a broad range of industries.

11:51AM B37.00004 EPR spectral study and modeling of lithium borovanadate $\text{RLi}_2\text{OB}_2\text{O}_3\text{KV}_2\text{O}_5$ glasses¹, BRANDON POLLPETER, BLANE BAKER, BIKESH DAHAL, William Jewell College, STEVE FELLER, Coe College — Utilizing electron paramagnetic resonance EPR spectroscopy, lithium borovanadate $\text{RLi}_2\text{OB}_2\text{O}_3\text{KV}_2\text{O}_5$ glasses with R = 0.4 and K ranging from 0.1 to 0.5 were analyzed in order to elucidate the environment of unpaired $3d^1$ electrons. Transitions associated with coupling of such electrons to vanadium nuclear spins were identified and modeled to reveal both g factor and A factor values. For a system with K = 0.3, representative data include: $g_{\parallel} = 1.9242$, $g_{\perp} = 1.9693$, $A_{\parallel} = 184.3768 \text{ cm}^{-1}$, $A_{\perp} = 64.6568 \text{ cm}^{-1}$, $\Delta g_{\parallel} = 0.0781$, $\Delta g_{\perp} = 0.0330$, and $\Delta g_{\parallel}/\Delta g_{\perp} = 2.3670$. A comparison revealing $g_{\parallel} < g_{\perp} < g_e$ is indicative of localized electrons residing in tetragonally-distorted octahedral sites. A slight increase observed in $\Delta g_{\parallel}/\Delta g_{\perp}$ values when K = 0.1 to K = 0.3 is further evidence of a possible elongation of the octahedral site associated with increasing K values. This pattern, however, is not present in systems with K values greater than 0.3, suggesting that perhaps no further elongation of the site is possible due to bond constraints. A comprehensive model will be presented to summarize data for the entire family of lithium borovanadates studied here.

¹This work was supported in part by NSF-DMR 0904615.

12:03PM B37.00005 Metal-Metal Oxide Nanocomposite for Solar Cell Applications¹, H. GEMAR, K. GHOSH, Department of Physics, Astronomy and Materials Science, Missouri State University, Springfield, MO 65897 — Currently, there is a large need for alternative energies and one good option is solar cells. A High efficiency solar cell generally consists of a number of thin layers: active layer consisting of a material having high absorption in the solar spectrum, transparent conducting layer, *p*- and *n*-type materials used to fabricate the junction, and electrodes for good Ohmic contacts. The presence of metal nanoparticles in metal oxide films improves significantly the solar absorbance of metal oxide films. The absorption depends on the bandgap of metal oxides which can be tuned by incorporation of metal nanoparticles. Tuning of the bandgap and absorption are the very important parameters to fabricate the solar cell devices. Thin films of M-MO (M = transition metals Co and Ni) nanocomposite have been grown on quartz substrate using pulse laser deposition technique. Structural properties have been characterized using X-ray diffraction and scanning electron microscopy. Electrical properties with and without light and absorption spectra have been measured using I-V characterization and UV-VIS spectroscopy techniques. Detailed results will be discussed in the presentation.

¹This work is supported by National Science Foundation (Award Number DMR-0907037).

12:15PM B37.00006 Electrical Characterization of Flexible Titanium Dioxide Memristors, VICTORIA ROSBOROUGH, NADINE GERGEL-HACKETT, Mary Baldwin College — The memristor is a new fundamental circuit element with a resistance that depends on the magnitude and polarity of the voltage applied to it and the length of time that voltage is applied. Memristors are also nonvolatile, which means that when the bias is removed, a memristor retains its last resistive state. While memristors have potential applications ranging from alternative computer architectures to memory in inexpensive lightweight wearable sensors, the mechanism behind its switching is not well understood. One of the major questions to be resolved is whether memristive switching is electric field dependent or charge dependent. In the former case, a minimum bias is needed for switching to occur. In the latter case, a minimum amount of charge needs to pass through the device to cause switching. I will present the results of electrically characterizing flexible memristors that consist of a nm-thick layer of titanium dioxide sandwiched between two metal contacts in an effort to help establish whether their switching is charge or field-driven.

12:27PM B37.00007 Two-Dimensional Ordering of DNA Origami Using Stacking Bonds, YOSUKE SUGISHITA, LEE WIZDA, PRASHANT SHARMA, Department of Physics, Suffolk University — Utilizing the DNA Origami method we have designed nano-scale self-assembled structures. These structures are made using a 7000 base pair long single stranded DNA as a scaffold that is held in place by shorter single stranded DNA molecules using Watson-Crick DNA base pairings. The staples were chosen to attach at certain specific sites of the scaffold DNA so that a well-defined planar structure of double stranded DNA can be created at room temperature. In designing these origami structures we made use of the computer application caDNAo. Two geometrical structures with differing symmetries were created using the same scaffold. Edges of these structures were modified in such a way that the double stranded DNA of one structure's edge can stack onto the edge of the second structure. Similar modifications were recently shown by Woo and Rothmund (Nat Chem., 1755-4330, 2011) to enable the formation of extended DNA origami structures. We intend to extend this method to create two-dimensional square and triangular lattice structures. We discuss our experimental results and implications of this method for nano-scale self-assembly.

12:39PM B37.00008 Synthesis of Magnetic Nanoparticles for Biosensing Studies Using Magneto-Impedance Technology¹, ROSEMARY SHELLEN, Covenant College, RAMON RUIZ, KRISTEN STOJAK, NICHOLAS LAURITA, ANURAG CHATURVEDI, University of South Florida, PHILLIP BROUSSARD, Covenant College, MANH-HUONG PHAN, HARIHARAN SRIKANTH, University of South Florida — Polymer nanocomposites (PNCs) have been shown to be a compact and durable solution for applications such as electromagnetic interference shielding and magnetically tunable microwave devices. We report studies aimed at exploring applications of PNCs to aid in bio-sensing, using the Giant Magneto-Impedance (GMI) effect. GMI is a change in the ac impedance of a ferromagnetic conductor in a varying dc magnetic field, and has been shown to be about 500 times more sensitive than its counterpart, Giant Magneto-Resistance (GMR). In our study, magnetite (Fe_3O_4) nanoparticles (mean size, $6 \pm 2 \text{ nm}$) were synthesized by thermal decomposition and dispersed in a polymer provided by the Rogers Corporation to create PNCs with 20, 50, and 80 wt% compositions. The GMI of an amorphous magnetic ribbon was measured with and without the PNCs layered on the ribbon. The effects of nanoparticle concentration on the GMI sensitivity were studied, with a view toward applications in highly sensitive bio-molecular detection.

¹This work was supported by NSF REU program (award No DMR-1004873).

12:51PM B37.00009 Development of a Protocol to Study the Conformational Stability of Protein Using the Model Protein Cytochrome *c*¹, JESSICA STAVOLE, BENJAMIN OPPERMAN, Department of Biology, Xavier University, JUSTIN LINK, Department of Physics, Xavier University — The function of a protein is inherently dependent upon the proper folding and the resulting tertiary structure of the molecule. The development of an unfolding procedure is desirable so that the structural stability of a protein molecule can be determined through the change in thermodynamic properties of the unfolding reaction. The protein cytochrome *c* has long been used in protein structural studies and monitored by circular dichroism (CD), absorption, and fluorescence spectroscopic techniques. Single amino acid mutations of wild type cytochrome *c* were unfolded both chemically and thermally using the developed protocol and the unfolding was monitored by CD spectroscopy. Thermodynamic properties such as Gibbs free energy, enthalpy and melting temperature were used to interpret the results. The mutant proteins were calculated to have different thermodynamic properties than that of the native cytochrome *c* during the unfolding process. When denatured at a lower pH, the proteins thermally unfolded more readily. The objective of this session is to present recent work addressing the denaturation of wild type and mutant proteins.

¹This work was supported by The John A. Hauck Foundation and Xavier University.

1:03PM B37.00010 Genotyping and phenotyping of an epigenetic modifier *Unstable factor for orange1 (Ufo1)* in maize, KARISA BOWERSOX, Lock Haven University of Pennsylvania, SURINDER CHOPRA, Penn State University — Pericarp color 1 is a model system for the study of epigenetic gene regulation. It has more than 100 alleles that contribute to the color of the pericarp and cob glume of maize. Unstable factor for orange 1 (Ufo1) is a spontaneous dominant mutation that leads to a gain in pigmentation due to a decrease in methylation in *p1* genes. This decrease in methylation of cytosine in the DNA leads to changes in chromatin structure. Finding the mechanism for this spontaneous mutation can lead to way of preventing the mutation increasing production colorless maize for food production. Through genotyping and phenotyping fine gene mapping, gene expression and whole genome profiling can be accomplished for plants with the Ufo1 mutation present.

1:15PM B37.00011 Computational and Electronic Analog Implementation of the Hodgkin-Huxley Model of Action Potentials in Neurons¹, PETER SMITH, JUSTIN LINK, Xavier University — Alan Loyd Hodgkin and Andrew Huxley's mathematical model of action potential initiation and propagation in neurons is one of the greatest hallmarks of biophysics. Two techniques for implementing the Hodgkin-Huxley model were explored: computational and electronic analog. Computational modeling was done using NEURON 7.1. NEURON is a free, robust, and relatively user friendly simulation environment that enables quantitatively accurate computational modeling of neurons and neural networks. An analog electronic circuit was built using field-effect transistors (FETs) to simulate the non-linear, voltage-dependent (sodium and potassium) conductances that are responsible for membrane excitability. While the electronic analog qualitatively reproduces many of the key features of the action potential including overall shape, inactivation period, and propagation, it was difficult to quantitatively reproduce the Hodgkin-Huxley model. In addition, while the relative cost to build circuits equivalent to small membrane patches is minimal (~\$50), implementation of larger cells or networks would prove uneconomical. Still, both techniques are viable avenues toward introducing interdisciplinary research into either a computational or electronics lab setting at the undergraduate level.

¹This work was supported by The John A. Hauck Foundation and Xavier University.

1:27PM B37.00012 First-principles calculation of structural and electronic properties of memantine (Alzheimer's disease) and adamantane (anti-flu) drugs¹, KIRSTEN MIDDLETON, GUOPING ZHANG, Department of Physics, Indiana State University, THOMAS F. GEORGE, University of Missouri-St. Louis — Memantine is currently used as a treatment for mild to severe Alzheimer's disease, although its functionality is complicated. Using various density functional theory calculations and basis sets, we first examine memantine alone and then add ions which are present in the human body. This provides clues as to how the compound may react in the calcium ion channel, where it is believed to treat the disease. In order to understand the difference between calcium and magnesium ions interacting with memantine, we compute the electron affinity of each complex. We find that memantine is more strongly attracted to magnesium ions than calcium ions within the channel. By observing the HOMO-LUMO gap within memantine in comparison to adamantane, we find that memantine is more excitable than the anti-flu drug. We believe these factors to affect the efficiency of memantine as a treatment of Alzheimer's disease.

¹Thanks to the Department of Energy grant #DE-FG02-06ER46304, the Department of Chemistry and Physics at Indiana State University, Eric Glendening for his help with Gaussian and other calculations, and Payton Kuhnle for her calculations with memantine.

1:39PM B37.00013 Construction and Operation of a Differential Hall Element Magnetometer¹, MATTHEW W. CALKINS, Dept. Physics, Univ. Florida, PHILIP D. JAVERNICK, Dept. Chem. and Physics, Augusta State Univ., PEDRO A. QUINTERO, YITZI M. CALM, MARK W. MEISEL, Dept. Physics, Univ. Florida and NHMFL — A Differential Hall Element Magnetometer (DHEM) was constructed to measure the magnetic saturation and coercive fields of small samples consisting of magnetic nanoparticles that may have biomedical applications. The device consists of two matched Hall elements that can be moved through the room temperature bore of a 9 Tesla superconducting magnet. The Hall elements are wired in opposition such that a null response, to within a small offset, is measured in the absence of a sample that may be located on top of one unit. A LabVIEW program controls the current through the Hall elements and measures the net Hall voltage while simultaneously moving the probe through the magnetic field by regulating a linear stepper motor. Ultimately, the system will be tested to obtain a figure of merit using successively smaller samples. Details of the apparatus will be provided along with preliminary data.

¹We acknowledge early contributions to this work by Alex M. Sincore and Elisabeth S. Knowles. Supported by NSF DMR-0701400 (MWM), UF Dept. Physics REU (DMR-0851707), NHMFL REU (DMR-0654118), and the State of Florida

1:51PM B37.00014 Magnetostriction of engineered magnetorheological elastomers, WILLIAM RIEGER, CHRIS KASSNER, PARIS VON LOCKETTE, SAMUEL LOFLAND, Rowan University — We have completed a study of the magnetostriction and poison ratio of several types of magnetorheological elastomers (MREs), including both hard and soft magnetic materials in silicone rubber matrices. While both random and aligned soft magnetic particles gave large (~1%) magnetostriction, hard magnetic powders provided minimal actuation, regardless of whether they were aligned or not. In addition, we have created engineered lattices of magnetic wires and find the actuation highly dependent on the sample shape, and the angle of the magnetic field with respect to the alignment axis. We also propose some new structures based on hard magnetic wires which should provide piezomagnetic response.

2:03PM B37.00015 Physical Patterns Associated with 27 April 2011 Tornado Outbreak¹, FERNANDA RAMOS, University of Puerto Rico at Mayaguez, THOMAS SALEM, National Weather Service, Memphis, TN — The National Weather Service office in Memphis, Tennessee has aimed their efforts to improve severe tornado forecasting. Everything is not known about tornadogenesis, but one thing is: tornadoes tend to form within supercell thunderstorms. Hence, 27 April 2011 and 25 May 2011 were days when a Tornado Outbreak was expected to arise. Although 22 tornadoes struck the region on 27 April 2011, only 1 impacted the area on 25 May 2011. In order to understand both events, comparisons of their physical features were made. These parameters were studied using the Weather Event Simulator system and the NOAA/NWS Storm Prediction database. This research concentrated on the Surface Frontal Analysis, NAM40 700mb Dew-Points, NAM80 250mb Wind Speed and NAM20 500mb Vorticity images as well as 0-6 km Shear, MUCAPE and VGP mesoscale patterns. As result of this research a Dry-Line ahead of a Cold Front, Dew-points $\sim 5^{\circ}\text{C}$ and higher, and high Vorticity values were synoptic patterns that influenced to the formation of supercell tornadoes. Finally, MUCAPE and VGP favored the possibility of tornadoes occurrence on 25 May 2011, but shear was the factor that made 27 April 2011 a day for a Tornado Outbreak weather event.

¹Meteorology Program at University of Puerto Rico at Mayaguez

Monday, February 27, 2012 11:15AM - 2:15PM – Session B39 DCOMP: Electronic Structure: Calculations I 109B

11:15AM B39.00001 Acceleration of Hartree-Fock Exchange Computations using Recursive Subspace Bisection¹, IVAN DUCHEMIN, Department of Applied Science, University of California Davis, Davis CA 95616, FRANCOIS GYGI, Department of Computer Science, University of California Davis, Davis CA 95616 — We use the recursive subspace bisection algorithm [1] to accelerate the computation of the Hartree-Fock exchange operator in electronic structure computations involving hybrid density functionals. This approach leads to a reduction of the computational cost of the exchange operator from $O(N^3 \log N)$ to $O(N^2 \log N)$ and allows for controlled accuracy through a threshold parameter. The subspace bisection method is extended to invariant subspaces including excited states. Applications to molecular dynamics simulations and computations of energy band gaps in large systems using the PBE0 hybrid functional will be presented.

[1] F. Gygi, Phys. Rev. Lett. 102, 166406 (2009).

¹Supported by NSF OCI 0749217 and DOE SciDAC DE-FC02-06ER25794

11:27AM B39.00002 A Discontinuous Galerkin Framework for Electronic Structure Calculations, ANDREW BACZEWSKI, BALASUBRAMANIAM SHANKER, SUBHENDRA MAHANTI, BENJAMIN LEVINE, Michigan State University — It is generally accepted that a good basis set for any calculation should possess a number of salient features, including systematic improvability, adaptive resolution of multiscale features, and fidelity in capturing the pertinent physics. Considering the progenitors of most modern electronic structure basis sets to be Gaussian-type orbitals or plane waves, descendants of these methods have inherited features that address either systematic improvability (plane waves) or adaptive resolution (Gaussians) separately, and use a variety of tricks to differentiate the core and valence physics. Discontinuous Galerkin methods provide a framework for defining adaptive local basis sets, that may be based on these canonical basis sets, that can be mixed and matched to simultaneously achieve all of these goals. Our group is presently developing a new electronic structure code to enable Density Functional and Hartree-Fock calculations within this framework, particularly in the context of all-electron formulations wherein the accurate resolution of both core and valence states is necessary. Numerous implementation details will be addressed, including the incorporation of hardware- and software-based acceleration, such as GPU-based parallelism, and fast electrostatics solvers.

11:39AM B39.00003 New method of optimizing the Jastrow factor for solids with the transcorrelated method, MASAYUKI OCHI, Department of Physics, The University of Tokyo, SHINJI TSUNEYUKI, Department of Physics, The University of Tokyo, ISSP, The University of Tokyo — Transcorrelated (TC) method[1-5] is one of the promising theories for *ab initio* electronic structure calculation of solids. It is one of the wave-function-based approaches which are considered to be advantageous for high-accuracy calculation. In the TC method, the total wave function is approximated as the Jastrow-Slater-type wave function, and the many-body Hamiltonian is similarity-transformed by the Jastrow factor. Then we solve an SCF equation and optimize one-body orbitals in the Slater determinant with relatively low computational cost. On the other hand, optimization of the Jastrow factor has been computationally much more demanding although it is indispensable to high-accuracy calculation. In this study, a new method of optimizing the Jastrow factor is developed by use of variance minimization of the total energy. It is demonstrated that, by truncating the basis-set expansion of the variance, the optimization is realized with low computational cost. [1] S. F. Boys and N. C. Handy, Proc. R. Soc. London Ser. A 309, 209 (1969). [2] S. Ten-no, Chem. Phys. Lett. 330, 169 (2000). [3] N. Umezawa and S. Tsuneyuki, J. Chem. Phys. 119, 10015 (2003). [4] R. Sakuma and S. Tsuneyuki, J. Phys. Soc. Jpn. 75, 103705 (2006). [5] H. Luo, J. Chem. Phys. 133, 154109 (2010).

11:51AM B39.00004 Adaptive local basis set for Kohn-Sham density functional theory in a discontinuous Galerkin framework, LIN LIN, Lawrence Berkeley National Laboratory, JIANFENG LU, Courant Institute, New York University, LEXING YING, The University of Texas at Austin, WEINAN E, Princeton University — Uniform discretization of the Kohn-Sham Hamiltonian generally results in a large number of basis functions per atom in order to resolve the rapid oscillations of the Kohn-Sham orbitals around the nuclei even in the pseudopotential framework. Atomic orbitals and similar objects significantly reduces the number of basis functions, but these basis sets generally require fine tuning of the parameters in order to reach high accuracy. We present a novel discretization scheme that adaptively and systematically builds the rapid oscillations of the Kohn-Sham orbitals around the nuclei as well as environmental effects into the basis functions. The resulting basis functions are localized in the real space, and are discontinuous in the global domain. The continuous Kohn-Sham orbitals and the electron density are evaluated from the discontinuous basis functions using the discontinuous Galerkin (DG) framework. Our method is implemented in parallel and the current implementation is able to handle systems with at least thousands of atoms. Numerical examples indicate that our method can reach very high accuracy (less than 1meV) with a very small number ($4 \sim 40$) of basis functions per atom.

12:03PM B39.00005 Retrofit of the HSE density functional¹, JONATHAN MOUSSA, PETER SCHULTZ, Sandia National Labs, JAMES CHELIKOWSKY, UT Austin — The original parameterization of the Heyd-Scuseria-Ernzerhof (HSE) density functional was dependent on the choice of a hybrid fraction and a range-separation length for separating out a portion of the exchange energy to compute exactly. For backward compatibility with the PBE0 functional, the hybrid fraction was fixed to 0.25. Here, we examine the full hybrid fraction / separation length phase space. With respect to multiple error metrics, the phase space does not have a well-developed point of minimum error. Instead, there is a “valley” of functionals with increasing hybrid fraction and decreasing separation length of similarly good quality. This enables a reduction of the separation length without degrading the accuracy of the HSE06 parameterization, which in turn reduces the computational cost of evaluating the exchange energy.

¹Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's NNSA under contract DE-AC04-94AL85000.

12:15PM B39.00006 Projector Augmented Wave formulation of orbital-dependent exchange-correlation functionals¹, XIAO XU, N.A.W. HOLZWARTH, Wake Forest University — The use of orbital-dependent exchange-correlation functionals within electronic structure calculations has recently received renewed attention for improving the accuracy of the calculations, especially correcting self-interaction errors. Since the Projector Augmented Wave (PAW) method² is an efficient pseudopotential-like scheme which ensures accurate evaluation of all multipole moments of direct and exchange Coulomb integrals, it is a natural choice for implementing orbital-dependent formalisms. Using Fock exchange as an example of an orbital-dependent functional, we developed the formulation and numerical implementation of the approximate optimized effective potential formalism of Kreiger, Li, and Iafrate (KLI)³ within the PAW method, comparing results with the analogous Hartree-Fock treatment.⁴ Test results are presented for ground state properties of two well-known materials – diamond and LiF. This formalism can be extended to treat orbital-dependent functionals more generally.

¹Supported by NSF Grants 0427055 and 0705239

² P. Blöchl, *Phys. Rev. B* **50**, 17953 (1994).

³ J. B. Krieger, Y. Li, and G. J. Iafrate *Phys. Rev. A* **45**, 101 (1992).

⁴ Xiao Xu and N. A. W. Holzwarth, *Phys. Rev. B* **81**, 245105 (2010); **84**, 155113 (2011).

12:27PM B39.00007 Solution of the Bethe-Salpeter equation without empty electronic states: Applications to solids, nanostructures and molecules¹, DARIO ROCCA, YUAN PING, UC Davis, DEYU LU, Brookhaven National Laboratory, GIULIA GALLI, UC Davis — A method to solve the Bethe-Salpeter equation that avoids the explicit calculation of empty electronic states and the storage and inversion of dielectric matrices has been recently introduced [1-3]. This approach is suitable to compute the absorption spectra of large systems in a wide energy range and without relying on the Tamm-Dancoff approximation. We show the accuracy and scalability of this method by presenting calculations of absorption spectra of solids, molecules and nanostructures, including Si quantum dots and nanowires. In the case of nanowires, we discuss the influence of size and surface reconstruction on the optical properties.

[1] D. Rocca, D. Lu, and G. Galli, *J. Chem. Phys.* **133**, 164109 (2010)

[2] D. Rocca, Y. Ping, R. Gebauer, and G. Galli, submitted to PRB

[3] Y. Ping, D. Rocca, D. Lu, and G. Galli, submitted to PRB

¹ Work supported by NSF CHE-0802907 and DOE BES-FG02-06ER46262 grants.

12:39PM B39.00008 Iterative diagonalization of non-Hermitian eigenproblems in time-dependent density-functional and many-body perturbation theory¹, ZHAOJUN BAI, DARIO ROCCA, UC Davis, REN-CANG LI, UT Arlington, GIULIA GALLI, UC Davis — We present a technique for the iterative diagonalization of random-phase approximation (RPA) matrices, which are encountered in the framework of time-dependent density-functional theory (TDDFT) and in the solution of the Bethe-Salpeter equation (BSE) [1]. The non-Hermitian character of these matrices does not permit a straightforward application of standard iterative techniques used, i.e., for the diagonalization of ground state Hamiltonians. We first introduce a new block variational principle for RPA matrices. We then develop an algorithm for the simultaneous calculation of multiple eigenvalues and eigenvectors, with convergence and stability properties similar to techniques used to iteratively diagonalize Hermitian matrices. The algorithm is validated by computing multiple low-lying excitation energies of molecules at both the TDDFT and BSE level.

[1] D. Rocca, Z. Bai, R.-C. Li, and G. Galli, submitted to *J. Chem. Phys.*

¹Work supported by NSF OCI-0749217 and DOE BES-FG02-06ER46262 grants.

12:51PM B39.00009 New *ab initio* approaches for calculating the microscopic electron-density response matrix, KATHLEEN SCHWARZ, Cornell University Department of Chemistry, JEEHYE LEE, T.A. ARIAS, Cornell University, Department of Physics — The electron-density response matrix is a key quantity for excitation calculations such as GW-BSE. Typically, the response matrix is obtained at the level of the random phase approximation (RPA), with the wavefunction from local density approximation (LDA) density functional theory. The expense of this approach grows quickly with the number of atoms, and its accuracy depends on both the accuracy of the LDA and the RPA. We investigate a series of approaches to overcome these difficulties, based on an eigenvalue decomposition of the molecular response matrix.

1:03PM B39.00010 Cluster expansion of the electron-density response function: GW+BSE with molecular environments, JEEHYE LEE, T.A. ARIAS, Cornell University, Department of Physics — Molecular excitations in dielectric environments have drawn great interest because environmental manipulation provides the possibility to engineer photo-excitation processes. In exciton calculation the environments often are replaced by dielectric continuum media. These approaches have been successful for solvated molecules, but they lack molecular detail, and hence miss microscopic features. We present a new method to represent environments that allows a more accurate treatment of a wide range of systems by employing cluster expansions of environmental response functions. This initial work, at the GW+BSE level, presents results for shifts in excitation energies due to environments consisting of either individual molecules or conjugated polymers.

1:15PM B39.00011 Unified description of ground and excited states of finite systems: the self-consistent *GW* approach, FABIO CARUSO, PATRICK RINKE, XINGUO REN, Fritz Haber Institute, Berlin, Germany, ANGEL RUBIO, Universidad del Pais Vasco, San Sebastian, Spain, MATTHIAS SCHEFFLER, Fritz Haber Institute, Berlin, Germany — Fully self-consistent *GW* calculations – based on the iterative solution of the Dyson equation – provide an approach for consistently describing ground and excited states on the same quantum mechanical level. Based on our implementation in the all-electron localized basis code FHI-aims [1], we show that for finite systems self-consistent *GW* reaches the same final Green function regardless of the starting point. The results show that self-consistency systematically improves ionization energies and total energies of closed shell systems compared to perturbative *GW* calculations (G_0W_0) based on Hartree-Fock or (semi)local density-functional theory. These improvements also translate to the electron density as demonstrated by a better description of the dipole moments of hetero-atomic dimers and the similarity with the coupled cluster singles doubles (CCSD) density. The starting-point independence of the self-consistent Green function facilitates a systematic and unbiased assessment of the performance of the *GW* approximation for finite systems. It therefore constitutes an unambiguous reference for the future development of vertex corrections and beyond *GW* schemes. [1] V. Blum *et al.*, *Comp. Phys. Comm.* **180**, 2175 (2009).

1:27PM B39.00012 Stress formulation in the all-electron full-potential linearized augmented plane wave method, NAUYUKI NAGASAKO, Toyota Central R&D labs., Inc., TAMIO OGUCHI, ISIR, Osaka University — Stress formulation in the linearized augmented plane wave (LAPW) method has been proposed in 2002 [1] as an extension of the force formulation in the LAPW method [2]. However, pressure calculations only for Al and Si were reported in Ref.[1] and even now stress calculations have not yet been fully established in the LAPW method. In order to make it possible to efficiently relax lattice shape and atomic positions simultaneously and to precisely evaluate the elastic constants in the LAPW method, we reformulate stress formula in the LAPW method with the Soler-Williams representation [3]. Validity of the formulation is tested by comparing the pressure obtained as the trace of stress tensor with that estimated from total energies for a wide variety of material systems. Results show that pressure is estimated within the accuracy of less than 0.1 GPa. Calculations of the shear elastic constant show that the shear components of the stress tensor are also precisely computed with the present formulation [4].

[1] T. Thonhauser *et al.*, Solid State Commun. **124**, 275 (2002).

[2] R. Yu *et al.*, Phys. Rev. B **43**, 6411 (1991).

[3] J. M. Soler and A. R. Williams, Phys. Rev. B **40**, 1560 (1989).

[4] N. Nagasako and T. Oguchi, J. Phys. Soc. Jpn. **80**, 024701 (2011).

1:39PM B39.00013 Real Space DFT by Locally Optimal Block Preconditioned Conjugate Gradient Method, VINCENT MICHAUD, HONG GUO, McGill University — Real space approaches solve the Kohn-Sham (KS) DFT problem as a system of partial differential equations (PDE) in real space numerical grids. In such techniques, the Hamiltonian matrix is typically much larger but sparser than the matrix arising in state-of-the-art DFT codes which are often based on directly minimizing the total energy functional. Evidence of good performance of real space methods - by Chebyshev filtered subspace iteration (CFSI) - was reported by Zhou, Saad, Tiago and Chelikowsky [1]. We found that the performance of the locally optimal block preconditioned conjugate gradient method (LOGPCG) introduced by Knyazev [2], when used in conjunction with CFSI, generally exceeds that of CFSI for solving the KS equations. We will present our implementation of the LOGPCG based real space electronic structure calculator.

[1] Y. Zhou, Y. Saad, M. L. Tiago, and J. R. Chelikowsky, "Self-consistent-field calculations using Chebyshev-filtered subspace iteration," J. Comput. Phys., vol. 219, pp. 172-184, November 2006.

[2] A. V. Knyazev, "Toward the optimal preconditioned eigensolver: Locally optimal block preconditioned conjugate gradient method," SIAM J. Sci. Comput., vol. 23, pp. 517-541, 2001.

1:51PM B39.00014 Bridging density-functional and many-body perturbation theory: orbital-density dependence in electronic-structure functionals, ANDREA FERRETTI, S3 Center, CNR - Istituto Nanoscienze, Modena, Italy., ISMAILA DABO, CERMICS, Universite Paris-Est, MATTEO COCCIONI, CEMS, University of Minnesota, NICOLA MARZARI, Department of Materials, Oxford University — Energy functionals which depend explicitly on the orbital densities (ODD), instead of the total charge density, appear when applying self-interaction corrections to density-functional theory. In these cases (e.g. the Perdew-Zunger [1] and the non-Koopmans [2] approaches) the total energy loses invariance under unitary rotations of the orbitals, and the minimization of the functionals leads to orbital-dependent Hamiltonians. We show that it is possible to identify the orbital-dependency of densities and potentials with an effective and discretized frequency-dependency, in close analogy to the quasi-particle approximation of frequency-dependent self-energies and naturally oriented to interpret electronic spectroscopies [3]. Some of the existing ODD functionals are analyzed from this new perspective. Numerical results for the electronic structure of gas-phase molecules (within the Koopmans-corrected class of functionals) are computed and found in excellent agreement with photoemission (UPS) data. [1] J.-P. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981). [2] I. Dabo, A. Ferretti, N. Poilvert, Y. Li, N. Marzari, M. Cococcioni, Phys. Rev. B **82**, 115121 (2010). [3] M. Gatti, V. Olevano, L. Reining, I.-V. Tokatly, Phys. Rev. Lett. **99**, 057401 (2007).

2:03PM B39.00015 A new type of pseudopotentials: effective atomic pseudopotentials, JAIRO RICARDO CARDENAS, ROBY CHERIAN, GABRIEL BESTER, Max Planck Institute for Solid State Research — We derive a new type of pseudopotentials from conventional norm-conserving pseudopotentials for the treatment of a large number of atoms. The pseudopotentials are not aimed at the calculation of the total energy, but of band edge states relevant for optical processes. We describe the pseudopotential construction and benchmark its quality and transferability by comparison to standard DFT calculations.

Monday, February 27, 2012 11:15AM - 2:15PM –
Session B40 DBIO DPOLY: Focus Session: Cytoskeleton and Biomechanics - Entanglement and Crosslinking 156A

11:15AM B40.00001 Seeing is believing: New insight into structure-mechanics relationships in entangled and crosslinked microtubule networks, MEGAN VALENTINE, Department of Mechanical Engineering, University of California Santa Barbara — The microtubule cytoskeleton is essential in maintaining the shape, strength and organization of cells and its misregulation has been implicated in neurological disorders and cancers. To better understand the structure-mechanics relationships in microtubule networks, we measure the force-dependent viscoelastic responses of entangled and sparsely crosslinked microtubule networks to precise microscale manipulation. We use magnetic tweezers devices to apply calibrated step stresses and measure the resultant strain as a function of time. At short times the material behaves as an elastic solid. The linear regime is large, with gentle stiffening observed in entangled networks above ~70% strains. Crosslinked networks are stiffer, and show an extended linear regime. At longer times, we find a creeping regime, suggesting that structural rearrangements of the network dominate the mechanical response. To understand the molecular origins of this behavior, we use a newly-developed portable magnetic tweezers device to observe the network morphology using a confocal microscope while simultaneously applying point-like stresses to embedded magnetic particles. We observe substantial network compression in front of the bead with no evidence of long-length scale filament flow, and find that the spatial extent of the deformation field depends sensitively on network architecture and connectivity. Our results are important to understanding the role of the cytoskeleton in regulating cargo transport in vivo, as well as the basic physics of non-affine deformations in rigid rod polymer networks.

11:51AM B40.00002 Actin filament curvature biases branching direction, EVAN WANG, VIVIANA RISCA, UC Berkeley, OVIJIT CHAUDHURI, Harvard University, JIA-JUN CHIA, Johns Hopkins University, PHILLIP GEISSLER, DANIEL FLETCHER, UC Berkeley — Actin filaments are key components of the cellular machinery, vital for a wide range of processes ranging from cell motility to endocytosis. Actin filaments can branch, and essential in this process is a protein complex known as the Arp2/3 complex, which nucleate new "daughter" filaments from pre-existing "mother" filaments by attaching itself to the mother filament. Though much progress has been made in understanding the Arp2/3-actin junction, some very interesting questions remain. In particular, F-actin is a dynamic polymer that undergoes a wide range of fluctuations. Prior studies of the Arp2/3-actin junction provides a very static notion of Arp2/3 binding. The question we ask is how differently does the Arp2/3 complex interact with a straight filament compared to a bent filament? In this study, we used Monte Carlo simulations of a surface-tethered worm-like chain to explore possible mechanisms underlying the experimental observation that there exists preferential branch formation by the Arp2/3 complex on the convex face of a curved filament. We show that a fluctuation gating model in which Arp2/3 binding to the actin filament is dependent upon a rare high-local-curvature shape fluctuation of the filament is consistent with the experimental data.

12:03PM B40.00003 Condensation of F-Actin by Dimensional Reduction, ROBIJN BRUINSMA, Department of Physics and Astronomy, UCLA, CYRON CHRISTIAN, KEI MUELLER, Mechanical Engineering, Technical University, Munich, Germany, ANDREAS BAUSCH, Chair Cell Biophysics E27, Technical University, Muenchen, Germany, WOLFGANG WALL, Mechanical Engineering, Technical University, Munich, Germany — We present a Brownian Dynamics simulation of the equilibrium condensation of F-actin in the presence of linker molecules. The filaments are modeled as worm-like chains, using finite element analysis. At low linker concentrations, the systems forms a gel whose physical properties do not depend on the linker molecules. If the linker concentration is increased then for isotropic linkers only a single mode of condensation is encountered: bundle formation. If the linker molecules impose a preferential angle between F-actin filaments, then condensation takes place either into a either a hexatic or squaratic two-dimensional liquid crystal phase or into a heterogeneous cluster. Condensation is driven by competition between linker and filament entropy, which imposes dimensional reduction on the F-actin aggregate.

12:15PM B40.00004 Stress Enhanced Gelation in α -Actinin-4 Cross-linked Actin Networks, NORMAN YAO, Harvard University, CHASE BROEDERSZ, Princeton University, MARTIN DEPKEN, Vrije Universiteit, DANIEL BECKER, Brigham and Women's Hospital and Harvard Medical School, MARTIN POLLAK, Beth Israel Deaconess Medical Center and Harvard Medical School, FREDERICK MACK-INTOSH, Vrije Universiteit, DAVID WEITZ, Harvard University — A hallmark of biopolymer networks is their exquisite sensitivity to stress, demonstrated for example, by pronounced nonlinear elastic stiffening. Typically, they also yield under increased static load, providing a mechanism to achieve fluid-like behavior. In this talk, I will demonstrate an unexpected dynamical behavior in biopolymer networks consisting of F-actin cross-linked by a physiological actin binding protein, α -Actinin-4. Applied stress actually enhances gelation of these networks by delaying the onset of structural relaxation and network flow, thereby extending the regime of solid-like behavior to much lower frequencies. By using human kidney disease-associated mutant cross-linkers with varying binding affinities, we propose a molecular origin for this stress-enhanced gelation: It arises from the increased binding affinity of the cross-linker under load, characteristic of catch-bond-like behavior. This property may have important biological implications for intracellular mechanics, representing as it does a qualitatively new class of material behavior.

12:27PM B40.00005 Simulations and theory of model microtubule self-assembly¹, MARK STEVENS, SHENGFENG CHENG, Sandia National Labs, ANKUSH AGGARWAL, U. California at Los Angeles — We used molecular dynamics simulations to study the self-assembly of artificial microtubules. The model monomer has a wedge-shape to promote formation of rings that stack to form tubules. Attractive interaction sites are on the sides for ring formation and top/bottom for filament growth. We have studied the assembly kinetics and dynamics as a function of these lateral and vertical interaction strengths. A full structure diagram was calculated. The range of interaction strengths that best form tubules has been determined. We found that tubules form better when the lateral strength is stronger than the filamental strength, which contrast the picture for microtubules. The interaction strengths must be weak enough to allow for reformation of the clusters that initially form. Besides tubules, a variety of structures form depending on the interaction parameters. Interestingly, helical tubes and other helical structures are frequently observed despite the fact that the minimum energy substructure is a nonhelical ring. We have used a simple Flory-Huggins type theory to characterize the structure diagram.

¹Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE

12:39PM B40.00006 Dynamical Length-Regulation of Microtubules, ANNA MELBINGER, LOUIS REESE, ERWIN FREY, Ludwig-Maximilians University, Munich — Microtubules (MTs) are vital constituents of the cytoskeleton. These stiff filaments are not only needed for mechanical support. They also fulfill highly dynamic tasks. For instance MTs build the mitotic spindle, which pulls the doubled set of chromosomes apart during mitosis. Hence, a well-regulated and adjustable MT length is essential for cell division. Extending a recently introduced model [1], we here study length-regulation of MTs. Thereby we account for both spontaneous polymerization and depolymerization triggered by motor proteins. In contrast to the polymerization rate, the effective depolymerization rate depends on the presence of molecular motors at the tip and thereby on crowding effects which in turn depend on the MT length. We show that these antagonistic effects result in a well-defined MT length. Stochastic simulations and analytic calculations reveal the exact regimes where regulation is feasible. Furthermore, the adjusted MT length and the ensuing strength of fluctuations are analyzed. Taken together, we make quantitative predictions which can be tested experimentally. These results should help to obtain deeper insights in the microscopic mechanisms underlying length-regulation.

[1] L.Reese, A.Melbinger, E.Frey, Biophys. J., **101**, 9, 2190 (2011)

12:51PM B40.00007 On the origins and extent of mechanical variation among cells, JOHN MALONEY¹, Massachusetts Institute of Technology, ERIC LEHNHARDT², Arizona State University, KRISTYN VAN VLIET³, Massachusetts Institute of Technology — Why would any one biological cell be mechanically different from another from the same population? Prompted by findings of broad distributions of cell stiffness within populations, we investigate possible origins of intrinsic mechanical heterogeneity among single cells. Through optical stretching, a non-contact technique for deforming cells in the suspended state, we obtain the creep compliance and complex modulus of single cells. Measurements of hundreds of human mesenchymal stem cells and murine fibroblasts in the time and frequency domains reveal that mechanical heterogeneity is not detectably dependent on cell lineage, cell cycle, cytoskeletal crosslinking, or repeated loading. However, adenosine triphosphate (ATP) depletion reduces heterogeneity of both stiffness and fluidity values. We explore the connection between these two parameters by positing that mechanical variation predominantly arises from Gaussian fluctuations in cell fluidity, which can be interpreted as emergent agitation in the energy landscape of soft glassy materials. Our findings ultimately link relatively small structural variations within cytoskeletal networks to large mechanical differences among cells and cell populations.

¹Department of Materials Science and Engineering

²Department of Biomedical Engineering

³Department of Materials Science and Engineering and Department of Biological Engineering

1:03PM B40.00008 Non-Equilibrium Cell Mechanics Studied with a Dual Optical Trap, FLORIAN SCHLOSSER, FLORIAN REHFELDT, CHRISTOPH F. SCHMIDT, Drittes Physikalisches Institut, Georg-August-Universitaet Goettingen, Germany — Cells communicate with their surroundings biochemically, but at the same time also sense the active and passive mechanical properties of their micro-environment. Cells can “feel” mechanical stress and they generate contractile forces through their actomyosin network to actively probe the mechanical response of the material they adhere to or are embedded in. These mechanosensory interactions result in cellular responses. We have used a dual optical trap to perform force measurements on cells suspended between two fibronectin-coated beads. We analyzed the correlated fluctuations of the beads with high spatial and temporal resolution. Using a combination of active and passive microrheology, we can simultaneously determine the (non-thermal) forces generated by the cells and actively probe their visco-elastic response properties. Here, we present data on contractile forces and elastic response of 3T3 fibroblasts, demonstrating that the transmitted force depends on the trap stiffness (i.e. rigidity of the environment). Using biochemical perturbations, we have studied the contributions of different cytoskeletal elements to the active and passive mechanical properties of the cell.

1:15PM B40.00009 M & M's: Mechanosensitivity and Mechanotransduction in Myoblasts¹, ZEINAB AL-REKABI, ANDREW PELLING, University of Ottawa — The effect of external mechanical stimulation of muscle precursor cells (myoblasts) during exercise is a crucial step in myogenesis. This effect takes place many hours later while muscles are in a resting state; however it remains unclear to what extent the role of force application has on the promotion of myogenesis. Here, we combine Traction Force Microscopy (TFM) and Atomic Force Microscopy (AFM) to directly measure the magnitude of generated cellular traction forces (CTFs) in myoblasts, as a result of controlled mechanical loading. Precise nanonewton forces (1 & 10 nN) were applied to live cells with the AFM tip while simultaneous TFM measurements were performed. The experiment was performed on substrates ranging in elastic moduli (E), (16-89 kPa) mimicking resting and active muscle tissue, respectively. The results of this analysis demonstrated that the magnitude of CTFs was dependent on substrate E , as expected. However, CTFs only increased in response to applied force (compared to controls) on substrates with E greater than 62 kPa. Our results suggest that muscle precursor cells are most sensitive to mechanical force when the surrounding muscle tissue is stiff and contracted, whereas myogenesis itself proceeds optimally on softer, resting tissue.

¹NSERC Create in Quantitative Biomedicine

1:27PM B40.00010 Polymer Coated Surface Acoustic Wave Biosensor for Living Cells, LIAN DAI, ECE U. Mass Lowell, JIANPING ZHANG, ABICHE DEWILDE, GANG WANG, Biology U. Mass Lowell, KENNETH MARX, Chemistry U. Mass Lowell, SUSAN BRAUNHUT, Biology U. Mass Lowell, JOEL THERRIEN, ECE U. Mass Lowell — A shear horizontal surface acoustic wave (SH-SAW) biosensor is fabricated on quartz wafer for measurement of mechanical properties of living cells. The SAW device was fabricated with a top film of polymer (PMMA, SU-8) to avoid immense attenuation in aqueous media. Several models were designed to operate under different frequencies such as 20MHz, 40MHz and 80MHz and higher in order to identify how frequency affect the sensitivity. A network analyzer was used to capture the resonant frequency of inter-digitated transducers (IDT) of SAW, and it is found that resonant frequency shift is closely correlated to the cell deposition on the sensing area of SAW.

1:39PM B40.00011 Modeling spinal cord biomechanics¹, CARLOS LUNA, Fischell Department of Bioengineering, University of Maryland, SAMEER SHAH, Departments of Orthopaedic Surgery and Bioengineering University of California, San Diego, AVIS COHEN, Department of Biology and Institute of Systems Research, University of Maryland, HELIM ARANDA-ESPINOZA, Fischell Department of Bioengineering, University of Maryland — Regeneration after spinal cord injury is a serious health issue and there is no treatment for ailing patients. To understand regeneration of the spinal cord we used a system where regeneration occurs naturally, such as the lamprey. In this work, we analyzed the stress response of the spinal cord to tensile loading and obtained the mechanical properties of the cord both in vitro and in vivo. Physiological measurements showed that the spinal cord is pre-stressed to a strain of 10%, and during sinusoidal swimming, there is a local strain of 5% concentrated evenly at the mid-body and caudal sections. We found that the mechanical properties are homogeneous along the body and independent of the meninges. The mechanical behavior of the spinal cord can be characterized by a non-linear viscoelastic model, described by a modulus of 20 KPa for strains up to 15% and a modulus of 0.5 MPa for strains above 15%, in agreement with experimental data. However, this model does not offer a full understanding of the behavior of the spinal cord fibers. Using polymer physics we developed a model that relates the stress response as a function of the number of fibers.

¹HAE and CL acknowledge support from NSF CMMI-0643783. CL acknowledges support from CONACyT, Mexico.

1:51PM B40.00012 Matrix elasticity perturbation and Lamin-A/C expression in stem cells modulate their mechanics and lineage specification¹, IRENA IVANOVSKA, DENNIS DISCHER, University of Pennsylvania — Commitment of stem cells to different lineages is regulated by many cues in their local microenvironment. They are particularly sensitive to the mechanical properties of their extracellular matrix. Nuclear lamins are fibrous proteins providing structural function and transcriptional regulation in the cell nucleus. In particular Lamin A/C levels could influence cellular mechanical sensitivity. Here we show that perturbation of the extracellular matrix and nucleus mechanics can direct stem cells lineage specification. We studied the behavior of human mesenchymal stem cells (hMSC) cultured on thin highly ordered collagen nanofilms. To tune the mechanical properties of the nanofilms we used the enzyme transglutaminase as a crosslinking agent. AFM imaging and manipulation is used to examine the nano topography and mechanical properties of the films and cells. Film stiffening affects cells morphology, cytoskeleton organization and their elastic response. hMSCs cultured for two weeks on collagen nanofilms initially tune their stiffness with matrix elasticity but later continuously change it with time. We observed upregulation of osteogenic markers on cross-linked films and increased lamin A/C expression. We show that manipulating Lamin-A/C expression in stem cells also directs cell lineage with knockdown favoring adipogenesis and over expression favoring osteogenesis. We found positive correlation between matrix and nucleus mechanics and that they have a synergistic effect on hMSCs differentiation potential.

¹HFSP Long-Term Fellowship

2:03PM B40.00013 Simulation of Second Harmonic Generation from Heterogeneous Microtubule Structures, NOAH LANGOWITZ, CHE-HANG YU, DANIEL NEEDLEMAN, Harvard University — Second harmonic generation imaging is a coherent nonlinear microscopy with contrast arising from certain asymmetric endogenous structures in cells, including spindle microtubules. As a second-order nonlinear optical process, SHG requires a noncentrosymmetric macromolecular organization to generate signal, so it can be used as a measure of microtubule polarity within spindles or other microtubule structures. We developed a simulation of SHG microscopy accounting for 3-dimensional orientation and circularly polarized excitation in order to quantify the dependence of SHG signal on microtubule density, spacing, polarity, and rotational order. SHG can be used to assess spindle polarity in living cells using simultaneous ratio imaging with two-photon excited fluorescence from labeled tubulin. The results from simulation are used to quantify microtubule polarity from SHG and TPEF images of spindles in the one-cell *C. elegans* embryo and *Xenopus* oocyte extract.

Monday, February 27, 2012 11:15AM - 2:15PM –
Session B41 DBIO: Lipid Bilayers and Biological Membranes 156B

11:15AM B41.00001 Computer Simulation of Cytoskeleton-Induced Blebbing of Lipid Membranes¹, MOHAMED LARADJI, EIRC J. SPANGLER, University of Memphis, CAMERON W. HARVEY, University of Notre Dame, JOEL D. REVALEE, University of Michigan, P.B. SUNIL KUMAR, Indian Institute of Technology Madras, India — Blebs are balloon-shaped membrane protrusions that form during many physiological processes such as cytokinesis, cell motility and apoptosis. Using computer simulation of a particle-based model for self-assembled lipid bilayers coupled to an elastic meshwork, we investigated the phase behavior and kinetics of blebbing. We found that for small values of the mismatch parameter, defined as the ratio between the area of the lipid bilayer divided by the rest area of the cytoskeleton, the equilibrium state is that of a homogeneous vesicle with the cytoskeleton conforming to the bilayer. However, for large values of a mismatch parameter, the equilibrium state is that of a blebbed vesicle. We also found that blebbing can be induced when the cytoskeleton is subject to a localized ablation or a uniform compression. The obtained results are qualitatively in agreement with the experimental evidence and the model opens up the possibility to study the kinetics of bleb formation in detail. For more information see Spangler *et al.*, Phys. Rev. E **84**, 051906 (2011).

¹This work was supported by NSF (DMR-0812470 and DMR-0755447) and the Research Corporation (CC66879)

11:27AM B41.00002 Coarse-grained simulation of lipid vesicles with “n-atic” orientational order¹, JUN GENG, JONATHAN SELINGER, ROBIN SELINGER, Liquid Crystal Institute, Kent State University, Ohio 44242, USA — We perform coarse-grained simulation studies of fluid lipid vesicles with in-plane “n-atic” orientational order associated with the shape of lipid head group, to test the theoretical predictions of Park, Lubensky and MacKintosh [1] for resulting vesicle shape and defect structures. Our simulation model uses a single layer coarse-grained implicit-solvent approach proposed by Yuan et al [2], with addition of an extra vector degree of freedom representing in-plane orientational order. We carry out simulation studies for n=1 to 6, examining in each case the spatial distribution of defects and resulting deformation of the vesicle. An initially spherical vesicle (genus zero) with n-atic order has a ground state with 2n vortices of strength 1/n, as expected, but the observed equilibrium shapes are sometimes quite different from those predicted theoretically. For the n=1 case, we find that the vesicle may become trapped in a disordered, long-lived metastable state with extra +/- defects whose pair-annihilation is inhibited by local changes in membrane curvature, and thus may never reach its predicted ground state.

[1] J. Park, T. C. Lubensky, and F. C. MacKintosh, *Europhys. Lett.* 20, 279 (1992)

[2] H. Yuan, C. Huang, Ju Li, G. Lykotrafitis, and S. Zhang, *Phys. Rev. E* 82, 011905 (2010)

¹Work supported by NSF DMR-1106014.

11:39AM B41.00003 Morphologies of Elastic Membranes with Fluctuating Connectivity, CHLOE FUNKHOUSER, RASTKO SKNEPNEK, MONICA OLVERA DE LA CRUZ, Northwestern University — We numerically investigate the effects of topological defects in single-component two-dimensional elastic membranes with spherical topology allowing changes in shape. The membrane is simulated as a closed, triangulated elastic surface in three dimensions, where the vertices are permitted to move in space and the connectivity of the triangulation is able to fluctuate. Fluctuations in connectivity allow the creation of topological defects. A Monte Carlo simulated annealing method is utilized to explore optimal shapes and connectivities. The familiar defect-driven buckling transition [Seung & Nelson, *PRA* 1988, 38:1005] from a sphere to an icosahedron is shifted as a result of the fluctuating connectivity.

11:51AM B41.00004 Cooperative Motion in Lipid Bilayer Membranes, BENEDIKT HARTMANN, FRANCIS STARR, Wesleyan University — Lipid bilayer membranes, like the cell membrane, are complex biological systems. Transport of specific molecules in and out of cells are controlled by these membranes. Therefore, it is vital to understand the detailed dynamics that ultimately control membrane transport. We use molecular dynamics simulations of a coarse-grained and solvent-free lipid model that has been previously shown to spontaneously assemble a bilayer structure. Approaching the crossover to the gel-like state of the bilayer, the lipid dynamics become extremely slow. We analyze the cooperativity of the lipid motion and compare it with the cooperativity that has been well-characterized in liquids nearing a glass transition. Future simulations will examine the generality of this behavior using more realistic models, and comparing with experiments.

12:03PM B41.00005 How the antimicrobial peptides destroy bacteria cell membrane: Translocations vs. membrane buckling¹, LEONARDO GOLUBOVIC, West Virginia University, LIANGHUI GAO, LICUI CHEN, WEIHAI FANG, Beijing Normal University — In this study, coarse grained Dissipative Particle Dynamics simulation with implementation of electrostatic interactions is developed in constant pressure and surface tension ensemble to elucidate how the antimicrobial peptide molecules affect bilayer cell membrane structure and kill bacteria. We find that peptides with different chemical-physical properties exhibit different membrane obstructing mechanisms. Peptide molecules can destroy vital functions of the affected bacteria by translocating across their membranes via worm-holes, or by associating with membrane lipids to form hydrophilic cores trapped inside the hydrophobic domain of the membranes. In the latter scenario, the affected membranes are strongly corrugated (buckled) in accord with very recent experimental observations [G. E. Fantner *et al.*, *Nat. Nanotech.*, 5 (2010), pp. 280-285].

¹Supported by the National Science Foundation of China (Grant No. 20873007)

12:15PM B41.00006 Interaction of PLGA and trimethyl chitosan modified PLGA nanoparticles with mixed anionic/zwitterionic phospholipid bilayers studied using molecular dynamics simulations¹, BRIAN NOVAK, Louisiana State University, Center for Computation and Technology, CARLOS ASTETE, CRISTINA SABLIOV, Louisiana State University, Department of Biological and Agricultural Engineering, DOREL MOLDOVAN, Louisiana State University, Department of Mechanical Engineering — Poly(lactic-co-glycolic acid) (PLGA) is a biodegradable polymer. Nanoparticles of PLGA are commonly used for drug delivery applications. The interaction of the nanoparticles with the cell membrane may influence the rate of their uptake by cells. Both PLGA and cell membranes are negatively charged, so adding positively charged polymers such as trimethyl chitosan (TMC) which adheres to the PLGA particles improves their cellular uptake. The interaction of 3 nm PLGA and TMC-modified-PLGA nanoparticles with lipid bilayers composed of mixtures of phosphatidylcholine and phosphatidylserine lipids was studied using molecular dynamics simulations. The free energy profiles as function of nanoparticles position along the normal direction to the bilayers were calculated, the distribution of phosphatidylserine lipids as a function of distance of the particle from the bilayer was calculated, and the time scale for particle motion in the directions parallel to the bilayer surface was estimated.

¹Work supported by NSF-EPSCoR LA-SiGMA Grant #EPS-1003897, and by LONI and HPC@LSU.

12:27PM B41.00007 Atomic Force Microscopy Study of Changes to the Mechanical Properties of *Pseudomonas aeruginosa* Cells Induced By Antimicrobial Peptides, SHUN LU, JOHN DUTCHER, University of Guelph — The cell envelope of Gram-negative bacteria plays a key role in the maintenance of cell shape and the selective transfer of small molecules in and out of the cell. Both the inner and outer membranes of the cell envelope can be major targets for antimicrobial peptides, which can ultimately compromise the mechanical integrity of the cell. We have applied a new, AFM-based creep deformation technique (1) to study changes to the mechanical properties of individual *Pseudomonas aeruginosa* cells as a function of time of exposure to polymyxin B (PMB), a well-known cyclic antimicrobial peptide. The results can be understood in terms of simple viscoelastic models of arrangements of springs and dashpots. These measurements provide a direct measure of the mechanical integrity of the bacterial cell, and time-resolved creep deformation experiments reveal that the time of action for PMB is very fast (of the order of a minute). This measurement provides new insight into the mechanism of action of antimicrobial peptides. (1) V. Vadillo-Rodriguez, T. J. Beveridge, and J. R. Dutcher, *J. Bacteriol.* 190, 4225-4232 (2008).

12:39PM B41.00008 Interactions between HIV-1 Neutralizing Antibodies and Model Lipid Membranes imaged with AFM, STEFAN ZAUSCHER, GREGORY HARDY, MUNIR ALAM, Duke University, JOSEPH SHAPTER, Flinders University — Lipid membrane interactions with rare, broadly neutralizing antibodies (NABs), 2F5 and 4E10, play a critical role in HIV-1 neutralization. Our research is motivated by recent immunization studies that have shown that induction of antibodies that avidly bind the gp41-MPER antigen is not sufficient for neutralization. Rather, it is required that antigen designs induce polyreactive antibodies that recognize MPER antigens as well as the viral lipid membrane. However, the mechanistic details of how membrane properties influence NAb-lipid and NAb-antigen interactions remain unknown. Furthermore, it is well established that the native viral membrane is heterogeneous, representing a mosaic of lipid rafts and protein clustering. However, the size, physical properties, and dynamics of these regions are poorly characterized and their potential roles in HIV-1 neutralization are also unknown. To understand how membrane properties contribute to 2F5/4E10 membrane interactions, we have engineered biomimetic supported lipid bilayers (SLBs) and use atomic force microscopy to visualize membrane domains, antigen clustering, and antibody-membrane interactions at sub-nanometer z-resolution. Our results show that localized binding of HIV-1 antigens and NABs occur preferentially with the most fluid membrane domain. This supports the theory that NABs may interact with regions of low lateral lipid forces that allow antibody insertion into the bilayer.

12:51PM B41.00009 Modeling curvature-dependent subcellular localization of a small sporulation protein in *Bacillus subtilis*, VAIBHAV WASNIK, Department of Physics, Clark University, NED WINGREEN, Princeton University, RANJAN MUKHOPADHYAY, Department of Physics, Clark University — Recent experiments suggest that in the bacterium, *B. subtilis*, the cue for the localization of small sporulation protein, SpoVM, that plays a central role in spore coat formation, is curvature of the bacterial plasma membrane. This curvature-dependent localization is puzzling given the orders of magnitude difference in lengthscale of an individual protein and radius of curvature of the membrane. Here we develop a minimal model to study the relationship between curvature-dependent membrane absorption of SpoVM and clustering of membrane-associated SpoVM and compare our results with experiments.

1:03PM B41.00010 Relationship between peptide amino acid sequence and membrane curvature generation, NATHAN SCHMIDT, DAVID KUO, GHEE HWEE LAI, ABHIJIT MISHRA, GERARD WONG, Bioengineering Dept, UCLA — Amphipathic peptides and amphipathic domains in proteins can perturb and restructure biological membranes. For example, it is believed that the cationic, amphipathic motif found in membrane active antimicrobial peptides (AMPs) is responsible for their membrane disruption mechanisms of action. And ApoA-I, the main apolipoprotein in high density lipoprotein contains a series of amphipathic α -helical repeats which are responsible for its lipid associating properties. We use small angle x-ray scattering (SAXS) to investigate the interaction of model cell membranes with prototypical AMPs and consensus peptides derived from the helical structural motif of ApoA-I. The relationship between peptide sequence and the peptide-induced changes in membrane curvature and topology is examined. By comparing the membrane rearrangement and corresponding phase behavior induced by these two distinct classes of membrane restructuring peptides we will discuss the role of amino acid sequence on membrane curvature generation.

1:15PM B41.00011 Family of pH-Low-Insertion-Peptides (pHLIPs), DHAMMIKA WEERAKKODY, ANNA MOSHNIKOVA, Department of Physics, University of Rhode Island, VALENTINA MOSHNIKOVA, College of William and Mary, MAK THAKUR, BETHANY ROSSI, University of Rhode Island, DONALD ENGELMAN, Department of Molecular Biophysics and Biochemistry, Yale University, OLEG ANDREEV, YANA RESHETNYAK, Department of Physics, University of Rhode Island — pHLIP (pH (Low) Insertion Peptide) is a novel delivery system for targeting of acidic diseased tissue such as solid tumors, sites of inflammation, arthritis and other pathological states. The molecular mechanism of pHLIP action is based on pH-dependent insertion and folding of pHLIP in membrane. We performed sequence variation and investigated 16 pHLIP variants with main goals of understanding the main principles of peptide-lipid interactions and tune delivery capability of pHLIP. The biophysical studies including thermodynamics and kinetics of the peptides interaction with a lipid bilayer of liposomes and cellular membranes were carried out. We found that peptides association to membrane at neutral and low pH could be modulated by 3-4 times. The apparent pK of transition from surface bound to membrane-inserted state could be tuned from 6.5 to 4.5. The rate of peptide's insertion across a bilayer could be enhanced 100 times compared to parent pHLIP. As a result, blood clearance and tumor targeting were modulated in a significant degree. The work is supported by NIH grants CA133890 to OAA, DME, YRK.

1:27PM B41.00012 Membrane-associated peptide folding: pH triggered insertion and helical structure formation¹, ALEXANDER KARABADZHAK, Department of Molecular Biophysics and Biochemistry, Yale University, DHAMMIKA WEERAKKODY, MAK THAKUR, Physics Department, University of Rhode Island, DONALD ENGELMAN, Department of Molecular Biophysics and Biochemistry, Yale University, VLADISLAV MARKIN, Department of Neurology, University of Texas Southwestern Medical Center, OLEG ANDREEV, YANA RESHETNYAK, Physics Department, University of Rhode Island — We are interested in the molecular events that occur when a peptide inserts across a membrane or exits from it. pHLIP (pH (Low) Insertion Peptide) provides an opportunity to study membrane insertion/exit and folding/unfolding, since its insertion is modulated by pH and since it forms helical structure as it inserts. We found that pHLIP inserts across a POPC phospholipid bilayer in several steps: first is the rapid formation (100 ms) of an interfacial helix, which is then followed by a slow insertion pathway that contains several intermediates. We show that while the number of protonatable residues at the inserting end does not affect the formation of helical structure in the membrane, it correlates with the time for transmembrane insertion, the number of intermediate states on the folding pathway, and the rate of unfolding and exit. We conclude that particular intermediate states on the folding and unfolding pathways are not mandatory and, in the simple case of a polypeptide with a non-charged and non-polar inserting end, the folding and unfolding is well described as an all-or-none transition. A model for membrane-associated insertion/folding and exit/unfolding is proposed.

¹The work is supported by NIH grants CA133890 and GM073857 to OAA, DME, YRK.

1:39PM B41.00013 Modulation of the transmembrane helix insertion pathway by polar cargo, DAYANJALI WIJESINGHE, ALEXANDER KARABADZHAK, Department of Physics, University of Rhode Island, VLADISLAV MARKIN, Department of Neurology, University of Texas Southwestern Medical Center, DONALD ENGELMAN, Department of Molecular Biophysics and Biochemistry, Yale University, OLEG ANDREEV, YANA RESHETNYAK, Department of Physics, University of Rhode Island — In an earlier study, we found a series of kinetic steps in the pH-triggered insertion of the pHLIP® (pH (Low) Insertion Peptide). In the present work we observe that the polarity of the inserting end, including its cargo, modulates the number of intermediates, and that insertion can be described as a two state process for a simple case. Each investigated pHLIP variant preserve the pH-dependent properties of surface binding to membrane at neutral pH and insertion at low pH to form a transmembrane helix. However, there are thermodynamic and kinetic properties that are determined by the degree of cargo polarity. The presence of a polar cargo at the peptide's inserting end leads to the appearance of two additional intermediate states on the insertion pathway of the pHLIP-2E peptide, which itself (when no cargo is attached) shows an all-or-none transition from the partially unstructured membrane-surface to the transmembrane state described well by the two-state model at 800 ms timescale. We discuss the utility of our observations for the design of new delivery agents for the direct translocation of polar therapeutic and diagnostic cargo molecules across cellular membranes. The work is supported by NIH grants CA133890 to OAA, DME, YRK.

1:51PM B41.00014 Exploration of phase separation in heterogeneous lipid monolayers, CURT DECARO, SAMBUNATH BERA, Northern Illinois University, ZHANG JIANG, Argonne National Laboratory, MRINMAY MUKHOPADHYAY, Spring-8, CAROL THOMPSON, Northern Illinois University — A Langmuir monolayer is a well established model of a single leaflet of a lipid membrane. In this work, we investigate the phase separation behavior of a model Langmuir monolayer as a function of both Langmuir surface pressure and ratio of saturated lipid : unsaturated lipid : cholesterol. The specifics of domain separation behavior, or “rafting,” in membranes are generally thought to be responsible for much of the behavior of living membranes, specifically in protein integration and transport. Off-specular x-ray scattering is used to probe in-plane structure of the membrane at the sub-micron scale. Additionally, atomic force microscopy imaging is taken on samples transferred to a rigid support. In-plane order is found to grow as a function of surface pressure. Also, the in-plane order is found to depend on cholesterol concentration in the monolayer. The phase space of the in-plane order as a function of lipid and cholesterol concentration is presented.

2:03PM B41.00015 Domain formation in multicomponent lipid bilayers coupled to elastic substrate, MD ZULFIKAR ALI, RANJAN MUKHOPADHYAY, Clark University — We will discuss the physics that governs the lipid localization and domain formation in multicomponent lipid bilayers coupled to an elastic substrate. Lipid localization and domain formation has been studied extensively in biological cell membranes. In this talk we will extend a previous model for membrane energetics to account for the coupling between the bending and the local lipid composition of the two leaflets. Our aim is to determine the relationship between the localization and domain formation in the presence of lipid flip-flops between the two leaflets and the effect of intrinsic curvature of the lipids. Using a lattice model for the membrane, we simulate the system and study the effect of lipid flip-flop on lipid organization in the membrane.

Monday, February 27, 2012 11:15AM - 2:15PM —

Session B42 DBIO DFD: Focus Session: BioChip Physics-Detection and Transport 156C

11:15AM B42.00001 On-chip Metamaterials for Ultra-sensitive Spectroscopy and Identification of Biomolecules, HATICE ALTUG, Boston University — Infrared absorption spectroscopy is a unique tool for identifying and characterizing molecular bonds. For most organic and inorganic molecules (such as proteins, chemical toxins and gases), vibrational and rotational modes are spectroscopically accessible within the mid-infrared (mid-IR; 3-20 μm) regime of the electromagnetic spectrum. Characteristic vibrational modes are associated with unique IR absorption spectral bands that are bond-specific. Because of that, the IR wavelength range is also known as “finger print” region. However, because of the Beer-Lambert law, its sensitivity has been limited to perform analytical/functional studies on small samples often available from biological specimens. In this talk we will describe how we use plasmonic metamaterials to overcome these challenges. We will introduce tailoring of the resonances to selectively address fingerprint signatures of proteins. We will also describe novel designs and fabrication methods to exploit extreme near-field enhancements in small gaps for vibrational signal enhancements.

In collaboration with In collaboration with Ronen Adato, Serap Aksu, Alp Artar, Arif Cetin, and Boston University.

11:51AM B42.00002 Ultrasensitive Plasmonic Biosensors for Direct Detection of Biomarker Proteins with The Naked Eye, AHMET ALI YANIK, Harvard University Medical School and Massachusetts General Hospital, JOHN CONNOR, Boston University Medical School, GENNADY SHVETS, University of Texas, Austin, HATICE ALTUG, Boston University Electrical and Computer Engineering — We introduce an ultrasensitive label free biodetection technique based on asymmetric plasmonic Fano resonances. Our sensors bring a number of advantages: (i) ultrasensitive detection limits surpassing gold standard Kretschmann configuration plasmon sensors, (ii) detection of biomarker molecules with “the naked eye”, (iii) massive multiplexing capabilities. By exploiting extraordinary light transmission phenomena through high quality factor sub-radiant dark modes, we experimentally demonstrate record high figures of merits for intrinsic detection limits surpassing the gold standard BioCore devices. Our experiments show an order of magnitude improved device performances over the state of art metamaterial and other plasmonic biosensors. Steep dispersion of the plasmonic Fano resonance profiles in engineered plasmonic sensors exhibit dramatic light intensity changes to the slightest perturbations within their local environment. As a spectacular demonstration, we show direct detection of a single monolayer of biomolecules with naked eye using these Fano resonances and the associated Wood’s anomalies. The demonstrated sensing platform offers point-of-care diagnostics in resource poor settings by eliminating the need for fluorescent labeling and optical detection instrumentation (such camera, spectrometer, etc.).

12:03PM B42.00003 High-Throughput On-Chip Diagnostic System for Circulating Tumor Cells, JAEHOON CHUNG, HUILIN SHAO, RALPH WEISSLEDER, HAKHO LEE, Center for Systems Biology, Massachusetts General Hospital — We have developed a novel, low-cost and high-throughput microfluidic device for detection and molecular analysis of circulating tumor cells (CTCs). The operation is based upon a size-selective cell separation, which was enabled by a weir-style physical barrier with a gap in the fluidic channel. The new system is a versatile CTC analysis platform with many advantages. First, it supports extremely high throughput operation, since the use of weir structure reduces fluidic resistance and enables flow-through separation ($> 20,000$ -fold CTC enrichment from whole blood at the flow rate of 10 mL/h). Second, the CTC-chip facilitates visual verification and enumeration of CTCs during/after operation. By implementing microwell-shaped structures on the physical barrier, CTCs can be individually captured at sites for single-cell resolution analyses. Furthermore, the captured cells could be profiled in situ by introducing antibodies or small molecular probes. The chip thus assumes not only high detection sensitivity but also molecular specificity for CTC identification. Finally, the CTC-chip can retrieve captured CTCs. By reversing the flow direction, the cells can be dislodged from their capture sites and collected for downstream investigation.

12:15PM B42.00004 Mass transport to suspended waveguide biosensors, JASON GAMBA, CHAITANYA MURTHY, ANDREA ARMANI, University of Southern California — The response of a biosensor is controlled both by the kinetics of analyte adsorption as well as the mass transport to the device. Improving the affinity between a target molecule and the functionalized sensor can pose significant challenges in terms of biochemistry and surface chemistry. The careful design of sample flow systems presents a more convenient route for decreasing the time required for a measurement. Using finite element methods, we model mass transport to a novel integrated photonic biosensor suspended within a microfluidic channel in an effort to understand how boundary layer flow patterns may be engineered to improve the transient response of the device. By monitoring the surface concentration of bound analyte over a range of inlet concentrations and vertical positions within the channel, we compare the behavior of suspended devices to that of planar sensors located on the floor of the channel. Thinner boundary layers and increased effective sensing area lead to consistently faster transient responses for the suspended sensor, with optimal performance resulting from the symmetric placement of the sensor with respect to the channel height.

12:27PM B42.00005 Weighing single cells in two fluids: measuring mass, volume and density, FRANCISCO FEIJÓ DELGADO, WILLIAM GROVER, NATHAN CERMAK, ANDREA BRYAN, SCOTT MANALIS, Massachusetts Institute of Technology — The Suspended Microchannel Resonator (SMR) is a highly sensitive cantilever-based mass sensor shown to be capable of weighing the buoyant mass of living single cells. We have engineered SMR-based microfluidic systems to achieve consecutive weighing of single cells in two different fluids, with controlled exposure times. By choosing fluids of two different densities, the paired buoyant mass measurements are used to characterize single-cell volume, mass and density. With density precision of $0.001 \text{ g}\cdot\text{cm}^{-3}$, we explore the application of our techniques to samples ranging from bacterial to mammalian cells and show that cellular density is a tightly regulated biological property within populations, up to 100-fold more so than the other size parameters.

12:39PM B42.00006 Label-free screening of niche-to-niche variation in satellite stem cells using functionalized pores , MATTHEW R. CHAPMAN, Biophysics Graduate Group, UC Berkeley, KARTHIK BALAKRISHNAN, Dept. Mechanical Engineering, UC Berkeley, MICHAEL J. CONBOY, Dept. Bioengineering, UC Berkeley, SWOMITRA MOHANTY, Dept. Mechanical Engineering, UC Berkeley, ERIC JABART, Dept. Bioengineering, UC Berkeley, HAIYAN HUANG, Dept. Statistics, UC Berkeley, JAMES HACK, Dept. Mechanical Engineering, UC Berkeley, IRINA M. CONBOY, Dept. Bioengineering, UC Berkeley, LYDIA L. SOHN, Dept. Mechanical Engineering, UC Berkeley — Combinations of surface markers are currently used to identify muscle satellite cells. Using pores functionalized with specific antibodies and measuring the transit time of cells passing through these pores, we discovered remarkable heterogeneity in the expression of these markers in muscle (satellite) stem cells that reside in different single myofibers. Microniche-specific variation in stem cells of the same organ has not been previously described, as bulk analysis does not discriminate between separate myofibers or even separate hind-leg muscle groups. We found a significant population of Sca-1+ satellite cells that form myotubes, thereby demonstrating the myogenic potential of Sca-1+ cells, which are currently excluded in bulk sorting. Finally, using our label-free pore screening technique, we have been able to quantify directly surface expression of Notch1 without activation of the Notch pathway. We show for the first time Notch1-expression heterogeneity in unactivated satellite cells. The discovery of fiber-to-fiber variations prompts new research into the reasons for such diversity in muscle stem cells.

12:51PM B42.00007 Demonstration and analysis of the harmonic dithering technique for a high-sensitivity silicon waveguide biosensor , KANGBAEK KIM, ROBERT M. PAFCHECK, THOMAS L. KOCH, Lehigh University — A label-free biosensor readout technique is demonstrated based on a silicon-on-insulator ring resonators and a harmonic dithering technique using a distributed feedback (DFB) laser and a lock-in amplifier. The 400 μm ring resonator is integrated with a microfluidic sample delivery channel formed with Polydimethylsiloxane (PDMS). Dithering the frequency of the DFB laser across the Lorentzian lineshape of the drop port at high frequency eliminates $1/f$ noise, and broadband noise is reduced by narrow-band detection with the lock-in amplifier. Biosensor system noise is analyzed and compared with more conventional readout methods, and in our case is dominated by thermal noise of the receiver, shot noise, and relative intensity noise (RIN) of the DFB laser. Because the readout automatically latches onto the drop port and does not require a complex scanning process, this methodology may provide a pathway for high-sensitivity, real-time, and low-cost biosensing.

1:03PM B42.00008 Label-free detection of DNA on silicon surfaces using Brewster angle straddle interferometry (BASI) , XIAO WANG, University of Rochester School of Medicine and Dentistry, Department of Biochemistry and Biophysics, 601 Elmwood Ave., Box 712, Rochester, NY, 14642, LEWIS ROTHBERG, University of Rochester, Department of Chemistry, Rochester, NY 14627 — Label-free sensing of biomolecular interactions is of great importance for drug screening and a variety of clinical assays. Ultrasensitive detection of dsDNA on silicon substrates can be achieved using our new label-free sensing method - Brewster angle straddle interferometry (BASI) which exploits the removal of destructive interference to detect binding of target molecules on a silicon surface functionalized by probe molecules. By exploiting the fact that reflections of p-polarization undergo 180 degree phase shifts above the Brewster angle and none below it, we are able to use unprocessed silicon substrates with native oxide serving as the interference layer. Destructive interference in the geometry we use results in reflectivities $\sim 0.01\%$. Reflectivity from the chip is a quantitative measure of the amount of bound target molecules and can be imaged in real time in microarray format. We demonstrate detection of DNA intercalation on pyrene modified surfaces. The substrates are shown to exhibit excellent binding toward dsDNAs. This work provides an avenue for understanding the binding specificity of small molecule-DNA interactions that can be potentially helpful in developing anticancer agents.

1:15PM B42.00009 Real-time molecular detection using a nanoscale porous silicon waveguide biosensor , XING WEI, JEREMY MARES, SHARON WEISS, Vanderbilt University — A grating-coupled porous silicon waveguide with an integrated PDMS flow cell is demonstrated as a platform for real-time detection of chemical and biological molecules. This sensor platform not only allows for quantification of molecular binding events, but also provides a means to improve understanding of diffusion and binding mechanisms in constricted nanoscale geometries. The large internal surface area of porous silicon enables the capture of molecules inside the waveguide, which causes a large perturbation of the guided mode field and improves detection sensitivity by more than one order of magnitude as compared to evanescent wave-based detection methods. Molecular binding events in the waveguide are monitored by real-time angle-resolved reflectance measurements. Diffusion, adsorption and desorption coefficients of different sized chemical linker and nucleic acid molecules are determined based on the rate of change of the measured resonance angle. Both the magnitude of the waveguide resonance angle shift and kinetic parameters are observed to depend on molecule size. Experimental results are shown to be in good agreement with calculations based on rigorous coupled wave analysis and finite element simulation.

1:27PM B42.00010 On-chip Magnetic Separation and Cell Encapsulation in Droplets , A. CHEN, T. BYVANK, A. BHARDE, B.L. MILLER, J.J. CHALMERS, R. SOORYAKUMAR, The Ohio State University, W.-J. CHANG, University of Wisconsin-Milwaukee, R. BASHIR, University of Illinois at Urbana-Champaign — The demand for high-throughput single cell assays is gaining importance because of the heterogeneity of many cell suspensions, even after significant initial sorting. These suspensions may display cell-to-cell variability at the gene expression level that could impact single cell functional genomics, cancer, stem-cell research and drug screening. The on-chip monitoring of individual cells in an isolated environment could prevent cross-contamination, provide high recovery yield and ability to study biological traits at a single cell level. These advantages of on-chip biological experiments contrast to conventional methods, which require bulk samples that provide only averaged information on cell metabolism. We report on a device that integrates microfluidic technology with a magnetic tweezers array to combine the functionality of separation and encapsulation of objects such as immunomagnetically labeled cells or magnetic beads into pico-liter droplets on the same chip. The ability to control the separation throughput that is independent of the hydrodynamic droplet generation rate allows the encapsulation efficiency to be optimized. The device can potentially be integrated with on-chip labeling and/or bio-detection to become a powerful single-cell analysis device.

1:39PM B42.00011 Chip-based magnetic cytometer for high-throughput cellular profiling in unprocessed biological samples , DAVID ISSADORE, JAEHOON CHUNG, HUILIN SHAO, MONTY LIONG, RALPH WEISSELEDER, HAKHO LEE, Massachusetts General Hospital / Harvard Medical School — Quantitative, high-throughput measurement of biomarkers in individual cells is a cornerstone of biomedical research, but prohibitive size, cost, and requisite sample processing have kept this technology from being more widely adapted in the clinic. We have developed a miniaturized magnetic cytometer (μMCM), a hybrid semiconductor / microfluidic chip, to rapidly measure the magnetic moments of individual immunomagnetically tagged cells. The use of magnetic detection enables measurements to be done on native specimens, thus decreasing the loss of rare cells and removing the need for expensive sample processing equipment. Benefiting from the high speed and sensitivity of semiconductor technology, the μMCM offers high-throughput operation (upwards of 10^7 cells/sec) with a detection resolution of ~ 2000 magnetic nanoparticles/cell. The clinical utility of the μMCM was demonstrated by detecting scant tumor cells (20 cells) in whole blood and by molecularly profiling cells from solid tumor to monitor longitudinal drug efficacy.

1:51PM B42.00012 Miniature magnetic resonance system for robust and portable diagnostics¹, CHANGWOOK MIN, DAVID ISSADORE, JAEHOON CHUNG, HUILIN SHAO, MONTY LIONG, Massachusetts General Hospital, RALPH WEISSLEDER, Massachusetts General Hospital/Harvard Medical School, HAKHO LEE, Massachusetts General Hospital — We have recently developed a new diagnostic platform, microNMR(μ NMR), specifically designed for clinical applications. This new μ NMR system performs rapid, accurate, and robust measurements of cells, proteins and small molecules in point-of-care settings. The system utilizes magnetic nanoparticles (MNPs) to amplify the analytical signals in NMR detection. When molecularly-specific MNPs identify their targets, the particles induce large, amplified changes in the transverse relaxation of water protons by producing local magnetic fields. A major challenge in achieving reliable NMR detection is the fluctuation of NMR frequency (f_0) with temperature, which originates from the temperature-dependent drift of the magnetic field. To overcome the challenge, we have implemented a new, automated feedback controller that keeps track of f_0 and reconfigures measurement settings. The mechanism enables robust μ NMR measurements in realistic clinical environments (4-50 °C). Moreover, the μ NMR interfaces with mobile devices for its operation, maximizing the portability of μ NMR. The clinical utility of the new μ NMR system is demonstrated by detecting and molecularly profiling cancer cells from patient samples.

¹This work is supported in part by National Institutes of Health Grants 2R01-EB004626, HHSN268201000044C, U54-CA119349, and T32-CA79443.

2:03PM B42.00013 Paper Inside? - New Thinking for Biochip and Other Applications, ANDREW STECKL, University of Cincinnati — The drive to improve the performance and reduce the cost of electronic, photonic and fluidic devices is starting to focus on the use of materials that are exotic for these applications but actually readily available in other fields. In this talk the use of paper in biochip and other applications will be reviewed. Paper is a very attractive material for many device applications: very low cost, available in almost any size, versatile surface finishes, portable and flexible. From an environmental point of view, paper is a renewable resource and is readily disposable (incineration, biodegradable). Applications of paper-based electronics currently being considered or investigated include biochips, sensors, communication circuits, batteries, smart packaging, displays. The potential advantages of paper-based devices are in many cases very compelling. For example, biochips fabricated on paper can use the capillary properties of paper to operate without the need of external power sources, greatly simplifying the design and reducing the cost. For e-reader devices, in addition to flexibility, the ideal solution for providing the look-and-feel of ink on paper is to have *e-paper on paper*.

Monday, February 27, 2012 11:15AM - 2:15PM – Session B43 DBIO: Invited Session: Physical Mechanisms of Cell Growth 157AB

11:15AM B43.00001 Processive motions of MreB micro-filaments coordinate cell wall growth¹, ETHAN GARNER, Harvard — Rod-shaped bacteria elongate by the action of cell-wall synthesis complexes linked to underlying dynamic MreB filaments, but how these proteins function to allow continued elongation as a rod remains unknown. To understand how the movement of these filaments relates to cell wall synthesis, we characterized the dynamics of MreB and the cell wall elongation machinery using high-resolution particle tracking in *Bacillus subtilis*. We found that both MreB and the elongation machinery move in linear paths across the cell, moving at similar rates (~ 20 nm / second) and angles to the cell body, suggesting they function as single complexes. These proteins move circumferentially around the cell, principally perpendicular to its length. We find that the motions of these complexes are independent, as they can pause and reverse, and also as nearby complexes move independently in both directions across one surface of the cell. Inhibition of cell wall synthesis with antibiotics or depletions in the cell wall synthesis machinery blocked MreB movement, suggesting that the cell wall synthetic machinery is the motor in this system. We propose that bacteria elongate by the uncoordinated, circumferential movements of synthetic complexes that span the plasma membrane and insert radial hoops of new peptidoglycan during their transit.

¹Watching the motions of the cell wall synthesis machinery and underlying cytoskeleton in *B. subtilis* with high precision particle tracking.

11:51AM B43.00002 Spatial Patterning of Newly-Inserted Material during Bacterial Cell Growth¹, TRISTAN URSELL, Stanford University — In the life cycle of a bacterium, rudimentary microscopy demonstrates that cell growth and elongation are essential characteristics of cellular reproduction. The peptidoglycan cell wall is the main load-bearing structure that determines both cell shape and overall size. However, simple imaging of cellular growth gives no indication of the spatial patterning nor mechanism by which material is being incorporated into the pre-existing cell wall. We employ a combination of high-resolution pulse-chase fluorescence microscopy, 3D computational microscopy, and detailed mechanistic simulations to explore how spatial patterning results in uniform growth and maintenance of cell shape. We show that growth is happening in discrete bursts randomly distributed over the cell surface, with a well-defined mean size and average rate. We further use these techniques to explore the effects of division and cell wall disrupting antibiotics, like cephalaxin and A22, respectively, on the patterning of cell wall growth in *E. coli*. Finally, we explore the spatial correlation between presence of the bacterial actin-like cytoskeletal protein, MreB, and local cell wall growth. Together these techniques form a powerful method for exploring the detailed dynamics and involvement of antibiotics and cell wall-associated proteins in bacterial cell growth.

In collaboration with Kerwyn Huang, Stanford University.

¹Genentech Bio-X Fellowship

12:27PM B43.00003 Mechanics of cell division in fission yeast, FRED CHANG, Columbia University — Cytokinesis is the stage of cell division in which a cell divides into two. A paradigm of cytokinesis in animal cells is that the actomyosin contractile ring provides the primary force to squeeze the cell into two. In the fission yeast *Schizosaccharomyces pombe*, cytokinesis also requires an actomyosin ring, which has been generally assumed to provide the force for cleavage. However, in contrast to animal cells, yeast cells assemble a cell wall septum concomitant with ring contraction and possess large (MPa) internal turgor pressure. Here, we show that the inward force generated by the division apparatus opposes turgor pressure; a decrease in effective turgor pressure leads to an increase in cleavage rate. We show that the ring cannot be the primary force generator. Scaling arguments indicate that the contractile ring can only provide a tiny fraction of the mechanical stress required to overcome turgor. Further, we show that cleavage can occur even in the absence of the contractile ring. Instead of the contractile ring, scaling arguments and modeling suggest that the large forces for cytokinesis are produced by the assembly of cell wall polymers in the growing septum.

1:03PM B43.00004 Decoding the topology of vascular organization¹, ELENI KATIFORI, Rockefeller University — Distribution and structural networks permeate virtually all life, from the cellular to the organismic level. They have allowed organisms to grow in size and complexity by ensuring efficient distribution of nutrients and structural support. Given their importance, these vascular and structural webs have been under strong evolutionary selection and their form frequently reflects important aspects of their function. We discuss the design principles behind the evolution of the architecture and topology of vascular and structural networks and present some examples (leaf venation, arterial vasculature of the neocortex and others) that elucidate them.

¹This work was supported in part by the NSF under Grant PHY-1058899

1:39PM B43.00005 Mechanics and Dynamics of Plant Cell Division¹, JACQUES DUMAIS, Harvard University — The division of eukaryotic cells involves the assembly of complex cytoskeletal structures to exert the forces required for chromosome segregation and cytokinesis. In plants, tensional forces within the cytoskeleton constrain cells to divide according to a small number of area minimizing configurations. We have shown that the probability of observing a particular division configuration increases inversely with its relative area according to an exponential probability distribution known as the Gibbs measure. The distribution is universal up to experimental accuracy with a unique constant that applies for all plants studied irrespective of the shape and size of their cells. Using a maximum entropy formulation, we were able to demonstrate that the empirically observed division rule is predicted by the dynamics of the tense cytoskeletal elements controlling the positioning of the division plane. Finally, by framing this division rule as a dynamical system, we identified a broad class of attractors that are predictive of cell patterns observed in plants. Plant cell division thus offers a remarkable example of how interactions at the molecular level can lead to strikingly complex behaviors at the cellular and multicellular levels.

¹This research was funded by the Human Frontier Science Program and the National Science Foundation

Monday, February 27, 2012 11:15AM - 2:15PM –
Session B44 DPOLY DBIO: Focus Session: Translocation through Nanopores - Measurements and Theoretical Models 157C

11:15AM B44.00001 Sequence-dependent ion current modulations in biological and synthetic nanopores¹, ALEKSEI AKSIMENTIEV, University of Illinois at Urbana-Champaign — The possibility of DNA sequence detection by measuring the blockade ionic current in nanopores has been the driving force for the spectacular development of the nanopore research field. Nevertheless, fifteen years after the first measurements, the molecular mechanism(s) of ion current modulation by the sequence of DNA nucleotides remains elusive. Here, we report the results of extensive all-atom molecular dynamics and Brownian dynamics simulations of three nanopore systems: a biological nanopore MspA, a solid-state nanopore and a graphene nanopore, aimed at elucidating the microscopic mechanism of the ion current modulation. In the case of solid-state and graphene nanopores, we determined the effect of sequence convolution on the ionic current value by simulating the ionic current blockades produced by all 64 permutations of the DNA nucleotide triplets. In the case of MspA, we determined the effect of the sequence, the global orientation, and the conformation of a DNA strand on the distribution of the ion current blockades. Based on the results of our simulations, we suggest possible routes for increasing the resolution of DNA sequence detection by measuring the nanopore ionic current and describe the inherent limitations of the method.

¹Support by grants from NSF (DMR-0955959) and NIH (R01-HG005115).

11:51AM B44.00002 Unexpected stop-and-go when DNA is pulled through a network, JUAN GUAN, BO WANG, SUNG CHUL BAE, STEVE GRANICK, University of Illinois Urbana Champaign — We perform single-molecule imaging of lambda-DNA chains when DC electric fields drive them through agarose networks in which they are heavily entangled. Velocity is decidedly unsteady. Exhaustive statistics reveal how motion switches between “mobile” and “pause” states, the latter differing from well-known “hooking.” As these observations appear to be inconsistent with the prevailing theories of DNA electrophoresis, we are also engaged in measurements that discriminate between motion of the chain ends and the chain centers, by direct two-color fluorescence imaging.

12:03PM B44.00003 Non-Equilibrium DNA Dynamics Probed by Delayed Capture and Recapture by a Solid-State Nanopore¹, MIRNA MIHOVILOVIC, ERIN TEICH, NICHOLAS HAGERTY, DEREK STEIN, Brown University — We studied the relaxation of λ -DNA following its translocation through a voltage-biased solid-state nanopore. The translocation process drives DNA into a non-equilibrium state because the ~ 2 ms translocation time is roughly fifty times shorter than the polymer's characteristic (Zimm) relaxation time. By reversing the applied voltage at controlled delay times after a translocation event, the nanopore probed the configurations of recaptured molecules at various stages of relaxation. We monitored the disruptions of the ionic current through the nanopore and computed the integrated charge deficits (ECDs) resulting from DNA translocations. As the delay time between voltage reversals was decreased from 50 ms to 5 ms, the distribution of ECDs shifted to lower values. Furthermore, an increasing fraction of recapture events occurred in a shorter interval from the voltage reversal than the delay time. These observations are explained by the expansion of the DNA coil as it approaches equilibrium. Finally, we show that recapturing a molecule multiple times and averaging the ECDs reduces the measurement error, which is useful for molecular diagnostic applications. The variance decreases approximately as the inverse number of passes through the pore.

¹This material is based upon work supported by the National Science Foundation under Grant No. CBET0846505 and Intel Corp.

12:15PM B44.00004 Forced Translocation of Polymer through Nanopore: Deterministic Model and Simulations, YANQIAN WANG, UNC-Chapel Hill, SERGEY PANYUKOV, P. N. Lebedev Phys. Inst., Russ. Acad. of Sci., QI LIAO, Inst. of Chem., Chin. Acad. of Sci., MICHAEL RUBINSTEIN, UNC-Chapel Hill — We propose a new theoretical model of forced translocation of a polymer chain through a nanopore. We assume that DNA translocation at high fields proceeds too fast for the chain to relax, and thus the chain unravels loop by loop in an almost deterministic way. So the distribution of translocation times of a given monomer is controlled by the initial conformation of the chain (the distribution of its loops). Our model predicts the translocation time of each monomer as an explicit function of initial polymer conformation. We refer to this concept as “fingerprinting”. The width of the translocation time distribution is determined by the loop distribution in initial conformation as well as by the thermal fluctuations of the polymer chain during the translocation process. We show that the conformational broadening Δt of translocation times of m -th monomer $\Delta t \propto m^{1.5}$ is stronger than the thermal broadening $\delta t \propto m^{1.25}$. The predictions of our deterministic model were verified by extensive molecular dynamics simulations.

12:27PM B44.00005 Force-Driven Translocation of a Polymer through a Nanopore, PAYAM ROWGHANIAN, PhD student, ALEXANDER GROSBERG, Professor, NYU CSMR TEAM¹ — We study the far from equilibrium translocation of a DNA molecule through a nanopore. The pore is much narrower than the DNA, so the electrically driven DNA undergoes dramatic deformations during its passage. Using an idealized model in which the DNA is assumed to be a very long and flexible homopolymer driven by a force exerted only in the pore, we modify a previously developed method by introducing the concept of “iso-flux trumpet”. We show that although the speed of the process is determined by the friction of the trailing part with the solvent, friction dissipates a small portion of the work performed by the electric field on the polymer, and the work is mostly dissipated by the irreversible stretching and destretching of the polymer squeezed into the small pore. Moreover, due to such stretches essentially caused by the membrane, a net heat transfer occurs during translocation from the post-translocation to the pre-translocation side of the membrane. The current theory can be improved by accounting for the nonzero field outside the pore and by considering the coupling between electric and hydrodynamic fields. The forces exerted by such fields on the DNA bulk not only alter the passage dynamics, but also introduce deformations on the initial conformation of the polymer.

¹I am Professor Grosberg's student at the Center for Soft Matter Research at NYU's physics department.

12:39PM B44.00006 Non-equilibrium tension propagation as a unifying description of driven polymer translocation, TIMO IKONEN, TAPPIO ALA-NISSILA, Aalto University School of Science, Finland, ANIKET BHATTACHARYA, University of Central Florida, WOKYUNG SUNG, Pohang University of Science and Technology, South Korea — We present results from a new Brownian dynamics model of driven polymer translocation¹, in which non-equilibrium memory effects due to tension propagation (TP) along the cis side subchain are included as a time-dependent friction. To solve the effective friction, we develop a finite chain length TP formalism, expanding on the work of Sakaue^{1,2}. The model yields results in excellent quantitative agreement with molecular dynamics simulations in a wide range of parameters. Our results show that non-equilibrium TP along the cis side subchain dominates the dynamics of driven translocation. In addition, the model explains the different scaling of translocation time with chain length observed both in experiments and simulations as a combined effect of finite chain length and pore-polymer interactions.

¹T. Ikonen, A. Bhattacharya, T. Ala-Nissila and W. Sung, submitted.

²T. Sakaue, Phys. Rev. E **76**, 021803 (2007)

³T. Sakaue, Phys. Rev. E **81**, 041808 (2010).

12:51PM B44.00007 Graphene Nano-Electrodes for DNA Sequencing: an Ab initio Perspective, R.H. SCHEICHER, J. PRASONGKIT, A. GRIGORIEV, Uppsala University, Y. HE, M. LIU, Institute of Microelectronics, Chinese Academy of Sciences, R. AHUJA, Uppsala University — The proposal was made that a graphene nanogap could be used to probe the transverse conductance of individual nucleotides in DNA to rapidly identify the associated base sequence. Experimentally, the characteristic drop in ionic current associated with translocation events of DNA passing through a graphene nanopore was measured. Using first-principles methods, we evaluated the performance of two graphene nano-electrodes configurations for nucleobase identification. In the first study, Nano Lett. **11**, 1941 (2011), we investigated the electronic transport properties of the four nucleotides when located in a graphene nanogap by employing density functional theory and the non-equilibrium Green's function method. In particular, we determined the electrical current variation at finite bias due to changes in the nucleotides orientation. Our second study, Adv. Funct. Mater. **21**, 2674 (2011), utilized molecular dynamics simulations in conjunction with electronic transport calculations to explore specifically the effect of the hydrogenated graphene edges on the translocating DNA. It is found that edge-hydrogenated graphene electrodes facilitate the temporary formation of weak H-bonds with suitable atomic sites in the nucleotides.

1:03PM B44.00008 Preprotein translocation across the endoplasmic reticulum membrane in milieus crowded by proteins, JOSÉ ANTONIO VÉLEZ, ORLANDO GUZMÁN, Universidad Autónoma Metropolitana Iztapalapa, FERNANDO NAVARRO, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional — Translocation of preproteins chains between the cytoplasm and the endoplasmic reticulum lumen takes place in a milieu crowded primarily by proteins. We compute translocation and retrotranslocation times for chains of different length in a milieu crowded by spherical agents at volume fractions equivalent to that found in cells. These numerical times obtained from a diffusion-equation model subject to a potential given by the free energy of one chain, indicate that crowding increases the translocation time by up to five times compared to those in dilute conditions for average-size chains and by up to a thousand times for long chains. Retrotranslocation times become smaller than translocation ones, in approximately 75%. Translocation rates obtained in this work are similar to those found in a theoretical model for Brownian-ratchet translocation and coincide with in vitro experimental results (1-8 aminoacid/s) only in the limit of very long chains; for shorter chains, translocation rates are much faster. Our prediction that for long chains translocation rates would be significantly slowed by crowding can be tested experimentally using vesicles. Discrepancy of time-scales with experiments for short chains indicates that other factors beside crowding must be included in our model.

1:15PM B44.00009 Nanopore Mass Spectrometry¹, DEREK STEIN, JOSEPH BUSH, MIRNA MIHOVILOVIC, WILLIAM MAULBETSCH, WOYOUNG MOON, CARTHENE BAZEMORE-WALKER, PETER WEBER, Brown University — We describe a concept for single-DNA analysis called nanopore mass spectrometry, which seeks to combine the benefits of nanopores with the speed, sensitivity, and robustness of single base detection by mass spectrometry. The basic idea is to cleave the individual nucleotides from a DNA polymer as they transit a nanopore in sequence, and to identify each one by determining its charge-to-mass ratio in a mass spectrometer. We describe how nanopore mass spectrometry can address the challenges faced by other nanopore-based DNA analysis approaches. We also describe the design, construction, and testing of a prototype instrument that interfaces a nanopore ion source with a quadrupole mass filter and a single ion detector. We are using this new instrument to test the key scientific questions bearing on our analysis strategy: 1) Can DNA nucleotides be reliably transferred from their native liquid phase into the vacuum environment of a mass spectrometer? 2) Can nucleotides be detected with near 100% efficiency? 3) Can DNA polymers be controllably cleaved to isolate ionized bases or nucleotides in the mass spectrometer?

¹This work was supported by NIH through grant R21HG005100.

1:27PM B44.00010 Direct observation of DNA translocation influenced by electrically gated nanopores, GENKI ANDO, HIROKI MORIYA, KENTA TSUKAHIRA, SATOSHI YANO, TOSHIYUKI MITSUI, Department of Physics and Mathematics, Aoyama Gakuin University — One of remarkable recent developments in the solid state nanopore based DNA analysis is adding the ability to control electric potential near nanopore as a gate electrode by patterning metal in or on nanopore. In this approach, better control of DNA translocations for example, slowing down the translocation speed might be expected. We have fabricated insulator-metal-insulator nanopores of rather large 100 nm pore in diameter. The 100 nm diameter pores allow us to observe the translocation of lambda-DNA molecules directly by means of fluorescence microscopy without heavy clogging of the DNA molecules into the pores. By controlling gate voltage on metal relative to the cis and trans voltages, the translocation rates of DNA are able to change. Interestingly, applying pulse voltage to the gate metal near 100 ms to reverse the direction of the electric field near the cis side of nanopore reverses the direction of the DNA translocation instantaneously. This in fact provides us a new way to repeat translocation of the same DNA molecule. Furthermore, repeating the pulse tends to clear off the clogged DNA molecules in nanopore. We will present more details of these phenomena caused by the gate voltages.

1:39PM B44.00011 Thermophoretic stretch of a polymer confined to a nanofluidic channel, MARTIN BERTRAND, BELA JOOS, University of Ottawa — The precise manipulation of macromolecules by thermophoresis is quite promising. Indeed, Thamdrup *et al.* (Nano Lett., **10**, 2010) successfully moved double-stranded DNA (dsDNA) filaments in microfluidic geometries and subsequently inserted them into nano-channels using thermophoretic forces originating from highly localized thermal gradients and also showed that once in the channel, DNA can be symmetrically stretched under thermophoresis. This last procedure could be used to better expose the backbone of a nano-confined polymer to study its properties or the binding activity of some enzyme. We present a novel approach to model this symmetric stretch using blobs and the Flory free-energy of a polymer chain. Our model describes the monomer concentration profile reported in the aforementioned study. A value close to what is found in the literature is obtained for the Soret coefficient of the segments of dsDNA, characterizing thermophoresis. We further corroborate the validity of our model using molecular dynamics simulations. In these calculations, excluded volume interactions are shown to play a key role especially when temperatures are close to the solvent's θ value.

1:51PM B44.00012 Small Interfering RNA Transfection Across a Phospholipid Membrane, KEN-ICHI NOMURA, VAN NGO, AMIT CHOUBEY, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, Collaboratory for Advanced Computing and Simulations, Department of Physics and Astronomy, University of Southern California, Los Angeles, California — Small interfering RNA (siRNA) molecules play a pivotal role in silencing gene expression via the RNA interference mechanism. We have performed steered MD simulations to study the transfection of a bare siRNA and siRNA/Oleic Acid (OA) complex across the dipalmitoylphosphatidylcholine (DPPC) bilayer at $T = 323$ K. Bare siRNA induces the formation of frustrated lipid gel domains, whereas in the presence of siRNA/OA complex the membrane is found to be in the liquid-ordered phase. In both cases the stress profiles across the membrane indicate that the membrane is under tension near the head groups and highly compressed at the water-hydrophobic interface. During transfection, the membrane is deformed and the lateral stress is significantly lowered for the bare siRNA and siRNA/OA complex. The bare siRNA transfects through a lipid-nanopore of hydrophilic head-groups and hydrophobic carbon chains, whereas the siRNA/OA complex transfects through a lipid-nanopore of hydrophilic head groups.

2:03PM B44.00013 DNA base-specific modulation of μ A transverse edge currents through a metallic graphene nanoribbon with a nanopore, KAMAL K. SAHA, Department of Physics and Astronomy, University of Delaware, Newark, DE 19716, MARIJA DRNDIĆ, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104, BRANISLAV K. NIKOLIĆ, Department of Physics and Astronomy, University of Delaware, Newark, DE 19716 — We study two-terminal devices for DNA sequencing which consist of a zigzag graphene nanoribbon (ZGNR) and a nanopore in its interior through which the DNA molecule is translocated. Using the nonequilibrium Green functions combined with density functional theory, we demonstrate that each of the four DNA nucleobases inserted into the nanopore, whose edge carbon atoms are passivated by either hydrogen or nitrogen, will lead to a unique change in the device conductance. Unlike other recent biosensors based on transverse electronic transport through translocated DNA, which utilize small (of the order of pA) tunneling current across a nanogap or a nanopore yielding a poor signal-to-noise ratio, our device concept relies on the fact that in ZGNRs local current density is peaked around the edges so that drilling a nanopore away from the edges will not diminish the conductance. Inserting a nucleobase into the nanopore affects the charge density in the surrounding area, thereby modulating edge conduction currents whose magnitude is of the order of μ A at bias voltage $\simeq 0.1$ V. The proposed biosensors could also be realized with other nanowires supporting transverse edge currents, such as chiral GNRs or wires made of two-dimensional topological insulators.

Monday, February 27, 2012 11:15AM - 2:15PM —

Session B45 DPOLY: Focus Session: Thin Film Block Copolymers - Swelling and Ordering 159

11:15AM B45.00001 ABSTRACT WITHDRAWN —

11:27AM B45.00002 Effect of Solvent Removal Rate on the Morphology of Solvent Vapor Annealed ABA Triblock Copolymer Thin Films, JULIE N. L. ALBERT, WEN-SHIUE YOUNG, RONALD L. LEWIS, III, TIMOTHY D. BOGART¹, JASMINE R. SMITH², THOMAS H. EPPS, III, University of Delaware — Solvent vapor annealing (SVA) treatments can be used to kinetically trap unique self-assembled nanostructures in block copolymer thin films that are not achievable by traditional thermal annealing methods. In this work, we kinetically trapped the thin film morphologies of a cylinder-forming ABA triblock copolymer at key points during the solvent removal process following SVA in order to gain insight into the re-ordering mechanisms associated with solvent removal. Specifically, we identified morphology transformations as a function of solvent removal rate, showed that the mechanism for cylinder reorientation involved the propagation of changes at the free surface through the film as a front, and validated a film etching scheme to image the through-film morphology using successive ultra-violet ozone (UVO) etching steps followed by atomic force microscopy (AFM). This facile real-space analysis of the thin film internal structure is more easily implemented in comparison to cross-sectional imaging. The results and methodology of our work are significant not only for improving our understanding of block copolymer thin film self-assembly, but also for tailoring solution processing methods to fabricate nanostructured materials (e.g., for nanotemplate and membrane applications) in general.

¹Current location: University of Texas at Austin

²Current location: Delaware State University

11:39AM B45.00003 Obtaining Perpendicular Block Copolymer Morphologies with Solvent Annealing, KEVIN GOTRIK, JEONG GON SON, ADAM HANNON, CAROLINE ROSS, Massachusetts Institute of Technology — Being able to control block copolymer (BCP) thin film morphology and orientation is of interest for lithographic applications where creation of feature sizes ranging from 10-100nm is desirable. Perpendicular oriented cylinders and lamellae are especially valuable due to their high aspect ratios but are difficult to achieve in BCP systems with a large Flory-Huggins interaction parameter (χ). We explore the morphological phase behavior that films (30-200nm) of poly(styrene-*b*-dimethylsiloxane) (PS-PDMS, 45kg/mol, $\chi=0.26$) exhibit under different solvent conditions with focus on conditions that produce perpendicular microdomains. The microdomains are revealed by selectively etching the PS with an oxygen plasma (50W CF4). Variation in the solvent vapor conditions results in selective swelling of the different blocks of the copolymer depending on the relative Hildebrand solubility parameters (e.g. PS- 18.5, toluene-18.3 MPa^{1/2}), affecting the microdomain morphologies, and the solvent evaporation and deswelling process influences the orientation of the microdomains. Two different strategies are presented involving solvent vapor annealing that result in perpendicular morphologies in films of PS-PDMS and the results are compared with self-consistent field theory modeling of solvent-polymer systems.

11:51AM B45.00004 Mesoscale Dynamics of Solvent Evaporation in Block Copolymer Thin Films, SEAN PARADISO, SU-MI HUR, KRIS DELANEY, HECTOR CENICEROS, CARLOS GARCIA-CERVERA, GLENN FREDRICKSON, University of California, Santa Barbara — Block copolymer thin films are being investigated for a wide variety of applications ranging from separation membranes, organic photovoltaics, and lithographic masks. In order to accelerate defect annihilation in the periodic structures that develop within these films, solvent annealing techniques are often employed that exploit control over solvent atmosphere to modify the free surface thermodynamics and evaporation rate in an attempt to influence the alignment of ordered domains. The inherently non-equilibrium nature of this problem complicates standard theoretical treatments based on relative free energy calculations, so we have employed a dynamical extension of Self-Consistent Field Theory coupled with a solvent evaporation mechanism to gain insights into the interplay between component-surface interactions, evaporation rate, and observed film morphology. The effects of these factors on the micro-phase separation trajectory of the film will be discussed.

12:03PM B45.00005 Optimizing the Combination of Solvent Annealing and Directed Self-Assembly in Thin Film Block Copolymer Systems Using Self-Consistent Field Theory, ADAM HANNON, KEVIN GOTRIK, ALFREDO ALEXANDER-KÄTZ, CAROLINE ROSS, Massachusetts Institute of Technology — We show how self-consistent field theory simulations can be used to optimize the combination of solvent annealing and directed self-assembly using topographical and chemical templating in order to achieve an ultimate goal of arbitrary pattern generation in thin film block copolymer systems. The simulations use a combination of field boundary conditions to model topographical features such as posts and chemically distinct surfaces along with a variety of compositions to model a range of solvent, homopolymer, and block copolymer multi-component blends [Macromolecules 2010, 43, 8290–8295]. Computational results are compared with experimental systems that use polydimethylsiloxane, polystyrene, and polyferrocenylsilane polymers, heptane, toluene, and chloroform solvents, and electron beam lithography created hydrogen silsesquioxane posts. By varying the different polymers used and thus their χ interaction parameters, the relative fractions of solvent and different polymer blocks, and surface feature affinity and shape, the optimal requirements to create arbitrary complex features for nanolithography applications will be demonstrated.

12:15PM B45.00006 Sub-10 nm block copolymer patterns with mixed morphology and period using electron irradiation and solvent annealing, JEONG GON SON, Korea Institute of Science and Technology, JAE-BYUM CHANG, KARL K. BERGGREN, CAROLINE A. ROSS, MIT — High resolution patterns with controllable period and feature geometry are of intense interest for nanolithography applications, but to date this has been challenging to accomplish from a single block copolymer, which produces patterns of a fixed period and morphology. Here we show how patterns consisting of coexisting sub-10 nm spheres and cylinders and sphere patterns with a range of periods can be created using a combination of serial solvent anneal processes and electron-beam irradiation of selected areas of a film of poly(styrene-block-dimethylsiloxane). We also additionally combined with topographical templates consisting of either removable polymeric regions to make patterns with highly aligned lines, dots and featureless regions, or post arrays which can simultaneously align and register the line and dot arrays. These techniques offer the possibility of forming a wide range of aperiodic pattern geometries including single lines or ordered line segments, and significantly extend the ability of block copolymer lithography to produce patterns essential for nanoscale device fabrication.

12:27PM B45.00007 Raster solvent vapor annealing of block copolymer thin films, JONATHAN SEPPALA, RONALD LEWIS, THOMAS EPPS, University of Delaware — Nanoscale phase separation in block copolymer (BCP) thin films makes them attractive for a variety of applications such as membranes, organic electronics, and nanoscale templating. Annealing BCP thin films (thermal or solvent) promotes ordering of their microphase-separated structures into useful patterns. Solvent vapor annealing (SVA) is an attractive approach as it avoids thermal degradation and provides greater flexibility in morphology control compared to thermal annealing through overall film swelling and preferential swelling of one or more blocks. SVA is typically conducted in an annealing chamber that permits exposure of the film to a controlled vapor environment. However, control over the vapor environment locally may be more desirable for nano-patterning applications. In this work we introduce raster solvent vapor annealing, a method that gives us precise control over the annealed region and excellent point control of the resulting morphology allowing for specific mixed morphologies on a single sample. The simplest setup, needle directed solvent vapor with controlled solvent flow rate and rastering speed, allows “drawn” ordered parallel and perpendicular cylinders in a cylinder forming BCP thin film. The efficacy of this method will be discussed in the oral presentation.

12:39PM B45.00008 Confined drying of copolymer solutions¹, DAUBERSIES LAURE, LENG JACQUES, SALMON JEAN-BAPTISTE, None — We developed a simple tool for the rapid screening of phase diagrams of polymer and surfactant solutions. Our technique is based on the controlled drying of a droplet solution in a confined geometry. A μL -sized droplet of an aqueous solution is confined between two wafers (diameter 3 cm), separated by a controlled thickness ($\approx 150 \mu\text{m}$). The confinement casts a well-defined timescale to the drying kinetics, mainly governed by the wafer area. Indeed, water removal only occurs through a diffusive process from the edge of droplet to the edge of the wafer. Confinement also permits a simple 2D description, and allows simple observations of the drying. We studied the drying of an aqueous solution of a triblock copolymer (Pluronic, P104) thanks to three different techniques: polarized microscopy, fluorescent microscopy, and Raman imaging. With our tool and techniques, we not only build an accurate phase diagram of the solution (with one microliter only) but also measure both the mutual diffusion coefficient and the activity of the solution as a function of its concentration, including the Flory-Huggins parameter.

¹towards thermodynamical and kinetics data.

12:51PM B45.00009 Rapid Self- Assembly and Perpendicular Alignment in lamellar PS-b-PEO System for Fabrication of Sub 20 nm Nanolithography Templates, PARVANEH MOKARIAN-TABARI, University College Cork and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Ireland, TIMOTHY W. COLLINS, University College Cork and Tyndall National Institute, RAMSANKAR SENTHAMARAIKANNAN, JUSTIN D. HOLMES, MICHAEL A. MORRIS, University College Cork and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Ireland — Creating perpendicular alignment in lamellar block copolymer systems has considerable industrial and commercial significance. In general, these lamellar systems require careful interface engineering to obtain vertical orientation of the blocks. To avoid the strong preferential adsorption of one block to either the substrate or the polymer/air interface, the surface must be ‘neutralised’ by chemical brushes or external forces e.g. solvent fields. Reported here is a stepwise thermo/solvent annealing process called “combinatorial annealing” allowing the formation of perpendicular domains of polystyrene-b-polyethylene oxide (PS-b-PEO) lamellar structures while avoiding brush or other surface modification. The Thermo/solvent annealing is done in a commercial microwave reactor and perpendicular alignment is observed within a few minutes. This BCP has a very small minimum feature size, relevant to the fabrication of nano-features in electronic devices and results are presented here.

1:03PM B45.00010 Controlled Deposition of Ordered Block Copolymer Thin Films by Electrospray¹, HANQIONG HU, Department of Chemical Engineering, Yale University, SOFIA RANGOU, APOSTOLOS AVERGOPOULOS, Department of Materials Science and Engineering, University of Ioannina, Greece, CHINEDUM OSUJI, Department of Chemical Engineering, Yale University — Electrospray offers a potentially useful platform for the controlled delivery of a variety of materials, but surprisingly, its application to block copolymer thin film deposition remains unexplored. Here we show that under appropriate conditions, well ordered films of PEO cylinder-forming poly(styrene-b-ethylene oxide) may be continuously deposited by electrospray. Ordered film formation is predicated on fast thermal equilibration relative to rate of deposition. We conduct time-resolved observations and investigate the effects of process parameters that underpin film morphology including solvent selectivity, substrate temperature and flow rate of the electrospray feed solution. For the particular system studied, we uncover a wide temperature window from 90°C to 160°C and an ideal flow rate (2 $\mu\text{L}/\text{min}$) for ordered film growth, but no strong influence of solvent selectivity was observed. PEO cylinders were observed to align with their long axes perpendicular to the substrate at optimal spray conditions.

¹NSF support (DMR-0847534) is gratefully acknowledged.

1:15PM B45.00011 Two distinct timescales in the ordering of symmetric diblock copolymer films, ROBERT D. PETERS, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1 — At equilibrium, an ordered symmetric diblock copolymer film forms lamellae parallel to the substrate interface. Furthermore, unless a film's thickness is exactly commensurate with the intrinsic height of the layered structure, the free surface will break up into holes or islands with a thickness corresponding to one lamellae. This ensures that the preferred lamellar spacing of the film is achieved while volume is conserved. We study the internal dynamics of ordering as a lamellar forming thin film transitions from the disordered state to its equilibrium morphology. In particular, before the free surface nucleates to form islands or holes, a film must begin by ordering internally. Using ellipsometry, we measure small changes in the internal film structure as the diblock orders prior to any change of the free surface topology. We probe two distinct timescales along the pathway to an equilibrium state: 1) An initial ordering time where molecules begin to align and form lamellae; and 2) an incubation time where the structure remains constant before nucleation of holes or islands. We will show the effect that film height and commensurability has on these two timescales, allowing us to better understand the effect of confinement on the ordering dynamics of lamellar forming thin films.

1:27PM B45.00012 The hydration and ordering of lamellar block copolymer films prior to the formation of polymer vesicles¹, YOHEI KAMATA, Kuraray Co., Ltd., ANDREW PARNELL, Department of Physics and Astronomy, University of Sheffield, ANDREW DENNISON, ROBERT BARKER, PHILIPP GUTFREUND, Institut Laue-Langevin, MAXIMILIAN SKODA, ISIS, STFC, Rutherford-Appleton Lab, SHAOMIN MAI, Department of Chemistry, University of Sheffield, RICHARD JONES, Department of Physics and Astronomy, University of Sheffield — Polymersomes – vesicles based on self-assembled bilayers in turn composed of amphiphilic copolymers – are good candidates for molecular delivery systems; hydrophilic molecules can be enclosed within the aqueous core, to be released by a trigger, which disrupts the vesicle's wall. The key to the use of these polymer vesicles as effective molecular delivery system is in the ability to efficiently encapsulate a molecular payload within the vesicle. To understand the formation mechanism of polymer vesicles via the thin film rehydration method, we have evaluated the hydration and ordering of PEO-PBO diblock copolymer thin films in a controlled water vapor atmosphere. We have performed Neutron Reflectivity, Ellipsometry and Atomic Force Microscopy measurements during the hydration process. These results show that the film swells slowly in the initial stage. It then swells rapidly at a certain critical point and makes ordered structure at the same time. The lamellae are gradually oriented parallel to the substrate with increasing water absorption.

¹We acknowledge ISIS and ILL neutron sources for access to these facilities.

1:39PM B45.00013 Effect of thickness on microdomain orientation in shear-aligned, cylinder-forming PS-PHMA thin films, RALEIGH DAVIS, Princeton University, PAUL CHAIKIN, New York University, RICHARD REGISTER, Princeton University — Previous work has shown that application of a shear stress can impart well-defined orientational order to the microdomains of cylinder-forming poly(styrene)-b-poly(n-hexylmethacrylate) (PS-PHMA) thin films. Unlike many block copolymer thin films, PS-PHMA tend not to form terraces (islands/holes). As a result, film thickness plays an important role in determining the orientation of the cylindrical microdomains. Here we study the effect of film thickness on the morphology of aligned and unaligned PS-PHMA films. Films with a gradient in thickness were generated, via flow coating, and then imaged using atomic force microscopy to examine the microdomain morphology before and after shear alignment. As a function of thickness the unsheared film morphology oscillated between dots (either spheres or cylinders oriented perpendicularly to the substrate) and lines (cylinders oriented parallel to the substrate), with the highest fraction of lines occurring at film thicknesses corresponding to an integral number of cylinder domain spacings. For thicknesses larger than three domain spacings, the oscillation ceased and complete coverage by line patterns was observed. Once shear-aligned, the thicknesses that exhibited the largest fraction of lines pre-shear, showed the highest quality of alignment post-shear.

1:51PM B45.00014 GISAXS simulation and analysis on GPU clusters¹, SLIM CHOUROU, ABHINAV SARJE, XIAOYE LI, Computational Research Division, Lawrence Berkeley National Laboratory, ELAINE CHAN, ALEXANDER HEXEMER, Advanced Light Source, Lawrence Berkeley National Laboratory — We have implemented a flexible Grazing Incidence Small-Angle Scattering (GISAXS) simulation code based on the Distorted Wave Born Approximation (DWBA) theory that effectively utilizes the parallel processing power provided by the GPUs. This constitutes a handy tool for experimentalists facing a massive flux of data, allowing them to accurately simulate the GISAXS process and analyze the produced data. The software computes the diffraction image for any given superposition of custom shapes or morphologies (e.g. obtained graphically via a discretization scheme) in a user-defined region of k-space (or region of the area detector) for all possible grazing incidence angles and in-plane sample rotations. This flexibility then allows to easily tackle a wide range of possible sample geometries such as nanostructures on top of or embedded in a substrate or a multilayered structure. In cases where the sample displays regions of significant refractive index contrast, an algorithm has been implemented to perform an optimal slicing of the sample along the vertical direction and compute the averaged refractive index profile to be used as the reference geometry of the unperturbed system. Preliminary tests on a single GPU show a speedup of over 200 times compared to the sequential code.

¹This work was supported by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

2:03PM B45.00015 Modeling Line Edge Roughness in Lamellar Block Copolymer Systems¹, PAUL PATRONE, University of Maryland, College Park; and NIST Gaithersburg, GREGG GALLATIN, NIST Gaithersburg — Block copolymers offer an appealing alternative to current lithographic techniques with regard to fabrication of the next generation microprocessors. However, if copolymers are to be useful on an industrial manufacturing scale, they must meet or exceed lithography specifications for placement and line edge roughness (LER) of resist features. Here we discuss a field theoretic approach to modeling the LER in the lamellar phase of a strongly segregated block copolymer system. Our model is based on the Leibler-Ohta-Kawasaki free energy functional, which takes the Flory-Huggins parameter and index of polymerization as inputs. We consider a domain with a finite number of phase separated microdomains; at the system boundary, we apply conditions akin to a chemical pinning field. Using a path integral formalism, we determine how fluctuations of the microdomain boundaries depend on distance from the system boundary, number of microdomains, the Flory-Huggins parameter, and index of polymerization.

¹Supported by NIST-ARRA Grant 70NANB10H026

Monday, February 27, 2012 11:15AM - 2:15PM –
Session B46 DPOLY: Invited Session: Industrial Applications of Advanced Polymer-Based Nanomaterials 160AB

11:15AM B46.00001 Polymer and Material Design for Lithography From 50 nm Node to the sub-16 nm Node¹, PETER TREFONAS, The Dow Chemical Company — Microlithography is one of the technologies which enabled the Information Age. Developing at the intersection of optical physics, polymer science and photochemistry, the need for ever smaller high fidelity patterns to build integrated circuits is currently pushing the technology evolution from 193 nm immersion lithography to extreme ultraviolet lithography (13.5 nm) to alternate patterning technologies such as directed self assembly (DSA) of block copolymers. Essential to the success of this progression is a rapid application of new concepts and materials in polymer science. We will discuss the requirements for 193 immersion lithography and how advanced acrylic random polymers are being designed with chemical amplification functionality to meet these needs. The special requirements of a water immersion lithography led to the invention and rapid commercial application of surface assembled embedded barrier layer polymers. Design of polymers for EUV lithography is having to respond to much different challenges, prominent being the dearth of photons in the exposure step, and the other being how to maximize the efficiency of photoacid production. In parallel, alternative lithographic approaches are being developed using directed self assembly of block copolymers which realize pattern frequency multiplication. We will update with our progress in the applications of polymers designed for DSA.

¹In collaboration with Phillip D. Hustad, George Barclay, Jim Thackeray, Deyan Wang, Shih Wei Chuang, Vivian P. Chuang, Valeriy Ginzburg, Jeffrey D. Weinhold, and Rahul Sharma, The Dow Chemical Company.

11:51AM B46.00002 Development of nanostructured surfaces for ice protection applications¹, AZAR ALIZADEH, GE Global Research — Ice accretion on surfaces of aircrafts, wind turbine blades, oil and gas rigs and heat exchangers, to name a few examples, presents long recognized problems with respect to efficiency and cost of operation. For instance, significant ice accretion on critical surfaces of an aircraft will cause problems during lift off (and will change the aerodynamics of the wings during flight). On the other hand, ice built up on wind turbine blades in cold climates ($T < -20^{\circ}\text{C}$) drastically reduces the efficiency of power generation. Despite considerable number of studies and significant progress toward development of icephobic coatings, development of *robust ice-resistance* or *anti-icing coatings* is still elusive. Several approaches towards development of anti-icing surfaces have recently postulated that the superhydrophobic properties of hierarchically textured coatings, with contact angles $> 150^{\circ}$, may lead to a significant reduction and perhaps elimination of snow and ice accretion. However, the exact mechanism of delayed icing on these surfaces is still under debate. Here we present a systematic study of early stages of ice formation upon water droplet impact on a range of hydrophobic, hydrophilic, textured and chemically patterned surfaces. We show that, in addition to a significant reduction in ice-adhesion strength on superhydrophobic surfaces, decreasing the water-substrate contact area plays a *dual* role in delaying ice nucleation: first by reducing heat-transfer and second by reducing the probability of heterogeneous nucleation at the water-substrate interface. The study presented here also offers a comprehensive perspective on the efficacy of textured surfaces for practical non-icing applications.

¹The Nanotechnology Advanced Technology Program at GE Global Research and the Department of Energy (Grant Award Number: DE-AC07-05ID14517) are acknowledged for financial support.

12:27PM B46.00003 Tough Block Copolymer Organogels and Elastomers as Short Fiber Composites¹, EDWARD J. KRAMER, Departments of Materials and Chemical Engineering, UCSB — The origins of the exceptional toughness and elastomeric properties of gels and elastomers from block copolymers with semicrystalline syndiotactic polypropylene blocks will be discussed. Using synchrotron X-radiation small angle (SAXS) and wide angle X-ray scattering (WAXS) experiments were simultaneously performed during step cycle tensile deformation of these elastomers and gels. From these results the toughness can be attributed to the formation, orientation and elongation of the crystalline fibrils along the tensile direction. The true stress and true strain ε_H during each cycle were recorded, including the true strain at zero load $\varepsilon_{H,p}$ after each cycle that resulted from the plastic deformation of the sPP crystals in the gel or elastomer. The initial Young's modulus E_{init} and maximum tangent modulus E_{max} in each cycle undergo dramatic changes as a function of $\varepsilon_{H,p}$, with E_{init} decreasing for $\varepsilon_{H,p} \leq 0.1$ and then increasing slowly as $\varepsilon_{H,p}$ increases to 1 while E_{max} increases rapidly over the entire range of $\varepsilon_{H,p}$ resulting in a ratio of $E_{max}/E_{init} > 100$ to 1000 at the highest maximum (nominal) strain. Based on SAXS patterns from the deformed and relaxed gels, as well as on previous results on deformation of semicrystalline random copolymers by Strobl and coworkers, we propose that the initial decrease in E_{init} and increase in E_{max} with $\varepsilon_{H,p}$ are due to a breakup of the network of the original sPP crystal lamellae and the conversion of the sPP lamellae into fibrils whose aspect ratio increases with further plastic deformation, respectively. The gel elastic properties can be understood quantitatively as those of a short fiber composite with a highly deformable matrix. At zero stress the random copolymer midblock chains that connect the fibrils cause these to make all angles to the tensile axis (low E_{init}), while at the maximum strain the stiff, crystalline sPP fibrils align with the tensile axis producing a strong, relatively stiff gel. The evolution of the crystalline structure during deformation is confirmed by WAXS and FTIR measurements.

¹I thank my collaborators F. Deplace, G. H. Fredrickson, G. W. Coates, H. Ohtaki, Y.-W. Shin, F. Shimizu, L. Rong and B. S. Hsiao.

1:03PM B46.00004 Interfacial, Thin Film, and Structural Measurements to Facilitate Polymer Nanomanufacturing, CHRISTOPHER SOLES, NIST Polymers Division — There is a growing interest in coupling the relatively mature roll-to-roll manufacturing processes with advanced lithographic patterning methods to enable high volume manufacturing of technologies with the added functionality that can only be realized by nanoscale patterning. Nanoimprint lithography is particularly attractive for roll-to-roll processes because the patterning is achieved through a simple embossing technique that relies upon the mechanical deformation of a liquid, melt, or solid material via a squeeze-flow process. Embossing techniques on a roll-to-roll substrate are routinely encountered in the graphic arts community. The difference with nanoimprint lithography is that the printed features can be on the order of 10 nm or smaller. In this presentation we will look at some of the difficulties encountered when these roll-to-roll embossing processes are scaled to the nanoscale. In particular we will look at issues related to the viscous flow of high molecular mass polymer melts into the nanoscale cavities with high throughput. We will show how fast nanoscale squeeze-flow patterning can lead to significant plastic deformation of the polymer melt. This can have implications on the ability of the material to fill the mold and the residual stresses that are generated in the pattern through the imprint process. Techniques to quantitatively evaluate these processes will be discussed and related to fundamental concepts of polymer physics.

1:39PM B46.00005 Self-Healing Polymer Networks, FRANCOIS TOURNILHAC, Ecole Supérieure de Physique et Chimie Industrielles (Paris) — Supramolecular chemistry teaches us to control non-covalent interactions between organic molecules, particularly through the use of optimized building blocks able to establish several hydrogen bonds in parallel. This discipline has emerged as a powerful tool in the design of new materials through the concept of supramolecular polymers. One of the fascinating aspects of such materials is the possibility of controlling the structure, adding functionalities, adjusting the macroscopic properties of and taking profit of the non-trivial dynamics associated to the reversibility of H-bond links. Applications of these compounds may include adhesives, coatings, rheology additives, high performance materials, etc. However, the synthesis of such polymers at the industrial scale still remains a challenge. Our first ambition is to design supramolecular polymers with original properties, the second ambition is to devise simple and environmentally friendly methods for their industrial production. In our endeavours to create novel supramolecular networks with rubbery elasticity, self-healing ability and as little as possible creep, the strategy to prolongate the relaxation time and in the same time, keep the system flexible was to synthesize rather than a single molecule, an assembly of randomly branched H-bonding oligomers. We propose a strategy to obtain through a facile one-pot synthesis a large variety of supramolecular materials that can behave as differently as associating low-viscosity liquids, semi-crystalline or amorphous thermoplastics, viscoelastic melts or self-healing rubbers.

Monday, February 27, 2012 11:15AM - 2:15PM –

Session B47 DPOLY: Focus Session: Jamming, Glass Transition, and Gelation in Colloids and Soft Matter Systems 160C

11:15AM B47.00001 Geometrical analysis of suspension flows near jamming¹, MATTHIEU WYART, New York University — The viscosity of suspensions was computed early on by Einstein and Batchelor in the dilute regime. At high density however, their rheology remains mystifying. As the packing fraction increases, steric hindrance becomes dominant and particles move under stress in a more and more coordinated way. Eventually, the viscosity diverges as the suspension jams into an amorphous solid. Such a jamming transition is reminiscent of critical points: the rheology displays scaling and a diverging length scale. Jamming bears similarities with the glass transition where steric hindrance is enhanced under cooling, and where the dynamics is also observed to become more and more collective as it slows down. In all these examples, understanding the nature of the collective dynamics and the associated rheology remains a challenge. Recent progress has been made however on a related problem, the unjamming transition where a solid made of repulsive soft particles is isotropically decompressed toward vanishing pressure. In this situation various properties of the amorphous solid, such as elasticity, transport or force propagation, display scaling with the distance to threshold. Theoretically these observations can be shown to stem from the presence of soft modes in the vibrational spectrum, a result that can be extended to thermal colloidal glasses as well. Here we focus on particles driven by shear at zero temperature. We show that if hydrodynamical interactions are neglected an analogy can be made between the rheology of such a suspension and the elasticity of simple networks, building a link between the jamming and the unjamming transition. This analogy enables us to unify in a common framework key aspects of the elasticity of amorphous solids with the rheology of dense suspensions, and to relate features of the latter to the geometry of configurations visited under flow.

¹Supported by NSF (DMR-1105387), the Petroleum Research Fund (52031-DNI9) and the Sloan Fellowship

11:51AM B47.00002 Finite Size Effects at the Jamming Transition, CARL GOODRICH, University of Pennsylvania, SIDNEY NAGEL, University of Chicago, ANDREA LIU, University of Pennsylvania — Packings of spheres at zero temperature and shear stress exhibit a jamming/unjamming transition as a function of density. For spheres that repel when they overlap and do not otherwise interact, packings are jammed with a nonzero static shear modulus when the density, ϕ , exceeds a critical density, ϕ_c . This jamming transition displays characteristics of both first and second order phase transitions with, for example, a discontinuous jump in the coordination number (average number of interacting neighbors per particle) and a power-law increase in the shear modulus. In addition, multiple length scales have been identified that diverge as ϕ decreases towards ϕ_c , emphasizing the second order nature of the transition. The existence of diverging length scales suggests that quantities such as the coordination number and shear modulus should exhibit finite size scaling as ϕ_c is approached, but until now this has not been observed. We report the first measurements of finite size scaling at the jamming transition of soft frictionless repulsive spheres and explore the implications of these results on our current understanding of the jamming transition.

12:03PM B47.00003 ABSTRACT HAS BEEN MOVED TO Y50.00015 –

12:15PM B47.00004 Stability of jammed systems to generalized boundary deformations¹, OLEG KOGAN, SAM SCHOENHOLZ, ANDREA LIU, University of Pennsylvania, SIDNEY NAGEL, University of Chicago, LIU GROUP, UNIV. OF PENNSYLVANIA COLLABORATION, NAGEL GROUP, UNIV. OF CHICAGO COLLABORATION — At zero temperature and applied stress, amorphous packings of repulsive spheres exhibit a jamming transition to rigidity. As pointed out by Torquato and Stillinger, some of these “collectively jammed” configurations may not be stable with respect to boundary deformations, while others, “strictly jammed,” may be stable with respect to any change of the boundaries. We explore this by considering systems with periodic boundary conditions at packing fractions above the jamming transition as comprising the basis of an infinite square (or cubic) lattice. The displacement fields of particles corresponding to normal modes of vibration are generally not consistent with the periodic boundary conditions used to construct the basis packing. Therefore, by studying the vibrational modes we determine the linear response to boundary deformations that do not respect the periodicity of the initial system. Hence, we are able to explore the stability of packings with respect to a large class of boundary deformations. We discover that some configurations have modes with negative energies, indicating instability. We report the effects of system size and packing fraction upon the probability that a collectively jammed packing is also stable with respect to boundary deformations.

¹Acknowledging the support from Department of Energy

12:27PM B47.00005 Vestige of $T = 0$ jamming transition at finite temperature in 3D, THOMAS CASWELL, MARGARET GARDEL, SIDNEY NAGEL, University of Chicago, ZEXIN ZHANG, ARJUN YODH, University of Pennsylvania — When a random packing of spheres at $T = 0$ is compressed to the jamming transition, the system becomes rigid and the first peak of the pair-correlation function, $g(r)$, diverges [1]. We study the manifestation of this signature and the associated particle dynamics when the temperature, T , is no longer negligible. To this end, we employ a three-dimensional packing of monodisperse, micron-size, colloids made from n-isopropyl acrylimide (NIPAM). NIPAM particles change size and hence the packing fraction of the system in response to environmental temperature. Thus by changing sample temperature we can probe all packing fractions of interest using a single sample. These particles are compressible so the system can reach packing fractions and configurations inaccessible to hard colloids. We observe a vestige of the $T = 0$ divergence as a maximum in the first peak of $g(r)$ versus packing fraction coincident with dynamical arrest of the particles. The general features in 3D are in agreement with a previous study in a two-dimensional bi-disperse NIPAM system [2]. We report the dependence of $g(r)$ and particle motion on packing fraction.

[1] C. S. O'Hern, et al., Phys. Rev. E 68, 011306 (2003). [2] Z. Zhang, N. Xu, et al., Nature 459, 230 (2009).

12:39PM B47.00006 Localization model for relaxation in glass-forming materials¹, DAVID S. SIMMONS, MARCUS T. CICERONE, JACK F. DOUGLAS, National Institute of Standards and Technology — As a material approaches its glass transition, its structural relaxation time τ rapidly increases as its particles become localized. A model relating this relaxation time increase to an experimentally accessible measure of localization (e.g. the Debye-Waller factor $\langle u^2 \rangle$) would have a fundamental impact on our understanding of glass formation and would be practically useful in the design of new materials. After examining such a relationship proposed by Leporini and coworkers and finding it to be inadequate, we develop an activated transport model that accurately describes relaxation data from a variety of simulated and experimental glass-forming materials. This model naturally extends the Hall-Wolynes and free volume models relating τ to $\langle u^2 \rangle$ (or free volume). The model parameters are physically meaningful and reflect the anharmonicity and anisotropy of particle localization. The Vogel-Fulcher-Tamman relation also describes relaxation in the simulated and experimental glass-forming materials we considered, and by exploring consistency between these two relations we gain new insight into the characteristic temperatures of glass formation in terms of the extent of particle localization.

¹This work was funded in part under NIH/NIBIB Grant R01 EB006398-01A1. DSS acknowledges financial support from the National Research Council Postdoctoral Research Associateship Program.

12:51PM B47.00007 Lattice Model of Dynamic Heterogeneity in Glassy Systems¹ , NICHOLAS B. TITO, JANE E.G. LIPSON, Dartmouth College, SCOTT T. MILNER, The Pennsylvania State University — Free volume in a fluid provides space for molecular motion; this creates local mobility and avoids “kinetic jamming” as the sample is rapidly cooled towards its glass transition. This physical picture has recently garnered significant interest in the polymer materials realm, where free volume is suspected to be the key factor in suppressing the glass transition of a polymer thin film near its exposed surfaces. We have developed a simple kinetic model that describes how free volume is transported in a near-glassy liquid. Model simulation results reveal that spatial fluctuations of free volume grow large near the glass transition, and this gives rise to hallmark glassy characteristics such as dynamic heterogeneity, intermittency and, ultimately, kinetic arrest. We will also discuss the response of glassy and molten states to perturbations, as a probe for characterising fluctuations near the glass transition.

¹work supported by the National Science Foundation.

1:03PM B47.00008 Building a Colloidal Proxy for Binary Metallic Glasses , RYAN KRAMB, National Research Council, KATHARINE JENSEN, Harvard University, LOGAN WARD, Ohio State University, RICHARD VAIA, DANIEL MIRACLE, Air Force Research Laboratory — Current experimental techniques for determining the atomic structure of metallic glasses and testing structural theories such as the efficient cluster packing model are limited to diffraction and scattering. These techniques give only average structural information that could result from many different unique structures. Simulations of metallic glasses, on the other hand, give the exact structure of every atom in the system, but are limited by computing power to a few thousand atoms which are equilibrated over a few nanoseconds. This leads to uncertainties in the reliability of reproducing real metallic glass structures. To overcome these deficiencies, we have created a proxy experimental system that can be treated much like a simulation. We have synthesized suspensions of larger, colloidal scale particles (2-3 μ m in diameter) to build pseudo binary metallic glasses. Using confocal microscopy imaging techniques, we determine the three dimensional position of hundreds of thousands of individual particles (atoms), and calculate structural information such as the radial distribution function, Voronoi volume, and partial coordination numbers. We compare these results to both theoretical calculations and experimental results of real metallic glasses. The focus here will be on a building a proxy for the CuZr binary system.

1:15PM B47.00009 Contact processes in crowded environments , SHILYANG XU, Physics Department, Syracuse University, B. CHAKRABARTI, Physics Department, Rutgers University, J.M. SCHWARZ, Physics Department, Syracuse University — Periodically sheared colloids at low densities demonstrate a dynamical phase transition from an inactive to active phase as the strain amplitude is increased. To begin to answer the question of what happens to this system at higher densities, we investigate a conserved-particle-number contact process with a three-body interaction as opposed to the usual two-body interaction. In particular, one active (diffusing) particle collides with two inactive (non-diffusing) particles such that they can become active. In mean-field, this system exhibits a continuous absorbing phase transition belonging to conserved directed percolation universality class. Simulations on 2D lattices support our result. In contrast, the three-body interaction with two active particles colliding and activating one inactive particle exhibits a first-order transition. Inspired by kinetically-constrained models of the glass transition, we investigate the “caging effect” at even higher particle densities to look for a second dynamical phase transition back to an inactive phase. While mean-field calculations demonstrate a continuous transition, 2D lattice simulations show a hint of a first-order transition, suggesting a possible fluctuation-driven transition due to the highly localized geometric constraint.

1:27PM B47.00010 Experiments on Rearrangements and Forces in 2D Emulsion Hopper Flow , XIA HONG, KENNETH DESMOND, DANDAN CHEN, ERIC WEEKS, Physics Dept., Emory University, WEEKS' LAB TEAM — We did experiments with a quasi-two-dimensional binary emulsion flowing through a hopper. Our samples are oil-in-water emulsion confined between two close-spaced parallel plates, so that the droplets are deformed into pancake shapes. In this system, there is only viscous friction and no static friction between droplets. The hopper flow induces a high rate of rearrangement events allowing us to understand how stresses and forces change during the process. By imaging the droplets during flow, we observed T1 events, which are topological changes when droplets exchange neighbors. Simultaneously, we measured forces between the droplets using a technique we have developed and studied the evolution of forces between droplets during rearrangements.

1:39PM B47.00011 The Role of Solvent-Solute Interactions on The Behavior of Low Molecular Mass Organo-Gelators , KEVIN CAVICCHI, LI FENG, Department of Polymer Engineering, University of Akron — Low molecular mass organo-gelators (LMOGs) are a class of small molecules that can self-assemble in organic solvents to form three-dimensional fibrillar networks. This has a profound effect on the viscoelastic properties of the solution causing physical gelation. These gels have uses in a range of industries including cosmetics, foodstuffs, plastics, petroleum and pharmaceuticals. A fundamental question in this field is: What makes a good LMOG? This talk will discuss the relationships between the viscoelastic properties and thermodynamic phase behavior of LMOG/solvent solutions. The regular solution model was used to fit the liquidus line and sol/gel transition temperature vs. concentration in different solvents to determine LMOG-solvent interaction parameters ($\chi = A/T$). This parameter A was found to scale with the solubility parameter of the solvent, especially for non-polar solvents. This demonstrates that gelation is strongly linked to LMOG solubility and indicates that the bulk thermodynamic parameters of the LMOG (solubility parameter and melting temperature) are useful to predict the solution behavior of LMOGs.

1:51PM B47.00012 Effects of penalty function type on the history-penalized metabasin escape algorithm for supercooled liquids , RAVI HEUGLE, XI LIN, Boston University — The history-penalized metabasin escape algorithm provides an autonomous transition state pathway for a trapped system to escape from deep metastable energy minima and larger basins of attraction. The effects of penalty function type on the efficiency of the algorithm are demonstrated by sampling portions of the potential energy surface of a binary Lennard-Jones liquid close to the glass transition temperature. Our results indicate that optimal penalty functions prefer both large 3N+1 dimensional volumes and the ability to force the system over a large range. The Gaussian, which until now has served as the standard penalty function used for activation, serves as the benchmark against other representative penalty function types. Analysis shows that the triangle function results in four fold improvements in efficiency over the Gaussian, thereby furthering the reach of simulation into timescale regimes largely inaccessible to molecular dynamics.

2:03PM B47.00013 Nonlinear effective medium theory of disordered spring networks , M. SHEINMAN, VU University, C.P. BROEDERSZ, Princeton University, F.C. MACKINTOSH, VU University — Disordered soft materials, such as fibrous networks in biological contexts exhibit a nonlinear elastic response. We study such nonlinear behavior with a minimal model for networks of simple Hookian elements with disordered spring constant. We develop a mean-field approach to calculate the differential elastic bulk modulus for the macroscopic network response of such networks under large isotropic deformations. We find that the nonlinear mechanics depends only weakly on the lattice geometry and is governed by the average network connectivity. In particular, the nonlinear response is controlled by the isostatic connectivity, which depends strongly on the applied strain. Our predictions for the strain dependence of the isostatic point as well as the strain-dependent differential bulk modulus agree well with numerical results in both two and three dimensions. In addition, by using a mapping between the disordered network and a regular network with random forces, we calculate the non-affine fluctuations of the deformation field and compare it to the numerical results. Finally, we discuss the limitations and implications of the developed theory.

Monday, February 27, 2012 11:15AM - 2:15PM —
Session B48 DPOLY: Electrically and Optically Active Polymers 161

11:15AM B48.00001 Micellar Electrolytes in Organic Electrochemical Transistors, FABIO CICOIRA, Ecole Polytechnique de Montréal, TARABELLA GIUSEPPE, CNR-IMEM Parma, GAURAV NANDA, Ecole Polytechnique de Montréal, SALVATORE IANNOTTA, CNR-IMEM Parma, CLARA SANTATO, Ecole Polytechnique de Montréal — Organic electrochemical transistors (OECTs) are promising for applications in sensing and bioelectronics. OECTs consist of a conducting polymer film (transistor channel) in contact with an electrolyte. A gate electrode immersed in the electrolyte controls the doping/dedoping level of the conducting polymer. OECTs can be operated in aqueous electrolytes, making possible the implementation of organic electronic materials at the interface with biology. The inherent signal amplification of OECTs has the potential to yield sensors with low detection limits and high sensitivity. In this talk we will present recent studies on OECTs using ionic surfactants (such as hexadecyl-trimethyl-ammonium bromide) as electrolytes. As the conducting polymer we used PEDOT:PSS, i.e. (Poly(3,4 ethylenedioxythiophene) doped with Poly(styrene sulphonate). Interestingly, ionic surfactant electrolytes result in large transistor current modulation, especially beyond the critical micellar concentration (CMC). Since micelles play a primary role in biological processes and drug-delivery systems, the use for micellar electrolytes opens new exciting opportunities for the use of OECTs in bioelectronics.

11:27AM B48.00002 Quadratic Electro-Optic Effect in the Nonconjugated Conductive Co-polymer Iodine-doped Styrene-Butadiene-Rubber Measured at 633 nm and 1550 nm, GURUDUTT TELANG, MRINAL THAKUR, Photonic Materials Research Laboratory, Auburn University, AL — The quadratic electro-optic effect in the nonconjugated conductive co-polymer film of styrene-butadiene-rubber (SBR) has been measured using field-induced birefringence method. Thin films of styrene-butadiene-rubber have been prepared on various substrates from a chloroform solution and characterized using optical absorption spectroscopy, FTIR and DSC before and after doping with iodine. The optical absorption spectrum at low doping shows two peaks: one at 4.27 eV and the other at 3.2 eV corresponding to the radical cation and charge-transfer transition. FTIR data indicate C-H vibration bands (964 cm^{-1} and 910 cm^{-1}) of polybutadiene decrease upon doping due to transformation of the double bonds into radical cations. The Kerr coefficients as measured at 633 nm and at 1550 nm are $3.1 \times 10^{-10}\text{ m/V}^2$ and $1.3 \times 10^{-10}\text{ m/V}^2$ respectively. These exceptionally large values have been attributed to the subnanometer metallic domains formed upon doping and charge-transfer involving isolated double-bonds.

11:39AM B48.00003 Photoluminescence of P3HT nanoparticles¹, IRENE DUJOVNE, JOELLE LABASTIDE, UMass Amherst, Chem. Dept., MINA BAGHGAR, UMass Amherst, Phys. Dept., AIDAN MCKENNA, UMass Amherst, Chem. Eng. Dept., AUSTIN M. BARNES, UMass Amherst, Phys. Dept., D. VENKATARAMAN, MICHAEL D. BARNES, UMass Amherst, Chem. Dept. — Polythiophenes are semiconducting polymers that have been designed to crystallize. The photophysics of semicrystalline polythiophene and polythiophene-blends are the focus of intense research efforts across different disciplines. In these systems there is a competition between charge separation and recombination. Exciton diffusion length in organic-semiconductors is a major road-block for efficient solar energy harvesting devices since, for direct bandgap organic materials, this distance is about 10 nanometers. Thus, efficient extraction of photogenerated electrons and holes requires engineering polymer domain dimensions in this size range. In our initial investigations of the photophysics of isolated P3HT nanoparticles (15 - 130 nm), we have observed several intriguing size-dependent features in the single-particle photoluminescence (PL) connected with exciton diffusion and dissociation dynamics. In addition to the short-time behavior, we also observe size-dependent differences in PL decay at long times. In the 10 - 100 ns time regime, the PL originates not from radiative transitions of bound excitons, but rather from charge-separation followed by bi-polaron recombination—and thus provides an interesting measure of exciton fission probability within the nanoparticle.

¹This material is based upon work supported in part by DOE-EFRC Award Number DE-SC0001087 and DOE award DE-FG02-05ER15965

11:51AM B48.00004 Crystallizing Conjugated Polymer Chains of P3HT Stretched for Dramatic Enhancements in Optoelectronic Efficiencies, CHIH-HUNG CHANG, ARNOLD C.-M. YANG, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu 300, Taiwan — Previously the amorphous conjugated polymer MEH-PPV was shown to illustrate huge enhancement in photoluminescence (PL) efficiencies upon stretching to large molecular strains. In this work the crystallizing polymer of poly(3-hexylthiophene) (P3HT), dispersed in the polystyrene (PS) matrix, was stretched in the PS local deformation zones to study the effect of molecular deformation. A huge enhancement of the PL intensity was observed that when normalized to the fraction of the strained polymer corresponded to an increase of 15 folds, significantly larger than that of the stretched MEH-PPV. Moreover, when examined under a con-focal micro-PL (spot size $\sim 5\mu\text{m}$), the emission from the local deformation zones subject to a high stress ($\sim 40\text{MPa}$) manifested marked increase of the intrachain emission relative to the effect on the interchain. These emission peak positions, however, were unaffected by the stretching. The PL enhancements were attributed to the depression of electron-phonon interactions of the stretched P3HT chains. Constraining conjugated polymers to yield high efficiencies thus may provide a feasible way for improving the performance of polymer-based devices.

12:03PM B48.00005 Manipulating meso-structure and electrical conductivity in polymer-acid doped polyaniline by exploiting redox chemistry, JACOB TARVER, JOLINE FAN, YUEH-LIN LOO, Department of Chemical & Biological Engineering, Princeton University — Template synthesis of polyaniline on poly(2-acrylamido-2-methyl-1-propane sulfonic acid) yields electrostatically stabilized particles that can be aqueously dispersed and cast into thin films; electrical conductivity in these films scales with inter-particle connectivity. Solvent annealing with dichloroacetic acid induces structural relaxation of the polymer acid, thereby eliminating the particulate nature of thin films and consequently increasing their conductivity by up to two orders of magnitude (from 0.4 to 40 S/cm). Alternatively, the electrostatic interactions between polyaniline and its template can be neutralized through chemical reduction with hydrazine monohydrate, after which the polymer acid can be plasticized by water vapor to encourage structural relaxation. Exposure to nitric oxide leads to oxidation of polyaniline and concurrent reassociation with its polymer acid dopant. Enhanced conductivity is observed following this redox process, and is attributed to extensive polymer chain relaxation and the simultaneous elimination of the particulate nature of template-synthesized polyaniline.

12:15PM B48.00006 An Integrated Electrochromic Nanoplasmonic Optical Switch, ALEC TALIN, ERICH WALTER, NIST, AMIT AGRAWAL, Syracuse University, TING XU, HENRI LEZEC, NIST — We describe an electrochemically-driven optical switch based on absorption modulation of surface plasmon polaritons (SPPs) propagating in a metallic nanoslit array waveguides containing the electrochemical polymer polyaniline (PANI). Optical transmission modulation of near 100% is achieved by electrochemically switching PANi between oxidized and reduced states using voltages below 1 V. High spatial overlap and long interaction length between the SPP and the active material are achieved by preferential growth of PANi on the nanoslit sidewalls. The resulting orthogonalization between the directions of light propagation, and that of charge transport from the electrolyte to ultra-thin active material inside the nanoslit waveguide offers significant promise for the realization of electrochromic devices with record switching speeds.

12:27PM B48.00007 Resistive Switching in Ag Nanowire/Polymer Composite Materials, JAMIE FORD, ROSE MUTISO, KAREN WINEY, University of Pennsylvania — Bulk composites of electrically conductive nanoparticles within an insulating polymer matrix are insulating when the conductive particle concentration is below the electrical percolation threshold and conductive above it. However, we have observed reversible resistive switching with increasing voltage at room temperature in Ag nanowire/polystyrene composites with nanowire concentrations close to the percolation threshold. We have found the reversibility of the observed switching behavior to be temperature dependent which implies a diffusive process is involved. We propose the basis for resistive switching in these materials is the formation of field-induced filaments between adjacent nanowires that extend the percolated electrical network and increase the overall conductivity of the system. Here, we will compare our observations of resistive switching in Ag nanowire/polystyrene and Ag nanowire/poly(methylmethacrylate) bulk nanocomposites, explore the breadth of metal nanowire and polymer systems that exhibit resistive switching, and explore the underlying mechanism for filament formation.

12:39PM B48.00008 Far-infrared through visible optical characterization of polymer-based electrochromic devices on single-walled carbon nanotube electrodes¹, ZAHRA NASROLLAHI, SVETLANA V. VASILYEVA, EVAN P. DONOGHUE, ANDREW G. RINZLER, D.B. TANNER, Department of Physics, University of Florida, Gainesville, Florida 32611 — Electrochromic polymers (ECPs) exhibit reversible optical modulation in a wide spectral range as a function of an externally applied voltage. In this work, ECPs have been used in absorptive/transmissive electrochromic devices as candidates for smart window applications. The electrochromic devices were fabricated on flexible polyethylene substrates and used ECPs sandwiched between thin films of single-walled carbon nanotubes serving as conductive and flexible electrodes. Unlike ITO, the nanotube films are highly transmissive in the visible and infrared region of the spectrum. The transmission and reflection of the individual device components as well as assembled devices were measured over a wide spectral range (FIR to UV). The devices were switched in situ in the spectrometers. The optical constants of the constituent layers were calculated using the Drude-Lorentz model. The devices demonstrated high transmission contrasts between their colored and bleached states in the VIS, NIR, and MIR spectra, enabling electrically tunable control over the transmission or reflection of both light and heat. This control could lead to reduced heating or cooling costs in real world applications and the flexible nature of the device components allows many applications.

¹The authors gratefully acknowledge Nanoholdings LLC for funding of this research.

12:51PM B48.00009 Consequence of the miscibility and mesostructure of the photoactive layer on organic solar cell performance, ENRIQUE GOMEZ, DEREK KOZUB, KIARASH VAKHSHOURI, The Pennsylvania State University — Recent work has found that mixed phases exist in polythiophene/fullerene solar cells. Nevertheless, the consequence of miscibility between the electron donor and acceptor is not fully understood. Through model polythiophene/fullerene mixtures, we have characterized charge transport in amorphous mixed phases. These results suggest that partial miscibility may be important for device performance, due to the interplay between minimizing large scale phase separation and maximizing charge transport in the photoactive layer. However, in some systems crystallization of either the electron donor or acceptor complicates the role of miscibility on device performance by modifying the composition of amorphous phases. As a result, we utilize grazing-incidence small angle X-ray scattering results to quantitatively describe solar cell device performance from the structure of the photoactive layer.

1:03PM B48.00010 Magnetic field alignment of supramolecular perylene/block copolymer complexes for electro-optic thin films¹, MANESH GOPINADHAN, PAWEL MAJEWSKI, Department of Chemical Engineering, Yale University, RYAN SHADE, EMMA DELL, NALINI GUPTA, LUIS CAMPOS, Department of Chemistry, Columbia University, CHINEDUM OSUJI, Department of Chemical Engineering, Yale University — The realization of nanostructured electro-optic materials by self-assembly is complicated by the persistence of structural defects which render the system properties isotropic on macroscopic length scales. Here we demonstrate the use of magnetic fields to facilitate large area alignment of a supramolecular system consisting of a poly(styrene-*b*-acrylic acid) (PS-*b*-PAA) diblock copolymer host and a semiconducting perylene ligand. Hydrogen bonding between the carboxylic acid groups of PAA and imidazole head group of the perylene species results in hierarchically ordered materials with smectic perylene layers in a matrix of hexagonally packed PS cylinders at appropriate stoichiometries. The smectic layers and the PS domains are strongly aligned by the application of large ($> 2T$) magnetic fields in a manner reflective of the positive diamagnetic anisotropy and the planar anchoring of perylene units at the PS interface. We use a combination of SAXS studies in-situ with applied magnetic fields, GISAXS and polarized optical transmission measurements to characterize the system. Magnetic fields thus offer a viable route for directing the self-assembly of functional materials based on rigid chromophores and further, that supramolecular approaches can be complementary to such efforts.

¹NSF support (DMR-0847534) is gratefully acknowledged.

1:15PM B48.00011 Structure/property relationships in high hole mobility regioregular PT based copolymers, LOUIS PEREZ, LEI YING, GUILLERMO BAZAN, EDWARD KRAMER, University of California - Santa Barbara — The synthesis of novel solution processable conjugated polymers with high hole mobilities is an active field of study due to the potential to fabricate low cost, high through-put, lightweight organic field effect transistors (OFET). Two regioregular copolymers, based on cyclopenta[2,1-*b*:3,4-*b'*]dithiophene (CDT) and pyridal[2,1,3]thiadiazole (PT) structural units, have been prepared by using polymerization reactions involving reactants specifically designed to avoid random orientation of the PT heterocycle. Compared to their regiorandom counterpart, the regioregular polymers exhibit a two orders of magnitude increase in hole mobility from 0.005 to 0.6 cm²V⁻¹ s⁻¹. Grazing incidence wide angle X-ray scattering (GIWAXS), near edge X-ray absorption fine structure (NEXAFS) spectroscopy, and transmission electron microscopy were carried out to obtain further insight into possible differences of structural order within the bulk and interfaces of the thin films. It was found that the backbone regioregularity leads to significant differences in the structural arrangement of the chains and indicates the importance of regioregularity for achieving optimal electronic properties.

1:27PM B48.00012 Electric Field Effect on Adhesion of Poly(ethylene oxide) Physical Hydrogels, VICTOR BARINOV, BILAL MARIE, Polytechnic Institute of New York University — The objective of this study was to characterize the effect of electric field on adhesion of poly(ethylene oxide) physical hydrogels to an aluminum substrate. The normal load necessary to disbond two plain aluminum surfaces joined by a thin layer of a poly(ethylene oxide) physical hydrogel can be reduced by about at least one order of magnitude if a reduced normal load is applied to aluminum-hydrogel interfaces simultaneously with an electric potential difference. Two aluminum surfaces joined by the hydrogel serve as a cathode and an anode. The current densities of about ten amperes per square meter determine the tenths-of-watt power dissipated in a sample. The effect of electric field on the adhesion strength of poly(ethylene oxide) hydrogels to aluminum depends on polymer concentration.

1:39PM B48.00013 Optical behavior of the conjugated polymer MEH-PPV thin films stretched in bi-layer dewetting by an unstable layer, PO-TSUN CHEN, ARNOLD C.-M. YANG, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan 30013 — Molecular packing and chain conformation play important roles in the optoelectronic performance of conjugated polymer thin films. It has been shown that by virtue of stretching via dewetting, the photoluminescence (PL) efficiencies of rarefied MEH-PPV thin films may be dramatically enhanced. To result similar effects in the stable non-diluted pristine MEH-PPV thin films, bi-layer dewetting was attempted in samples of MEH-PPV thin films (~7nm) covered by one layer of polystyrene (PS) (~40nm) that dewetted in toluene vapor to form droplets (height ~300 nm) and ultrathin residual layer (~3nm) on the substrate. The instability was initiated from the PS layer in which small pinholes first emerged upon the intake of the solvent vapor. The pinholes then expanded and deepened into the underlying MEH-PPV, forcing the conjugated film to dewet. As a result of the stretching induced by the dewetting, the PL peak blue-shifted 20 nm to 540 nm and the intensity was enhanced around 10 times. Revealed by the position-sensitive confocal PL data, the huge enhancement came from both the droplet and residual layer, caused by molecular separation and stretching. Electroluminescence devices are being made based on these stretched MEH-PPV films.

1:51PM B48.00014 High pressure optical studies of donor-acceptor polymer heterojunctions, KESHAB PAUDEL, MEERA CHANDRASEKHAR, SUCHI GUHA, University of Missouri, Columbia — Bulk heterojunction polymer solar cells are based on a composite blend of two materials with electron donating and electron accepting properties. We present optical studies of a ladder-type poly(para-phenylene) and a regioregular poly(3-hexylthiophene) polymer blended with a fullerene derivative under hydrostatic pressure. The photoluminescence and absorption spectra reveal different pressure coefficients for the pristine polymer compared with the blended system. Using a phenomenological model to determine the volume change of the system under pressure, we attribute the difference in the pressure coefficient to a change in the band-edge offset at the heterojunction upon enhanced interaction. The band-edge offset is found to increase with increasing pressures for both the ladder-type and thiophene systems.

2:03PM B48.00015 Electrical transport properties of FeCl₃ doped poly(phenylenevinylene-co-3,4-ethylenedioxythiophene), KYUNG HO KIM, AJEONG CHOI, JUN-MO PARK, SUNG JU HONG, JOON BEOM SHIM, TAE-LIM CHOI, YUNG WOO PARK, Seoul National University — Poly(arylenevinylene) copolymers, in which 3,4-ethylenedioxythiophene (EDOT) and dialkoxy phenylenes are alternatively linked by vinylene unit, were synthesized by the Horner-Emmons reaction. The samples were doped with FeCl₃ and the temperature dependence of conductivity, magnetoresistance (MR), and thermoelectric power (TEP) were measured. The temperature dependence of conductivity follows $\exp[-(T_0/T)^{1/2}]$ and positive MR is observed up to $H = 14$ tesla. The TEP can be described by $S(T) = A + B/T + CT$. These behaviors are understood in the frame of charging energy limited tunneling conduction between metallic islands separated by insulating barriers.

Monday, February 27, 2012 11:15AM - 2:15PM –

Session B49 DPOLY: Focus Session: Long-time, Entangled Dynamics in Polymers - Rods, Rings, Fibers, Particle Tracking 162A

11:15AM B49.00001 An improved dissipative particle dynamics model for simulation of entangled polymers, JAN ANDZELM, YELENA SLOZBERG, TIMOTHY SIRK, JOHN BRENNAN, Army Research Laboratory, MARTIN LISAL, Academy of Sciences of the Czech Republic, ARL COLLABORATION, PRAGUE COLLABORATION — We develop an improved polymer model to capture entanglements within the DPD framework by using simplified bond-bond repulsive interactions to prevent bond crossings. We show that structural and thermodynamic properties can be improved by applying a segmental repulsive potential (SRP) that is a function of the distance between the midpoints of the segments, rather than the minimum distance between segments. The alternative approach, termed the modified segmental repulsive potential (mSRP), is shown to produce chain structures and thermodynamic properties that are similar to the softly-repulsive, flexible chains of standard DPD. Parameters for the mSRP are determined from topological, structural and thermodynamic considerations. The effectiveness of the mSRP in capturing entanglements is demonstrated by calculating the diffusion and mechanical properties of an entangled polymer melt. This improved DPD method was used in simulations for entangled polymer networks to explore impact of branched architectures on the mechanical response to the tensile and compressive deformation.

11:27AM B49.00002 Theory of the nonlinear rheology of topologically entangled rod fluids, KEN SCHWEIZER, DANIEL SUSSMAN, University of Illinois at Urbana-Champaign — Our first-principles microscopic theory of the tube confinement field and dynamics of topologically entangled rod fluids is extended to describe nonlinear rheology. Stress generically weakens tube constraints, resulting in a competition between reptation and transverse activated entropic barrier hopping. For a step-strain deformation, four distinct nonlinear relaxation regimes are predicted with increasing strain amplitude: quiescent-like reptation, strongly accelerated reptation due to stress-induced tube dilation, relaxation dominated by lateral barrier hopping, and, beyond a critical strain of order unity, an initially complete destruction of the tube constraint (microscopic yielding) followed by a re-entanglement process with complex kinetics and multi-step stress relaxation. A theory for continuous start up shear has also been formulated. In the nonlinear regime, deformation-rate-dependent stress overshoots are predicted. In the nonequilibrium steady state, strong shear thinning occurs determined largely by the rate-dependent dilated tube diameter. At very high Weissenberg numbers, a stress plateau in the flow curve is predicted and relaxation is controlled by a convective-constraint-release-like process that self-consistently emerges within the theory.

11:39AM B49.00003 Theoretical and computational studies of entangled rod-coil block copolymer diffusion, MUZHOU WANG, ALFREDO ALEXANDER-KATZ, B.D. OLSEN, Massachusetts Institute of Technology — Despite continued interest in the thermodynamics of rod-coil block copolymers for functional nanostructured materials in organic electronics and biomaterials, relatively few studies have investigated the dynamics of these systems which are important for understanding diffusion, mechanics, and self-assembly kinetics. Here, the diffusion of coil-rod-coil block copolymers through entangled melts is simulated using the Kremer-Grest molecular dynamics model, demonstrating that the mismatch between the curvature of the rod and coil blocks results in dramatically slower reptation through the entanglement tube. For rod lengths near the tube diameter, this hindered diffusion is explained by a local curvature-dependent free energy penalty produced by the curvature mismatch, resulting in a rough energy surface as the rod moves along the tube contour. Compared to coil homopolymers which reptate freely along the tube, rod-coil block copolymers undergo an activated diffusion process which is considerably slower as the rod length increases. For large rods, diffusion of the rod through the tube only occurs when the coil blocks occupy straight entanglement tubes, which requires “arm retraction” as the dominant relaxation mechanism.

11:51AM B49.00004 Memory and transient forces in coarse grain simulations of complex polymers, WIM BRIELS, University of Twente — No abstract available.

12:27PM B49.00005 Self-Consistent Field Theory of Gaussian Ring Polymers¹, JAEUP KIM, YONG-BIAO YANG, UNIST, WON BO LEE, Sogang University — Ring polymers, being free from chain ends, have fundamental importance in understanding the polymer statics and dynamics which are strongly influenced by the chain end effects. At a glance, their theoretical treatment may not seem particularly difficult, but the absence of chain ends and the topological constraints make the problem non-trivial, which results in limited success in the analytical or semi-analytical formulation of ring polymer theory. Here, I present a self-consistent field theory (SCFT) formalism of Gaussian (topologically unconstrained) ring polymers for the first time. The resulting static property of homogeneous and inhomogeneous ring polymers are compared with the random phase approximation (RPA) results. The critical point for ring homopolymer system is exactly the same as the linear polymer case, $\chi N = 2$, since a critical point does not depend on local structures of polymers. The critical point for ring diblock copolymer melts is $\chi N \approx 17.795$, which is approximately 1.7 times of that of linear diblock copolymer melts, $\chi N \approx 10.495$. The difference is due to the ring structure constraint.

¹This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MEST) (No. 2011-0027260 and 2011-0005403).

12:39PM B49.00006 Self-consistent field theory for polymer dynamics, DOUG GRZETIC, ROBERT WICK-HAM, Department of Physics, University of Guelph, AN-CHANG SHI, Department of Physics and Astronomy, McMaster University — We develop a self-consistent field theory (SCFT) for polymer dynamics. We reformulate a Rouse model for interacting monomers as a dynamical functional integral over field variables, using standard techniques. Novel aspects include our use of the functional Fokker-Planck equation to describe single-chain dynamics, and our extremization of the functional integral, resulting in a set of self-consistent equations for the time-dependent monomer density and the mean force field on a monomer. Our theory is distinct from published dynamical SCFTs that combine elements of equilibrium SCFT with phenomenological dynamical evolution schemes. The time scale in our theory is known exactly; no phenomenological kinetic coefficient needs to be introduced. Dynamical quantities in our theory have analogs in equilibrium SCFT, allowing sophisticated numerical techniques developed for equilibrium SCFT to be applied directly to study the dynamics. Our approach is flexible and can be used, for example, to study polymer melt dynamics. To test the self-consistent nature of the theory in space-time, we examine the simple case of the dynamics of trapped, interacting particles, and binary mixtures, in one dimension.

12:51PM B49.00007 Structure Formation in Semi-Dilute Polymer Solution during Electrospinning, EYAL ZUSSMAN, YAKOV PALEY, ARKADII ARINSTEIN, KIM SHUSTER, Department of Mechanical Engineering, Technion-Israel Institute of Technology — In our recent work it was shown that longitudinal stretching of electrospun highly entangled semi-dilute polymer solution caused by jet hydrodynamic forces, transforms the topological network to an almost fully-stretched state within less than 1 mm from the jet start (PRE, 2011). Further evolution of the polymer network is related to a disentanglement of polymer chains and transformation of the topological network structure. As was shown by Malkin et al., (Rheol. Acta, 2011) high deformation rate of a topological polymer network, results in reptations of macromolecules caused by uncompensated local forces, whereas Brownian motion effect is negligible. Based on this conclusion, we examine the disentanglement process, using a mechanical pulley-block system assembled from multiple pulleys suspended by elastic springs, and taut string connecting two blocks. Each pulley corresponds to a topological knot; the taut string corresponds to a reptated chain; the springs correspond to surrounded polymer chains; and the blocks correspond to local deformation force. It turned out that the system is sensitive to system parameters. The pulleys can approach each other and the string stops to move. Such a behavior corresponds to formation of bundle of knots of entangled chains. In other conditions, the string continuously moves while the pulleys do not approach each other which corresponds to disentanglement of polymer chains. These experiments clarify the disentanglement kinetics in rapid-deformed polymer system.

1:03PM B49.00008 Edge electrospinning from a fluid-filled bowl for high throughput production of quality nanofibers, J.R. BOCHINSKI, Department of Physics, NC State University, N.M. THOPPEY, R.E. GORGA, Fiber and Polymer Science Program, NC State University, L.I. CLARKE, Department of Physics, NC State University — We present a stationary, edge-cylinder geometry for high throughput electrospinning that utilizes a reservoir filled with polymer solution and a concentric cylindrical collector [Nanotechnology 22, 345303 (2011)]. In this “bowl” electrospinning configuration, under high voltage initiation, multiple jets spontaneously form on the fluid surface, rearrange until they are approximately equidistant along the reservoir-edge and spin towards the collector, producing high quality fibers after the voltage is reduced to a working value. The technique produced poly(ethylene oxide) nanofibers with average diameter of 225 nm and a demonstrated throughput ~ 40 times higher than traditional single-needle electrospinning. The electric field patterns generated by traditional, bowl, and our previously reported edge-plate [Polymer 51, 4928 (2010)] geometries show significant similarity in field magnitude and gradient along a path towards the collector, which may underlie the ability to form similar quality fibers. We discuss how the interaction between fluid properties and the applied electric field determines the effective flow rate, jet stability versus time, throughput, and fiber quality.

1:15PM B49.00009 Size-dependent behavior of as-spun nanofiber vs. polymer molecular weight, ARKADII ARINSTEIN, Department of Mechanical Engineering, Technion - Israel Institute of Technology — The size-dependent behavior of nano-objects is a well-known and widely-accepted phenomenon, but up to now it has no satisfactory explanation. From the physical point of view, such a behavior is to be related to an internal scale parameter which is comparable with the scale of the system. Recently Ji et al. showed that the elastic moduli of polystyrene nano-fibers of different molecular weights can be described by one universal curve as a function of fiber radius, scaled by radius of gyration R_g (EPL, 84, 56002, 2008). However, the crossover to the size-dependent behavior in the above dependence occurs at $R/R_g \sim 25 - 30$, therefore the radius of gyration, R_g , is too small in order to play a role of the required scale parameter. This discrepancy requires an explanation. Utilizing a number of well-known scaling dependences, on the base of the model of confinement mechanism of polymer nanofiber reinforcement, proposed by us earlier, it is demonstrated that elastic modulus of polymer nanofibers is described by the function $F[(R/R_g)^\alpha]$ ($\alpha \sim 1.5$). This function, conforming to experimental observation, increases at small argument values, whereas for large argument values tends to value of the bulk elastic modulus, in doing so the crossover scale to the size-dependent behavior also agrees with experimental data.

1:27PM B49.00010 Mechanical properties and morphology of polymer gels, YELENA SLOZBERG, TIMOTHY SIRK, JOHN BRENNAN, JAN ANDZELM, RANDY MROZEK, JOSEPH LENHART, Army Research Laboratory, Aberdeen, Maryland, USA — Understanding morphology and mechanical response of polymeric gels is of particular importance to design materials with required energy dissipation characteristics. We will present our latest results for polymer gels based on 1) self-assembled block copolymers and 2) chemically cross-linked polymers. The dissipative particle dynamics (DPD) was used to predict morphology in good agreement with atomic force microscopy. We have performed DPD non-equilibrium oscillatory shear calculations predicting elastic modulus of unentangled gels that correlates well with experimental rheology data. However, this methodology fails to predict mechanics of entangled polymer networks due to unphysical chain crossing brought by the soft potentials used in DPD simulations. Recently, we have introduced an improved segmental repulsion potential that removes the bond crossing allowing for reptation dynamics. The improved DPD method was used in simulations for entangled gels to explore impact of branched architecture of solvent on the mechanical response to the tensile deformation. Novel architectures of solvent resulting in a dramatic increase of the elastic modulus were identified. The topological analysis was applied to understand contributions of chemical cross-links and entanglements to the stress.

1:39PM B49.00011 Rapid, accurate single particle tracking based on radial symmetry center determination, RAGHUVeer PARTHASARATHY, University of Oregon, Dept. of Physics — Accurately tracking particles in images is a crucial task for applications as diverse as super-resolution microscopy, membrane biophysics, and microrheology. Tracking errors can easily propagate into flawed conclusions about mechanisms underlying particle dynamics. The commonly used method of locating the center of a particle by direct fitting a Gaussian function to a measured intensity profile is very accurate, but is computationally intensive and not generalizable to non-point-like particles. Its slowness is a necessary consequence of numerically searching a large parameter space. I introduce a new approach to sub-pixel particle tracking based on exploiting radial symmetry, valid for any radially symmetric particle intensity profile. I provide an algorithm that analytically, non-iteratively calculates the best-fit symmetry center to determine the particle location. Over a wide range of signal-to-noise ratios, this approach yields accuracies nearly identical to those of Gaussian fitting with execution times over two orders of magnitude faster and with greater robustness in the presence of nearby particles. This algorithm is tested on simulated data as well as real images from several experimental systems, including colloidal assemblies and single fluorescent proteins.

1:51PM B49.00012 Molecular Simulations of Passive Particle Rheology, RAJESH KHARE, MIR KARIM, Department of Chemical Engineering, Texas Tech University, TSUTOMU INDEI, JAY SCHIEBER, Department of Chemical and Biological Engineering, Illinois Institute of Technology — In this work, we demonstrate that nanoscale viscoelastic properties of polymer melts can be obtained from molecular dynamics (MD) simulations by using an approach analogous to the experimental passive microrheology. We carry out MD simulations of a system consisting of a probe particle that is embedded in a polymer melt represented using the bead-spring model. The mean squared displacement of the probe particle determined from these MD simulations is analyzed to calculate the storage and the loss moduli of the medium. Our results indicate that calculation of the viscoelastic properties from the straightforward Generalized Stokes Einstein Relationship leads to unphysical values for these quantities in the high frequency regime. We show that this problem can be alleviated by accounting for the inertial effects in the system. Our particle rheology simulation results are quantitatively compared with the literature results that were obtained from other simulation approaches. Results will also be presented for the effects of the particle size, rigidity and the chain length on the viscoelastic properties.

2:03PM B49.00013 NMR-based Molecular Rheology of Entangled Polymers in Bulk and in Nanoscopic Confinement¹, KAY SAALWACHTER, MARIE-LUISE TRUTSCHER, FABIAN VACA CHAVEZ², Martin-Luther-Univ. Halle-Wittenberg — We demonstrate the use of simple proton low-field NMR to probe the validity of the tube model of polymer dynamics. The method yields a time-domain measure of the segmental orientation autocorrelation function $C(t)$, which in turn is directly related to the stress relaxation modulus $G(t)$, thus providing a true molecular measure of rheologically relevant quantities. The fixed-tube model does not describe actual data well, and current work focuses on deuteron labeling schemes to investigate the relevance of contour-length fluctuation (CLF) or constraint release (CR) effects. As first results, we found that unexpectedly, CR processes are responsible for modified chain modes faster than actual reptation [1], and also that the dynamics is inhomogeneous along a given chain, stressing also the significance of CLF. We also present recent results for melt dynamics in nanoscopic confinement of long cylindrical channels of 20-400 nm diameter [2]. We consistently observe a fraction of chains whose dynamics is less isotropic on long time scales, i.e., in the Doi-Edwards regimes III (reptation) and IV (disentangled dynamics)
[1] F. Vaca Chávez, K. Saalwächter, *Phys. Rev. Lett.* **104**, 198305 (2010), [2] S. Ok et al., *Macromolecules* **43**, 4429 (2010)

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Monday, February 27, 2012 11:15AM - 2:15PM –
Session B50 DPOLY: Focus Session: Nano to Mesoscale Structures in Ordered Systems: Liquid Crystalline Structure and Interactions 162B

11:15AM B50.00001 Molecular Assembly and Liquid Crystal Properties of a Near-IR Absorbing Dye, PETER COLLINGS, ELIZABETH MILLS, Swarthmore College — The molecules of the near-IR absorbing dye IR-806 spontaneously assemble in water at very low concentrations, forming a liquid crystal phase at room temperature when the concentration is above 0.6 wt%. Unlike most chromonic liquid crystal systems, macroscopic phase separation between the isotropic and liquid crystal phases is not observed. Also unlike most chromonic liquid crystal systems, the absorption spectrum of IR-806 changes dramatically as the concentration increases and molecular assembly proceeds. Analysis of the absorption spectra provides evidence of an isodesmic assembly process at an extremely low concentration, followed by a second non-isodesmic assembly process at a higher concentration just before the liquid crystal phase appears.

11:27AM B50.00002 Studies on Sunset Yellow Chromonic liquid crystals by Polarized Raman and X-ray Scattering¹, MOHAN SRINIVASARAO, Georgia Institute of Technology, XUXIA YAO, Intel Corp., JUNG OK PARK, Georgia Institute of Technology, LEELA JOSHI, Kent State University, SHIN-WOONG KANG, Chonbuk National University, DENA MAE AGRA-KOOIJMAN, SATYENDRA KUMAR, Kent State University — Sunset Yellow FCF (SSY) molecules aggregate into columns in water and form chromonic liquid crystalline phases. Nematic SSY is aligned both in a flat capillary and in the magnetic field with columns pointing perpendicular to the long axis of capillary and perpendicular to the magnetic field direction, respectively. Temperature and concentration dependence of order parameters, both $\langle P_{200} \rangle$ and $\langle P_{400} \rangle$, are calculated based on polarized Raman measurement. The scission energy, E , determined from the Arrhenius thermal evolution of the longitudinal correlation length, is found to be around $4.3k_B T$ in the nematic N phase based on x-ray measurement. Flow behavior of 1.1 M nematic SSY chromonic solution under steady shear is predicted using the order parameters measured and the aspect ratios of columns.

¹This study was partially supported by NSF (DMR-0706235) and DOE (Office of Basic Energy Sciences, DE-SC0001412).

11:39AM B50.00003 Photoisometric liquid crystals integrated with plasmonic nano-structures, GARY WALSH, Electrical Engineering Boston University; US Army NSRDEC, SYLVANUS LEE, Mechanical Engineering Boston University, BRIAN KIMBALL, US Army NSRDEC, LUCA DAL NEGRO, Electrical Engineering and Materials Science Boston University — Optically switching photoisometric liquid crystals can be used for a variety of applications. However, the dependence of the efficiency of photoisometric processes on optical fluence requires power levels too high for many practical applications. Recently it has been shown that symmetry breaking in deterministic aperiodic plasmonic nano-structures boosts the efficiency of nonlinear processes by producing significant spatial field localization. This technology has the potential to dramatically enhance the performance of photoisometric liquid crystal devices. In this work, we combine photoisometric liquid crystals with lithographically fabricated periodic and aperiodic plasmonic nano-particle arrays in microfluidic channels to enhance their all optical switching properties. Using rigorous analytical multiple scattering methods we engineer particle arrays for near field enhancement at a control wavelength and the diffraction properties of a probe beam at another. Optical pump probe measurements of retardance and absorption are used to characterize the liquid crystal's structure factor as function pump power. The effects of plasmonic particle arrays on the switching dynamics on the photoisometric liquid crystals are also experimentally explored.

11:51AM B50.00004 Elasticity of lyotropic chromonic liquid crystal Sunset Yellow probed by magnetic Frederiks transition¹, SHUANG ZHOU, YU. A. NASTISHIN², M.M. OMELCHENKO, L. TORTORA, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, Kent, OH 44242, V.G. NAZARENKO, O.P. BOIKO, Institute of Physics, prospect Nauky 46, Kiev-39, 03039, Ukraine, T. OSTAPENKO, S.N. SPRUNT, J.T. GLEESON, Department of Physics, Kent State University, Kent, OH 44242, O.D. LAVRETOVICH³, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, Kent, OH 44242 — By using director reorientation in the magnetic field, we determine the concentration and temperature dependencies of the splay K_1 , twist K_2 , and bend K_3 elastic constants (normalized by the anisotropy of the diamagnetic susceptibility) for a nematic lyotropic chromonic liquid crystal (LCLC) Sunset Yellow. In a sharp contrast to thermotropic liquid crystals, the Frederiks effects in LCLC show a hysteresis, which is more pronounced at high concentration and low temperatures. We attribute the hysteresis to the changes in self-assembled structure of LCLC aggregates under the influence of field-imposed deformations.

¹This work was supported by NSF MWN Lyotropic Chromonic Liquid Crystals grant DMR076290.

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12:03PM B50.00005 Electric Field Induced Stable Micro Rotor in Nematic Liquid Crystal Drops Constrained on Thin Cellulosic Fibers, MARIA HELENA GODINHO, YONG GENG, PEDRO ALMEIDA, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, JOÃO FIGUEIRINHAS, IST - Technical University of Lisbon, EUGENE TERENTJEV, Cavendish Laboratory, University of Cambridge, FCT/UNL TEAM, FCT/UNL TEAM, IST TEAM, CAVENDISH LABORATORY TEAM — We directly visualize the response of nematic liquid crystal drops of toroidal topology constrained on thin fibers, suspended in air, to an AC applied electric field $\mathbf{E}$. This new localized liquid crystal system can exhibit non-trivial point defects, which may become energetically unstable against expanding into ring disclinations depending on the fiber constraining geometries. The director anchoring tangential near the fiber surface and homeotropic at the air interface, making a hybrid shell distribution that in turn causes a ring of disclination line around the main axis of the fiber at the center of the droplet. Upon application of $\mathbf{E}$, the disclination ring first expands and slightly moves along the fiber main axis, followed by the appearance of a stable “spherical particle” orbiting around the fiber at the center of the liquid crystal drop. The rotation speed of this particle was found to vary linearly with the applied voltage. This constrained liquid crystal geometry seems to meet the essential requirements in which soliton like particles can develop and exhibit stable orbiting in three dimensions upon application of an external electric field. This is another example of a soft energy transducer system which allows, at the micro scale, the transfer in a continuous way of electrical to mechanical energy.

12:15PM B50.00006 Synthesis and investigations of mesogen encapsulated gold nanoparticles¹, CHIH-HAO YU, CHRIS J. WELCH, BAI J. TANG, CHRIS J. SCHUBERT, GEORG H. MEHL, Department of Chemistry, University of Hull, UK — Nematic mesogen encapsulated gold nanoparticles with defined size and shapes are currently of great interest for a wide range of applications for electro-optical device or metamaterials. However the synthesis of most of the materials reported so far is quite cumbersome. Thus there is the need for new routes to synthesize more advanced compounds. A suitable strategy could be based on functionalizing the organic shell. In this contribution we report a new method to prepare gold nanoparticles with a bifunctional capping agent enabling control over their size and also act as a linking group for the connection with the mesogenic groups. The result showed monolayer coated gold nanoparticles without any co-ligands and lower the isotropic point. Physical and optical properties of the nematic gold nanoparticles have been characterized by HRTEM, EDS, NMR, DSC, TGA, XRD, and OPM. The results show stable nematic mesophase formation at room temperature. The investigate system displays a typical nematic schlieren texture, and a decreased viscosity when compared to other LC Au NPs. Structure properties relationships will be discussed and the materials will be compared to earlier research.

¹Found by EU FP7 (NANOGOLD) no 228455

12:27PM B50.00007 Nonlinear Diffusion on a Sphere¹, XIAOYU ZHENG, Dept. of Mathematical Sciences, Kent State University, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University — We are interested in describing orientation of non-spherical particles such as liquid crystal molecules, nanoparticles and colloidal particles due to interactions with each other and with external fields. Since the orientation of a rod-like particle corresponds to a point on a unit sphere, the time evolution of the orientational distribution function corresponds to nonlinear diffusion on a sphere. We use a direct cell-based method to solve the Smoluchowski equation describing the behavior. We construct the Voronoi tessellation on the sphere, and regularize it. We then use a finite volume method to compute the particle density in the cells. Numerical results show the time evolution of the orientational probability density function. These results can describe the behavior of nanorod suspensions in electric fields.

¹This work was supported under NSF DMS-0908470.

12:39PM B50.00008 Elastic Torque on a Ferromagnetic Disk within a Nematic Liquid Crystal, JOEL B. ROVNER, DAN S. BORGNIA, CLAYTON P. LAPOINTE, DANIEL H. REICH, ROBERT L. LEHENY, Department of Physics and Astronomy, Johns Hopkins University — An aspherical particle suspended in a nematic liquid crystal will impose an orientationally dependent energy due to coupling to the nematic elasticity. This energy depends strongly on the anchoring conditions on the surface of the inclusion, its shape, as well as the proximity of other boundary conditions on the fluid such as those set by the container. To study these properties, ferromagnetic nickel disks with homeotropic surface anchoring were suspended in the liquid crystal 4-cyano-4'-pentylbiphenyl (5CB) in a planar cell. The disks, 300 nm in thickness and 10 μm in diameter, possess a permanent magnetic moment confined to the disk's plane. In the absence of any external torque the disks align with the normal to their faces parallel to the director. Rotating of the disks from this preferred orientation creates an elastic deformation that is manifested by an opposing torque. Balancing this torque with the torque from an external magnetic field for various angles of rotation, we have mapped out the orientationally dependent energy. Over a large range of angles the torque shows a linear dependence as predicted by an electrostatic analogy.

12:51PM B50.00009 Anomalous diffusion of colloidal particles in a nematic liquid crystal¹, ISRAEL LAZO, OLEG D. LAVRETOVICH², Kent State University, TARAS TURIV, ALEXANDER BRODIN, VASSILI NAZARENKO, Institute of Physics NAS Ukraine — We explore the Brownian motion of colloidal microspheres in a nematic liquid crystal within time scales below 100ms that was not accessible in previous experiments. Our experimental results point towards an apparent sub-diffusion of the colloids with a mean square displacement $\text{MSD} \propto t^{1/2}$. For longer time scales, the particles exhibit normal diffusion with two anisotropic diffusion constants parallel and perpendicular to the nematic director $\mathbf{n}$ [1]. The nonlinear effect vanishes when the host is heated up to the isotropic phase; therefore the subdiffusive behavior can be attributed to the coupling of slow director fluctuations of the nematic with the colloidal particle dynamics. We also discuss the role of finite accuracy of measurements.

[1] J. C. Loudet, P. Hanusse and P. Poulin, Science 306, (2004).

¹The work was supported by NSF DMR 1104850.

²Corresponding author

1:03PM B50.00010 Colloids at a Chiral Liquid Crystal-Isotropic Liquid Interface, ANNE PAWSEY, JUHO LINTUVUORI, TIFFANY WOOD, JOB THIJSEN, DAVIDE MARENUZZO, PAUL CLEGG, University of Edinburgh — Whilst the behavior of particles trapped at liquid-liquid interfaces is relatively well understood the behavior as one of the phases begins to break translational symmetry is almost completely unexplored. Here the particles seed defects in the partially ordered liquid and new, effective, particle-particle interactions are induced. We use a chiral (cholesteric) liquid crystal which has a characteristic length scale, the pitch length, similar to the particle size. Our system consists of particles with planar anchoring which are trapped at an interface between the liquid crystal and an isotropic liquid (silicone oil which induces homeotropic anchoring). The creation of the cholesteric "fingerprint" texture allows the deformation of the cholesteric around a particle to be easily visualized. This allows us to determine the nature of the defects created and their symmetries. We have clear trends for the distribution of particles with respect to the interface as a function of particle size. Inspired by computer simulations we study the position of small particles (diameter < pitch length) within the fingerprint texture. The behavior of the unadorned interface between the chiral liquid crystal and the oil is also explored.

1:15PM B50.00011 Deformable Colloids in the Presence of a Liquid Crystal, FRANCES MACKAY, COLIN DENNISTON, University of Western Ontario — Spherical colloidal particles immersed in a liquid crystal experience a non-uniform pressure, as well as directional interactions among one another due to the defects they induce in the surrounding liquid crystal. Here, we use a lattice-Boltzmann algorithm to investigate the behavior of initially circular, 2D deformable colloids placed in a nematic liquid crystal. The colloidal particles, which are represented using a bead-spring model, are of a sufficient physical size to ensure that the anchoring of the liquid crystal molecules on their surface has a significant impact on the background liquid crystal. We present the resulting equilibrium particle shapes for a range of surface elasticities, and investigate the interaction between pairs of particles.

1:27PM B50.00012 Multistable alignment of nematic liquid crystals on patterned surfaces, TIMOTHY ATHERTON, Tufts University — A nematic in contact with a substrate patterned to promote a spatially-varying easy axis experiences a large elastic distortion adjacent to the surface and relaxes to a uniform state in the bulk. The bulk ordering may be thought of as an effective easy axis which, unlike conventional surface treatments, can be easily controlled by adjusting the geometry of the pattern. In this work, the behavior of a nematic film confined between substrates periodically patterned with rectangles is examined analytically. It is shown that multiple stable configurations exist and the effective azimuthal anchoring energy may be arbitrarily controlled by changing the aspect ratio of the rectangles. The various effects of flexoelectricity and saddle-splay elasticity, both important because of large spatial gradients in molecular orientation near the surface, are also considered. Prospects for applications of these surfaces in electrooptic devices such as displays are discussed.

1:39PM B50.00013 Direct Nanomechanical Measurement of an Anchoring Transition in a Nematic Liquid Crystal Subject to Hybrid Anchoring Conditions, BRUNO ZAPPONE, CNR-IPCF, Liquid Crystal Lab., Univ. of Calabria, Italy, MARINA RUTHS, Dept. of Chemistry, Univ. of Massachusetts Lowell — A Surface Forces Apparatus was used to measure the normal force between two solid curved surfaces confining a film of nematic liquid crystal (5CB, 4'-n-pentyl-4-cyanobiphenyl) under hybrid planar-homeotropic anchoring conditions. Upon reduction of the surface separation D , we measured an increasingly repulsive force in the range $D = 35\text{--}80$ nm, reaching a plateau in the range $D = 10\text{--}35$ nm, followed by a short-range oscillatory force at $D < 5$ nm. The oscillation period was comparable to the cross-sectional diameter of the liquid crystal molecule and characteristic of a configuration with the molecules parallel to the surfaces. These results show that the director field underwent a confinement-induced transition from a splay-bend distorted configuration at large D , which produces elastic repulsive forces, to a uniform planar configuration with broken homeotropic anchoring, which does not produce additional elastic forces as D is decreased. These findings, supported by measurements of the birefringence of the confined film at different film thicknesses, provide the first direct visualization of an anchoring transition at the nanometer scale.

1:51PM B50.00014 Unified theory of chiral smectic A monolayers and π -wall defects, C. NADIR KAPLAN, MARK J. ZAKHARY, THOMAS GIBAUD, EDWARD BARRY, ROBERT B. MEYER, ZVONIMIR DOGIC, Brandeis University — Monodisperse suspensions of the rodlike chiral fd viruses are condensed into one rod length thick colloidal monolayers of aligned rods by depletion forces. Twist deformations of the molecules are expelled to the monolayer edge as in a chiral smectic A (Sm-A*) liquid crystal, and a cholesteric (Ch) region forms at the edge. Coalescence of two such isolated monolayers results in a cholesteric wall sandwiched between two regions of aligned fd viruses, dubbed π -wall defects. Based on the analogy of Sm-A* with superconductors, we develop a unified theory of the π -wall defects and the monolayer edge structure. Our model yields the molecular tilt profiles, the local thickness change, and the crossover from Sm-A*-to-Ch behavior across the monolayer and the π -wall. These allow us to determine the line tension as a function of the depletant polymer concentration and the chirality of the viruses, in agreement with experiment.

2:03PM B50.00015 Molecular Tilt on Monolayer-Protected Nanoparticles, XU MA, Department of Physics, Syracuse University, Syracuse, New York, USA, LUCA GIOMI, School of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts, USA, MARK BOWICK, Department of Physics, Syracuse University, Syracuse, New York, USA, APALA MAJUMDAR, Oxford Centre for Collaborative Applied Mathematics, University of Oxford, OX1 3LB, UK — We present a simple Ginzburg-Landau model to describe the order of ligands coating small metal nanoparticles (NPs). Two dimensionless parameters are introduced: a preferential tilt angle and a ratio epsilon between the energy cost due to spatial variations in the tilt of the coating molecules and that of the van der Waals interactions which favors uniform tilt. Even for the ground state, topological defects are present due to the topology of the NPs. The ground state for spherical particles is an ordered bipolar defective texture (B) for small epsilon and an untilted phase (U) for large epsilon. Octahedral particles have an additional phase (6V) at small epsilon characterized by the presence of six topological defects.

Monday, February 27, 2012 11:15AM - 2:15PM –
Session B51 DBIO GSNP: Focus Session: Evolutionary Systems Biology I - Evolutionary Dynamics and Rugged Fitness Landscapes 154

11:15AM B51.00001 Optimal lineage principle for age-structured populations, EDO KUSSELL, New York University — Populations whose individuals exhibit age-dependent growth have often been studied using temporal dynamics of age distributions. In this talk, I examine the dynamics of age along lineages. We will see that the lineage point-of-view provides fundamental insights into evolutionary pressures on individuals' aging profiles. I will describe a variational principle that enables exact results for lineage statistics, in a variety of models. I will also discuss measurements on continuously dividing bacterial populations growing in microfluidics devices.

11:51AM B51.00002 Why Do Complex Systems Age?, DERVIS VURAL, Harvard University and University of Illinois at Urbana Champaign, GREGORY MORRISON, L. MAHADEVAN, Harvard University — Aging can be defined as the increase in probability of death with time. The observation that organisms, colonies, ecosystems, as well as larger social structures age and die in very similar ways suggest that the reasons underlying aging does not depend sensitively on molecular or cellular details. In this work we argue that aging is an inevitable outcome of the neutral co-evolution of non-aging components which with time become increasingly interdependent. Starting from this hypothesis, we construct generic dependency networks and obtain mortality rate as a function of time, as well as mean life expectancy as a function of organism size, complexity and metabolic rate.

12:03PM B51.00003 Learning about evolution from sequence data, ADEL DAYARIAN, BORIS SHRAIMAN, KITP — Recent advances in sequencing and in laboratory evolution experiments have made possible to obtain quantitative data on genetic diversity of populations and on the dynamics of evolution. This dynamics is shaped by the interplay between selection acting on beneficial and deleterious mutations and recombination which reshuffles genotypes. Mounting evidence suggests that natural populations harbor extensive fitness diversity, yet most of the currently available tools for analyzing polymorphism data are based on the neutral theory. Our aim is to develop methods to analyze genomic data for populations in the presence of the above-mentioned factors. We consider different evolutionary regimes - Muller's ratchet, mutation-recombination-selection balance and positive adaption rate - and revisit a number of observables considered in the nearly-neutral theory of evolution. In particular, we examine the coalescent structure in the presence of recombination and calculate quantities such as the distribution of the coalescent times along the genome, the distribution of haplotype block sizes and the correlation between ancestors of different loci along the genome. In addition, we characterize the probability and time of fixation of mutations as a function of their fitness effect.

12:15PM B51.00004 Population genetics inside a cell: Mutations and mitochondrial genome maintenance, SIDHARTHA GOYAL, Kavli Institute for Theoretical Physics, University of California Santa Barbara, BORIS SHRAIMAN, University of California Santa Barbara, DAN GOTTSCHLING, Fred Hutchinson Cancer Research Center — In realistic ecological and evolutionary systems natural selection acts on multiple levels, i.e. it acts on individuals as well as on collection of individuals. An understanding of evolutionary dynamics of such systems is limited in large part due to the lack of experimental systems that can challenge theoretical models. Mitochondrial genomes (mtDNA) are subjected to selection acting on cellular as well as organelle levels. It is well accepted that mtDNA in yeast *Saccharomyces cerevisiae* is unstable and can degrade over time scales comparable to yeast cell division time. We utilize a recent technology designed in Gottschling lab to extract DNA from populations of aged yeast cells and deep sequencing to characterize mtDNA variation in a population of young and old cells. In tandem, we developed a stochastic model that includes the essential features of mitochondrial biology that provides a null model for expected mtDNA variation. Overall, we find approximately 2% of the polymorphic loci that show significant increase in frequency as cells age providing direct evidence for organelle level selection. Such quantitative study of mtDNA dynamics is absolutely essential to understand the propagation of mtDNA mutations linked to a spectrum of age-related diseases in humans.

12:27PM B51.00005 Rare beneficial mutations can halt Muller's ratchet, DANIEL BALICK, Physics Department, University of California, Santa Barbara, SIDHARTHA GOYAL, KITP, UCSB, ELIZABETH JERISON, Physics Department, Harvard University, RICHARD NEHER, MPI for Developmental Biology, Tübingen, BORIS SHRAIMAN, KITP and Physics Department, UCSB, MICHAEL DESAI, Physics Department and OEB, Harvard University — In viral, bacterial, and other asexual populations, the vast majority of non-neutral mutations are deleterious. This motivates the application of models without beneficial mutations. Here we show that the presence of surprisingly few compensatory mutations halts fitness decay in these models. Production of deleterious mutations is balanced by purifying selection, stabilizing the fitness distribution. However, stochastic vanishing of fitness classes can lead to slow fitness decay (i.e. Muller's ratchet). For weakly deleterious mutations, production overwhelms purification, rapidly decreasing population fitness. We show that when beneficial mutations are introduced, a stable steady state emerges in the form of a dynamic mutation-selection balance. We argue this state is generic for all mutation rates and population sizes, and is reached as an end state as genomes become saturated by either beneficial or deleterious mutations. Assuming all mutations have the same magnitude selective effect, we calculate the fraction of beneficial mutations necessary to maintain the dynamic balance. This may explain the unexpected maintenance of asexual genomes, as in mitochondria, in the presence of selection. This will affect in the statistics of genetic diversity in these populations.

12:39PM B51.00006 Clustering and Phase Transitions on a Neutral Landscape¹, ADAM SCOTT, DAWN KING, Center for Neurodynamics - Department of Physics & Astronomy - University of Missouri at St. Louis, NEVENA MARIC, Department of Mathematics & Computer Science - University of Missouri at St. Louis, SONYA BAHAR, Center for Neurodynamics - Department of Physics & Astronomy - University of Missouri at St. Louis — The problem of speciation and species aggregation on a neutral landscape, subject to random mutational fluctuations rather than selective drive, has been a focus of research since the seminal work of Kimura on genetic drift. These ideas have received increased attention due to the more recent development of a neutral ecological theory by Hubbell. De Aguiar et al. recently demonstrated, in a computational model, that speciation can occur under neutral conditions; this study bears some comparison with more mathematical studies of clustering on neutral landscapes in the context of branching and annihilating random walks. Here, we show that clustering can occur on a neutral landscape where the dimensions specify the simulated organisms' phenotypes. Unlike the De Aguiar et al. model, we simulate *sympatric* speciation: the organisms cluster phenotypically, but are not spatially separated. Moreover, we find that clustering occurs not only in the case of assortative mating, but also in the case of asexual fission. Clustering is not observed in a control case where organisms can mate randomly. We find that the population size and the number of clusters undergo phase-transition-like behavior as the maximum mutation size is varied.

¹Funding provided by the University of Missouri Research Board and the James S. McDonnell Foundation.

12:51PM B51.00007 Mutational pathways to drug resistance through a maximally-rugged fitness landscape, ADAM PALMER, ERDAL TOPRAK, Department of Systems Biology, Harvard Medical School, Boston, MA, USA, SEUNGSOO KIM, ADRIAN VERES, Faculty of Arts and Sciences, Harvard University, Cambridge, MA, USA, SHIMON BERSHTEIN, Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, USA, ROY KISHONY, Department of Systems Biology, Harvard Medical School, Boston, MA, USA — Recent laboratory evolution experiments have identified surprising properties in the evolution of trimethoprim resistance in *E.coli* through mutation of the drug's target, DHFR: (1) mutations are acquired in a reproducibly ordered manner; (2) multiple resistant endpoints exist; and (3) some pathways include mutation reversion or conversion. Here we investigate how these properties emerge from the fitness landscape of DHFR by characterizing all combinations of observed DHFR mutations. We see that the effects of mutations are so profoundly dependent on other mutations that sign-epistasis is nearly maximised, and the distributions of most mutations' effects are indistinguishable from randomly increasing or decreasing resistance. This almost 'maximally-rugged' fitness landscape contains multiple separated peaks in drug resistance, and 20% of favourable mutational steps are the loss or conversion of a previously acquired mutation. Select pathways through the rugged landscape avoid a common tradeoff between growth and resistance. Empirical characterization of this fitness landscape has identified that ordered but sometimes indirect mutational pathways to multiple endpoints arises from near-maximal levels of sign epistasis.

1:03PM B51.00008 Hidden Randomness between Fitness Landscapes Limits Reverse Evolution, LONGZHI TAN, STEPHEN SERENE, HUI XIAO CHAO, JEFF GORE, Massachusetts Institute of Technology — Natural populations must constantly adapt to the ever-changing environment. A fundamental question in evolutionary biology is whether adaptations can be reversed by returning the population to its ancestral environment. Traditionally, reverse evolution is defined as restoring an ancestral phenotype (physical characteristics such as body size), and the classic Dollo's Law has hypothesized the impossibility of reversing complex adaptations. However, this "law" remains ambiguous unless reverse evolution can be studied at the level of genotypes (the underlying genome sequence). We measured the fitness landscapes of a bacterial antibiotic-resistance gene and analyzed the reversibility of evolution as a global, statistical feature of the landscapes. In both experiments and simulations, we find that an adaptation's reversibility declines as the number of mutations it involves increases, suggesting a probabilistic form of Dollo's Law at the molecular level. We also show computationally that slowly switching between environments facilitates reverse evolution in small populations, where clonal interference is negligible or moderate. This is an analogy to thermodynamics, where the reversibility of a physical process is maximized when conditions are modified infinitely slowly.

1:15PM B51.00009 Exploring the fitness landscape of poliovirus, SIMONE BIANCO, ASHELY ACEVEDO, RAUL ANDINO, CHAO TANG, University of California San Francisco — RNA viruses are known to display extraordinary adaptation capabilities to different environments, due to high mutation rates. Their very dynamical evolution is captured by the quasispecies concept, according to which the viral population forms a swarm of genetic variants linked through mutation, which cooperatively interact at a functional level and collectively contribute to the characteristics of the population. The description of the viral fitness landscape becomes paramount towards a more thorough understanding of the virus evolution and spread. The high mutation rate, together with the cooperative nature of the quasispecies, makes it particularly challenging to explore its fitness landscape. I will present an investigation of the dynamical properties of poliovirus fitness landscape, through both the adoption of new experimental techniques and theoretical models.

1:27PM B51.00010 Scaling laws and universality for the strength of genetic interactions in yeast, ANDREA VELENICH, M.I.T., MINGJIE DAI, Harvard University, JEFF GORE, M.I.T. — Genetic interactions provide a window to the organization of the thousands of biochemical reactions in living cells. If two mutations affect unrelated cellular functions, the fitness effects of their combination can be easily predicted from the two separate fitness effects. However, because of interactions, for some pairs of mutations their combined fitness effect deviates from the naive prediction. We study genetic interactions in yeast cells by analyzing a publicly available database containing experimental growth rates of 5 million double mutants. We show that the characteristic strength of genetic interactions has a simple power law dependence on the fitness effects of the two interacting mutations and that the probability distribution of genetic interactions is a universal function. We further argue that the strength of genetic interactions depends only on the fitness effects of the interacting mutations and not on their biological origin in terms of single point mutations, entire gene knockouts or even more complicated physiological perturbations. Finally, we discuss the implications of the power law scaling of genetic interactions on the ruggedness of fitness landscapes and the consequent evolutionary dynamics.

1:39PM B51.00011 Speeding up Evolutionary Search by Small Fitness Fluctuations, JAKUB OTWINOWSKI, Department of Physics, Emory University, SORIN TANASE-NICOLA, Department for Cell and Molecular Biology, Uppsala University, ILYA NEMENMAN, Departments of Physics and Biology and Computational and Life Sciences Initiative, Emory University — We consider a fixed size population that undergoes an evolutionary adaptation in the weak mutation rate limit, which we model as a biased Langevin process in the genotype space. We show analytically and numerically that, if the fitness landscape has a small highly epistatic (rough) and time-varying component, then the population genotype exhibits a high effective diffusion in the genotype space and is able to escape local fitness minima with a large probability. We argue that our principal finding that even very small time-dependent fluctuations of fitness can substantially speed up evolution is valid for a wide class of models.

1:51PM B51.00012 ABSTRACT HAS BEEN MOVED TO J42.00011 —

2:03PM B51.00013 Experimental observation of critical slowing down as an early warning of population collapse, DAAN VORSELEN, Department of Physics and Astronomy, VU University, Amsterdam, The Netherlands., LEI DAI, KIRILL KOROLEV, JEFF GORE, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA — Near tipping points marking population collapse or other critical transitions in complex systems small changes in conditions can result in drastic shifts in the system state. In theoretical models it is known that early warning signals can be used to predict the approach of these tipping points (bifurcations), but little is known about how these signals can be detected in practice. Here we use the budding yeast *Saccharomyces cerevisiae* to study these early warning signals in controlled experimental populations. We grow yeast in the sugar sucrose, where cooperative feeding dynamics causes a fold bifurcation; falling below a critical population size results in sudden collapse. We demonstrate the experimental observation of an increase in both the size and timescale of the fluctuations of population density near this fold bifurcation. Furthermore, we test the utility of theoretically predicted warning signals by observing them in two different slowly deteriorating environments. These findings suggest that these generic indicators of critical slowing down can be useful in predicting catastrophic changes in population biology.

Monday, February 27, 2012 11:15AM - 2:15PM —
Session B52 GSNP: Granular Media: Flow and Structure 153C

11:15AM B52.00001 Simulations of Granular Particles Under Cyclic Shear, JOHN ROYER, PAUL CHAIKIN, Center for Soft Matter Research, New York University — We perform molecular dynamics (MD) simulations of spherical grains subjected to cyclic, quasi-static shear in a 3D parallelepiped shear cell. This virtual shear cell is constructed out of rough, bumpy walls in order to minimize wall-induced ordering and has an open top surface to allow the packing to readily dilate or compact. Using a standard routine for MD simulations of frictional grains, we simulate over 1000 shear cycles, measuring grain displacements, the local packing density and changes in the contact network. Varying the shear amplitude and the friction coefficient between grains, we map out a phase diagram for the different types of behavior exhibited by these sheared grains. With low friction and high enough shear, the grains can spontaneously order into densely packed crystals. With low shear and increasing friction the packing remains disordered, yet the grains arrange themselves into configurations which exhibit limit cycles where all grains return to the same position after each full shear cycle. At higher shear and friction there is a transition to a diffusive state, where grains continue rearrange and move throughout the shear cell.

11:27AM B52.00002 A Continuous Time Random Walk Description of Monodisperse, Hard-Sphere Colloids below the Ordering Transition, JEREMY LECHMAN, FLINT PIERCE, Sandia National Laboratories — Diffusive transport is a ubiquitous process that is typically understood in terms of a classical random walk of non-interacting particles. Here we present the results for a model of hard-sphere colloids in a Newtonian incompressible solvent at various volume fractions below the ordering transition ($\sim 50\%$). We numerically simulate the colloidal systems via Fast Lubrication Dynamics — a Brownian Dynamics approach with corrected mean-field hydrodynamic interactions. Colloid-colloid interactions are also included so that we effectively solve a system of interacting Langevin equations. The results of the simulations are analyzed in terms of the diffusion coefficient as a function of time with the early and late time diffusion coefficients comparing well with experimental results. An interpretation of the full time dependent behavior of the diffusion coefficient and mean-squared displacement is given in terms of a continuous time random walk. Therefore, the deterministic, continuum diffusion equation which arises from the discrete, interacting random walkers is presented. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

11:39AM B52.00003 Shear failure of granular materials, ERIC DEGIULI, NEIL BALMFORTH, Dept. Mathematics, UBC, JIM MCELWAINE, DAMTP, University of Cambridge, CHRISTIAN SCHOOF, Dept. Earth and Ocean Sciences, UBC, IAN HEWITT, Dept. Mathematics, UBC — Connecting the macroscopic behavior of granular materials with the microstructure remains a great challenge. Recent work connects these scales with a discrete calculus [1]. In this work we generalize this formalism from monodisperse packings of disks to 2D assemblies of arbitrarily shaped grains. In particular, we derive Airy's expression for a symmetric, divergence-free stress tensor. Using these tools, we derive, from first-principles and in a mean-field approximation, the entropy of frictional force configurations in the Force Network Ensemble. As a macroscopic consequence of the Coulomb friction condition at contacts, we predict shear failure at a critical shear stress, in accordance with the Mohr-Coulomb failure condition well known in engineering. Results are compared with numerical simulations, and the dependence on the microscopic geometric configuration is discussed.

[1] E. DeGiuli & J. McElwaine, PRE 2011. doi: 10.1103/PhysRevE.84.041310

11:51AM B52.00004 A simple analytic theory for the statistics of avalanches in sheared granular materials, KARIN DAHMEN, University of Illinois at Urbana Champaign, YEHUDA BEN-ZION, University of Southern California, Los Angeles, JONATHAN UHL, private — Slowly sheared granular materials at high packing fractions deform via slip avalanches with a broad range of sizes. Conventional continuum descriptions are not expected to apply to such highly inhomogeneous, intermittent deformations. Here, we show that it is possible to analytically compute the dynamics using a simple model that is inherently discrete. This model predicts quantities such as the avalanche size distribution, power spectra and temporal avalanche profiles as functions of the grain number fraction and the frictional weakening. A dynamical phase diagram emerges with quasi-static avalanches at high number fractions, and more regular, fluid-like flow at lower number fractions. The predictions agree with experiments and simulations for different granular materials, motivate future experiments and provide a fresh approach to data analysis. The simplicity of the model reveals quantitative connections to plasticity and earthquake statistics. (Reference: K.A. Dahmen, Y. Ben-Zion, J.T. Uhl, Nature Physics 7, 554-557 (2011).)

12:03PM B52.00005 Simulation of 2D Granular Hopper Flow¹, ZHUSONG LI, MARK SHATTUCK, CUNY Graduate Center and the Benjamin Levich Institute and Physics Department of The City College of New York — Jamming and intermittent granular flow are big problems in industry, and the vertical hopper is a canonical example of these difficulties. We simulate gravity driven flow and jamming of 2D disks in a vertical hopper and compare with identical companion experiments presented in this session. We measure and compare the flow rate and probability for jamming as a function of particle properties and geometry. We evaluate the ability of standard Hertz-Mindlin contact mode to quantitatively predict the experimental flow.

¹Supported by NSF (CBET-0968013)

12:15PM B52.00006 Forces on intruders in granular media, IBAR DELACRUZ, STEPHAN KOEHLER, WPI — We measure the forces acting on intruders moving in different directions in a granular medium consisting of mono-disperse spherical glass beads. We present the dependence of the drag force on the intruder's geometry and surface roughness, bead size, dragging speed and immersion depth. We also determine the distribution of the forces on the intruder's surfaces. We compare our results with lithostatic pressure ($p = \rho gz$).

12:27PM B52.00007 2D Granular Impact Dynamics with Photoelastic Particles¹, ABE CLARK, Duke University, LOU KONDIS, New Jersey Institute of Technology, R.P. BEHRINGER, Duke University — What is the response of a granular material to a high speed impact from a foreign object? To answer this question, we use a large 2D granular system which is impacted from above by an intruder. Using photoelastic discs and a high-speed camera (frame rates at 7,000-775,00 fps at varied resolution, typically 40,000 fps at 584x256 pixels), we are able to observe the dynamics in this process in a way which has not been done previously. Data consists of the trajectory of the intruder, as well as either particle positions or interparticle force information. High frame rates allow observation of complex acoustic waves during the impact process. We examine the effects of varying the initial velocity, density, shape, and size of the intruder, with the goal of extracting the grain-scale mechanisms responsible for the dissipation of the intruder's kinetic energy. In comparing our data to macroscopic frictional models used in past work, we observe good agreement with the low-frequency behavior in our experiments, but we also observe large high-frequency fluctuations in the acceleration which are inherently granular, and not captured by these models. The large fluctuations are well correlated to the emission of localized intermittent stress pulses, seen in the photoelastic response.

¹This work is supported by DTRA, grant HDTRA1-10-0021

12:39PM B52.00008 Cooperative rotations of 2d frictional disks under oscillatory shear, MITCHELL MAILMAN, MICHELLE GIRVAN, WOLFGANG LOSERT, university of Maryland — We explore the dynamics of the contact network under cyclic shear, with a particular focus on cooperative rolling and sliding contacts, using a molecular dynamics (MD) simulation approach and external fixed pressure. We systematically study the formation and persistence of clusters of cooperatively rolling grains for a range of reversal amplitudes. The propensity for cooperative rotation dictates structural properties of the contact network: loop configurations of even numbers of grains are able to rotate without sliding, while odd numbers of grains must have at least one sliding contact. We report on the statistics of loop structures in the contact network, as well as their relationships to cooperatively rotating grains. Finally, we demonstrate a characteristic scale over which grains can cooperatively rotate as well as the dependence on friction parameters.

12:51PM B52.00009 High-speed measurement of axial grain transport in a rotating drum¹, FRANK VAN BUSSEL, Max Planck Institute for Dynamics and Self-Organization, ZEINA KHAN, Chemical Engineering, Texas Tech University, MARC SCHABER, RALF SEEMANN, Experimental Physics, Saarland University, MARIO SCHEEL, MARCO DIMICHIEL, European Synchrotron Radiation Facility — Over short timescales granular mixtures separate by size when tumbled in a partially filled horizontal drum. The smaller grains move toward the axis of rotation to form a central core; undulations in this core gradually increase in amplitude until they grow into axial bands. Using non-invasive high-speed synchrotron x-ray particle tracking, we investigate the axial transport properties of tracer particles traveling amongst glass spheres. This new technique allows us to gather data on time scales not previously possible. When the tracers are present in larger proportions the mixtures we used should have different tendencies to segregate axially according to size ratio; one of our findings, however, is that when the tracer concentration is low the single-particle dynamics of these mixtures do not depend on the relative particle sizes in any appreciable way. This implies that the potential for a mixture to axially segregate cannot be inferred from the microscopic dynamics of individual small particles. A second finding is that while the slope of the mean-squared displacement is close to that expected from diffusive transport, as determined from the single-particle dynamics, more detailed analyses indicate anomalous transport.

¹The authors thank the ESRF for providing the synchrotron radiation facilities under proposal LTP MA-800.

1:03PM B52.00010 Jamming of Cylindrical Grains in Vertical Channels¹, G. WILLIAM BAXTER, GREGORY SPIER, NICHOLAS BARR, FIONA STEEL, Penn State Erie, The Behrend College — We study jamming of low aspect-ratio cylindrical Delrin grains in a vertical channel. These cylindrical grains resemble antacid tablets, poker chips, or coins since their height is less than their diameter. Grains are allowed to fall through a vertical channel with a square cross section where the channel width is greater than the diameter of a grain and constant throughout the length of the channel with no obstructions or constrictions. Within this channel, grains are sometimes observed to form jams, stable structures supported by the channel walls with no support beneath them. The probability of jam occurrence and the strength or robustness of a jam is effected by the grain dimensions and channel size. We will present experimental measurements of the jamming probability and jam strength in this system and discuss the relationship of these results to other experiments and theories.

¹Supported by an Undergraduate Research Grant from Penn State Erie, The Behrend College.

1:15PM B52.00011 Ordered and disordered granular sphere packings obtained by epitaxial growth, ANDREEA PANAITESCU, ARSHAD KUDROLI, Clark University — We study granular packings obtained by depositing spheres on a substrate under the influence of gravity. By exploiting the direct particle tracking enabled by X-ray tomography, the nature of the order and disorder is investigated using statistical measures including density pair correlation function, and the orientational order parameter. We find that by using a low deposition rate, impinging particles with sufficient energy can overcome friction and come to rest in a potential minimum of a periodic substrate, giving rise to ordered face-centered cubic structures. However, impinging particles with large kinetic energy can dislodge particles in the substrate leading to disorder as mobile particles cooperatively form arches while they come to rest. Thus, a wide range of volume fractions and packing structures is accessed by simply controlling the nature of the substrate and deposition rate and energy, along with the shape of the impinging particles. We contrast the ordered and disordered phases observed as a function of packing fraction with our previous study with cyclically sheared packings. In that study, compaction, nucleation and growth of face centered cubic and hexagonal close packed crystalline order was observed after hundreds of thousands of shear cycles.

1:27PM B52.00012 Tunable acoustic switching and rectification in one-dimensional granular crystals, NICHOLAS BOECHLER, Massachusetts Institute of Technology, GEORGIOS THEOCHARIS, CHIARA DARAI, California Institute of Technology — We study a new mechanism for tunable acoustic switching and rectification, which we experimentally demonstrate in a one-dimensional granular crystal. The granular crystal is composed of an array of statically compressed elastic spherical particles that interact nonlinearly via Hertzian contact. The granular crystal is uniform except for a single light-mass defect placed near one boundary of the crystal. Because of the interplay of the periodicity, nonlinearity, dissipation, and asymmetry of the granular crystal, vibrations applied near the defect position cause the system response to bifurcate from periodic non-transmitting states to quasiperiodic and chaotic transmitting states with broadband frequency content. We illustrate the nature of this bifurcation using numerical simulations and compare these results to experimental observations. Because the bifurcation causes a sharp transition between states, this mechanism can lead to phononic switching and sensing. Furthermore, as switches and rectification devices are fundamental components used for controlling the flow of energy in numerous applications, we envision that this mechanism could more generally enable the design of advanced photonic, thermal, and acoustic materials and devices.

1:39PM B52.00013 Granular compaction under confinement, NATHAN MUEGGENBURG, Lake Forest College — A granular pack that is vertically vibrated undergoes rearrangements and often progresses to more dense configurations. The experiments presented here study the role of dilation in this granular compaction process. By applying a confining force to the granular pack during vibration, the dilation is inhibited and the compaction is greatly reduced. In general, systems with different accelerations during vibration will compact differently. However, these systems will compact in the same manner if the confining force is tuned to result in the same amount of dilation. Under large confining forces, there is very little dilation. In this regime, the compaction is significantly slowed and may approach a steady state packing fraction of approximately 0.60, consistent with ideas of a critical packing fraction for the onset of dilation.

1:51PM B52.00014 Densest columnar structures of hard spheres from sequential deposition¹, HO-KEI CHAN, Foams & Complex Systems, School of Physics, Trinity College Dublin, Ireland, ABERYSTWYTH UNIVERSITY COLLABORATION — The rich variety of densest columnar structures of identical hard spheres inside a cylinder can surprisingly be constructed from a simple and computationally fast sequential deposition of cylinder-touching spheres, if the cylinder-to-sphere diameter ratio D is within $[1, 2.7013]$. This provides a direction for theoretically deriving all these densest structures and for constructing such densest packings with nano-, micro-, colloidal or charged particles, which all self-assemble like hard spheres [*Rapid Communication*, Physical Review E (in press)].

¹Funded by IRCSET

2:03PM B52.00015 Discrete Calculus as a Bridge between Scales, ERIC DEGIULI, Dept. Mathematics, UBC, JIM MCELWAINE, DAMTP, University of Cambridge — Understanding how continuum descriptions of disordered media emerge from the microscopic scale is a fundamental challenge in condensed matter physics. In many systems, it is necessary to coarse-grain balance equations at the microscopic scale to obtain macroscopic equations. We report development of an exact, discrete calculus, which allows identification of discrete microscopic equations with their continuum equivalent [1]. This allows the application of powerful techniques of calculus, such as the Helmholtz decomposition, the Divergence Theorem, and Stokes' Theorem. We illustrate our results with granular materials. In particular, we show how Newton's laws for a single grain reproduce their continuum equivalent in the calculus. This allows introduction of a discrete Airy stress function, exactly as in the continuum. As an application of the formalism, we show how these results give the natural mean-field variation of discrete quantities, in agreement with numerical simulations. The discrete calculus thus acts as a bridge between discrete microscale quantities and continuous macroscale quantities.

[1] E. DeGiuli & J. McElwaine, PRE 2011. doi: 10.1103/PhysRevE.84.041310

Monday, February 27, 2012 11:15AM - 2:15PM — Session B53 GSNP: Disordered and Glassy Systems II 153B

11:15AM B53.00001 Nanoscale dynamics of binary metallic glass $\text{Cu}_x\text{Hf}_{1-x}$ films¹, JACOB BURGESS, University of Alberta Department of Physics, National Institute for Nanotechnology, CHRIS HOLT, University of Alberta Department of Chemical and Materials Engineering, National Institute for Nanotechnology, DAVID FORTIN, GREG POPOWICH, University of Alberta Department of Physics, ERIK LUBER, DAVID MITLIN, University of Alberta Department of Chemical and Materials Engineering, National Institute for Nanotechnology, MARK FREEMAN, University of Alberta Department of Physics, National Institute for Nanotechnology — Scanning probe microscopy provides a valuable tool for investigating nanoscale structure of thin films. Less commonly it can be applied to study the low speed dynamical behavior of these systems as well. Presented here are scanning tunneling microscope investigations of sputtered glass $\text{Cu}_x\text{Hf}_{1-x}$ films which reveal the nanocrystalline structure of the films as well as hopping dynamics of crystal clusters on the surface. A correction for limited bandwidth and a range of activation energies is developed in the context of an Arrhenius process to allow extraction of the average energy barrier for cluster hopping. Concentration of the component metals in the films was varied allowing observation of the change in cluster size as well as the transition to the amorphous state. A second form of dynamics, more diffusive in character, was found for amorphous samples.

¹This work was supported by NSERC, CIFAR, NRC, Alberta Innovates, and CRC

11:27AM B53.00002 Isothermal Pressurizations and Glass Transition Dynamics in the Intermediate Glass-Forming Liquid Glycerol¹, WILLIAM OLIVER, University of Arkansas, Department of Physics, TITUS MORRIS, Michigan State University, Department of Physics and Astronomy, TIM RANSOM, University of Arkansas, Department of Physics — Brillouin scattering data along both a 75 °C and 100 °C isotherm to pressures as high 6 GPa are reported for glycerol an intermediate strength glass forming liquid. This represents the highest pressure data of any type reported for glycerol, and enables us to probe directly the alpha relaxation process at these high pressures. Acoustic mode frequencies and linewidths are obtained from fits to the spectra. These frequency shifts and linewidths are fit for each isotherm with an iterative technique in which parameters are adjusted until self consistency is obtained. The Tait equation of state along with a complex expression for the dynamical longitudinal modulus, $M(\omega)$, and quantitative models for other physical quantities such as the adiabatic index are used in our analysis. A Cole-Davidson function is used to model the dynamical modulus, and self-consistent fits indicate that the stretching parameter, β , is pressure independent with a value of 0.37 consistent with other low pressure acoustic results in the literature. Final values for the pressure dependent dynamical longitudinal modulus and relaxation time are obtained. In contrast to the results of recent pressure-dependent dielectric studies, there does not appear to be a second process that obscures the alpha process.

¹We gratefully acknowledge support from the NSF under grant NO.: DMR-0552944

11:39AM B53.00003 Fast Scanning Calorimetry study of non-equilibrium relaxation in 2-Ethyl-1-Hexanol¹, VLAD SADTCHENKO, DEEPANJAN BHATTACHARYA, The George Washington University, Department of Chemistry, CANDACE PANE, The University of Aberdeen — Fast scanning calorimetry (FSC), capable of heating rates in excess of 1000000 K/s, was combined with vapor deposition technique to investigate non-equilibrium relaxation in micrometer thick ultraviscous of 2-Ethyl-1-Hexanol (2E1H) films under high vacuum conditions. Rapid heating of 2E1H samples prepared at temperatures above approximately 145 K (standard glass transition temperature of 2E1H, T_{gs}), resulted in well manifested dynamic glass transitions at temperatures tens of degrees higher than T_{gs}. Furthermore, strong and complex dependence of dynamic glass transition temperature on the sample's initial state, i.e., the starting temperature of FSC scan was also observed. We discuss implications of these results for contemporary models of non-equilibrium relaxation in glasses and supercooled liquids.

¹Supported by National Science Foundation grant 1012692.

11:51AM B53.00004 Fluctuating Relaxation Times in Glass-forming Liquids, GCINA A. MAVIMBELA, HORACIO E. CASTILLO, Department of Physics and Astronomy, Ohio University, Athens OH, AZITA PARSAEIAN, Materials Research Center, Northwestern University, Evanston IL — The presence of fluctuating local relaxation times, $\tau(\vec{r}, t)$ has been used for some time as a conceptual tool to describe dynamical heterogeneities [?]. Here we report on a new method for determining the local phase field, $\phi(\vec{r}, t) \equiv \int^t \frac{dt'}{\tau(\vec{r}, t')}$ from snapshots $\{\vec{r}(t_i)\}_{i=1\dots M}$ of the positions of the particles in a system, and we apply it to extract $\phi(\vec{r}, t)$ from simulations of glass forming models. By studying how the phase field depends on the number of snapshots, we find that it is a well defined quantity. By studying fluctuations of the phase field, we find that they describe heterogeneities well at long distance scales. We also determine how the stretching exponent β depends on the coarse graining volume, in order to test the hypothesis that relaxation in small regions is exponential and it only becomes non-exponential when considering large regions of the system.

[1] M. D. Ediger, 2000 Annu. Rev. Phys. Chem. **51** 99

12:03PM B53.00005 Mapping dynamical heterogeneity in structural glasses to correlated fluctuations of the time variables, KARINA E. AVILA, HORACIO E. CASTILLO, Ohio University, AZITA PARSAEIAN, Northwestern University — Dynamical heterogeneity is believed to play an important role in the dynamical behavior of slowly relaxing disordered materials. In this work, we test one hypothesis for its origin, namely that it emerges from soft (Goldstone) modes associated with a broken continuous symmetry under time reparametrizations. We do this by constructing coarse grained observables and decomposing the fluctuations of these observables into transverse components, which are associated with the postulated time-fluctuation soft modes, and a longitudinal component, which is unrelated to them. We perform our test on data obtained in simulations of four models of structural glasses. We find that as temperature is lowered and timescales are increased, the time reparametrization fluctuations become increasingly dominant. In particular, the ratio between the strengths of the transverse fluctuations and the longitudinal fluctuations grows as a function of the dynamical susceptibility χ_4 , which represents the strength of the dynamical heterogeneity; and the correlation volumes for the transverse fluctuations are approximately proportional to those for the dynamical heterogeneity, while the correlation volumes for the longitudinal fluctuations remain small and approximately constant.

12:15PM B53.00006 High Pressure Brillouin Scattering in the Fragile Glass Former Cumene¹, TIM RANSOM, WILLIAM OLIVER, University of Arkansas — In recent years full-spectrum analysis in light-scattering has been utilized to explore the liquid-glass transition at variable temperature and ambient pressure. In this study we present temperature- and pressure-dependent Brillouin scattering results for the fragile glass-former cumene. Both equal-angle forward scattering and depolarized backscattering geometries are used, and high pressures are attained by the use of a diamond anvil cell mounted in a custom temperature-controlled housing. Opening up the variable pressure regime to full-spectrum analysis will allow more stringent tests of mode-coupling theory as well as greater insight into the behavior of glass-forming systems.

¹We gratefully acknowledge support from NSF under grant NO.: DMR-0552944

12:27PM B53.00007 Molecular modeling of ultra-stable vapor deposited glasses, SADANAND SINGH, DEVIN AVERETT, CHI-CHENG CHIU, JUAN J. DE PABLO, University of Wisconsin-Madison — Recent studies have shown that physical vapor deposition can be used to prepare glasses of small organic molecules with remarkably high kinetic stability and low enthalpy, particularly when compared to ordinary glasses prepared by cooling the supercooled liquid. The thermophysical properties of these new ultra-stable glasses are equivalent to those of common glasses after thousands of years of aging. However, experimental studies have so far been limited to relatively few types of molecules. We propose a molecular modeling scheme to prepare stable glasses that mimics the experimental procedure of vapor deposition. For simple disaccharides, such as trehalose, the thermophysical properties of our simulated glasses are consistent with those measured experimentally. We also prepare stable glasses of trehalose and glycerol mixtures, which are of interest for their use in stabilization of biomolecules in the glass state. Results for model binary Lennard-Jones glasses, which have been studied extensively in the literature, are also discussed. We find that the most stable glasses formed by vapor deposition are equivalent to ordinary glasses formed by cooling at a rate approximately 10 orders of magnitude slower than those accessible by ordinary cooling methods.

12:39PM B53.00008 Dynamic heterogeneity above and below the mode-coupling temperature

, ELIJAH FLENNER, GRZEGORZ SZAMEL, Chemistry Department, Colorado State University — We study the temperature dependence of the spatial extent of the dynamic heterogeneity in a soft sphere system near the so-called mode-coupling temperature T_c . We utilize a recently introduced procedure¹ to calculate the ensemble independent dynamic susceptibility $\chi_4(\tau_\alpha)$ and the dynamic correlation length $\xi(\tau_\alpha)$ at the alpha relaxation time τ_α . Above T_c , we find that $\chi_4(\tau_\alpha) \sim \xi(\tau_\alpha)^3$ and $\xi(\tau_\alpha) \sim \ln(\tau_\alpha)$, which is the same behavior found in a binary hard-sphere system. We track these relationships below T_c to examine the recently reported non-monotonic temperature dependence of dynamic correlations found in the same system². Finally, we examine the relationship between dynamic susceptibilities that can be determined from experiments and the dynamic correlation length $\xi(\tau_\alpha)$.

¹E. Flenner and G. Szamel, Phys. Rev. Lett. **105**, 217801 (2010)

²W. Kob, S. Roland-Vargas and L. Berthier, Nat. Phys. DOI:10.1038/NPHYS2133

12:51PM B53.00009 Fast Scanning Calorimetry studies of glassy and supercooled water¹

, DEEPANJAN BHATTACHARYA, The George Washington University, CANDACE PAYNE, The University of Aberdeen, VLAD SADTCHENKO, The George Washington University — Despite intense efforts, development of a comprehensive system of relationships between various condensed phases of water remains an illusive goal. The lack of consensus on the nature of supercooled and glassy water is due primarily to the lack of kinetic and thermodynamic data at temperatures from 150 to 235 K. Because supercooled water undergoes rapid crystallization near 235 K, application of standard experimental methods is virtually impossible. With the objective of gaining insights into properties of water, we have developed an experimental approach which relies on rapid (1000000 K/s) heating of micro- and mesoscopic aqueous samples prepared by vapor deposition in vacuum at cryogenic temperatures. Due to high heating rates, this Fast Scanning Calorimetry approach, makes it possible to bypass crystallization and to obtain new data on molecular kinetics and thermodynamics in glassy water in previously inaccessible temperature interval. We will report the results of our FSC studies and discuss their impact on fundamental and applied research areas where glassy and supercooled water plays significant role.

¹Supported by National Science Foundation Grant 1012692

1:03PM B53.00010 Volume and structural analysis of super-cooled water under high pressure

, SOLOMON F. DUKI¹, Department of Physics and Astronomy, Rowan University, 201 Mullica Hill Road, Glassboro, NJ 08028-1701, MESFIN TSIGE², Department of Polymer Science, Goodyear Polymer Center 1021, The University of Akron, Akron, OH 44325-3909 — Motivated by recent experimental study of super-cooled water at high pressure [1], we performed atomistic molecular dynamic simulations study on bulk water molecules at isothermal-isobaric ensemble. These simulations are performed at temperatures that range from 40 K to 380 K using two different cooling rates, 10K/ns and 10K/5ns, and pressure that ranges from 1atm to 10000 atm. Our analysis for the variation of the volume of the bulk sample against temperature indicates a downward concave shape for pressures above certain values, as reported in [1]. The same downward concave behavior is observed at high pressure on the mean-squared-displacements (MSD) of the water molecules when the MSD is plotted against time. To get further insight on the effect of the pressure on the sample we have also performed a structural analysis of the sample.

[1] O. Mishima, J. Chem. Phys. **133**, 144503 (2010);

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1:15PM B53.00011 A field theory approach to the dynamics of classical particles

, DAVID MCCOWAN, GENE MAZENKO, University of Chicago — For nearly 30 years, mode-coupling theory (MCT) has been regarded as the *de facto* theoretic description of dense fluids and the transition from the fluid to glassy state. But MCT is limited by its ad hoc construction and lacks a mechanism to institute corrections. We present a new fundamental theory for the kinetics of systems of classical particles which represents a unification of kinetic theory, Brownian motion and field theory. It is developed from first principles via a self-consistent perturbation in terms of an effective two-body potential, and we use this theory to investigate the existence of ergodic-nonergodic (ENE) transitions near the liquid-glass transition. After a brief introduction of the theory, we will address the development of a kinetic equation of the memory function form. The memory function kernel (or self-energy) determined by the theory shares properties with the MCT form, however our theory provides the crucial advantage of well-defined, perturbative corrections.

1:27PM B53.00012 N.Q.R measurements of low energy Chiral structures in powdered glassy

As_2Se_3 , CHRIS NELSON, A.P.S — Experimental and theoretical work on the As-chalcogen glasses have shown that in the glassy state the local cylindrical symmetry associated with the elemental pyramidal unit is preserved. Here we introduce a local paracrystalline model of glassy As_2Se_3 . This model is based on a tight binding calculation of the electric field gradient (EFG) at the core of an As atom located at the apex of the pyramidal structure. This EFG is shown to be hyper sensitive to the bond angles and bond lengths the As atom forms with the chalcogen nearest neighbors, as well as the hybrid angle formed with second neighbor As atoms. A continuous variation of the bonding parameters produces a unique set of these pyramidal units which are shown to fit the NQR data for powdered glassy samples. The best fit to the NQR data indicates that the pyramidal units organize themselves into Chiral structures in the glass. A plot of the electronic energy per molecular site shows that the chiral structures have on average a lower electronic energy than a random configuration.

1:39PM B53.00013 Slow relaxations in glasses: full aging and beyond

, YOSEPH IMRY, The Weizmann Institute of Science, ARIEL AMIR, Harvard University, YUVAL OREG, The Weizmann Institute of Science, STEFANO BORINI, INRIM, Torino — Experiments performed in the last years demonstrated slow relaxations and aging in the conductance of a large variety of materials. Here, we present experimental and theoretical results for conductance relaxation and aging for the case-study example of porous silicon. The relaxations are experimentally observed even at room temperature over time scales of hours, and when a strong electric field is applied for a time t_w , the ensuing relaxation depends on t_w . We derive a theoretical curve and show that all experimental data collapse onto it with a single time scale as a fitting parameter. This time scale is found to be of the order of thousands of seconds at room temperature. The generic theory suggested is not fine-tuned to porous silicon, and thus we believe the results should be universal, and the presented method should be applicable for many other systems manifesting memory and other glassy effects. Reference: Phys. Rev. Lett. **107**, 186407 (2011)

1:51PM B53.00014 Voids and molecuar hydrogen in hydrogenated amorphous silicon

, RAJENDRA TIMILSINA, PARTHAPRATIM BISWAS, The University of Southern Mississippi — Nuclear magnetic resonance (NMR) and Infrared (IR) spectroscopy experiments show that hydrogen microstructure consists of clustered and diluted hydrogen atoms as well as voids and hydrogen molecules in hydrogenated amorphous silicon. Several theoretical studies have also attempted that whether the microstructure incorporates voids and hydrogen molecules or not, by introducing hydrogen atoms within artificially created cavities, after relaxing the models of hydrogenated amorphous silicon. However, no theoretical study, up until now, has conclusively demonstrated that the voids and molecular hydrogen are built-in features of the microstructure. We generate several realistic models of hydrogenated amorphous silicon at different hydrogen concentrations by developing an information-based inverse method. The models not only satisfy structural and electronic properties but also provide correct NMR line spectra as compare to NMR experiments. The microstructure at high (>15%) hydrogen concentration shows the presence of voids and some hydrogen molecules within the voids. The voids with molecular hydrogen are built-in configurations of the microstructure because they evolve themselves while relaxing the models via the first-principles density functional method.

2:03PM B53.00015 Structural and microscopic relaxations in glycerol: an IXS study, ALESSANDRO CUNSOLO, Brookhaven National Laboratory — We present an Inelastic X Ray Scattering study of the THz dynamics of room temperature glycerol at pressures spanning the 0.66-3 Kbar range. We propose a comparison with ultrasound absorption results available in literature, which leads to infer the presence of two distinct relaxation phenomena, a slow and a fast one. Although the former relaxation has been thoroughly studied in glycerol by lower frequency spectroscopic techniques, no experimental evidences of the latter were so far reported in literature. A line-shape modeling based upon the memory function formalism allows us to observe that the characteristic timescale of the fast relaxation ranges in the sub-picosecond, tends to decrease with increasing the wave-vector and is rather insensitive to pressure changes. More in general, the observed phenomenology definitely reveals the microscopic, single particle, nature of this additional relaxation process.

Monday, February 27, 2012 11:15AM - 2:15PM —
Session B54 GSNP: Focus Session: Complex and co-evolving networks - Modeling Social and Biological Networks 152

11:15AM B54.00001 Human travel and time spent at destination: impact on the epidemic invasion dynamics, CHIARA POLETTI, MICHELE TIZZONI, ISI Foundation, Turin, Italy, VITTORIA COLIZZA, INSERM and Univ Pierre et Marie Curie, UMR-S 707, Paris, France — Human mobility has a strong impact on the spatial spread of infectious diseases. Analyses of metapopulation models, that consider the epidemic spreading on a network of populations, show that topological and traffic fluctuations favor the global epidemic invasion. These studies consider markovian mobility (i.e. the memory of the origin of traveling individuals is lost) or non-markovian mobility with homogeneous timescales (i.e. individuals travel to a destination and come back with a homogenous rate). However, the time spent at destination is found to exhibit wide fluctuations. Such varying length of stay crucially affects the mixing among individuals and hence the disease transmission dynamics. In order to explore this aspect, we present a modeling framework that, by using a time-scale separation technique, allows analyzing the behavior of spreading processes on a complex metapopulation network with non-markovian mobility characterized by heterogeneously distributed timescales. Analytical and numerical results show how the degree of heterogeneity of the length of stay is able, alone, to drive a phase transition between local outbreak and global invasion. This highlights the importance of the interplay between mobility and disease timescales in the propagation of an epidemic.

11:27AM B54.00002 Effect of Spatial-Dependent Utility on Social Group Domination, NATHANIEL RODRIGUEZ, ANDREW MEYERTHOLEN, University of Redlands — The mathematical modeling of social group competition has garnered much attention. We consider a model originated by Abrams and Strogatz [Nature 424, 900 (2003)] that predicts the extinction of one of two social groups. This model assigns a utility to each social group, which is constant over the entire society. We find by allowing this utility to vary over a society, through the introduction of a network or spatial dependence, this model may result in the coexistence of the two social groups.

11:39AM B54.00003 Evolution of opinions on social networks in the presence of competing committed groups, SAMEET SREENIVASAN, Dept. of Computer Science, Dept. of Physics, Rensselaer Polytechnic Institute, JIERUI XIE, BOLESŁAW SZYMANSKI, Dept. of Computer Science, Rensselaer Polytechnic Institute, JEFF EMENHEISER, MATT KIRBY, GYORGY KORNISS, Dept. of Physics, Rensselaer Polytechnic Institute — Using a model of pairwise social influence, the *binary agreement* model (Xie et. al, Phys. Rev. E 84, 011130 (2011)), we study how the presence of two groups of individuals committed to competing opinions, affect the steady-state opinion of influencable individuals on a social network. We assume that two groups committed to distinct opinions A and B , and constituting fractions p_A , p_B of the total population respectively, are present in the network. We show using mean-field theory that the phase diagram of this system in parameter space (p_A, p_B) consists of two regions, one where two stable steady-states coexist, and the remaining where only a single stable steady-state exists. For finite networks (complete graphs, Erdős-Rényi networks and Barabási-Albert networks), these two regions are separated by two first order transition lines which terminate and meet tangentially at $p_A = p_B \approx 0.1623$, which constitutes a second-order transition point. Finally, we quantify how the exponentially large switching times between steady states in the co-existence region depend on the distance from the second-order transition point for equal committed fractions.

11:51AM B54.00004 Strategy of Competition between Two Groups based on an Inflexible Contrarian Opinion Model, QIAN LI, Boston University, LIDIA BRAUNSTEIN, Universidat Nacional de Mar del Plate-CONICET, SHLOMO HAVLIN, Bar Ilan University, GENE STANLEY, Boston University — We introduce an inflexible contrarian opinion (ICO) model in which a fraction p of inflexible contrarians within a group holds a strong opinion opposite to the opinion held by the rest of the group. At the initial stage, stable clusters of two opinions, A and B exist. Then we introduce inflexible contrarians which hold a strong B opinion into the opinion A group. Through their interactions, the inflexible contrarians are able to decrease the size of the largest A opinion cluster, and even destroy it. We see this kind of method in operation, when companies send free new products to potential customers in order to convince them to adopt their product and influence others to buy it. We study the ICO model, using two different strategies, on both ER and SF networks. In strategy I, the inflexible contrarians are positioned at random. In strategy II, the inflexible contrarians are chosen to be the highest degrees nodes. We find that for both strategies the size of the largest A cluster decreases to zero as p increases as in a phase transition. At a critical threshold value p_c the system undergoes a second-order phase transition that belongs to the same universality class of mean field percolation. We find that even for an ER type model, strategy II is significantly more effective.

12:03PM B54.00005 Consensus in evolving networks of mobile agents, ANDREA BARONCHELLI, Universitat Politecnica de Catalunya, ALBERT DÍAZ-GUILERA, Universitat de Barcelona — Populations of mobile and communicating agents describe a vast array of technological and natural systems, ranging from sensor networks to animal groups. Here, we investigate how a group-level agreement may emerge in the continuously evolving networks defined by the local interactions of the moving individuals. We adopt a general scheme of motion in two dimensions and we let the individuals interact through the minimal naming game, a prototypical scheme to investigate social consensus. We distinguish different regimes of convergence determined by the emission range of the agents and by their mobility, and we identify the corresponding scaling behaviors of the consensus time. In the same way, we rationalize also the behavior of the maximum memory used during the convergence process, which determines the minimum cognitive/storage capacity needed by the individuals. Overall, we believe that the simple and general model presented in this talk can represent a helpful reference for a better understanding of the behavior of populations of mobile agents.

12:15PM B54.00006 Epidemic and information co-spreading in adaptive social networks, YUNHAN LONG, The College of William and Mary, THILO GROSS COLLABORATION, LEAH B. SHAW TEAM — We model simultaneous evolution of an epidemic and information about the epidemic on an adaptive social network. The classical Susceptible-Infectious-Susceptible (SIS) model is extended. Susceptible and infectious nodes are each divided into informed and uninformed types. Informed nodes affect the network structure by rewiring their network connections adaptively to avoid disease exposure. The impacts of mass media information and communication on the disease spreading and network structure are explored, and stochastic simulations are compared with a moment closure approximation. When the rewiring rate is high, the infection and information levels of the population show periodic oscillations for certain ranges of contact rate, and the moment closure approximation predicts similar dynamics. The epidemic threshold in the presence of rewiring and information is considered. Our results indicate that information can play a significant role in minimizing disease spread.

12:27PM B54.00007 Asymptotically inspired moment-closure approximation for adaptive networks, MAXIM SHKARAYEV, LEAH SHAW, College of William and Mary — Adaptive social networks, in which nodes and network structure co-evolve, are often described using a mean-field system of equations for the density of node and link types. These equations constitute an open system due to dependence on higher order topological structures. We propose a moment-closure approximation based on the analytical description of the system in an asymptotic regime. We apply the proposed approach to two examples of adaptive networks: recruitment to a cause model and epidemic spread model. We show a good agreement between the improved mean-field prediction and simulations of the full network system.

12:39PM B54.00008 Epidemics on Interacting Networks, MARK DICKISON, Boston University, SHLOMO HAVLIN, Bar-Ilan University, H.E. STANLEY, Boston University — Epidemic spreading is of great importance in public health, as well as in related fields such as infrastructure. While complex network models have been used with great success to analyze epidemic behavior on single networks, the reality is that our world is made up of a system of interacting networks that do not necessarily share common characteristics. I introduce a model for constructing interacting networks and show that the phase transition depends on the parameters κ_T , κ_A and κ_B , where $\kappa_T = \langle k^2 \rangle / \langle k \rangle$ over the nodes in both networks, including internetwork links, and κ_A and κ_B are over the networks considered individually, with no internetwork links. For strongly interacting networks ($\kappa_T > \kappa_A$ and κ_B), there exists only one phase transition, between a disease-free phase and an epidemic phase across both networks. For weakly interacting networks ($\kappa_T < \kappa_A$ or κ_B), a third, “mixed,” phase exists, where the disease enters an epidemic on one network alone. The analytic predictions are confirmed by Monte-Carlo simulations.

12:51PM B54.00009 Epidemic spreading on interacting networks with preferred degrees¹, SHIVAKUMAR JOLAD, R.K.P. ZIA, B. SCHMITTMANN, Virginia Tech — We discuss the SIS contact process on a network of two interacting communities, each with its own preferred degree of connections. Postulating various rules for an individuals to form intra-community and inter-community links, we find novel stationary (active) states, in addition to the expected absorbing states. The dynamics of infected individuals in the two communities can be quite different. Using Monte Carlo techniques, we explore the effects on both the network structure and the contact process due to different types of interactions between the communities. We will also present a mean field analysis of contact processes on a generic M interacting communities and compare these results with the simulation data.

¹Supported in part by NSF DMR- 1005417 and ICTAS- Virginia Tech.

1:03PM B54.00010 Scaling theory of human dynamics and network science, CHAOMING SONG, DASHUN WANG, ALBERT-LASZLO BARABASI, Center for Complex Network Research, Northeastern University — The increasing availability of large-scale real data has fueled simultaneous advances in network theory, aiming to characterize the scaling of complex networks, and human dynamics, capturing the temporal characteristics of human activity patterns. Yet, these two areas remain disjoint, with their separate scaling laws and modeling framework. Here we show that the exponents characterizing the degree and link weight distribution of the underlying social network can be expressed in terms of the dynamical exponents characterizing human activity patterns, establishing the first formal link between the two areas.

1:15PM B54.00011 Network model explains why cancer cells use inefficient pathway to produce energy, JOO SANG LEE, Department of Physics and Astronomy, Northwestern University, JOHN MARKO, Department of Molecular Biosciences, Northwestern University, ADILSON MOTTER, Department of Physics and Astronomy, Northwestern University — The Warburg effect—the use of the (energetically inefficient) fermentative pathway as opposed to (energetically efficient) respiration even in the presence of oxygen—is a common property of cancer metabolism. Here, we propose that the Warburg effect is in fact a consequence of a trade-off between the benefit of rapid growth and the cost for protein synthesis. Using genome-scale metabolic networks, we have modeled the cellular resources for protein synthesis as a growth defect that increases with enzyme concentration. Based on our model, we demonstrate that the cost of protein production during rapid growth drives the cell to rely on fermentation to produce ATP. We also identify an intimate link between extensive fermentation and rapid biosynthesis. Our findings emphasize the importance of protein synthesis as a limiting factor on cell proliferation and provide a novel mathematical framework to analyze cancer metabolism.

1:27PM B54.00012 Physiological Networks: towards systems physiology¹, RONNY P. BARTSCH, Harvard Medical School and Division of Sleep Medicine, Brigham and Womens Hospital, Boston, MA 02115, USA, AMIR BASHAN, Department of Physics, Bar-Ilan University, Ramat-Gan, Israel, JAN W. KANTELHARDT, Institute of Physics, Martin-Luther-Universitaet Halle-Wittenberg, Halle (Saale), Germany, SHLOMO HAVLIN, Department of Physics, Bar-Ilan University, Ramat-Gan, Israel, PLAMEN CH. IVANOV, Harvard Medical School and Division of Sleep Medicine, Brigham and Womens Hospital, Boston, MA 02115, USA — The human organism is an integrated network where complex physiologic systems, each with its own regulatory mechanisms, continuously interact, and where failure of one system can trigger a breakdown of the entire network. Identifying and quantifying dynamical networks of diverse systems with different types of interactions is a challenge. Here, we develop a framework to probe interactions among diverse systems, and we identify a physiologic network. We find that each physiologic state is characterized by a specific network structure, demonstrating a robust interplay between network topology and function. Across physiologic states the network undergoes topological transitions associated with fast reorganization of physiologic interactions on time scales of a few minutes, indicating high network flexibility in response to perturbations. The proposed system-wide integrative approach may facilitate new dimensions to the field of systems physiology.

¹Supported by: NIH Grant 1R01HL098437-01A1, Office of Naval Research Grant 000141010078, BWH BRI Fund, US-Israel BSF Grant 2008137 and the German Academic Exchange Service (DAAD).

1:39PM B54.00013 Detecting and evaluating communities in complex human and biological networks, GREG MORRISON, L. MAHADEVAN, Harvard University School of Engineering and Applied Sciences — We develop a simple method for detecting the community structure in a network can by utilizing a measure of closeness between nodes. This approach readily leads to a method of coarse graining the network, which allows the detection of the natural hierarchy (or hierarchies) of community structure without appealing to an unknown resolution parameter. The closeness measure can also be used to evaluate the robustness of an individual node's assignment to its community (rather than evaluating only the quality of the global structure). Each of these methods in community detection and evaluation are illustrated using a variety of real world networks of either biological or sociological importance and illustrate the power and flexibility of the approach.

1:51PM B54.00014 Small-world organization of self-similar modules in functional brain networks, MARIANO SIGMAN, Buenos Aires University, LAZAROS GALLOS, HERNAN MAKSE, City College of New York — The modular organization of the brain implies the parallel nature of brain computations. These modules have to remain functionally independent, but at the same time they need to be sufficiently connected to guarantee the unitary nature of brain perception. Small-world architectures have been suggested as probable structures explaining this behavior. However, there is intrinsic tension between shortcuts generating small-worlds and the persistence of modularity. In this talk, we study correlations between the activity in different brain areas. We suggest that the functional brain network formed by the percolation of strong links is highly modular. Contrary to the common view, modules are self-similar and therefore are very far from being small-world. Incorporating the weak ties to the network converts it into a small-world preserving an underlying backbone of well-defined modules. Weak ties are shown to follow a pattern that maximizes information transfer with minimal wiring costs. This architecture is reminiscent of the concept of weak-ties strength in social networks and provides a natural solution to the puzzle of efficient information flow in the highly modular structure of the brain.

2:03PM B54.00015 Unraveling the rules of evolution in the yeast protein-protein interaction network, YULIANG JIN, HERNAN MAKSE, Levich Institute and Physics Department, the City College of New York, THOMAS WEINMAIER, DMITRIJ TURAEV, THOMAS RATTEL, Department of Computational Systems Biology, University of Vienna — A question of fundamental importance is to understand the dynamical principles according to which biological networks have acquired their topological structures and functional modules. Here, we perform an empirical study of the yeast protein-protein interactions (PPI), combined with theoretical modeling of the genomic duplication-divergence processes. Our duplication-divergence model agrees with experimental data, and provides a novel approach to reconstruct ancestral PPI networks. Following the phylogenetic tree, our analysis unravels that the ancient networks evolve into the present day yeast network by a multiplicative growth. The rule of multiplicative growth demonstrates the relationship between the topological exponents and the evolution growth rates of interactions. An important consequence of this evolutionary principle is the emergence of self-similar modular structure, which is confirmed by the analysis of functional modules of proteins.

2:00PM - 2:00PM —
Session C1 Poster Session I (2:00-5:00PM) Exhibit Hall C

C1.00001 POLYMERS AND SOFT MATTER PHYSICS —

C1.00002 Partition function zeros and phase transitions of a square-well polymer¹, PYIE-PHYO AUNG, Hiram College, MARK TAYLOR, Department of Physics, Hiram College, OH, 44234 — The zeros of the canonical partition functions for flexible square-well polymer chains have been computed for chains up to length 256 for a range of square-well diameters. We have previously shown that such chain molecules can undergo a coil-globule and globule-crystal transition as well as a direct coil-crystal transition [1]. Here we show that each of these transitions has a well-defined signature in the complex-plane map of the partition function zeros. The freezing transitions are characterized by nearly circular rings of uniformly spaced roots, indicative of a discontinuous transition. The collapse transition is signaled by the coalescence of roots onto an elliptical horse-shoe segment pinching down towards the positive real axis. For sufficiently small square-well diameter the elliptical collapse ring merges with the circular freezing ring yielding the direct coil-crystal transition. The root density of all rings increases with increasing chain length and the leading roots move towards the positive real axis, implying a divergence of the specific heat in the thermodynamic limit (as originally proposed by Yang and Lee).

[1] M.P. Taylor, W. Paul, and K. Binder, J. Chem. Phys. **131**, 114907 (2009).

¹Funded by NSF

C1.00003 Modeling Amphiphilic Solutes in a Jagla Solvent, ZHIQIANG SU, Center for Polymer Studies and Dept of Physics, Boston University, SERGEY V. BULDYREV, Dept of Physics, Yeshiva University, PABLO G. DEBENEDETTI, Dept of Chemical and Biological Engineering, Princeton University, PETER J. ROSSKY, Dept of Chemistry and Biochemistry, College of Natural Science, The University of Texas at Austin, H.EUGENE STANLEY, Center for Polymer Studies and Dept of Physics, Boston University — Methanol is an amphiphilic solute whose aqueous solutions exhibit distinctive physical properties. The volume change upon mixing, for example, is negative across the entire composition range, indicating strong association. We explore the corresponding behavior of a Jagla solvent, which has been previously shown to exhibit many of the anomalous properties of water. We consider two models of an amphiphilic solute: (i) a “dimer” model, which consists of one hydrophobic hard sphere linked to a Jagla particle with a permanent bond, and (ii) a “monomer” model, which is a limiting case of the dimer, formed by concentrically overlapping a hard sphere and a Jagla particle. Using discrete molecular dynamics, we calculate the thermodynamic properties of the resulting solutions. We systematically vary the set of parameters of the dimer and monomer models and find that one can readily reproduce the experimental behavior of the excess volume of the methanol-water system as a function of methanol volume fraction. We compare the pressure and temperature dependence of the excess volume and the excess enthalpy of both models with experimental data on methanol-water solutions and find qualitative agreement in most cases. We also investigate the solute effect on the temperature of maximum density and find that the effect of concentration is orders of magnitude stronger than measured experimentally.

C1.00004 Localized entrapment of green fluorescent protein within nanostructured polymer films¹, JOHN ANKNER, Oak Ridge National Laboratory, VERONIKA KOZLOVSKAYA, University of Alabama at Birmingham, HUGH O'NEILL, QIU ZHANG, Oak Ridge National Laboratory, EUGENIA KHARLAMPIEVA, University of Alabama at Birmingham — Protein entrapment within ultrathin polymer films is of interest for applications in biosensing, drug delivery, and bioconversion, but controlling protein distribution within the films is difficult. We report on nanostructured protein/polyelectrolyte (PE) materials obtained through incorporation of green fluorescent protein (GFP) within poly(styrene sulfonate)/poly(allylamine hydrochloride) multilayer films assembled via the spin-assisted layer-by-layer method. By using deuterated GFP as a marker for neutron scattering contrast we have inferred the architecture of the films in both normal and lateral directions. We find that films assembled with a single GFP layer exhibit a strong localization of the GFP without intermixing into the PE matrix. The GFP volume fraction approaches the monolayer density of close-packed randomly oriented GFP molecules. However, intermixing of the GFP with the PE matrix occurs in multiple-GFP layer films. Our results yield new insight into the organization of immobilized proteins within polyelectrolyte matrices and open opportunities for fabrication of protein-containing films with well-organized structure and controllable function, a crucial requirement for advanced sensing applications.

¹Supported by AFOSR FA9550-09-1-0162 and FA9550-11-1-0233 (V. Tsukruk, Georgia Tech); at ORNL, US DOE DE-AC05-00OR22725 and ORNL CSMB project ERKP291 US DOE OBER.

C1.00005 Time-resolved WAXD/SAXS Characterization on the Crystallization of Silica Filled HDPE Nanocomposite¹, XIAOWEI LI, CHRISTIAN BURGER, YIMIN MAO, BENJAMIN HSIAO, Stony Brook University — The isothermal crystallization behavior of high density polyethylene/silica (HDPE-SiO₂) with different SiO₂ loading of 2% and 5%, along with the pure HDPE sample was studied by using the time-resolved wide angle X-ray diffraction (WAXD) and small angle X-ray scattering (SAXS) techniques. For isothermal crystallization at 120 °C, WAXD profiles show HDPE-Si₂% has the highest ending crystallinity index, while HDPE-Si₅% has the lowest value. Avrami exponent of pure HDPE is about 3.9, while HDPE-Si₂% has a value of 3.2 which is typically heterogeneous nucleation behavior due to the addition of silica in HDPE. SAXS patterns show that the silica inside HDPE has mass fractal structure. The mass fractal dimension is determined by using the fitting method and the value is less than 3 for all HDPE-SiO₂ samples. The structure of HDPE-SiO₂ is sketched based on the obtained results.

¹We thank National Science Foundation for financial support and Andy H. Tsou from ExxonMobil company for providing nanocomposite samples.

C1.00006 The CHX Beamline at NSLS-II: a Tool to probe Structure and Dynamics in Soft-Condensed Matter, ANDREI FLUERASU¹, LUTZ WIEGART², Brookhaven National Laboratory — The Coherent Hard X-ray (CHX) beamline currently under construction at NSLS-II (Brookhaven National Laboratory) will serve as an optimized tool for the study of structure and dynamics in soft condensed matter. The unprecedented coherent flux will enable the study of dynamics in soft matter systems down to microsecond time scales via X-ray Photon Correlation Spectroscopy (XPCS). The available scattering geometries such as (GI)SAXS and (GI)WAXS can be used in a simultaneous fashion to collect static and dynamic scattering information on length scales ranging from supramolecular assemblies to atomic distances.

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C1.00007 Ionic conductivity of imidazole-functionalized liquid crystal mesogens, SUPACHAREE ROD-DECHA, MITCHELL ANTHAMATTEN, University of Rochester — Imidazole has been investigated as a novel anhydrous proton conducting functional group that could enable higher temperature operation ($> 120\text{ }^{\circ}\text{C}$) of polymer electrolyte fuel cells. Its amphoteric behavior can support Grotthuss-like proton transport; however molecular mobility and a high concentration of imidazole groups are needed to achieve high ionic conductivity. Our hypothesis is that liquid crystal ordering, particularly in layered smectic phase, can facilitate formation of 2D proton transport and promote proton conductivity. We have designed and synthesized two imidazole-terminated liquid crystal mesogens, and the ionic conductivities in the liquid crystalline and isotropic states have been measured. Here we report on synthesis and characterization of diacylhydrazine liquid crystals bearing imidazole terminal groups. The proton conductivity of products is compared to pure liquid imidazole and to liquid crystal mesogens without imidazole groups.

C1.00008 New Soft Matter Soft X-ray Scattering Facility and the Advanced Light Source with Real Time Analysis, ELIOT GANN, North Carolina State University, ANTHONY YOUNG, Lawrence Berkeley National Laboratory, BRIAN COLLINS, HONGPING YAN, North Carolina State University, HOWARD PADMORE, Lawrence Berkeley National Laboratory, HARALD ADE, North Carolina State University, ALEX HEXEMER, CHENG WANG, Lawrence Berkeley National Laboratory — We present the development and first experiments at a new user scattering facility at the Advanced Light Source at Lawrence Berkeley National Laboratory designed to elucidate the structure of polymer thin films, including a number of systems important for understanding organic devices. These experiments utilize enhanced contrast mechanisms available due to resonance effects to gain sensitivity to morphology which other probes and harder X-ray beams cannot probe. We present the development of new characterization and calibration techniques as well as procedures to mitigate the unique problems that come with scattering in this energy range. These allow us to obtain quantitative scattering profiles and thus ensemble morphological information of these devices. In addition, we present a live analysis package which does initial data reduction in real time while scattering data is being collected.

C1.00009 Phase behavior of silica-polypeptide colloidal particles immersed in liquid crystal forming mesogens, MELISSA COLLINS, ERICK SOTO-CANTU, PAUL RUSSO, Louisiana State University — Silica-polypeptide composite particles (Silica-PCPs) are core-shell colloids. The size and function of the silica core are easily controlled. Established synthesis methods ensure uniformly sized cores and provide the ability to have magnetic or fluorescent inclusions within them. The interactions of the polypeptides in the shell with those unbound in solution can be explored by small/wide angle x-ray scattering (SAXS/WAXS) and polarized optical microscopy (POM) to identify the concentration at which the solution changes from isotropic to ordered. Silica-PCPs/untethered polymer/solvent systems are studied to determine the phase behavior in a non-aqueous environment, free from complications arising from electrostatic effects. The tendency of poly(γ -benzyl-L-glutamate) to form liquid crystalline phases on its own is affected by the presence of Silica-PCPs.

C1.00010 ABSTRACT WITHDRAWN —

C1.00011 A Novel 3D-Lattice Model of Fibrillar Polymeric Material, C. BRAD BENNETT, JAMES KRUCZEK, D.A. RABSON, W. GARRETT MATTHEWS, SAGAR A. PANDIT, University of South Florida — To elucidate a possible mechanism for simple material properties of fibrillar polymeric bulk material containing cross-links between constituent components, we introduce a 3D-lattice model that depends on cross-link number density (ρ) and the ratio (χ) of cross-link bond strength to thermal energy. The model predicts a phase transition in specific heat capacity occurring for χ between approximately 0.5 and 1.5, dependent on ρ . We present evidence that the properties of the represented phases are consistent with those of a solid phase and a liquid phase. These results indicate that variations in ρ or χ alone may provide a convenient basis for Nature to provide a range of material properties with limited resources.

C1.00012 PolyGraph: a Polymer Visualization system¹, ASHOK CUTKOSKY*, NAJEEB TARAZI*, EREZ LIEBERMAN AIDEN, Harvard University — Rapid advances in computational hardware and parallelization have made complex simulations of large polymers increasingly ubiquitous. However, visualizing such simulations remains a challenge. Here we present PolyGraph, a Blender-powered visualization system for complex polymer simulations. As a specific example, we study molecular dynamics simulations of condensing polymers. We illustrate our initial simulation results, suggesting that formation of local beads is an initial step in the condensation process. (This finding is consistent with earlier conjectures about polymer condensation.) PolyGraph makes it possible to create precise and visually appealing clips of polymer simulations. *contributed equally

¹This work is supported by NIH Grants 1P50HG006193-01 (Center for Cell Circuits) and 1DP2OD008540-01 (NIH New Innovator Award).

C1.00013 Confinement of Block Copolymer Nanocomposites within Nanoporous Templates, SEYEDALI MONEMIAN, LASHANDA KORLEY, Department of Macromolecular Science and Engineering, Case Western Reserve University — This research investigates the impact of surface-functionalized nanoparticles (NPs) on self-assembly of confined block copolymer (BCP) systems. Lamellar and cylindrical BCP morphologies were explored with variations in NP diameters and functional groups. The bulk and templated microphase-separated structures were characterized. The addition of addition of NPs resulted in a variety of morphological transitions due to a combination of selective localization of NPs and confinement.

C1.00014 Surface Modification for Controlling the Orientation of Block Copolymers in thin film and in Cylindrical Nanopores¹, XIN-GUAN LIN, FENG-CHENG LIN, SHIH-HUANG TUNG, Institute of Polymer Science and Engineering National Taiwan University, SOFT NANOMATERIALS GROUP TEAM — A series of benzocyclobutene-functionalized random copolymers of styrene and 4-vinylpyridine were synthesized by nitroxide-mediated controlled radical polymerization with BPO and TEMPO. Our research was to use these random copolymers of P(S-r-BCB-r-4VP) to control the orientation of microdomains in block copolymers (BCPs) of poly(styrene-*b*-4-vinylpyridine) (PS-*b*-P4VP) thin films and in cylindrical nanopores of anodized aluminum oxide (AAO) membranes. On P(S-r-BCB-r-4VP)-modified substrate, we found that in some particular compositions of random copolymer, the parallel orientation of the microdomains is switched to be perpendicular in PS-*b*-P4VP thin film. We also introduced P(S-r-BCB-r-4VP) solution into the nanopores of the AAO and nanotubes formed after solvent evaporation and pyrolysis. And then BCPs of PS-*b*-P4VP were drawn into the P(S-r-BCB-r-4VP)-modified nanopores in the melt via capillary action to form P(S-r-BCB-r-4VP) coated nanorods of PS-*b*-P4VP. Similarly, in some particular compositions of random copolymer, we observed that the interactions of the blocks with the walls are not strong or if the interactions are balanced, then the orientation of the microdomains will change from being parallel to being perpendicular to the confining walls.

¹Financial support from National Science Council under Contract NSC 99-2221-E-002-021-MY3.

C1.00015 Fast Fabrication of Hierarchically-Structured Nanocomposites in Thin Films, JOSEPH KAO, PETER BAI, SEONG-JUN JEONG, VIVIAN PENG-WEI CHUANG, TING XU, UC Berkeley — Significant attention has been given to developing bottom-up routes to direct hierarchical assemblies of nanoparticles in thin films for applications such as novel electronics, energy harvesting modules, and photonic materials. It remains challenging to control the self-assembly of the nanocomposites in a short period of time using methods compatible with scalable manufacturing. Here, we report a facile method utilizing solvent vapor annealing to precisely control the morphologies of nanocomposite thin films (PS-*b*-P4VP(PDP)_x with nanoparticles) in the time scale of minutes. By controlling the solvent vapor pressure during the annealing process, the orientations of the microdomains and the nanoparticles can be tailored. Long range-ordered lateral morphologies of the nanocomposites can be obtained. In-situ GISAXS experiments show that the fast assembly process may be attributed to the nature of the supramolecules. The rate of solvent evaporation has been identified as a critical factor in controlling the final morphologies of the nanocomposites.

C1.00016 Fabrication of Three-Dimensional Bilayered Nanostructures via Block Copolymers¹, SANGHOON WOO, Korea University, SUMI LEE, EUN AE KWAK, Samsung Electronics, HYUNJUNG JUNG, Korea University, FRANK LEIBFARTH, CRAIG HAWKER, University of California, Santa Barbara, JUNE HU, DU YEOL RYU, Yonsei University, JOONA BANG, Korea University — The self-assembly of block copolymers (BCPs) has been received wide attention because of their great potentials in various advanced lithographic applications. For specific applications, one of the most significant is controlling the orientation of the microdomains. In this study, we synthesized ketene-based cross-linkable cylinder forming BCPs, PMMA-*b*-P(S-r-ketene), in which 3.0 mol

¹Samsung Electronics

C1.00017 Fabrication of square arrays of inverted pyramids using ABC triblock terpolymer, HONG KYOON CHOI, CAROLINE ROSS, HANG YU, CARL THOMPSON, Department of Materials Science and Engineering, MIT — Nanolithography using Self-assembly of block copolymer thin film is promising technique to fabricate a wide range of useful devices. Previously, we have reported that we could achieve square array which is one of most important device geometry by using Polyisoprene-*b*-polystyrene-*b*-polyferrocenylsilane triblock terpolymer. In this presentation, self-assembled PI-*b*-PS-*b*-PFS triblock terpolymer thin film was used as an etching mask to fabricate array of silicon inverted pyramids. Solvent annealed thin film PI-*b*-PS-*b*-PFS triblock terpolymer forms a square array of PFS and PI alternation cylinders in a PS matrix with a period of 44 nm. When this square arrayed polymer film immersed into hexane, a good solvent for PI and poor solvent for PS and PFS, an ordered square array of holes was produced by PI phase coming out from its cylindrical post and covering the surface. By using this hole patterned polymer film as an etching mask, KOH anisotropic silicon etching produce square array of inverted pyramids of period 44nm etched into silicon substrate. These square arrays of inverted pyramids are used to template the dewetting of metal film to form metal nanoparticle arrays. Produced ordered metal nanoparticles can be used as magnetic memory arrays and also useful as catalysts for nanowires/nanotube growth.

C1.00018 Hierarchical buckling of block copolymer thin films on PDMS substrates, DOKYEONG KWON, HYO SEON SUH, KOOKHEON CHAR, Seoul National University, THE NATIONAL CREATIVE RESEARCH INITIATIVE CENTER FOR INTELLIGENT HYBRIDS TEAM — Buckling of thin films on low modulus substrates such as polydimethylsiloxane (PDMS) is the well-known phenomenon in buckling instability originating from moduli mismatch between the substrate and a top film. Recently, many studies on the microstructure created by the buckling have been reported but most of the work has typically employed either metal or semiconductor thin films and few utilized the block copolymers (BCP) as the covering films. Here, we present the buckling of oriented BCP thin films, placed by a novel off-set printing, on PDMS substrates. Buckling instability was induced by either swelling of the PDMS substrate with chemical vapor or the mechanical strain, resulting in the hierarchical structure of BCP microdomains. Due to the buckling of the BCP thin films, we observed the structural change or transitions of the films depending on the alignment of BCP domains with respect to the buckled direction of the substrates.

C1.00019 Surface Properties of Bottlebrush Copolymer Thin Films¹, XIANYU LI, STACY PRUKOP, RAFAEL VERDUZCO, Rice University — Bottlebrush polymers are novel macromolecules with polymeric side-chains. Due to their large size and densely crowded side-chains, bottlebrush polymers are candidates for a number of potential applications, including rheological modifiers, drug-delivery vehicles, and polymeric photonics. However, the structural details of bottlebrush polymers in solution and in the bulk are poorly understood. For example, while the overall size of bottlebrush polymers has been measured, the polymer stiffness and side-chain conformation have not been quantified. Here, we present a study of the surface properties of well-defined bottlebrush polymer and copolymer thin films. Surface property measurements provide a method to investigate polymeric side-chain conformation and flexibility. Bottlebrush polymers with mixed and copolymer side-chains are prepared via living ring-opening metathesis polymerization of norbornene-functionalized macromonomers. Contact angle measurements, x-ray photoelectron spectroscopy, and atomic force microscopy measurements on bottlebrush polymer thin films show that polymeric side-chains have significant conformational flexibility and that bottlebrush polymers with mixed and copolymer side-chains can be used to prepare stimuli-responsive surfaces.

¹This work was supported by the Louis Owen Foundation

C1.00020 Self-assembled nanostructures in a cross-linkable block copolymer, CHUNLIN HE, Department of Chemical & Biochemical Engineering, University of Colorado at Boulder, IAN CAMPBELL, University of Colorado at Boulder, MARK STOYKOVICH, Department of Chemical & Biochemical Engineering, University of Colorado at Boulder — The self-assembly of block copolymers in films 50~100 nm thick provides an attractive approach to patterning nanoscale features. Chemical and thermal stability of the morphology in thin films is critical for the generation of robust templates for subsequent fabrication processes, and can be improved by cross-linking the copolymer domains. Atom transfer radical polymerization was used to synthesize PS/PMMA block copolymers with cross-linkable units capable of reacting through an acid-catalyzed mechanism or by photoinitiation with UV exposure. The self-assembly behavior of lamellar-forming block copolymers with or without cross-linkable units were compared in thin films through top-down characterization. We have developed approaches to decouple the self-assembly process from the cross-linking process, and characterized the cross-linking density and reaction rates within the nanostructured domains. The cross-linked nanostructures exhibit enhanced solvent and thermal stability, and have been demonstrated for the fabrication of three-dimensional block copolymer nanostructures in thick films using a layer-by-layer approach.

C1.00021 Tuning the Morphology of Solvent Annealed Thin Films of Polystyrene-b-Polyethylene Oxide with Controlled Saturations of Water and Toluene Vapors, BRIAN C. STAHL, EDWARD J. KRAMER, CRAIG J. HAWKER, University of California, Santa Barbara — Solvent annealing can be used to facilitate the self-assembly of block copolymer thin films and has several advantages over thermal annealing including room-temperature processing, domain orientation control and the ability to anneal polymers not amenable to thermal processing. We have developed a controlled process design for performing solvent annealing that incorporates continuous flows of solvent-saturated carrier gas, multiple simultaneous co-solvents and in-situ metrology. This new method is modular and applicable to a wide range of block copolymer and solvent systems. The control over annealing and quenching conditions afforded by this new technique allows us to reproducibly control the domain orientation and periodicity in thin films of cylinder-forming polystyrene-b-polyethylene oxide (PS-b-PEO) annealed in environments with high saturations of water and toluene vapors without modifying the block copolymer or substrate. By adjusting the humidity of the quenching gas flow we are able to control the orientation of the PEO cylinders, and by adjusting the humidity during annealing we are able to tune the domain spacing of PEO cylinders oriented perpendicular to the substrate.

C1.00022 Laterally confined diblock copolymers, ROBERTA DESSI, MARCO PINNA, ANDREI ZVELINDOVSKY, University of Central Lancashire — With the help of cell dynamics simulation we investigate the self-assembly of cylinder-forming diblock copolymer thin films laterally confined within square and non-square geometries. The size of the confinement affects the ordering of the block copolymer domains and their symmetry. We found hexagonally packed cylinders and square packed cylinders by changing the box size of the system. In particular we performed several simulations to find that if the size of the pattern is comparable with the natural bulk period of the copolymer the packing symmetry changes from hexagonal to square. In this case the ordering induced by the pattern edges becomes dominant allowing the square lattice to be more stable than the hexagonal one.

C1.00023 Self-Assemble Behavior of Polystyrene-tethered Hydrophilic POSS Nanoparticle in Thin Film, I-FAN HSIEH, XINFEI YU, KAN YUE, STEPHEN CHENG, The University of Akron, DEPARTMENT OF POLYMER SCIENCE, THE UNIVERSITY OF AKRON TEAM — Recently, block copolymer thin films are of great interest in their applications of surface patterning. However, due to the restriction of the polymer material properties, the etch contrast between two phases is usually low and the smallest pattern block copolymer can create is around 10 nm. By taking the advantage of the hybrid property of POSS nanoparticle, we can produce the thin film pattern with great etch contrast with only a few nanometers in size. PS-tethered hydrophilic POSS can self assemble to form nano-pattern in both bulk and thin film state. As the PS molecular weight increases, the thin film morphology can transfer from lamella to cylinder then to sphere as block copolymer does. But because of the nature of the POSS particle, we discover a new packing symmetry in the cylinder phase that has not been discovered in block copolymer thin film system. Unlike block copolymer which has higher order-disorder transition temperature in thin film, PS-POSS thin film also shows some unique phase transition behavior during heating, and this transition behavior also affected by the different functional group attached on POSS particles.

C1.00024 Morphology of ABC linear triblock polymer melts: self-consistent-field theoretic simulation approach¹, MOUGE MOHAGHEGHI, BAMIN KHOMAMI, Dept. of Chemical and Biomolecular Eng., University of Tennessee, Knoxville, TN — It is well known that block copolymer morphologies resulting from microphase separation finds wide spread use in many applications, including nanolithographic templates, membranes, and electronic arrays. In this study, we have performed self-consistent field theoretic based simulations to examine the plethora of self-assembled morphologies obtained in symmetric linear ABC Tri-block polymer melts in bulk and confined films. Specifically in bulk systems, the conditions leading to lamellae, tetragonal cylinders, sphere, perforated lamellae, and network morphologies have been elucidated at various volume fractions of middle (B) block. In general, the predicted morphologies are in good agreement with the limited number of published experimental studies. The effect of confinement on the microphase separation is also studied by performing simulations of two neutral parallel walls. Overall, we observe lamellar and cylindrical domains that are oriented parallel to the walls; however, lamellar domains could become perpendicular to the neutral walls when the natural period of lamellae is incommensurate with the film thickness. Our calculations form the basis for understanding the stability of parallel and perpendicular orientations in thin films of ABC tri-block polymeric systems.

¹This work is supported by NSF through funding grant EPS-1004083.

C1.00025 Hierarchical silver concentric ring patterns of block copolymer microdomains for high efficient SERS, DUSIK BAE, JIN KON KIM, Pohang University of Science and Technology — We fabricated the half-onion like microdomains of polystyrene-block-poly(methyl methacrylate) copolymer (PS-b-PMMA) when it was confined within hemi-spherical anodic aluminum oxide (AAO) template. The ring number of the concentric ring patterns was easily controlled by changing the molecular weights of the block copolymers, which was verified by scanning and transmission electron microscopes and atomic force microscope. We also deposited silver with 6nm height selectively on the PS microdomains. A number of silver ring patterns were varied from 5 to 8 depending on the molecule weights of the block copolymer. This silver ring structures showed high surface enhanced Raman scattering (SERS) with a maximum enhancement factor of 10^7 .

C1.00026 Effect of tacticity on the interfacial structural properties of adsorbed polystyrene thin films, YERGOU TATEK, Addis Ababa University, MESFIN TSIGE, The University of Akron — We have carried out atomistic Molecular Dynamics simulations to investigate interfacial structural properties of thin films of polystyrene (PS) adsorbed onto solid substrates. The films are made of PS stereoregular chains, that are, isotactic PS or syndiotactic PS. Three types of surfaces of different phobicity and roughness were considered in the present work: hydroxylated silica, graphite and amorphous silica. The structural properties were studied in terms of side chains, end groups and backbone concentration and orientation in the interfacial regions (substrate/film and film/vacuum). Moreover the effect of temperature was investigated by adsorbing the films at different temperatures, below and above the glass transition temperature. Our results were compared to results obtained previously by our group on the adsorption of films made of atactic polystyrene.

C1.00027 Memory Effects of Multistage Crosslinking and Scission on Stress in Polymer Networks, JOANNE BUDZIEN, Physics and Engineering Department, Frostburg State University — While the independent network model (INM) typically used for polymers is excellent for networks that truly are independent, the model has to be modified for networks that are not independent. Such dependent networks can be the result of scission occurring in strain states where crosslinking also occurs. The overall material retains a memory of the strain/crosslinking/scission history because of the bias in how the crosslinks are introduced. These memory effects mean that the resulting zero-stress state (the shape to which the sample will return at equilibrium) varies depending on the sample preparation history, in contrast to the INM where only the number of crosslinks in each network should matter. In this talk, I will present recent results of molecular dynamics simulations where coarse-grained polymer models undergo sequential crosslinking and scission in multiple strain states. The effects of entanglements will also be considered.

C1.00028 Reduction of Dielectric Hysteresis in Multilayered Film via Nanoconfinement¹, LEI ZHU, MATHEW MACKEY, DONALD SCHUELE, Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, Ohio 44106-7202, LIONEL FLANDIN, LEPMI, UMR 5279, CNRS, Université de Savoie, F-73376 Le Bourget Du Lac Cedex, France, MASON WOLAK, JAMES SHIRK, US Naval Research Laboratory, Washington, DC 20375, USA, ANNE HILTNER, ERIC BAER, Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, Ohio 44106-7202 — Micro-/nano-layer coextrusion was used to fabricate polycarbonate (PC)/poly(vinylidene fluoride) (PVDF) layered films with significantly reduced dielectric losses while maintaining high energy density. The high-field polarization hysteresis was characterized for layered films as a function of PVDF layer thickness (6000 to 10 nm) and composition (10 to 70 vol.% PVDF), and was found to decrease with decreasing layer thickness and PVDF content. To gain a mechanistic understanding of the layer thickness (or nanoconfinement) effect, wide angle X-ray diffraction, polarized Fourier transform infrared spectroscopy, and broadband dielectric spectroscopy were employed. The results revealed that charge migration, instead of dipole flipping, was responsible for the hysteresis in multilayered films.

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C1.00029 Fullerene-based shape amphiphiles towards hierarchical supramolecular assemblies, CHIH-HAO HSU, The University of Akron, CHIEN-LUNG WANG, National Chiao Tung University, HAO-JAN SUN, The University of Akron, YINGFENG TU, Soochow University, STEPHEN CHENG, The University of Akron — Self-assembly is an elegant strategy which is used to create assemblies with tunable properties in nature as well as the artificial supramolecular systems. The self-assembly of [60]fullerene (C60) has drawn an tremendous amount of interest due to the exceptional optical and optoelectronic properties of C60. By constructing hierarchical supramolecular structures of C60 derivatives, the molecular functionality of C60 can be accumulated, amplified, and then transferred to bulk material properties. This research focuses on manipulating the balance of non-covalent interactions among C60 derivatives into molecular alignments in the supramolecular structure. The aliphatic tails and spacers in the C60 derivatives will improve the solubility and provide sufficient mobility for the effective packing of C60s. The differences in shape and intermolecular interaction between C60s and alkyl chains allow these molecules to arrange themselves in microphase-separated mesostructures. The hierarchical structure built up by C60 derivatives can be obtained via the highly-ordered packing of C60 in mesostructures. By adding an additional bisamide group to the molecular structure, the balance of the intermolecular interactions and the spatial packing can be tuned to exhibit supramolecular polymorphism.

C1.00030 Chain Packing and Trajectory of Isotactic Polypropylene α Crystals studied by Solid-State NMR¹, ZHEN LI, YAN CAO, TOSHIKAZU MIYOSHI, STEPHEN CHENG, The University of Akron — Isotactic polypropylene (ipp) is one of the simplest polyolefins and the crystalline structures, have been extensively studied. Ipp crystallizes as α form via isothermal crystallization from the melt state. Packing structures of α form has been used as structural markers of crystallization process. With the development of high resolution solid-state NMR (SS-NMR) technique, it becomes a powerful tool to investigate order-disorder of chain packing in the crystalline regions. We performed a series of experiments on different samples crystallized at different temperatures and studied the formation of α crystals influenced by different parameters, such as molecular weight, catalyst type and stereo, region regularity. Using selectively ¹³C enriched ipp samples we detect inter-nuclear correlations between the neighboring stems. This information provides chain reentry information. We figure out relationship between the chain reentry and chain packing of ipp α crystals. The recent discovery of the ipp α_2 single crystal offers a great opportunity to understand this topic also.

¹NSF-DMR1105829

C1.00031 Tube Visualization and Properties from Isoconfigurational Averaging, JIAN QIN, WINDSOR BISBEE, SCOTT MILNER, Dept. of Ch. E. at Penn. State Univ. — We introduce a simulation method to visualize the confining tube in polymer melts and measure its properties. We studied bead-spring ring polymers, which conveniently suppresses constraint release and contour length fluctuations. We allow molecules to cross and reach topologically equilibrated states by invoking various molecular rebridging moves in Monte Carlo simulations. To reveal the confining tube, we start with a well equilibrated configuration, turn off rebridging moves, and run molecular dynamics simulation multiple times, each with different initial velocities. The resulting set of “movies” of molecular trajectories defines an isoconfigurational ensemble, with the bead positions at different times and in different “movies” giving rise to a cloud. The cloud shows the shape, range and strength of the tube confinement, which enables us to study the statistical properties of tube. Using this approach, we studied the effects of free surface, and found that the tube diameter near the surface is greater than the bulk value by about 25%.

C1.00032 Unfolding of Collapsed Polymers in Shear Flow Enhanced by Colloidal Suspensions: Effect of Colloid Banding Structures in Confining Channels, HSIEH CHEN, ALFREDO ALEXANDER-KATZ, MIT — Very recently, using hydrodynamic simulations we have demonstrated that colloidal suspensions can greatly enhance the unfolding of collapsed single polymers in shear flow. Furthermore, we have shown that the enhancement may be suppressed if the colloid size is commensurate with the confining channel height, where the colloids form well-defined banding structures. In this study, we analyze the colloid banding structures in details and their relations to the polymer unfolding. We find that, for the colloid volume fractions up to 30%, the colloids form simple cubic (sc), hexagonal (hex), or the mixture of sc + hex structures depending on the commensurability of the colloid size and the channel height. By directly changing the height of the confining channels, we show that the collapsed polymers have the highest unfolding when the channel height is non-commensurate with either sc or hex structures.

C1.00033 Slippage of polymers: Influence of the chemical structure, MISCHA KLOS, Experimental Physics, Saarland University, OLIVER BÄUMCHEN, Dept. of Physics & Astronomy, McMaster University, MATTHIAS LESSEL, KARIN JACOBS, Experimental Physics, Saarland University — The continuing miniaturization of microfluidic devices causes a growing importance of the solid/liquid interface for the flow dynamics. Our experiments probe slippage using the dewetting process of thin polymer films on hydrophobic substrates. As hydrophobic coatings we use amorphous polymers (AF1600, AF2400) and different types of highly ordered self-assembled silane monolayers on top of ultraflat silicon substrates. Polystyrene (PS) of low molecular weight shows slip lengths between several hundreds of nanometers and even micrometers on silane surfaces [1], whereas on AF1600 nearly no slip is observable. However, slip can be induced by increasing the molecular weight of the PS [2]. Recent studies using scattering techniques showed an ordering effect of PS at the solid/liquid interface depending on the structure of the substrate [3]. Will the situation change if, instead of PS, polymethyl methacrylate (PMMA) is used? To probe the influence of the polymers composition on slippage, we show very first results of the dewetting dynamics of PMMA on AF2400.

[1] R. Fetzer, et. al., Europhys. Let., 75, no. 4, 638 (2006)

[2] O. Bäumchen, et al., PRL, 103, 247801 (2009)

[3] P. Gutfreund, et. al., arxiv.org 1104.0868v1 (2011, April 5)

C1.00034 Glass transition in ultra thin polymeric films measured by differential AC-Chip calorimetry, CHRISTOPH SCHICK, HEIKO HUTH, University of Rostock, DONGSHAN ZHOU, Nanjing University, MATHIAS AHRENBERG, University of Rostock — The film thickness dependency of glass transition in polymer films is still controversially discussed. For different experimental probes different dependencies are observed and a generally accepted link to molecular mobility is not yet established. Calorimetry has proven to provide useful information about glass transition, because it establishes a direct link to energetic characterization [1]. In several cases a direct comparison with results from other dynamic methods like dielectric spectroscopy is possible giving further insights. For thin films in the $\mu\text{m} \dots \text{nm}$ range standard calorimetric methods are mostly not applicable. We set up a differential AC-chip calorimeter capable to measure the glass transition in nanometer thin films with pJ/K sensitivity in a relative broad frequency range [2]. Changes in heat capacity can be measured for sample masses below one nanogram as needed for the study of the glass transition in nanometer thin polymeric films. The glass transition in thin films was determined at well defined experimental time scales. No thickness dependency of the glass transition temperature was observed within the error limits - neither at constant frequency nor for the traces in the activation diagrams. [1] C. Schick, Glass transition under confinement-what can be learned from calorimetry, *Eur. Phys. J. Special Topics* **189** (2010) 3-36. [2] H. Huth, A.A. Minakov, and C. Schick, Differential AC-Chip Calorimeter for Glass Transition Measurements in Ultrathin Films, *J. Polym. Sci. B Polym. Phys.* **44** (2006) 2996-3005.

C1.00035 Viscoelastic behavior of polymer in confined system, GUIDUK YU, BONG SEOCK KIM, JUNGWOOK KIM, KYUSOON SHIN, Department of Chemical and Biological Engineering, Seoul National University — Materials under nanoconfinement have been studied to exhibit interesting static and dynamic behaviors deviated from those in bulk state. In this study, we analyzed viscoelastic behavior of polymer confined to mesoscopic space. Polystyrene was adopted as the material to be probed, and anodized alumina was used as the substrates providing mesoscopic confinement. Controlling the confining conditions, the viscoelastic behavior of polystyrene was examined. Analyzing the surface tensions of the materials, we also considered the effect of interfacial tension on the thermodynamic stability of polymer in the confined geometry. In this presentation, we qualitatively explain the effects of confinement dimension and interface in comparison with that not in confined system.

C1.00036 Confinement effects on thermal frontal polymerization, PREETA DATTA, KIRILL EFIMENKO, JAN GENZER, NCSU — Frontal polymerization systems belong to the broader class of reaction-diffusion systems. In thermal frontal polymerization, the interplay of heat diffusion and Arrhenius reaction kinetics gives rise to a moving reactive front; propagation occurs through a positive feedback mechanism. We seek to understand how spatial confinement can change the system dynamics and cause to deviate the system from bulk behavior. In highly confined systems, the front propagates slower and the front profile is flatter than in bulk. The polymerization product shows a decrease in polydispersity index (<1.5) for high confinement. The molecular weights of the samples do not exhibit simple unimodal distributions, unlike bulk. In specimens at the highest degree of confinement the molecular weight of the resultant polymer decreases with increasing distance from the external heating source. In highly confined systems a smaller number of radicals are generated, resulting in a slower propagation step and polymer chains of more uniform length; front propagation is slow as it is reaction-limited. In contrast, for bulk or unconfined systems, higher heat generation rates, leading to faster polymerization with higher polydispersity in molecular weight; front propagation is fast as it is diffusion-limited.

C1.00037 Temperature Dependence of Polymer Diffusion in MWCNT/PS Nanocomposites¹, WEI-SHAO TUNG, University of Pennsylvania, NIGEL CLARKE, University of Sheffield, RUSSELL J. COMPOSTO, KAREN I. WINEY, University of Pennsylvania — Temperature dependence of homopolymer diffusion can be explained by the WLF equation. Here, we explore whether the WLF equation applies to polymer diffusion in nanocomposites. Previously, we found the diffusion coefficient shows a minimum with increasing MWCNT concentration. By studying the temperature dependence of polymer diffusion in this system, we will investigate the relative importance of entropic barriers or enthalpy interactions between polymer chain and fillers. Our composites contain MWCNT and polystyrene and are fabricated by a coagulation method. Using forward recoil elastic scattering (FRES), we probe the depth profile of tracer polymer (dPS) and obtain the diffusion coefficients by fitting the profile with Fick's second law.

¹National Science Foundation NSF/EPSRC Materials World Network DMR-0908449

C1.00038 Effect of confinement on reaction rates within polymer nanotemplates, CECILE MALARDIER-JUGROOT, XIA LI, Royal Military College of Canada — The most efficient catalysts have been developed and optimized by living systems. Indeed, in vivo enzyme-catalyzed reactions are several orders of magnitude more efficient than platinum based catalyzed reactions. However, the rate of reaction and equilibrium interactions are considerably reduced when the biological systems are studied in vitro. This phenomenon is largely attributed to the effect of confinement or macromolecular crowding present in the cell. Confinement can also be observed in an aqueous solution containing surfactants (amphiphilic copolymers). For example, copolymers can self-assemble into well defined ordered structures such as micelles, nanotubes, vesicles; and the geometries and shapes of a given copolymer can be controlled by their solvent affinity. The hollow nanoarchitectures obtained by self-assembly can be used as a model template to study confinement within a soft shell system to mimic biosystems. These systems provide a very controlled environment for the study of confinement. In this paper we will present the effect of confinement on polymerisation reactions combining both simulation and experimental characterisation for a comprehensive study of the effect of confinement on the interactions among confined molecules.

C1.00039 Influence of Thermal History in Crystallization of Physically Confined 2-Decanol, SAMUEL AMANUEL, ALEXANDREA SAFIQ, HILLARY BAUER, JARGALSAIKHAN DULMAA, AMER KHRAISAT, Department of Physics and Astronomy, Union College, Schenectady, NY 12308 — Bulk 2-decanol exhibits substantial hysteresis between its melting (-3°C) and freezing (-23°C) temperatures. When it is physically confined, the melting and freezing temperature are lowered and still exhibit hysteresis. Any presence of partially melted crystals, however, can trigger crystallization at higher temperatures upon subsequent cooling, suggesting that the hysteresis is thermal history dependant. The history, however, can be erased at temperatures higher than melting point. The lowest temperature at which the thermal history can be erased is physical size dependent. For example, 2-decanol physically confined in 100 nm has to be heated to a temperature between -10°C and -5°C to erase its history while 2-decanol confined in 300 nm has to be heated to a temperature between -2°C and 2°C .

C1.00040 Polymer Diffusion in Nanocomposites having attractive particle- polymer interactions¹, CHIA-CHUN LIN, SANGAH GAM, Department of Materials Science and Engineering, University of Pennsylvania, JEFFREY S. METH, DuPont Nanocomposite Technologies, Central Research & Development, E.I. DuPont de Nemours & Co., Inc, NIGEL CLARKE, Department of Physics and Astronomy, The University of Sheffield, KAREN I. WINEY, RUSSELL J. COMPOSTO, Department of Materials Science and Engineering, University of Pennsylvania — The addition of fillers into polymeric materials has drawn tremendous attention because of the remarkable mechanical and functional properties exhibited by these composites. Previously, we studied diffusion in a weakly interacting system and found that the reduced diffusion coefficient (D/D_0) scaled with the confinement parameter, defined as the inter-particle distance relative to the tracer size. Using elastic recoil detection, tracer diffusion of deuterated poly(methacrylate) is studied in a poly(methyl methacrylate) matrix containing silica nanoparticles with number average diameters of 12.8 and 28.8 nm. Because the silica contains surface hydroxyl groups, PMMA nanocomposites are a model system for studying diffusion in strongly attractive polymer-nanoparticle systems. In contrast to the weakly interacting system, the reduced diffusion coefficient in the matrix with smaller nanoparticles is less than that with larger nanoparticles and this difference increases as the confinement parameter decreases (i.e., more crowded system). The reduced diffusion coefficient is also analyzed in terms of the surface to volume ratio of the nanoparticles.

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C1.00041 Anomalous yet Brownian , SUNG CHUL BAE, BO WANG, JUAN GUAN, STEVE GRANICK, University of Illinois —

The items on the growing list of exceptions to Gaussian statistics have been given system-specific interpretations that fail to provide a universal picture of how Fickian diffusion can be non-Gaussian for diffusion over distances that much exceed the size of the diffusing object. Here, based on experiments in four separate systems, we present a general reasoning which indicates that the measured dynamics can be decomposed into a wide set of diffusivities that reflect slowly-varying, heterogeneous microscopic fluctuations. The identification of non-Gaussian yet Fickian diffusivity with long-lived environmental fluctuations allows us to conclude that non-Gaussian diffusivity should characterize much mobility in soft matter.

C1.00042 Glass Transition Temperature Gradient evidenced by NMR and Calorimetry , FRANCOIS LEQUEUX, HELENE MONTES, SIMM/ESPCI Paris France, AURELIE PAPON, SILCEA, LAURENT GUY, SILCEA Rhodia France, KAY SAALWAECHTER, Halle University Germany — Polymer, when confined, exhibit a dynamics different from the bulk one. However, measurements on unique films are rather difficult. One of the commonly accepted hypothesis is that there is a gradient of glass transition temperature in the vicinity of the solid surfaces. We have developed since ten years model nano-composite systems consisting in monodisperse spherical particles dispersed in an elastomer matrix. From Neutron Scattering, we can deduce the density of polymer located at any distance from any silica surface. We have then measured by NMR the magnetization relaxation at various temperatures above the glass transition temperature and its vicinity. From these measurements we were able to fit the whole set of data at various temperatures by a unique relation for the glass transition temperature T_g as a function of the distance z from a solid surface $T_g(z) = T_g(1 + \delta/z)$, with a unique parameter δ . In addition, the same law holds with the same parameter δ in the presence of solvent. Moreover, the parameter measured by NMR allows predicting quantitatively the Differential Scanning Calorimetry response, even after an aging step.

C1.00043 End Group Effects on the Hydrogel Formation of PEO-PPO-PEO Triblock Copolymers , AARON COHEN, CHANG Y. RYU, Rensselaer Polytechnic Institute, GYOO Y. JUNG, HEE SUNG HWANG, Postech — Pluronic F108, a triblock copolymer consisting of outer polyethylene oxide (PEO) chains and an inner polypropylene oxide (PPO) chains, has been shown to be an effective hydrogel matrix for DNA separation by capillary electrophoresis using single-stranded conformation polymorphism. This presentation will discuss a new pathway to potentially enhance the separation abilities of F108 by altering the chain end groups of the block copolymers. F108 is believed to form a micelle in aqueous solutions with the hydrophobic group in the interior, thus we expect considerable interaction between the DNA sample and the end groups found at the hydrophilic brush layers of the micelle. The rheological properties of end group derivatives of F108, in combination of small angle x-ray scattering, can reveal structural differences in the micelles. In particular, gelation temperature of the end group derivatives can be linked to differences in the micelle structure. Dynamic light scattering can also be used to determine the effects of chain end groups on the hydrodynamic size of the block copolymer micelles in dilute solution.

C1.00044 Self-assembly of polystyrene-*b*-poly(4-vinylpyridine) and polystyrene-*b*-poly(ethylene oxide) in small molecules melt¹ , CHENG-HAO YU, YU-HAO CHUANG, SHIH-HUANG TUNG, Institute of Polymer Science and Engineering, National Taiwan University, Taipei 10617, Taiwan, SOFT NANOMATERIALS GROUP TEAM — It is well known that amphiphilic block copolymers in selective solvents self-assemble into micellar structures, where solvophilic blocks tend to contact with solvents while solvophobic blocks are shielded from the solvents. Different from the conventional micellization in liquid systems, we report that block copolymer poly(styrene-*block*-4-vinylpyridine) (PS-*b*-P4VP) and poly(styrene-*block*-ethylene oxide) (PS-*b*-PEO) can self-assemble in melted small molecules at high temperature and the structures can be retained in “solid state” after being cooled down to room temperature. Transmission electron microscopy (TEM) was used to probe the structures and we found that a series of self-assembled structures, including spherical micelles, wormlike micelles and vesicles can be obtained by varying the length of block copolymers and the morphologies are dependent on annealing temperature and time. Since these nano-structures can be retained in solid state, we also demonstrate to extract the nano-structures by removing small molecules using appropriate solvents. These extracted structures, especially the vesicles, which are loaded with solid molecules, are potential applications of nanocapsules and controlled release

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C1.00045 Nanoparticle-Loaded Multifunctional Block Copolymer Micelles , JINHYE BAE, JIMMY LAWRENCE, CAROLINE MIESCH, ALEXANDER RIBBE, Polymer Science and Engineering Department at University of Massachusetts Amherst, WEIKUN LI, School of Chemistry and Chemical Engineering at Huazhong University of Science and Technology, TODD EMRICK, Polymer Science and Engineering Department at University of Massachusetts Amherst, JINTAO ZHU, School of Chemistry and Chemical Engineering at Huazhong University of Science and Technology, RYAN HAYWARD, Polymer Science and Engineering Department at University of Massachusetts Amherst — We have studied the incorporation of pre-synthesized hydrophobic inorganic nanoparticles within the cores of amphiphilic polystyrene-*block*-poly(ethylene oxide) (PS-PEO) diblock copolymer micelles formed through solvent-evaporation-induced interfacial instabilities of emulsion droplets. Using iron oxide, gold, and cadmium selenide nanoparticles coated with native alkane ligands, highly uniform encapsulation is obtained for cylindrical micelles, while spherical micelles can be enriched to ~ 90 % of loaded micelles through simple magnetic or centrifugal purification steps. Multiple different types of nanoparticles can easily be incorporated into each micelle, yielding multi-functional micelles. The ability to encapsulate both spherical and rod-like particles of different core chemistries and sizes ranging from ~ 1 to 20 nm, without the necessity of coating particles with specially designed ligands, makes this a versatile route to prepare hybrid micelle structures.

C1.00046 Phase Behavior of Star-shaped polystyrene-*block*-poly(methyl methacrylate) Copolymers , SANGSHIN JANG, HONGCHUL MOON, YOUNGMIN LEE, JIN KON KIM, Department of Chemical Engineering, Pohang University of Science and Technology — Star-shaped polystyrene-*block*-poly(methyl methacrylate) copolymer (PS-*b*-PMMA) was synthesized by utilizing α -cyclodextrin (α -CD) as a junction point of the star-shaped block copolymer. Eighteen hydroxyl groups on α -CD were substituted with bromine by the reaction with α -bromoisobutyl bromide for atom transfer radical polymerization. We found that the number of bromine substituted arms per one α -CD was higher than 16 measured by nuclear magnetic resonance and Matrix-assisted laser desorption/ionization. We could control molecular weight of this unusual kind of block copolymer depending on polymerization times. Those polymers were characterized by gel permeation chromatography and nuclear magnetic resonance. Phase behavior of these star-shaped block copolymers were investigated.

C1.00047 Kinetics of micellization for diblock copolymers in selective solvents studied using self-consistent field theory , RAGHURAM THIAGARAJAN, DAVID MORSE, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN — The kinetic barriers to association and dissociation of diblock copolymers in various selective solvents are calculated using self-consistent field theory. The variation of these kinetic barriers for both crew cut as well as hairy micelles are studied. The kinetic barriers are found to be very sensitive to temperature and become prohibitive except in a modest range of temperature near the critical micelle temperature. The dependence of kinetic barriers upon the chain and block lengths, and solvent quality are also studied.

C1.00048 Blending of Diblocks and Triblocks with identical hydrophilic block for multicompartment and multigeometry nanostructures, ZHENG ZENG, JIAHUA ZHU, YINGCHAO CHEN, University of Delaware, SHIYI ZHANG, Texas A&M University, DARRIN POCHAN, University of Delaware, KAREN WOOLEY, Texas A&M University, POCHAN'S GROUP TEAM, WOOLEY'S GROUP TEAM — Unique micellar morphologies, such as toroids, disks, and helices, have been obtained from a single triblock copolymer PAA-PMA-PS poly(acrylic acid)-b-poly(methyl acrylate)-b-poly(styrene) (PAA-PMA-PS) through a self-assembly process in dilute water/THF(tetrahydrofuran) solvent mixtures in the presence of organic multiamine molecules. Aiming to better understand their formation and explore novel structures, diblock copolymers, e.g. PAA-PMA and PAA-PS, were mixed with PAA-PMA-PS to co-assemble at desired solution conditions to produce known nanostructures (e.g. toroid, disk, helix formations). By taking advantage of the kinetic pathway of assembly and multiamine-PAA complexation, the additional diblock copolymers can be trapped in the same micelle with the triblock PAA-PMA-PS. Interesting transitions were found in toroid/disk/helix formations by changing the amount of the added diblock copolymers. The morphologies of the blended nanoparticles was characterized with cryogenic and conventional transmission electron microscopy, dynamic light scattering, and small angle neutron scattering.

C1.00049 Kinetic control of block copolymer self-assembly into multicompartment and novel geometry nanoparticles¹, YINGCHAO CHEN, University of Delaware, XIAOJUN WANG, University of Tennessee, KE ZHANG, Northwestern University, KAREN WOOLEY, Texas A&M University, JIMMY MAYS, University of Tennessee, VIRGIL PERCEC, University of Pennsylvania, DARRIN POCHAN, University of Delaware, UNIVERSITY OF DELAWARE COLLABORATION, TEXAS A&M UNIVERSITY COLLABORATION, UNIVERSITY OF TENNESSEE COLLABORATION, UNIVERSITY OF PENNSYLVANIA COLLABORATION — Micelles with the segregation of hydrophobic blocks trapped in the same nanoparticle core have been produced through co-self-assembly of two block copolymers in THF/water dilute solution. The dissolution of two block copolymer sharing the same polyacrylic acid PAA blocks in THF undergoes consequent aggregation and phase separation through either slow water titration or quick water addition that triggers the micellar formation. The combination and comparison of the two water addition kinetic pathways are the keys of forming multicompartment structures at high water content. Importantly, the addition of organic diamine provides for acid-base complexation with the PAA side chains which, in turn, plays the key role of trapping unlike hydrophobic blocks from different block copolymers into one nanoparticle core. The kinetic control of solution assembly can be applied to other molecular systems such as dendrimers as well as other block copolymer molecules. Transmission electron microscopy, cryogenic transmission electron microscopy, light scattering have been applied to characterize the micelle structures.

¹Thanks for the NSF grant MASC312153, Thanks for the keck lab in UD

C1.00050 Dynamic Processes in Diblock Copolymer Micelles with a Semi-Crystalline Core, AVANTIKA SINGH, MEGAN ROBERTSON, University of Houston — Amphiphilic diblock copolymers, which form micelle structures in selective solvents, offer a great advantage of tunability in physical characteristics as compared to low molecular weight surfactants. Their micelles in aqueous solvents have been a subject of great interest in drug delivery applications for their high loading capacity and targeted drug delivery. The aim of this work is to understand the dynamic processes underlying the self-assembly of diblock copolymer micelle systems which have a semi-crystalline core. The present work focuses on amphiphilic diblock copolymers containing blocks of poly(ethylene oxide) (a hydrophilic polymer) and polycaprolactone (a hydrophobic polymer), which spontaneously self-assemble into spherical micelles in water. Polycaprolactone is a semi-crystalline polymer. A variety of experimental techniques are used to probe the kinetic processes occurring during micelle self-assembly, including time-resolved neutron scattering, dynamic light scattering, pulsed field gradient nuclear magnetic resonance, and fluorescence resonance energy transfer experiments.

C1.00051 Long Circulating Micelles based on Helix Bundle-Forming Peptide-Polymer Conjugates, JESSICA SHU, UC Berkeley, HE DONG, Retired, NIKHIL DUBE, UC Berkeley, JAI WOONG SEO, UC Davis, YU FEI MA, UC Berkeley, KATHERINE FERRARA, UC Davis, TING XU, UC Berkeley — Stable, multi-functional organic nanoparticles that combine long in vivo circulation, the ability to cross vessel walls to reach tumor tissues and controlled disassembly for eventual clearance will have a significant impact in nanomedicine. Although current self-assemblies of amphiphiles provide a versatile platform to generate modular organic nanoparticles, it remains a significant challenge to simultaneously control nanoparticle size in the range of 10-30 nm, enhance particle stability and tailor disassembly within suitable timescales. We have advanced this goal by designing a new family of amphiphiles based on coiled-coil 3-helix bundle forming peptide-polymer conjugates. By attaching a polymer chain to the middle of a helical peptide, the protein tertiary structures are used to position entropic forces of compressed polymer chains comprising the headgroups so as to effectively slow down the subunit desorption rate and enhance the in vivo stability. The resultant monodispersed nanoparticles are composed of subunits, < 4 nm in size, that form highly stable 15-17 nm diameter particles and demonstrate an in vivo circulation half life-time of 28 hrs, minimal accumulation in the liver and spleen and effective urinary clearance. By uniquely combining the configurational entropy of a polymer chain with a common protein structure, i.e. coiled-coil helix bundle, and a lipid core, self-assembled nanoparticles have been engineered with tunable stability and disassembly.

C1.00052 Physics of Polymersomes: lateral segregation experiments and raft simulations, DENNIS DISCHER, Univ. Pennsylvania — Coupling between the inner and outer leaflets of a bilayer plays an important role in biomembrane function, particularly in inducing and registering rafts across leaflets for various cellular signals. However, mechanisms of raft registration remain elusive and several alternatives have been proposed, ranging from electrostatic coupling to chain interdigitation. A general mechanism has been suggested by recent experiments on Polymersomes in which binary mixtures of diblock copolymer amphiphiles exhibit domain registration upon ligand-induced segregation. Using coarse grained molecular dynamics (CGMD) simulations rooted in atomistics, raft registration arises spontaneously in bilayers with a calcium- or ligand-crosslinked ordered phase segregating from a liquid disordered phase. When rafts are not registered, a thickness mismatch between phases induces a “bump” in the apposing liquid phase leaflet, and the associated localized curvature guides rafts together stabilizing the registered state. The absence of explicit charge in the model and the fact that domain size modulates transmembrane coupling demonstrate that collective interactions are sufficient for raft registration. References: (1) D.A. Christian, et al. Spotted vesicles, striped micelles, and Janus assemblies induced by ligand binding. Nature Materials 8: 843–849 (2009). (2) D. Pantano, P.B. Moore, M.L. Klein, D.E. Discher. Raft registration across bilayers in a molecularly detailed model. Soft Matter 7, 8182-8191 (2011).

C1.00053 Controlling the Morphology of TiO2 Nanorods/Polythiophene Composites for Bulk Heterojunction Solar Cells Using H-Bonding¹, YING LIN, QINGSHUO WEI, JAMES J. WATKINS, Department of Polymer Science and Engineering, University of Massachusetts Amherst — We demonstrate how the morphology of solution-processable hybrid bulk heterojunction solar cells, within an active layer consisting of modified poly(3-hexylthiophene) (P3HT) and TiO2 nanorods, can be controlled by H-Bonding. The hybrid bulk heterojunction solar cells suffer from the problems of the aggregation of inorganic nanocrystals and the interface between nanocrystals and the polymer matrix. To address these issues, we utilize P3HT-based block copolymer (BCP), in which one block is P3HT and the other block is a P3HT derivative containing a poly(ethylene glycol) (PEG) oligomer side chain. In the mean time, we functionalized the TiO2 nanorods with dyes having multiple COOH groups. This design both enables self-assembly of the devices via micropase segregation into well-defined morphologies and provides a means for establishing strong preferential interaction between TiO2 nanorods and the PEG side chain. This strong, preferential H-bonding limits the aggregation of the TiO2 nanorods and modifies the interfacial properties between donor and acceptor. TEM showed the self-assembly structure of the TiO2 nanorods in polymer matrix. Using this modified thiophene copolymer, hybrid devices are made with power conversion efficiencies 50% higher than that of conventional P3HT homopolymer.

¹Funding from the NSF Center for Hierarchical Manufacturing (CMMI-0531171) and the Department of Energy supported Energy Frontier Research Center at the University of Massachusetts (DOE DE-PS02-08ER15944) are gratefully acknowledged.

C1.00054 Magnetic Nanoparticle/Block Copolymer Hybrid Materials for the Fabrication of Electromagnetic Devices¹, XINYU WANG, DAVID MESGUICH, JAMES WATKINS, University of Massachusetts Amherst — Significant efforts have been directed towards incorporating inorganic nanoscopic materials into well-defined, phase-separated block copolymer systems to create hybrid materials with intriguing optical, electrical or magnetic properties. Lin et al. recently reported the use of strong interactions between NPs and one segment of weakly segregated BCP systems to drive the assembly of well-ordered morphologies while confining the NPs specifically in the desired spherical, cylindrical or lamellar domains. Here we use this approach to assemble magnetic nanoparticles of high permeability into well ordered systems. Magnetic nanoparticles (MNPs) were synthesized and subsequent surface functionalization and/or ligand exchange reactions were carried out to decorate the NP surfaces with hydrogen-bonding donating groups and good particle dispersibility in polar solvents. The ligand attachment was confirmed by TGA and FTIR. The morphology evolution of BCP/MNPs composites was examined by SAXS. Such ferromagnetic structures with precise geometric control in nanoscale would enable the cost-effective fabrication of more advanced devices for AC electromagnetic applications such as miniaturized antennas with extended bandwidth, integrated microwave electronics and efficient power transformers.

¹This work was supported by the NSF Center for Hierarchical Manufacturing at the University of Massachusetts (CMMI-1025020)

C1.00055 Novel Approach to Quantify Dispersion of Spherical Nanoparticles in Polymer Nanocomposites¹, DENIZ RENDE, NIHAT BAYSAL, RAHMI OZISIK, Rensselaer Polytechnic Institute — Nanocomposites have emerged as promising materials due to improved conductivity, toughness, and permeability when compared to conventional bulk polymers. Controlling the dispersion of the nanoparticles in a polymer matrix is still one of the greatest challenges that limit our ability to achieve the aforementioned property enhancements. Nanoparticles tend to agglomerate due to strong interparticle interactions. The dispersion of nanoparticles in polymers is generally determined by transmission electron microscopy (TEM) or scanning electron microscopy (SEM). However, in these studies quantification of dispersion depends on the visual observations and is prone to subjective conclusions; thereby hampering possible comparison between samples. Considering its importance, little effort has been put forward to quantify the dispersion of nanoparticles in polymers. In the current study, we have applied network theory approach to quantify the dispersion of spherical particles. A network is a collection of nodes, which are entities (such as nanoparticles), and edges that connect pairs of nodes (distances between nanoparticles). By employing nodes and edges, we constructed interaction networks, which were then analyzed in terms of global topological measures: degree distribution, clustering coefficient, and average distance. We show that this approach is a powerful tool to quantify dispersion of spherical nanoparticles in a polymer matrix.

¹Partial support was provided by NSF Grant No. 1003574 and RPI. DR is also supported by TUBITAK 2219 program.

C1.00056 Mesoscopic Iron-Oxide Nanorod Polymer Nanocomposite Films, ROBERT FERRIER, University of Pennsylvania, KOHJI OHNO, University of Kyoto, RUSSELL COMPOSTO, University of Pennsylvania — Dispersion of nanostructures in polymer matrices is required in order to take advantage of the unique properties of the nano-sized filler. This work investigates the dispersion of mesoscopic (200 nm long) iron-oxide rods (FeNRs) grafted with poly(methyl methacrylate) (PMMA) brushes having molecular weights (MWs) of 3.7K, 32K and 160K. These rods were then dispersed in either a poly(methyl methacrylate) or poly(oxyethylene) (PEO) matrix film so that the matrix/brush interaction is either entropic (PMMA matrix) or enthalpic and entropic (PEO matrix). Transmission electron microscopy (TEM) was used to determine the dispersion of the FeNRs in the polymer matrix. The results show that the FeNRs with the largest brush were always dispersed in the matrix, whereas the rods with the shorter brushes always aggregated in the matrix. This suggests that the brush MW is a critical parameter to achieve dispersion of these mesoscopic materials. This work can be extended to understand the dispersion of other types of mesoscopic particles

C1.00057 Additive Driven Self Assembly in Poly(ethylene glycol) monomethyl ether monomethacrylate-block-Poly(ethyl methacrylate) Copolymers, CHENG LI, University of Massachusetts Amherst, WENXU ZHANG, UMass Amherst, EDWARD COUGHLIN, JAMES WATKINS, University of Massachusetts Amherst — Recent work in our labs has demonstrated the concept of additive driven assembly by hydrogen bond interactions between poly(ethylene oxide) segments of a disordered PEO containing block copolymer and a nanoparticle or organic additive induces strong segregation in the composite to yield well ordered morphologies. In some cases, these interactions were introduced by light-activated deprotection of functional groups on the additive to enable regioselective, photo-induced order in block copolymer films. While PEO crystallization in these polymers is suppressed by strong interaction between the additive and the PEO segments at high additive loadings, crystallization of the PEO block with no loading or at low additive loadings is highly undesirable for many applications. To remedy this issue, we prepared PEGMEMA-PEMA using RAFT living polymerization. This block copolymer phase mixed, noncrystallizable at room temperature. The incorporation of organic additives with multiple carboxylic acid groups or functionalized nanoparticles induces phase segregation in these systems. Furthermore, the use of additives in which the hydrogen bond donating group is protected with an acid labile group in combination with a photo acid generator enables photo-induced order of the composite films.

C1.00058 Correlating nanoscale structural changes to macromolecular gel formation in Laponite containing Pluronic F127 photogel systems, K. ANNE JUGGERNAUTH, Macromolecular Sci. & Eng. Research Center, Materials Sci & Eng Dept, University of Michigan, BRIAN LOVE, Materials Sci & Eng Dept, University of Michigan, UNIVERSITY OF MICHIGAN TEAM — Polymer nanocomposites has been a growing scientific field over the last 20 years. Recently, there has been increasing interest on nanocomposite systems with active responses to external stimuli such as heat, magnetic fields and light. The focus of this work is on a reversible thermoresponsive system, Pluronic F127 with added inorganic disk-shaped nanoparticles of Laponite. We further modify this system with the addition of a photoacid generator to enable photogelation. However, the nanoscale particle-particle and polymer-particle interactions within this Laponite/ block copolymer system are not well understood. We report on the photogelation kinetics of this system and further probe the interactions and rearrangement kinetics with heat and light exposure using in-situ synchrotron small angle x-ray scattering.

C1.00059 Gold-Decorated Supraspheres of Block Copolymer Micelles, M.P. KIM, D.J. KANG, A.G. KANNON, KAIST, D.-W. JUNG, G.R. YI, Chungbuk National Univ., B.J. KIM, KAIST — Gold-decorated supraspheres displaying various surface morphologies were prepared by infiltration of gold precursor into polystyrene-b-poly(2-vinylpyridine) (PS-b-P2VP) supraspheres under acidic condition. The supraspheres were fabricated by emulsifying PS-b-P2VP polymer solution into surfactant solution. Selective swelling of P2VP in the suprasphere by gold precursor under acidic condition resulted in the formation of gold-decorated supraspheres with various surface structures. As evidenced by TEM and SEM images, dot pattern was formed in the case of smaller supraspheres than 800 nm; whereas fingerprint-like pattern was observed in larger supraspheres than 800 nm. Gold nanoparticles were located inside P2VP domains near the surface of prepared supraspheres as confirmed by TEM. The optical property of the supraspheres was characterized using UV-vis absorption spectroscopy and the maximum absorption peak at around 580 nm was observed, which means that gold nanoparticles densely packed into P2VP domain on the suprasphere. Our approach to prepare gold-decorated supraspheres can be extended to other metallic particles such as iron oxide or platinum nanoparticles, and those precursors can be also selectively incorporated into the P2VP domain.

C1.00060 Self-Assembly of CdSe Nanorods by Controlled Solvent Evaporation and Applied Electric Field, SIRINYA CHANTARAK, TODD EMRICK, THOMAS P. RUSSELL, Polymer Science & Engineering Department, University of Massachusetts, Amherst — We report the synthesis of CdSe nanorods (NRs) having variable aspect ratios and their vertical alignment into a hexagonal arrays over a large area. NRs with a constant diameter of 6 nm and lengths, tunable to over 100 nm, were obtained by controlling the concentration of ligands in solution and injection of Se at defined time intervals. Hexagonal arrays of aligned, alkane covered CdSe nanorods within a polymer matrix were achieved by controlled solvent evaporation in the presence of an applied electric field. The nature of the solvent identity, substrate hydrophobicity, and strength of applied voltage were optimized such that close packing of nanorods was achieved over a large area. Such organized nanocomposites hold potential application in organic-inorganic bulk heterojunction photovoltaic devices.

C1.00061 Emulsions of Polymer Blends Stabilized by Janus Particles, KYLE BRYSON, RYAN HAYWARD, THOMAS RUSSELL, University of Massachusetts - Amherst — Particle-stabilized emulsions of both immiscible and partially miscible polymer blends have recently received renewed interest. In particular, bicontinuous stabilized emulsions are attractive for their three-dimensional expression of the properties of each component, but a true incarnation of this structure has yet to be demonstrated in polymer systems, due to the difficulties in preparing particles that neutrally wet both polymer phases. Janus particles, which possess different surface chemistries on two halves of the particles, afford a way to bypass the necessity of neutral wettability. Both theory and experiment have shown enhanced interfacial adsorption energies for Janus particles, in comparison to homogeneous particles. To investigate these concepts, silica particles were homogeneously and anisotropically functionalized and dispersed in fluid mixtures; interfaces were created by thermally induced phase separation or mechanical mixing. The resulting structures were characterized by laser-scanning confocal microscopy and transmission electron microscopy. The results elucidate the role of particle wettability on the structure of stabilized emulsions.

C1.00062 Crystallization of Polymers at liquid/liquid interface templated by single-walled carbon nanotubes, WENDA WANG, CHRISTOPHER LI, Drexel University, SOFT MATTER RESEARCH GROUP TEAM — Nanosized single-walled carbon nanotube rings were fabricated by using a Pickering emulsion-based method. By tuning a water/oil/SWNT miniemulsion system, SWNT rings with a diameter of ~200 nm can be readily achieved. The formation mechanism is attributed to the bending force induced by the curved liquid/liquid interface. Crystallization of polyethylene homo- and copolymers using this unique SWNT rings as the nucleation agent was conducted at the curved liquid/liquid interface. Crystal structure, hybrid morphology and crystallization kinetics were systematically studied. The structure of controlled alternating patterns on SWNT rings has great potential in various applications in large-scale integrated circuits and single-electron devices.

C1.00063 Effect of Nanoparticle Size on Nanoparticle Spatial Distribution in a Diblock Copolymer Supramolecular Thin Film, PETER BAI, JOSEPH KAO, MATTHEW LUCAS, PAUL ALIVISATOS, TING XU, University of California, Berkeley — The self-assembly of nanoparticles (NPs) opens many pathways towards generation of functional nanostructured materials with desirable optical, mechanical and electrical properties. A great challenge in this field is the effective control of NP spatial distribution within the block copolymer matrix, which is crucial in tailoring the macroscopic properties of the polymer/nanoparticle composites. We systematically investigated the effect of NP size on the spatial distribution of nanoparticles upon blending with a diblock copolymer based supramolecule in thin film. The spatial distribution of NPs in thin film was observed to be strongly dependent on NP size. These observations can be explained by the increase in entropic penalty of incorporating larger NPs associated with the deformation of the BCP block to accommodate the NPs. This effect is observed for NPs with different chemistries and could serve as a promising route to creating multifunctional thin film nanocomposites.

C1.00064 Direct Nanorod Assembly Using Block Copolymer-Based Supramolecules, KARI THORKESSON, ALEXANDER MASTROIANNI, Department of Materials Science and Engineering, UC Berkeley, PETER ERCIUS, National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, TING XU¹, Department of Materials Science and Engineering, UC Berkeley; Materials Sciences Division, Lawrence Berkeley National Laboratory — One-dimensional nanomaterials with high aspect ratios, such as nanorods, exhibit unique and useful anisotropic optical, magnetic, and electrical properties. The collective properties of 1-D nanomaterials depend on their spatial arrangements, interparticle ordering, and macroscopic alignment. Developing routes to control their organization with high precision is critical to generate functional materials. We have investigated the co-assemblies of nanorods and block copolymer (BCP)-based supramolecules that self-assemble into spherical, lamellar and cylindrical morphologies. By varying energetic contributions from the rod-rod interactions and the deformation of the supramolecule, a wide library of nanorod assemblies including highly aligned arrays, continuous networks, and clusters can be readily accessed. Since macroscopic alignment of BCP microdomains can be obtained by application of external fields, present studies open up a new route to manipulate macroscopic alignments of nanorods. Fundamentally, these studies have demonstrated that in these blends, the energetic contributions from the polymer chain deformation and rod-rod interactions are comparable and can be tailored to disperse nanorods with control over inter-rod ordering and their relative alignment.

¹Also: Department of Chemistry, UC Berkeley

C1.00065 Magnetically aligned polymers and nanocomposites for energy harvesting and energy storage applications¹, PAWEŁ MAJEWSKI, MANESH GOPINADHAN, CANDICE PELLIGRA, Yale University, SHANJU ZHANG, California Polytechnic State University, LISA PFEFFERLE, Yale University, LUIS CAMPOS, Columbia University, CHINEDUM OSUJI, Yale University — The realization of anisotropic, nanostructured, functional materials by self-assembly is impaired by the persistence of structural defects which render the properties of the system isotropic on macroscopic length scales. We present three distinct systems including ZnO nanowire-semiconducting polymer composites, Li-ion conducting block copolymer membranes, and perylene-based block copolymers where self-assembly under a magnetic field yields alignment and global anisotropy of their physical properties. The resulting aligned nanostructured systems are attractive for ordered heterojunction photovoltaics, high performance solid polymer electrolyte membranes and electro-optical devices, respectively. Our results demonstrate that magnetic fields offer a viable route for directing the self-assembly of certain soft functional materials. The ready scalability of this approach makes it potentially important from a technological standpoint.

¹The funding from NSF under DMR-0847534 and DMR-0934520 is gratefully acknowledged.

C1.00066 Absorption of nanoparticles onto curved surfaces, CHIH-YU JAO, Virginia Tech Dept of Physics, JIHAENG YI, ISHAC L. N. KANDAS, BO LIU, YONG XU, Virginia Tech ECE Dept., HANS D. ROBINSON, Virginia Tech Dept of Physics — We study the adsorption of gold nanospheres onto cylindrical and spherical glass surfaces from stagnant aqueous particle suspensions. The curved surfaces were obtained as tapers and microspheres fabricated from optical fibers and were coated with a nm-thick layer of the polycation polyallylamine hydrochloride, causing irreversible adsorption of the negatively charged spheres. Our results fit well with theory, which predicts that the rates of particle adsorption will depend strongly on the surface geometry. In particular, *adsorption is significantly faster on curved than on planar surfaces* at times long enough that the particle diffusion length is large compared to the surface curvature. This is of particular importance for plasmonic sensors and other devices where particles are deposited from a suspension onto surfaces which may have non-trivial geometries.

C1.00067 Thermodynamics of ligand-coated nanoparticle complexation with lipid bilayers, REID VAN LEHN, Massachusetts Institute of Technology, RANDY CARNEY, KISLON VOITCHOVSKY, FRANCESCO STELLACCI, MARIA RICCI, Ecole Polytechnique Federale de Lausanne, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — Recently, nanoparticles (NPs) coated with a mixed alkanethiol surface monolayer were observed to spontaneously penetrate cell membranes via a non-endocytotic mechanism. Penetration seems to depend on the structure of the ligand monolayer; particle uptake was greatest when the surface self-assembled into a striped morphology consisting of alternating domains of hydrophilic and hydrophobic ligands. Furthermore, these 'striped' particles form stable complexes with single component lipid bilayers, implying that cellular penetration may be related to bilayer interactions. Bilayer complexation is surprising, however, because the width of the striped domains is less than the thickness of the bilayer core, implying that charged ligands are exposed to hydrophobic lipid tails. In this work, we provide a thermodynamic analysis of NP-bilayer complexation supported by implicit bilayer simulations. Our results show that complexation is related to the deformation of both the ligand monolayer and the bilayer to maximize favorable hydrophobic interactions while minimizing unfavorable insertion of charges into the bilayer core. This study will improve our understanding of bilayer interactions and enable the design of ligand-coated nanoparticles for drug delivery and biosensing applications.

C1.00068 Morphological robustness in polythiophene/fullerene mixtures¹, SAMEER VAJJALA KESAVA, DEREK KOZUB², Pennsylvania State University, CHENG WANG, ALEXANDER HEXEMER, Advanced Light Source, Lawrence Berkeley National Laboratory, ENRIQUE GOMEZ, Pennsylvania State University, ENRIQUE GOMEZ TEAM, ALEXANDER HEXEMER TEAM — The morphology of the photoactive layer of organic solar cells evolves differently under different processing conditions such as annealing temperature, annealing time and casting solvent. Hence, characterizing it is crucial in understanding its effect on device performance. In our study, we used Grazing Incidence Small Angle X-ray Scattering (GISAXS) and Energy-Filtered Transmission Electron Microscopy (EFTEM) to characterize the in-plane morphology of poly(3-hexylthiophene-2,5-diyl) (P3HT)/[6,6]-phenyl-C₆₁-butyric acid methyl ester (PCBM) mixtures. We found that the characteristic length scale determined through GISAXS did not vary significantly for different processing conditions thus making P3HT/PCBM a robust system. For example, different spin-casting solvents did not significantly affect lateral phase separation, and consequently, device performance was similar once thickness effects are accounted for.

¹NSF, ALS LBNL, MRI Penn State

²Graduated in 2011

C1.00069 Thin-film fabrication and electric field induced poling of an azo dye-doped cyclic olefin copolymer¹, JONATHAN CHOI, The College of New Jersey, BASTIAN BRAEUER, Beuth University of Applied Sciences, PADMA GOPALAN, University of Wisconsin-Madison, DAVID MCGEE, The College of New Jersey — Cyclic olefin copolymers (COC) exhibit high transparency, low birefringence, and a high glass transition temperature, which make them promising as host materials for nonlinear optical chromophores. However, the non-polar COC environment limits chromophore loading, resulting in potentially weak nonlinear optical functionality. In this research, we fabricated COC films doped with the azo dye Disperse Red 1 (DR1), and corona poled the films to establish dipolar chromophore order. Second-harmonic generation experiments were used to probe chromophore orientational order during the poling process and to monitor the subsequent temporal relaxation. Preliminary experiments indicated a maximum loading of 5 wt% DR1 in COC, and that the effective second order nonlinear optical coefficient decayed by 50% within two weeks following poling.

¹Research supported by NSF-DMR award RUI 138416

C1.00070 Temperature Dependent Study of Regioregular and Regiorandom Poly (3-hexyl thiophene)s, XIAOBO SHEN, THOMAS RUSSELL, University of Massachusetts Amherst — Structure evolution of bulk regioregular (rr) and regiorandom (rra) poly (3-hexyl thiophene)s (P3HT) with temperature has been characterized by wide angle X-ray diffraction (WAXD). Different thermal behaviors associated with the inter- and intra-molecular packing were shown as regioregularity changes. Transition temperature of ~100°C for crystalline rr-P3HT has been assigned to side chain melting point where the thermal expansion along the edge-on direction shows a turning point separating solid and molten hexyl side chains. Meanwhile, $\pi - \pi$ stacking distance was observed to initially decrease and then increase upon heating, with a minimum at ~100°C. The average inter-molecular distance of rra-P3HT was independent of temperature while the average intra-molecular distance increased upon heating. Molten rr-P3HT and rra-P3HT show same inter- and intra-molecular distance. Temperature UV-Vis absorption and photovoltaic device performance were also measured.

C1.00071 Additive-Driven Assembly of Block Copolymer-Nanoparticle Hybrid Materials for Solution Processable Floating Gate Memory, QINGSHUO WEI, YING LIN, ERIC ANDERSON, ALEJANDRO BRISENO, SAMUEL GIDO, JAMES WATKINS, Department of Polymer Science and Engineering, University of Massachusetts Amherst — The preparation of well-ordered hybrid materials at nanoscale is not only fundamentally interesting but also of significant importance for the development of next generation functional devices. In this study, we present a simple approach for the preparation of well-ordered polymer/NP composites through the concept of additive-driven assembly, and its application for the fabrication of floating gate organic FET memory devices. The addition of gold NPs that selectively hydrogen bond with pyridine in poly(styrene-*b*-2-vinyl pyridine) is shown to induce an ordered structure. This enables the fabrication of well-ordered hybrid materials with lamellar domains at Au NP loadings of more than 40 wt%. The fabrication of floating gate memory devices was demonstrated by the ordered Au NPs / block copolymer hybrid film as a charge trapping layer, which is sandwiched between a SiO₂ dielectric layer and a poly(3-hexylthiophene) semiconductor layer. This approach enables us to fabricate well-ordered charge storage layers by solution processing and to achieve facile control of the memory windows by changing the density of gold NPs. The devices show high carrier mobility (> 0.1 cm²/Vs), controllable memory windows (0~50V), high *on/off* ratio (>10⁵) between memory states and long retention times (>10⁴ s). This approach is potentially suitable for roll-to-roll printing techniques to make flexible, large area and high density devices.

C1.00072 Classification of Semiconducting Polymeric Mesophases to Optimize Device Post-Processing, CHAD SNYDER, RYAN NIEUWENDAAL, DAVID VANDERHART, LEE RICHTER, R. JOSEPH KLINE, DEAN DELONGCHAMP, National Institute of Standards and Technology, MARTIN HEENEY, IAIN MCCULLOCH, Imperial College of London — Semiconducting polymers form a variety of phases and mesophases that respond differently to post-deposition solvent or thermal treatments. Here it is shown that classification of these materials into their appropriate mesophases can be a useful tool to optimize their post-deposition treatments. Calorimetry is used to quantify differences between very similar materials, using a well-established framework based on the kinetics and thermodynamics of phase changes. By way of example, this classification scheme is used to identify differences in the presence and distribution of mesophases in three polymers, poly(3-hexylthiophene) and two isomeric bithiophene-thiophene copolymers (pBTBT and pATBT). The diverse phase structure is notable in light of the molecular similarity of the three polymers, and it has impact on optimum post-processing conditions for maximum electrical performance in thin film transistor devices.

C1.00073 Conformation Effects on the Photoluminescence Behavior of Anchored MEH-PPV Pancakes and Brushes, KUO SHENG SHIH, PO-TSUN CHEN, ARNOLD C.-M. YANG, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan 30013 — Single molecular layer of poly[2-methoxy-5-(2'-ethylhexyloxy)-1,4-phenylenevinylene] (MEH-PPV) grafted on primed silicon wafer were synthesized, forming brushes (chain spacing 0.54 nm via graft-from) or pancakes (~7 nm to 34 nm via graft-to). For the tight-packed brushes, the PL emission peak, residing in the range from 434 nm to 550 nm depending on the chain length, was generally unchanged when transferring between the dry and solvent immersion states. However, for the pancakes, the emission peak blue-shifted dramatically (up to 100 nm) when dried in the air relative to that in the solvent. These shifts were fully reversible in the dry-wet cycles. The large blue shifts of the anchored pancakes were attributed to the mechanical stretching of entangled MEH-PPV segments in contact with substrate upon solvent loss. In contrast, the blue shifts disappeared and small red shifts emerged instead for extremely slowly drying (24 hrs drying time), revealing the stress-relaxation pathways in the equilibrium conditions. The drying-induced blue shift was also observed in the un-anchored drop-casting samples but the reversibility vanished. Finally, a large enhancement of PL intensity was accompanied with the blue shifts, manifesting the effect of the molecular constraints.

C1.00074 Properties of Alq₃ waveguides containing embedded metal layers, NIRANJALA WICKREMasinghe, XIAOSHENG WANG, JONATHAN THOMPSON, Department of Physics, University of Cincinnati, Cincinnati, OH 45221, HEIDRUN SCHMITZER, Department of Physics, Xavier University, Cincinnati, OH 45207, HANS PETER WAGNER, Department of Physics, University of Cincinnati, Cincinnati, OH 45221 — We study the properties of aluminum-quinoline (Alq₃) waveguides with embedded thin (few 10 nm thick) metal layers using the m-line technique at a wavelength of 633 nm. Our goal is to investigate how the guided TM and TE modes and their effective refractive indices are affected by the metal layers. The layered waveguides are fabricated on a glass substrate by organic molecular beam deposition (OMBD). A Mg_{0.9}Ag_{0.1} alloy is used for the metal layers. Pure Alq₃ waveguides serve as reference samples. Our experiments show that TM modes in an Alq₃ waveguide with a single centered metal film are nearly unaffected, except for a slight increase of the bulk refractive index in the sample. TE modes are more strongly affected. Compared to our reference sample, we do not observe the TE₀ and TE₂ mode. Other TE modes whose electric field nodes are at the location of the metal film are visible. A similar behavior is also found in waveguides with embedded multiple metal layers. Our experimental data is compared to a multi-layer model simulation and to an effective-medium model. The results indicate that strategically placed metal layers can potentially be used to tailor waveguides structures.

C1.00075 Mechanical deformations of the metal cathodes of polymer light emitting devices during stability tests¹, ZAC BARCIKOWSKI, JACOB COX, MARIAN TZOLOV², Department of Physics, Lock Haven University of Pennsylvania — The polymer light emitting devices (PLEDs) include materials with substantially different mechanical properties - oxides as anode, organic polymers as light emitter, and metals as cathode. The typical expectation is that this mix of materials would be a problem if there is an exposure to large temperature variation. Our studies on the stability of the PLEDs give evidence that even without substantial heating of the devices, mechanical deformations appear. They are manifested in delamination and loss of contact area with all associated negative impact on the light emission from the devices. Our optical and scanning electron microscopy images show round shaped cathode deformations with enhanced degradation of the polymer along their periphery. In order to check the hypothesis of build-up of mechanical stress in the metal films during their deposition, we have used thermally evaporated aluminum cathodes with different thickness. We have used anodes different than the traditionally used ITO film in order to verify if an oxygen evolution is responsible for the formation of the mechanical deformations. We will show results on how a buffer layer between the light emitting polymer and the cathode influences the formation of the mechanical deformations.

¹Supported by NSF Grant #0923047.

²Project Advisor

C1.00076 N-type Organic Field Effect Transistor Using Densely Aligned Carbon Nanotube Array Electrodes¹, EDWARDS G. JIMENEZ, School of Electrical Engineering and Computer Science, and Nanoscience Technology Center, University of Central Florida, BIDDUT K. SARKER, Nanoscience Technology Center, and Department of Physics, University of Central Florida, SAIFUL I. KHONDAKER, Nanoscience Technology Center, Department of Physics, and School of Electrical Engineering and Computer Science, University of Central Florida — We present fabrication of n-type organic field effect transistors (OFETs) using densely aligned array carbon nanotube (CNT) electrodes. The CNTs were aligned with a high linear density via dielectrophoresis (DEP) from an aqueous solution. In order to fabricate the CNT electrodes, aligned CNTs were cut by electron beam lithography (EBL) and precise oxygen plasma etching. The OFETs were fabricated in a bottom-contact configuration by depositing a thin film of C60 molecules between the CNT source and drain electrodes, and compared against a controlled OFET with gold electrodes. The room temperature electron transport measurements of the OFETs using CNT electrodes show better transistor characteristics compare to OFETs using gold electrodes due to improved charge injection from densely aligned and open-ended nanotube tips.

¹This work is partially supported by U.S. National Science Foundation under Grant ECCS 1102228.

C1.00077 Thermal Analysis of defects in Organic Light Emitting Diodes using Thermoreflectance imaging technique, ACHYUT SHRESTHA, Hampshire College, ANDREW DAVIS, KENNETH CARTER, University of Massachusetts-Amherst, JANICE HUDGINGS, Mt. Holyoke College — Organic light emitting diodes (OLEDs) have emerged as a next generation technology for flat panel displays. One of the factors inhibiting commercialization of this technology are their shorter life spans. Various defects induced during fabrication and operation tend to grow with time causing catastrophic failure of the device. In our work, we use thermoreflectance imaging (TR) to study defects in OLEDs. TR is based on measuring the change in reflectivity of the device as a function of temperature. We want to study the defects before catastrophic failure. We're interested in the physical origin of the defects, under what conditions failure occurs, and how defects affect current injection uniformity. Several defects including dark spots and bright spots on the surface of OLEDs are visible through the TR imaging. In our experiment, we are making controlled defects in OLEDs to study specific thermal maps of various kinds of defects. Understanding local temperatures and heat spread via TR imaging will provide better insight into formation of defects, which could be used to increase the lifetime and efficiency of OLEDs.

C1.00078 Correlation of interfacial width with device characteristics in all-polymer thin film transistors based on P(NDI2OD-T2), HONGPING YAN, NCSU, TORBEN SCHUETTERT, Cambridge, CHRISTOPHER MCNEILL, Monash Univ, HARALD ADE, NCSU — The interface between a conjugated polymer and a dielectric is critical to the performance of an organic thin-film transistor device, since charge transport occurs essentially along a 1 nm deep accumulation layer in the semiconducting polymer at the interface with the dielectric. Utilizing resonant soft x-ray reflectivity, we measure the interfacial widths of poly([N,N'-bis(2-octyldodecyl)-11 naphthalene-1,4,5,8-bis(dicarboximide)-2,6-diyl]-alt-5,5'-(2,2'-12 bithiophene)) and differentially cast dielectric layers of polystyrene (PS), poly(methyl methacrylate) (PMMA) or CYTOP, respectively. We demonstrate that devices with PMMA as the dielectric layer show the sharpest interface, whereas CYTOP has the largest. The measured widths correlate with the onset voltages of the thin-film transistor devices and anticorrelate with the activation energies in these three systems. A comparison to the surface roughness prior to differential casting furthermore indicates that deposition of the top dielectric layer affects the thus-formed interfaces to a different extent for various dielectric materials. Overall, the results suggest that further control of the interfacial properties during fabrication is required for ultimate performance.

C1.00079 Effect of bridging atom identity on the morphology of solution-processed small molecule bulk heterojunction photovoltaics, GREGORY SU, NANCY EISENMENGER, GREGORY WELCH, GUILLERMO BAZAN, EDWARD KRAMER, MICHAEL CHABINYC, University of California Santa Barbara — Organic bulk heterojunction photovoltaics have gained much attention based on their potential to be low-cost, large area modules. Solution-processable small molecules are attractive materials due to their well-defined nature and purity. We examine two small molecules that differ by the identity of one atom: 5,5'-bis{7-(4-(5-hexylthiophen-2-yl)thiophen-2-yl)-[1,2,5]thiadiazolo[3,4-c]pyridine}-3,3'-di-2-ethylhexylsilylene -2,2'-bithiophene, (SM_{Si}) and its carbon-bridged analog, (SM_C). Despite having similar absorption spectra and energy levels, SM_{Si} and SM_C have different thermal transitions and device performance. SM_{Si} melts at 215 °C, while SM_C melts at 145 °C, and similarly annealed devices based on blends of SM_{Si} or SM_C with [6,6]-phenyl-C₇₁-butyric acid methyl ester (PC₇₁BM) show power conversion efficiencies of ~3.4% and ~1.0%, respectively. To determine the origin of this difference, techniques including grazing incidence wide angle X-ray scattering, UV-Visible spectroscopy, optical microscopy, and *in situ* current-voltage measurements were employed to monitor morphological changes during thermal annealing. SM_C :PC₇₁BM devices exhibit a greater propensity to crystallize into large domains upon annealing, which is detrimental to performance. These results highlight the connections among structure, morphology, and performance and provide insight into the design and characterization of photovoltaic materials.

C1.00080 High Optical Quality Organic Thin Films for Nonlinear Photonics Fabricated by Molecular Beam Deposition, MARTEN BEELS, Lehigh University, IVAN BIAGGIO TEAM¹ — We use small donor-acceptor substituted organic molecules that sublimate without decomposition to fabricate organic thin films by organic molecular beam deposition. These thin films have thicknesses of the order of micrometers and are well adapted for integrated nonlinear optics. These films are essentially amorphous, without the formation of microcrystals. They combine a high third-order susceptibility of the order of 1000 times that of fused silica with a high optical quality. Surface roughness is below +/- 5 nm for micrometer thick films. The films have been shown to be durable and robust, with a long shelf life (>2 years). We successfully integrated such films with silicon-on-oxide waveguides which have been used to demonstrate ultrafast all-optical switching on the silicon photonics platform, successfully demultiplexing a 170 GBit/s signal to 42 GBit/s.

¹Lehigh University

C1.00081 Nanoscopic Assembly of Organic Semiconductors for Organoelectronic Devices, BENJAMIN J. RANCATORE, CLAYTON E. MAULDIN, Department of Chemistry, UC Berkeley, JEAN M.J. FRÉCHET, College of Chemistry, UC Berkeley, TING XU, Department of Materials Science and Engineering, UC Berkeley — Small molecule organic semiconductors have many advantages over their polymer counterparts, including high purity and well-defined electronic properties. To fabricate organoelectronic devices, they need to form smooth thin films with control over their spatial organization to tailor the electronic percolation pathway. A quaterthiophene (4T) containing alkyl and phenolic moieties was hydrogen-bonded to the 4-vinylpyridine groups of a block copolymer, polystyrene-*b*-poly(4-vinylpyridine) (PS-*b*-P4VP) or a homopolymer, P4VP. These supramolecules can be readily cast into uniform films where the 4Ts form oriented nanostructures without hindering the charge mobility. We also extended this supramolecular approach to blends of symmetrically and asymmetrically-functionalized organic semiconductors at various mixing ratios. Fundamentally, present studies shine light on how to synergize two self-assembly processes, i.e. molecular ordering of organic semiconductors and microphase separation of BCP, and provide useful guidance toward directed hierarchical assemblies in multi-component systems. Present studies may also open a new route for the fabrication of nanostructured thin films of organic semiconductors using solution processing.

C1.00082 Connecting the Nanodots: Programmable Nanofabrication of Fused Metal Shapes on DNA Templates, MAURICIO PILO-PAIS, SARAH GOLDBERG, ENRIQUE SAMANO, HENOK MEBRAHTU, Duke University, THOMAS LABEAN, North Carolina State University, GLEB FINKELSTEIN, Duke University — We present a novel method for producing complex metallic nanostructures of programmable design. DNA origami templates, modified to have DNA binding sites with a uniquely coded sequence, were adsorbed onto silicon dioxide substrates. Gold nanoparticles functionalized with the cDNA sequence were then attached. These seed nanoparticles were later enlarged, and even fused, by electroless deposition of silver. Using this method, we constructed a variety of metallic structures, including rings, pairs of bars, and H shapes. Due to the flexibility of the design these structures may offer great promise for electronic and plasmonic applications.

C1.00083 π -Conjugated Copolymers of Thiophene: Effect of Chain Architecture on the Physical and Optoelectronic Properties for Photovoltaic Applications, JOJO AMONOO, EMMANOUIL GLYNOS, CHELSEA CHEN, ANTON LI, JONAS LOCKE, ANNE MCNEIL, PETER GREEN, University of Michigan, Ann Arbor, JOJO AMONOO, EMMANOUIL GLYNOS, CHELSEA CHEN, ANTON LI COLLABORATION, JONAS R. LOCKE COLLABORATION — We found that polymer chain architecture strongly influences phase separation capabilities of the donor-acceptor blend in bulk heterojunction organic photovoltaic devices. Ni-catalyzed controlled polymerization was utilized to access new conjugated copolymers of 3-hexylthiophene and 3-(hexyloxy)methylthiophene, two donor polymers. Monomer sequence was controlled along the copolymer chain by the rate of addition of the comonomers, to achieve diblock, random and gradient copolymer chain architectures. This allowed us to study the effect of copolymer sequence of polythiophene based copolymer/[6,6]-phenyl-C₆₁-butyric acid methyl ester (PCBM) blend on the structure, nanoscale morphology and local charge transport properties using conductive and photoconductive atomic force microscopy. The gradient configuration showed the largest phase separation behavior with PCBM.

C1.00084 Organic-Inorganic Nanocomposites by Placing Conjugated Polymers in Intimate Contact with Quantum Rods, ZHIQUN LIN, XINCHANG PANG, LEI ZHAO, Georgia Institute of Technology — Semiconductor organic-inorganic nanocomposites were synthesized by directly grafting conjugated polymer poly(3-hexylthiophene) onto cadmium selenide nanorods surface (i.e., P3HT-CdSe NR nanocomposites). The direct grafting was accomplished by two simple yet robust coupling reactions: Heck coupling of vinyl-terminated P3HT with bromobenzylphosphonic acid functionalized CdSe NRs (i.e., BBPA-CdSe), and a newly developed catalyst-free click reaction of ethynyl-terminated P3HT with azide functionalized CdSe NRs. Such rationally designed nanocomposites possessed a well-defined interface between P3HT and CdSe NRs, thereby promoting the effective dispersion of CdSe NRs within the nanocomposites and facilitating their electronic interaction. The success of grafting was confirmed by nuclear magnetic resonance spectroscopy and dynamic light scattering. The occurrence of charge transfer at the P3HT/CdSe interface was evidenced by UV-Vis absorption, photoluminescence (PL), and time-resolved PL studies. Notably, the nanocomposites prepared by the catalyst-free click reaction exhibited a faster charge transfer from P3HT to CdSe. These nanocomposites offer a maximum interfacial area between the constituents for efficient exciton dissociation. As such, it represents a significant advance in rational design and fabrication of organic-inorganic hybrid solar cells with improved power conversion efficiency.

C1.00085 ABSTRACT WITHDRAWN —

C1.00086 Studies on Morphology of Three-component Polymer Solar Cells, YU GU, THOMAS RUSSELL, University of Massachusetts-Amherst — We prepared solar cells with an active layer that contains three components, including poly(3-hexylthiophene) (P3HT), a low bandgap polymer poly[2,6-(4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']-dithiophene)-alt-4,7-(2,1,3-benzothiadiazole)] (PCPDTBT) and [6,6]-phenyl C61-butyric acid methyl ester (PCBM). P3HT and PCPDTBT have complementary light absorption spectra such that, in parallel, the two cover a very broad range of the solar spectrum. It has been demonstrated that the power conversion efficiency of the P3HT/PCPDTBT/PCBM system is enhanced over that of either P3HT/PCBM or PCPDTBT/PCBM. Understanding the morphology developed for this system, therefore, can provide valuable insight into enhancing the performance of these technologically relevant and providing a fundamental challenge in controlling the phase behavior of such mixtures that undergo ordering. Morphological studies showed that the crystallization dynamics of P3HT was influenced by the presence of PCPDTBT. There are two domains existing in the thin films, one is pure P3HT domains and another is PCBM-rich domains mixed with amorphous PCPDTBT and P3HT.

C1.00087 Diketopyrrolopyrrole (DPP)-based low band gap polymers for efficient solar cells, FENG LIU, YU GU, UMASS-Amherst, CHENG WANG, LBNL, WEI ZHAO, DIAN CHEN, ALEJANDRO BRISENO, THOMAS RUSSELL, UMASS-Amherst — For bulk heterojunction (BHJ) organic photovoltaic (OPV) devices, effective strategies to maximize the performance have to be developed and fundamentally understood. In BHJ-type solar cells, the ability to control and optimize the active layer morphology is critical. A BHJ OPV of diketopyrrolopyrrole (DPP)-based low band gap polymer with phenyl-C71-butyric acid methyl ester (PCBM) was studied. DPP-based polymers are highly crystalline. The use of mixed solvents was critical in developing an optimal BHJ morphology, that was characterized by GISAXS and GIWAXS. In thin films, the polymer adopts an edge-on orientation and the blends are phase separated without thermal annealing. The diffusion of PCBM into the DPP polymer is markedly different from that observed with P3HT. The development of the morphology during solvent evaporation was studied in real-time by x-ray scattering and diffraction.

C1.00088 From carbon dioxide to organic compounds: Novel cathode materials for microbial electrosynthesis, MENG MENG CUI, TIAN ZHANG, HUARONG NIE, HAIYUN LU, DEREK LOVLEY, THOMAS RUSSELL, University of Massachusetts-Amherst — Electrode materials play an important role in the production of organic compound during microbial electrosynthesis, which uses bacteria as a catalysts to reduce carbon dioxide to organic compounds and stores electric energy in carbon-carbon bonds. An ideal electrode generally has high surface area, high electric conductivity, physical and chemical stability, and biocompatibility with bacteria. Based on these criteria, three types of materials were considered for the electrode design: CNTs, metal, and conductive polymers. Through a combination of these three materials, different properties were incorporated onto the electrodes for microbial electrosynthesis. The morphologies of the electrodes were characterized by high resolution TEM, SEM, and laser scanning confocal microscopy. The productivity of organic compounds was also verified.

C1.00089 Dynamics of Poly(ethyleneoxide) in the Presence of LiTFSI: Neutron Spin Echo and Dielectric Spectroscopy Study, CHANGWOO DO, Neutron Scattering Directorate, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, XIAO-GUANG SUN, Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, MICHAEL OHL, JÜRGEN ALLGAIER, Jülich Centre for Neutron Science, Forschungszentrum Jülich, 52425 Jülich, Germany, MARION GÖTZ, PETER LUNKENHEIMER, ALOIS LOIDL, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany, DIETER RICHTER, Jülich Centre for Neutron Science, Forschungszentrum Jülich, 52425 Jülich, Germany — Rechargeable lithium-ion batteries based on solid polymer electrolytes (SPEs) offer many advantages over their liquid counterparts. In comparison to a liquid electrolyte, the solid polymer is less flammable and more environmentally friendly. Issues such as microscopic dynamics of lithium ions and their dependence on their polymeric matrix are known to play a key role in determining the ionic conductivity in SPEs. Therefore, understanding of the microscopic dynamic characteristics of the lithium ions in relation with the dynamics of surrounding polymeric matrix is a crucial step for the interpretation of their transportation behavior and ultimately toward the control of their properties. Here, we investigated dynamics of poly(ethylene oxide) (PEO) in the presence of LiTFSI using neutron spin echo and dielectric spectroscopy techniques. Experimental results suggest that the dynamics of PEO is dramatically slowed down and strong correlation between ion transportation and alpha-relaxation of PEO.

C1.00090 Effect of Solvating Plasticizers on Ion Conduction of Polysiloxane Single-ion Conductors with Lithium Tetraphenyl Borate and Cyclic Carbonate Side Chains¹, U. HYEOK CHOI, SIWEI LIANG, Penn State University, MICHAEL O'REILLY, KAREN WINEY, University of Pennsylvania, JAMES RUNT, RALPH COLBY, Penn State University — We synthesize polysiloxane single-ion conductors containing two side groups: cyclic carbonates as a polar group and weak-binding tetraphenyl borate anions with Li⁺ counterions as an ionic group. With increasing ion content, the ionomer T_g increases because of ion aggregation, making the conductivity drop greatly. To enhance segmental mobility and decrease the tendency for ion aggregation, this ionomer was plasticized with poly(ethylene glycol) (M_n = 600, PEG600) to various extents. The room temperature conductivity of the plasticized ionomer is 3 orders of magnitude higher than that of the neat ionomer. Addition of PEG600 increases ion mobility by lowering T_g and increases conducting ion content due to raising the dielectric constant. This suggests that PEG600 plays an important role by solvating Li⁺ so as to lower T_g by dissolving ionic aggregates, consistent with X-ray scattering, which shows the ionomer aggregation peak decreases in intensity as PEG600 is added.

¹Supported by the Department of Energy under Grant BES-DE-FG02-07ER46409.

C1.00091 Fine-tuning Structures from Molecules to Nanophases: Insight into the Origin of Superior Organic Photovoltaic Efficiency¹, WEI CHEN, SETH DARLING, Center for Nanoscale Materials, Argonne National Laboratory — Organic photovoltaics (OPV) represent one of the most promising technologies for next-generation solar energy conversion due to their low-cost and scalability. To realize this potential, efficiencies must be improved for which a deeper understanding of the nanoscale morphology and molecular organization is required. Using the state-of-the-art PTB series of conjugated copolymers synthesized at the University of Chicago, we probed the internal structure of these materials both in solution and in films containing polymer/fullerene blends using a suite of tools spearheaded by neutron and x-ray scattering and, thereby, conceive the structural evolution from solution to thin films. Fine-tuning molecular structures via selective atomic replacement on the main chain of PTB copolymers, we gained unique insights into the structure-performance relationships, especially key features such as intermixing of polymers with fullerenes. Progress established in the course of these structural and morphological characterizations outline above will serve as the foundation for further improving the efficiency of polymer solar cells to realize their large-scale commercial use.

¹W. Chen gratefully acknowledges financial support from Argonne Director's Postdoctoral Fellowship. This work is partially supported by a University of Chicago-Argonne Strategic Collaborative Initiative Seed Grant.

C1.00092 Tuning Ion Conducting Pathways Using Holographic Polymerization¹, DERRICK SMITH, CHRISTOPHER LI, BIN DONG, Drexel University, TIMOTHY BUNNING, Air Force Research Lab — While much research has demonstrated repeatable characteristics of electrolyte membranes, the fundamentals behind the interactions during ionic diffusion in solid polymer electrolyte membranes for battery applications are not well understood, specifically the role of nanostructures, which hold the key to improving performance of energy storage devices such as fuel cells and Lithium ion batteries. The challenges in fabricating highly controlled model systems are largely responsible for the interdependent ambiguities between nanostructures and the corresponding ion conducting behavior. In this work, Holographic Polymer Electrolyte Membranes (hPEM) volume gratings comprised of alternating layers of crosslinked polymer resin and lithium ion salt were fabricated using holographic polymerization with an average d-spacing of approximately 200 nm. These one-dimensional confinement structures were used to quantitatively study the anisotropic ionic conductivity between the directions of in-plane and normal to the layers, and the unique ion conducting behavior was correlated with nanoscale phase separation. These volume gratings also offer an exciting route to fabricate multifunctional gratings for optic and sensing applications.

¹NSF DGE-0654313, CMMI-0900162 and DMR-0804838

C1.00093 Tuning interfacial interactions between conjugated polymers and inorganic nanocrystals for control over bulk thermoelectric properties, BORIS RUSS, NELSON COATES, SHANNON YEE, Department of Chemical Engineering, University of California, Berkeley, CA and Lawrence Berkeley National Laboratory, Berkeley, CA, JEFFREY URBAN, Lawrence Berkeley National Laboratory, Berkeley, CA, RACHEL A. SEGALMAN, Department of Chemical Engineering, University of California, Berkeley, CA and Lawrence Berkeley National Laboratory, Berkeley, CA — Electronic transport in conjugated polymers is highly dependent on doping level and chain conformation. Recent advances in next-generation thermoelectric devices rely on the fabrication of conjugated-polymer:inorganic-nanocrystal composites, but little is known about the how the thermoelectric properties are influenced by the doping level or morphology of the conjugated polymer at the organic-inorganic interface. A thorough understanding of the coupling between the molecular orbitals of conjugated polymers and the energy states of inorganic materials in such systems is, therefore, paramount for achieving improvements in these devices. In this study, we present our results on the coupling between Poly-(3-hexylthiophene) (P3HT), a well-studied conjugated polymer, with solution-processed lead selenide (PbSe) nanocrystals of controlled shape and morphology. Conjugated oligomeric ligands are used to tailor the organic/inorganic interface between P3HT/PbSe. Our results address the effects of polymer conformation on the nanocrystal surface, polymer doping levels, and organic-inorganic energy level alignment on the bulk thermoelectric properties of these hybrid materials.

C1.00094 Donor-acceptor block copolymer self-assembly in polymer-based photovoltaics, MICHAEL A. BRADY, SUNG-YU KU, JUSTIN E. COCHRAN, NEIL D. TREAT, CRAIG J. HAWKER, MICHAEL L. CHABINYC, EDWARD J. KRAMER, University of California, Santa Barbara — Polymer-based photovoltaics represent potentially low-cost, solution-processable devices for achieving sustainable energy generation. The optimal polymer-fullerene bulk heterojunction photovoltaic relies on a phase-separated microstructure in which domains of each component exist to allow for exciton dissociation at the interface and transport of each free electron (hole) through the n-type (p-type) domain to the cathode (anode). Due to the kinetically trapped, complex microstructure and phase-impure domains formed in this multi-component system, the development of a single-component material with pure n- and p-type domains is of great interest. Here we explore the microstructural evolution of a diblock copolymer of donor and acceptor segments, P3HT-b-DPP, due to various thermal treatments. Atomic force microscopy (AFM), resonant soft X-ray scattering (RSoXS), and grazing incidence wide-angle X-ray scattering (GIWAXS) are exploited to demonstrate that thermal treatments above the melting transition of each segment lead to an ordered domain structure containing both types of crystals. The effect of cooling rate from the melt on domain size and crystalline structure within those domains is investigated.

C1.00095 Synthesis and Characterization of a Systematic Series of All-Conjugated Diblock Copolymers¹, KENDALL SMITH, RAFAEL VERDUZCO, Rice University — All-conjugated block copolymers can potentially self-assemble into nanoscale structures beneficial for charge separation and transport, but due to synthetic challenges a comprehensive investigation of all-conjugated block copolymers has not been carried out. Here we detail a novel synthetic approach to all-conjugated block copolymers and characterize the structure of a systematic series of materials. The materials are prepared via copper-catalyzed azide-alkyne click chemistry followed by selective solvent removal of homopolymer impurities. This allows us to readily vary the molecular weight and type of each block in order to systematically study the properties of a family of block copolymers. As a system relevant to organic photovoltaics, we investigate a series of diblock copolymers based on poly(9,9-dioctyl-fluorene) and poly(3-alkylthiophene). This series of block copolymers is characterized with respect to phase behavior, including micro-phase segregation and crystallinity, optical properties, and charge mobilities.

¹This work was supported by the Welch Foundation for Chemical Research (Grant No. C-1750)

C1.00096 Incorporation of Functionalized Metal Oxides into Poly(Ethylene Oxide) Based Solid Polymer Electrolytes for Lithium-Ion Batteries, ERIC ANDERSON, YUYING TANG, University of Massachusetts Amherst Department of Polymer Science and Engineering, CRAIG VERSEK, MARK TUOMINEN, University of Massachusetts Amherst Department of Physics, SAMUEL GIDO, JAMES WATKINS, University of Massachusetts Amherst Department of Polymer Science and Engineering — A detailed study on the influence of size and shape as well as surface properties of metal oxides incorporated into poly(ethylene oxide) based solid polymer electrolytes for lithium-ion batteries is explored. The morphology of the solid polymer electrolyte is determined using small angle x-ray scattering and transmission electron microscopy. The surface properties of the metal oxide are modified through silane chemistry. Surfaces are modified to be hydrophobic, hydrophilic, high dielectric constants, as well as single-ion conductors. The electrochemical properties of the solid polymer electrolyte systems are investigated by electrochemical impedance spectroscopy and cyclic voltammetry. These functionalized metal oxide particles not only reduce crystallinity of poly(ethylene oxide) based solid polymer electrolytes, but also increase the conductivity.

C1.00097 Morphology Study of Bulk Heterojunction Solar Cells Based on PCDTBT, HSIN-WEI WANG, THOMAS RUSSELL, TODD EMRICK, UMass Amherst — To achieve high efficiency, the processing of conditions bulk heterojunction photovoltaic are important so that the desired morphology favoring efficient charge separation, electron and hole transportation can be generated. Solar cells based on poly[N-9'-hepta-decanyl-2,7-carbazole-alt-5,5-(4',7'-di-2-thienyl-2',1',3'-benzothiadiazole) (PCDTBT) as the donor system have been made. The effect of solvent, additives and annealing temperature have been systematically investigated. Grazing incidence small angle scattering (GI-SAXS), wide angle scattering (GI-WAXS), transmission electron microscopy (TEM), scanning electron microscopy (SEM) and atomic force microscopy (AFM) were utilized to study the morphology.

C1.00098 Comb-branched Polymer Electrolytes: Architectural Changes That Promote Increased Li^+ Transport, ROBERT DEMILLE, Department of Chemistry, University of Utah, SOWMYA MURTHY, DMITRY BEDROV, GRANT SMITH, Department of Materials Science and Engineering, University of Utah — The use of solid polymer electrolytes (SPEs) in the batteries of next generation technology applications is promising due to their safety and stability, yet is also hindered by low conductivity and high temperature requirements. Recent simulations of comb-branched poly(epoxide ether)-based SPEs have shown the comb-branched architecture to be able to overcome some of these hindrances. While providing the advantage of preventing crystallinity and allowing the optimization of the backbone to be decoupled from that of the side chain, the comb-branched SPE studied suffers from slow Li^+ cation dynamics due to coordination with the backbone. To improve Li^+ transport, we have modified the architecture of the comb-branched poly(epoxide ether) by attaching the side chains to the backbone with non-coordinating, flexible spacers. Inclusion of these spacers has resulted in a five-fold increase in the diffusion of Li^+ cation effected through 1) an increased side chain flexibility, 2) a decreased interaction of the cation with the dynamically slow backbone, and 3) quick conformational dynamics of the entire side chain. Additionally we report on other desirable architectural changes, such as including carbonate solvating moieties, to comb-branched SPEs allowing enhanced mobility of Li^+ .

C1.00099 Fluid Properties in Electromagnetic Fields¹, SEAN CANTU, University of Houston Clear Lake, SAMINA MASOOD, University of Houston Clear Lake — We study the effect of electromagnetic fields on the fluid properties to see if the modifications in the fluids properties are causing the effect of magnetic fields on the bacterial growth. For this purpose we design a simple experiment to study the changes in spectrum of light through the nutrient broth that is the fluid used to study the bacterial growth.

¹The authors will like to acknowledge TSGC grant for this submission

C1.00100 Electro-coflow as a route to drop generation, JOSEFA GUERRERO, ALBERTO FERNANDEZ-NIEVES, VENKATA R. GUNDABALA, Georgia Tech — We couple electric and hydrodynamic forces in glass-based microfluidic devices to generate droplets in steady state. The size of the drops can be larger, comparable and smaller than the tip diameter, which is the smallest geometric feature of the device.

C1.00101 Water nano-hydrodynamics: The interplay between interfacial viscosity, slip and chemistry, HSIANG-CHIH CHIU, School of Physics, Georgia Institute of Technology, DEBORAH ORTIZ-YOUNG, School of Chemistry, Georgia Institute of Technology, ELISA RIEDO, School of Physics, Georgia Institute of Technology — The understanding and the ability to manipulate fluids at the nanoscale is a matter of continuously growing scientific and technological interest. Fluid flow in nano-confined geometries is relevant for biology, polymer science and geophysics. The applications range from gene sequencing to protein segregation, cell sorting, sensors, nanotribology and diffusion through porous media. Here, we present experiments which show how the interfacial viscosity of water strongly depends on the wetting properties of the confining surfaces. This dependence is fully explained by considering water slippage at the stationary solid surface. The interfacial viscous forces as a function of six surfaces with different wettability are fitted with a modified form of the Newtonian definition of viscosity, which takes into consideration the fluid slip. This simple relationship can explain the viscosity measurements and permits us to extract a “slip parameter” for each investigated surface. This slip parameter is found to increase with the static contact angle of the solid surface as expected from previous work, bringing clear evidence of the relationship between viscosity and slip.

C1.00102 Investigating the hydrodynamics of asymmetrically driven polymer brushes in micro-channels¹, IBRAHIM SOUKI, MOHAMED LARADJI, University of Memphis, P.B. SUNIL KUMAR, Indian Institute of Technology Madras — The interfacial hydrodynamics between a polymer brush, under the influence of an asymmetric external driving field, and the surrounding solvent is explored across varying grafting densities, field strengths, and polymer chain lengths. A soft core model based on dissipative particle dynamics is used along with a 2-body FENE potential and a 3-body harmonic potential which define the internal mechanics of the polymer chains. The morphology of the polymer chains and the shearing produced at the interface layer between the polymer and solvent regimes is investigated as a function of hydrodynamic coupling to the external driving field. The momentum transfer and drag forces at the interface are shown to be the primary factors which lead to coupling and a directed non-zero net flow of the surrounding solvent through the coplanar nano-channel. The aim of the model is to introduce a novel mechanism to circumvent the large pressure gradients necessary to sustain fluid flow through micro/nano-pores as a consequence of Poiseuille's law.

¹This work was supported by NSF (EPS-1004083).

C1.00103 Solid Polymer Electrolytes by Self Assembly of Multi-Ionic Janus POSS Li-Salts in Polyethylene Oxide, STEPHANIE WUNDER, PARAMESWARA RAO CHINNAM, Temple University — Solid polymer electrolytes (SPEs), of which the most investigated has been polyethylene oxide (PEO), have low room temperature (RT) ionic conductivities and low lithium ion transport numbers. PEO is semicrystalline, with a glass transition temperature, T_g , of -60 °C and a melt temperature, T_m , of ~ 65 °C. Since lithium ion conduction occurs in the amorphous phase of PEO, conductivities $> 10^{-4}$ S/cm are only obtained after the crystalline domains have melted. Although high concentrations of lithium salts can eliminate the crystallization that causes the low conductivity at RT, the result is an amorphous liquid, not a solid. In order to impart structural rigidity to a noncrystalline PEO at RT, we have developed Janus-like multi-ionic lithium salts, in which one half of the salt is ionic in character, and the other half is hydrophobic. These salts are highly dissociative, imparting RT conductivities $> 10^{-4}$ S/cm and the hydrophobic ends aggregate. A phase separated morphology is formed in which the hydrophobic moieties form crosslink sites, and impart a solid state morphology, and the Li^+ ions dissociate into the conductive, amorphous PEO phase.

C1.00104 Molecular-based polyhedral crystalline colloids, MELINDA SINDORO, NOBUHIRO YANAI, STEVE GRANICK, University of Illinois at Urbana Champaign — We fabricate a new family of colloids with polyhedral morphology by controlled crystallization of metal ions and organic bridging ligands in the presence of capping reagents. The size and morphology of the crystalline colloids can be tuned by changing the ratio of the metal ions to the organic ligands and the amount of the capping reagents. Unlike spheres that isotropically interact along a curved surface, the polyhedral particles in suspension associate in a directional facet-to-facet fashion, forming clusters whose elemental units are orderly not only in interparticle distance but also mutual orientation. We also present unique supraparticle structures obtained by mixing different particles.

C1.00105 Molecular dynamic simulations of hydrophilically decorated poly-dots, SIDATH WJESINGHE, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — The structure and interfacial characteristics of nanoparticles formed by collapsed single conjugated polymer chains decorated with hydrophilic groups, poly *para* phenylene ethynylene (PPE) with substituted carboxylate side chains, have been studied by molecular dynamic simulations. These particles constitute a new type of light emitting/harvesting entities. Their interactions with the surrounding will determine their use where for example, directed interactions with membranes are essential for penetrating into organisms as bio markers. Trapping pre-decorated polymer chains into the nano dimensions with the expectations that some of the decorated groups will statistically reside at the nanoparticle interface has opened the way to control the surface decoration and hence the interactions of these particles. The effects of the distribution of the decorating groups along the polymer backbone on the conformation of the polymer chain within the poly dot and the resulting interfacial distribution of the COONa groups will be presented. The distribution of the hydrophilic groups at the surface of the particles will direct their interactions with the environment.

C1.00106 Optical Force Probe Microscopy of the Pericellular Matrix, LOUIS T. MCLANE, PATRICK CHANG, School of Physics, Georgia Institute of Technology, ANNA GRANQVIST, The Renal Center, The Wallenberg Laboratory for Cardiovascular Research, Sahlgrenska University Hospital, HEIKE BOEHM, New Materials and Biosystems, Max Planck Institute for Metals Research, Stuttgart, Germany, ANTHONY KRAMER, JENNIFER E. CURTIS, School of Physics, Georgia Institute of Technology — The pericellular matrix is a microns-thick grafted polymer film on the surface of cells. Its structure and mechanics influence processes as diverse as filtration, cell adhesion, proliferation, migration, cancer metastasis and possibly mechanotransduction. Optical force probe microscopy enables dynamic and equilibrium measurements of this polymer film on living cells. We show that equilibrium force measurements can be related to the osmotic pressure in the pericellular matrix, leading to a prediction of a spatially varying correlation length (mesh size) profile ranging from ~ 100 nm at the cell surface to 1000 nm near the edge of the cell coat. Assuming the film is brush-like, comparison to polymer brush theory provides estimates of the equilibrium brush length and the grafting density at the surface. The equilibrium length is consistent with that observed during dynamic force measurements, and the grafting density is close to that of maximal packing for the large, space filling molecules in the system - i.e. tethered polymers populated by semi-flexible side chains with cross sections $\sim 80 \times 400$ nm².

C1.00107 Mapping optical trapping energy of nanoparticles via confocal microscopy¹, MIN YAO LIM, Carleton College — Optical traps are highly focused laser beams that can hold and manipulate objects of microscopic scale. They are used to study the motion and energy of particles such as colloids or DNA molecules. In order to achieve this purpose we first propose to determine the energy of optical traps. We use a fluorescent nanoparticle ensemble within the optical trapping volume along with confocal microscopy to map the fluorescence intensity distribution of nanoparticles. This mapping allows us to calculate the trapping energy profile in three dimensions. We repeat this process with different trapping powers to find the depth of the trapping potential well as a function of trapping power. Trapping energy per trapping power thus measured is consistent with results obtained through previous methods such as fluorescence correlation spectroscopy conducted by our research group. With this technique of mapping trapping energy we can further study particle-particle interactions.

¹This research was funded by the National Science Foundation (NSF) Research Experience for Undergraduates (REU) grant PHY-0849416, NSF grant DMR-0923299 and the Karas Undergraduate Research Internship at Lehigh University.

C1.00108 Structural analysis of three-dimensional photonic crystals in nature¹, BEOM-JIN YOON, JUNG OK PARK, MOHAN SRINIVASARAO, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA — We studied the structural origin of the color and photonic band structure in exoskeletons of Eupholus weevils and dorsal wings of lycaenids butterflies. The internal structures of the insects were systematically investigated using focused ion beam (FIB) milling, and the optical response of the insects was observed by optical microscopy and a microspectrophotometer. A series of sequential SEM images were obtained during the FIB milling process and 3D structures were reconstructed by image processing. The correlation of the structures and the optical responses were studied by theoretical modeling. Diamond-based 3D photonic crystal lattice existed in Eupholus weevils, while gyroid structure was in lycaenids butterflies. The calculated photonic band structures matched the measured optical response. Aluminum oxide and titanium oxide were deposited on the weevils and the butterflies in order to study the effect of refractive index contrast to the photonic band structure and the optical response.

¹This work was partially supported by NSF funding (DMR-0907529).

C1.00109 Structure and Dynamics of Polymer-Coated Nanoparticles in Ionic Liquids Studied by In-Situ Electron Microscopy, PAUL KIM, THOMAS RUSSELL, DAVID HOAGLAND, Polymer Science and Engineering Department, University of Massachusetts, Amherst, MA 01002 — Ionic liquids (ILs) have unique solvent properties, including extremely low vapor pressure and high conductivity, which makes IL-solvated soft matter systems suitable to investigation by electron microscopy. ILs, as two-component solvents, may themselves organize into nanostructures, and these organizations can affect the behavior of dispersed polymers/particles. To understand these effects, the structure and dynamics of nanoparticles IL systems have been studied via multiple-particle tracking with electron microscopy. Several systems consisting of different polymer-coated nanoparticles, different ILs, and different substrates were prepared and analyzed with fluorescent microscopy, scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Spatial and temporal imaging information affords insight into particle-IL and polymer-IL interactions.

C1.00110 Polymer Conformation near the Critical Demixing Point of a Binary Solution, LILIN HE, Oak Ridge National Laboratory, GANG CHENG, Sandia National Laboratory, YURI MELNICHENKO, Oak Ridge National Laboratory — We have used Contrast Matching Small Angle Neutron Scattering (CMSANS) to probe directly the conformation change of polyethylene glycerol (PEO) chains in the critical demixing region of Acetonitrile-d₃ in (D₂O + H₂O) at concentration of the components corresponding to zero-average contrast condition. The d-PEO and h-PEO were mixed to match the scattering length density (SLD) of the critical liquid solution, which allowed us to extract single-chain dimension of polymer molecules in the aggregates near the critical point of the solvent. A non-monotonic variation of R_g was detected as temperature approached the critical temperature of phase demixing of acetonitrile- water solution, which was attributed to the interaction asymmetry of the solvent molecules with polymers predicted by Brochard and de Gennes two decades ago. To our best knowledge, this is the first direct experimental evidence supporting this prediction.

C1.00111 Fluorescent Polystyrene Sulfonate for Polyelectrolyte Studies, WAYNE HUBERTY, XIAOWEI TONG, SREELATHA BALAMURUGAN, DONGHUI ZHANG, PAUL RUSSO, Louisiana State University — The slow-mode decay found by dynamic light scattering for polyelectrolytes in low-salt conditions has perplexed investigators since its first observation. Many characterization methods have suggested temporary or transient aggregation, although there is still no consensus on the cause. Many different polyelectrolytes demonstrate the slow-mode decay, but the sodium salt of polystyrene sulfonate (NaPSS) is the most popular choice for study. Commercially available NaPSS may have hydrophobic patches due to incomplete sulfonation leading to associations apart from any putative ionic mechanisms. Therefore, essentially full sulfonation, or "patchless", NaPSS should be synthesized. To facilitate fluorescence measurements, which can provide new insights to the slow-mode phenomenon, the material must be rendered fluorescent (F-NaPSS). Several approaches to F-NaPSS have appeared; some labeled a previously synthesized NaPSS without concern for its hydrophobic patches. Other strategies include a free radical copolymerization of styrene sulfonate and a vinyl amine to provide side chains viable for labeling. This method is successful, but yields only small amounts of nearly monodisperse polymer after fractionation. In this presentation, a high-yield synthesis of fully sulfonated, low-polydispersity, fluorescently tagged polymer will be discussed.

C1.00112 Electromagnetic Propagation of Waves in Helical Stochastic, REYES ADRIAN, DAVID MENDEZ, Instituto de Fisica Universidad Nacional Autonoma de Mexico — We develop a model for studying the axial propagation of elliptically polarized electromagnetic waves in a spatially random helical media. We start by writing Maxwell equations for a structurally chiral medium whose helical angle contains both a stochastic contribution and a deterministic one, this latter corresponding to a uniform rotation. We write the electromagnetic equations into Marcuvitz Schwinger representation to transform them afterward by using the Oseen transformation. We exhibit that in the Oseen frame, Marcuvitz Schwinger equations turns out to be a linear vectorial stochastic system of equations with multiplicative noise. From this result and utilizing a well known formalism for treating stochastic differential equations, we find the governing equations for the first and second moments of the field amplitudes for a general correlation model for the slope angles, and calculate their corresponding band structure for a particular spectral noise density. We show that the average resulting electromagnetic fields exhibit dissipation and the appearance of a new reflection band whose chirality is the opposite of the one obtained for a simple cholesteric liquid crystals.

C1.00113 Flow Instability of Soft Gels from Pluronic F108 Aqueous Solution Under Steady Shear, HANJIN PARK, Rensselaer Polytechnic Institute, GYOO YEOL JUNG, Pohang University of Science and Technology, CHANG YEOL RYU, Rensselaer Polytechnic Institute — Nonionic surfactants of Pluronic tri-block copolymers have received special interest during the past decades because of the temperature dependent self-assembly characteristics that would lead to the formation of hydrogels upon heating. Here, we investigate the gelation behavior of Pluronic F108, (PEO)132-(PPO)50-(PEO)132, aqueous solution with an aim to elucidate how the shear affects the thermo-reversible transitions between micellar liquids and hydrogels. Specifically, we have studied the rheological characteristics of soft gels as an intermediate state between liquid to hard gels. From steady shear experiments, we found that there exists a shear rate window, where the flow instability of soft gels is observed. On the contrary, non-Newtonian behaviors following power-law are still observed at the shear rates above and below the shear rate window showing the flow instability. Small angle x-ray scattering and dynamic light scattering experiments had been performed to reveal how the temperature dependent rheological behavior correlates with the structural changes in the micellar aqueous solutions of F108.

C1.00114 Fourth-order Fluctuations near the Colloidal Glass Transition, CHRIS WAGENBACH, NATHAN ISRAELOFF, Northeastern University — Fourth-order statistical fluctuations are probed in order to determine the size of cooperative regions as the colloidal glass transition is approached. The experiment makes use of the electrical conductance of a colloidal fluid containing KCl measured through a micropore in a membrane placed in the colloid. The diameter of this micropore is adjusted to be at least ten times the diameter of the colloidal particles. The dynamics of the particles near and within the pore are revealed in the fluctuations of the conductance. For the largest particles, a polydisperse sample of 106 to 125 microns, the dynamics are driven by a mechanical shaking, while for the smaller particles, <10 microns, Brownian motion drives the dynamics. Using a spherical probe, we mapped the conductivity change near the pore which enabled us to determine that the effective volume for the fourth-order fluctuations was $\sim 1.5D^3$, where D is the diameter of the membrane pore. Thus, near the glass transition at a volume fraction of .58, the number of particles probed is about 1700 which is small enough to see the growth of fourth-order fluctuations. It is hoped that this technique can be applied to very small, ~ 100 nm, particles for which the cooperative length can be studied over a wide range of volume fractions.

C1.00115 Migration of Surfactant Vesicles during spontaneous emulsification, DOMINIK MICHLER, NOUSHINE SHAHIDZADEH, RUDOLF SPIRIK, PETER SCHALL, DANIEL BONN, Soft Matter, Van der Waals-Zeeman Instituut, Universiteit van Amsterdam, SHELL COLLABORATION — In aqueous AOT solutions, micrometer sized vesicles appear above the critical micelle concentration. These vesicle move spontaneously towards an oil interface and form an emulsion under the condition of ultra low interfacial tension. We discuss the probable mechanisms that lead to the migration behavior of these vesicles.

C1.00116 Controlling Droplet Impact with Polymer Additives, MICHAEL SMITH, University of Nottingham, VOLFANGO BERTOLA, University of Liverpool — When a water drop falls on to a hydrophobic surface, such as the waxy leaf of a plant, the drop often bounces off leading to wasted agrochemicals which harm the environment. However, adding small quantities ($\sim 100 \mu\text{gml}^{-1}$) of a flexible polymer can completely prevent rebound. This is surprising since the shear viscosity and surface tension of such drops are almost identical to those of pure water. The effect has for some time been explained in terms of the stretching of polymer chains by a velocity gradient in the fluid, resulting in a transient increase in the so-called “extensional viscosity.” We have developed an epi-fluorescent microscope system, to visualise the flow of fluid inside an impacting drop using tracer particles at 2000 fps. Analysis of the velocity as a function of radius showed negligible differences between water and polymer drops except near the edge, indicating that the extensional viscosity cannot be responsible for the anti-rebound effect. To probe the true mechanism, fluorescently labelled λ -DNA was used to visualise the edge of an impacting drop. During the retraction phase, DNA was shown to be stretched by the retreating droplet providing an “effective friction” at the contact line.

[1] M.I Smith and V. Bertola, Phys. Rev. Letts. 104, 154502 (2010).

C1.00117 Glints of light reveal properties of coiled electrospinning jets in flight, DARRELL H. RENEKER, KAIYI LIU, The University of Akron — Optical observations of jets provide information needed to control features of polymer nanofibers produced by electrospinning. Quantitative information about the location, vector velocity, and rotation of selected segments of the multiply coiled path of an electrospinning jet of polymer solution was provided by a combination of videography, stereography, and stop motion flash photography. Visual observations of a jet depend largely on glints of incident light that are specularly reflected from particular places on the multiply coiled jet path. The traces of moving glints bifurcate when a new turn is added to a coil, at an observed rate of 600 turns per second. The polarization of light, in glints reflected at Brewster's angle, allows measurement of the index of refraction of the fluid in a jet, in flight. Strategic placement of lights to either illuminate, or leave dark, parts of the coils, make both the handedness and changes in handedness of the electrical bending coils apparent to visual observation. The changes occurred at intervals of a few seconds in our experiments. Evidence was found, in the form of ribbon-like glint traces that were polarized, for the occurrence of undulations on the surface of some jets.

C1.00118 Digital Reconstruction of 3D Polydisperse Dry Foam, A. CHIECO, K. FEITOSA, Dept. of Physics and Astronomy, James Madison University, A.E. ROTH, P.T. KORDA, D.J. DÜRIAN, Dept. of Physics and Astronomy, University of Pennsylvania — Dry foam is a disordered packing of bubbles that distort into familiar polyhedral shapes. We have implemented a method that uses optical axial tomography to reconstruct the internal structure of a dry foam in three dimensions. The technique consists of taking a series of photographs of the dry foam against a uniformly illuminated background at successive angles. By summing the projections we create images of the foam cross section. Image analysis of the cross sections allows us to locate Plateau borders and vertices. The vertices are then connected according to Plateau's rules to reconstruct the internal structure of the foam. Using this technique we are able to visualize a large number of bubbles of real 3D foams and obtain statistics of faces and edges.

C1.00119 Asymptotic Behavior in Liquid Drop Coalescence, JOSEPH PAULSEN, JUSTIN BURTON, SIDNEY NAGEL, University of Chicago, SANTOSH APPATHURAI, MICHAEL HARRIS, OSMAN BASARAN, Purdue University — During coalescence, two drops first touch and then merge, as a liquid bridge grows from initially microscopic scales to a macroscopic size comparable to the drop diameter. The initial dynamics of coalescence are expected to be universal, owing to a singularity in the Laplace pressure, which diverges when the curvature of the liquid interface is infinite at the point where the drops first touch. Conventionally, this process has been thought to have just two regimes: a highly viscous one dominated by macroscopic flows pulling the two drops together and an inertial one described by local deformations near the growing neck. We use high-speed imaging, electrical measurements and full Navier-Stokes simulations to reveal a new regime that dominates the asymptotic dynamics of coalescence for any finite viscosity. The character of this new regime improves our understanding of the unexpectedly late viscous-to-inertial crossover [1]. An argument based on force balance and an appropriate choice of length-scales allow the construction of a new phase diagram of coalescence.

[1] J. D. Paulsen, J. C. Burton, S. R. Nagel, PRL 106, 114501 (2011).

C1.00120 Carbon nanotube-induced chirality and macroscopic helical twist in achiral liquid crystals, RAJRATAN BASU, KRYSTA BOCCUZZI, SAMEH FERJANI, Case Western Reserve University, ROBERT LEMIEUX, Queen's University, ROLFE PETSCHKE, CHARLES ROSENBLATT, Case Western Reserve University — A small quantity of carbon nanotubes was dispersed in an achiral liquid crystal, and the mixture was found to exhibit a weak degree of chirality both in the smectic and nematic phases. The induced chirality in the LC was probed by means of the electroclinic effect in the liquid crystal's smectic-*A* and nematic phases, which showed significant pretransitional behavior on approaching the smectic-*A* – smectic-*C* and the nematic – smectic-*A* transition temperatures, respectively, from above. The carbon nanotubes also were found to induce a bulk twist over macroscopic dimensions in an achiral nematic matrix. The nanotube-induced chiral pitch length *P* was determined as a function of average nanotube concentration by measuring the radii of curvature of reverse twist disclination lines in 90° twist nematic cells. The results reveal information about the nanotubes' spatial distribution inside the cells. A concentration for the onset of significant aggregation of the nanotubes can be quantified from the apparent saturation of P^{-1} at higher concentrations. The macroscopic helical twisting power of the nanotubes has been estimated from the results. The results indicate that there is a net chirality associated with the carbon nanotubes, which is transmitted into the achiral liquid crystal.

C1.00121 Pretransitional Clusters in Multicolor Liquid Crystalline Honeycombs¹, GORAN UNGAR, XIANGBIN ZENG, FENG LIU, Dept. Materials Sci. Eng., University of Sheffield, Sheffield, UK, ROBERT KIEFFER, CONSTANCE NÜRNBERGER, CARSTEN TSCHIERKE, Institute of Organic Chemistry, Martin Luther University, Halle, Germany, GILLIAN GEHRING, Dept. Physics & Astronomy, University of Sheffield, Sheffield, UK — X-shaped tetraphilic molecules consisting of a rod-like core with two hydrogen-bonding terminal groups and two mutually incompatible side-chains A and B form a range of honeycomb-like structures in which the rods act as bricks in the walls of polygonal cylinder cells containing the fluid side-chains. Some of these systems exhibit a 2nd-order transition from the high-temperature mixed ("1-color") phase to a low-temperature phase in which the side-chains are separated in A and B cells ("2-color"). This is the situation with triangular, rectangular and square honeycombs. Strong pre-transitional 2-color domains formation is observed above the transition temperature. Particularly interesting is the case of the hexagonal honeycomb, where no fully phase-separated ground state can exist. Here the 2-color "ordered" phase consists of [A] cells and [A(1/4)B(3/4)] cells. The situation is similar to frustrated ferro- and antiferromagnets on a kagome lattice. Instead of the spins flipping, it is the molecules that undergo 180 degree rotations about the axis of their rod-like cores [Science 331, 1302 (2011)].

¹This work was supported by EU FP7 project NANOGOLD grant 228455, ESF Eurocores project SCALES and WCU program of NRF Korea no. R31-10013.

C1.00122 Compaction of DNA with Lipid Modified Silica Nanoparticles, SUSHMA SAVARALA, STEPHANIE L WUNDER, MARC ILIES, Temple University — There is an increasing interest in modified inorganic nanoparticles, polymers or hybrid polymer-inorganic nanoparticles for use in DNA transfection, rather than viral vectors or liposomes. Adsorption of the DNA to the nanoparticles prevents enzymatic degradation of the DNA, although the reason for this protection is not completely understood. In order to compact the negatively charged DNA, a positively charged surface is required, and for transfection applications, the nanosystems must remain stable in suspension. It is also useful to minimize the amount of cytotoxic cationic lipid needed for DNA compaction in delivery applications. Here we investigate the colloidal stability of supported lipid bilayers (SLBs) composed of mixtures of 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC, 14:0 PC) and 1,2-dimyristoyl-3-trimethylammonium-propane (DMTAP, 14:0 TAP), and their ability to compact plasmid DNA. Ionic strengths and DMPC/DMTAP ratios that resulted in SLB formation, no excess small unilamellar vesicles (SUVs) in the suspensions, and colloidal stability, were determined. DNA/SLB/lipid ratios that resulted in compaction were then investigated.

C1.00123 Tunable and regenerative DNA zipper based spring, PRESTON LANDON, ALEXANDER MO, ALAN GILLMAN, BRIAN MECKES, SRINIVASAN RAMACHANDRAN, RATNESH LAL, Department of Bioengineering and Department of Mechanical and Aerospace Engineering, University of California, San Diego, La Jolla, CA 92093, U.S.A. — We report a DNA zipper based actuator device termed 'DNA- spring' with tunable and repeated cycles of extension and contraction ability. DNA zipper is a double-stranded DNA system engineered to open upon its specific interaction with appropriately designed single strand DNA (ssDNA), opening of the zipper is driven by binding energy differences between the DNA strands. The zipper system is incorporated with defined modifications to function like a spring, capable of delivering approximately 9 pN force over a distance of approximately 13 nm, producing approximately 116 kJ/mol of work. Time-lapse fluorescence and fluorescent DNA gel electrophoresis analysis is utilized to evaluate and confirm the spring action. A second zipper incorporated into the spring provides the ability to couple/decouple to an object/substrate. Such devices would have wide application, including for conditionally triggered molecular delivery systems and as actuators in nano-devices. zippers.

C1.00124 Single particle tracking for a particle in a thermo-osmotic trap, MARK NOLAN CONFESOR, PIK-YIN LAI, Department of Physics and Graduate Institute of Biophysics, National Central University, Taiwan, C.K. CHAN, Institute of Physics, Academia Sinica, Taiwan — Recently Jiang et al. (PRL 102, 2009) showed that colloidal particles in a polymer solution can be trapped by imposing a local temperature gradient. It is believed that the thermophoresis of the polymers leads to a polymer concentration gradient that drives the colloids to get trapped. We investigate the trapping force further by performing single particle tracking of a probe colloidal particle. Our system consists of Polystyrene beads immersed in PEG solution. We impose a temperature gradient by shining an IR laser to a chromium coated surface. We found the particle position distribution to have non-Gaussian tails but quiet symmetric for the radial positions. However we found quiet asymmetric distribution for the axial positions where the particle likes to stay very close to the heated surface. From the distribution we read out the trapping potential. We will present results for the dependence of the trapping potential to particle size and polymer concentration.

C1.00125 Controlled Transport of Functionalized Nanochannel through Lipid Membrane, MEENAKSHI DUTT, Dept of Chemical and Biochemical Engineering, Rutgers University, OLGA KUKSENOK, ANNA C. BALAZS, Chemical Engineering Dept, University of Pittsburgh — Via the Dissipative Particle Dynamics approach, we study the directed transport of a transmembrane nanochannel to a desired location within a lipid bilayer. Each nanochannel encompasses an ABA architecture, with a hydrophobic shaft (B) with two hydrophilic ends (A). One of the ends of the nanochannel is functionalized with hydrophilic functional groups, or hairs. The hydrophilic hairs serve a dual role: (a) control transport across the membrane barrier, and (b) enable the channel relocation to a specific membrane site. Our system comprises a lipid membrane with an embedded transmembrane nanochannel with the hairs extending into solution. First, we hold a suitably functionalized pipette above the membrane while the nanochannel freely diffuses within the membrane. For an optimal range of parameters, we demonstrate that the hairs find the pipette and spontaneously anchor onto it. We then show that by moving the pipette for a range of velocities, we can effectively transport the channel to any location within the membrane. This prototype assembly can provide guidelines for designing a number of systems for biomimetic applications.

C1.00126 Molecular Dynamics Simulations of Phosphatidylinositol Bisphosphate (PIP₂), DAVID SLOCHOWER, PAUL JANMEY, University of Pennsylvania — We are interested in the dynamics of membranes containing the highly charged phospholipid phosphatidylinositol bisphosphate (PIP₂ or PtdInsP₂). We performed a geometry optimization at the Hartree-Fock 6-31+G* level of theory to determine the biological conformation of the phospholipid headgroup in the presence of water and partial charge distribution. The angle between the headgroup and the acyl chains that form an anchor in the membrane is 94°, indicating that the inositol ring may lie flat along the surface of the inner plasma membrane. Next, we employed hybrid quantum mechanics/molecular mechanics simulations to investigate the protonation state of PIP₂ and its interactions with physiological divalent cations such as magnesium and calcium. Based on preliminary data, we propose that the binding of magnesium to PIP₂ is mediated by a water molecule that is absent when calcium binds. These results may explain the ability of calcium to induce the formation of PIP₂ clusters and phase separation from other phospholipids.

C1.00127 Divalent cation-induced cluster formation by polyphosphoinositides in model membranes¹, YU-HSIU WANG, PAUL JANMEY, University of Pennsylvania — Phosphatidylinositol-(4,5)-bisphosphate (PI4,5P2) binds with variable levels of specificity to hundreds of intracellular proteins in vitro. Such restricted targeting of proteins to PIP2 in cell membranes is thought to result in part from the formation of spatially distinct PIP2 pools. The hypothesis that PIP2 forms nanodomains in the membrane by electrostatic interactions with divalent cations is tested using lipid monolayer and bilayer model membranes. Competitive binding between Ca²⁺ and Mg²⁺ to PIP2 is quantified by surface pressure measurements and analyzed by a Langmuir competitive adsorption model. Addition of Ca²⁺, but not Mg²⁺, Zn²⁺ or polyamines to PIP2-coating monolayers induces surface pressure drops coincident with the formation of PIP2 nanodomains visualized by fluorescence, atomic force and electronic microscopy. Studies of bilayer membranes using probe-partitioning fluorescence resonance energy transfer (FRET) and fluorescence correlation spectroscopy (FCS) also reveal Me²⁺-induced domain formation or diffusion retardation which follows the trends: Ca²⁺ >> Mg²⁺ > Zn²⁺, while polyamines have minimal effects. These results suggest that divalent metal ions have substantial effects on PIP2 lateral organization under their physiological concentrations.

¹This work is supported by NIH grants GM083272 (PAJ) and HL067286 (Y-H W).

C1.00128 Driven Brownian transport through arrays of symmetric obstacles, STEFFEN MARTENS, Humboldt-University Berlin, Department of Physics, Newtonstr. 15, 12489 Berlin, Germany, PULAK K. GHOSH, Advanced Science Institute, RIKEN, Wako-shi, Saitama, 351-0198, Japan, PETER HÄNGGI, University Augsburg, Department of Physics, Universitätsstr. 1, 86135 Augsburg, Germany, FABIO MARCHESONI, Università di Camerino, Dipartimento di Fisica, 62032 Camerino, Italy, FRANCO NORI, Advanced Science Institute, RIKEN, Wako-shi, Saitama, 351-0198, Japan, LUTZ SCHIMANSKY-GEIER, Humboldt-University Berlin, Department of Physics, Newtonstr. 15, 12489 Berlin, Germany, GERHARD SCHMID, University Augsburg, Department of Physics, Universitätsstr. 1, 86135 Augsburg, Germany — The transport of a suspended overdamped Brownian particle driven through a two-dimensional rectangular array of circular obstacles with finite radius is numerically investigated [P. K. Ghosh et. al., *Phys. Rev. E*, submitted (2011)]. Two limiting cases are considered in detail, namely, when the constant drive is parallel to the principal or the diagonal array axes. This corresponds to studying the Brownian transport in periodic channels with reflecting walls of different topologies. The mobility and diffusivity of the transported particle in such channels are determined as functions of the drive and the array geometric parameters. Prominent transport features, like negative differential mobilities, excess diffusion peaks, and unconventional asymptotic behaviors, are explained in terms of two distinct lengths, the size of single obstacles (trapping length) and the lattice constant of the array (local correlation length). Local correlation effects are further analyzed by continuously rotating the drive between the two limiting orientations.

C1.00129 Hydrophobic Drug Encapsulation Mechanisms of an Injectable Self-Assembling Peptide Hydrogel, JESSIE E.P. SUN, University of Delaware, JOEL P. SCHNEIDER, National Cancer Institute at Frederick, DARRIN J. POCHAN, University of Delaware — We examined a beta-hairpin peptide network that is a shear thinning injectable solid with immediate rehealing behavior. These rheological properties result from the entangled and branched fibrillar nanostructure of the hydrogel networks. The fibrils are formed by the intramolecular folding and subsequent intermolecular assembly of the self-assembling peptides. Taking advantage of the nanofibrillar peptide structures, the hydrogel can be used to encapsulate curcumin, a hydrophobic, natural anticancer agent and indian spice. The hydrogel shields curcumin from the environment while depositing it exactly where it is intended through syringe injection, taking advantage of the hydrogel shear thinning and rehealing behavior. How the network envelopes and interacts with the curcumin is examined using fluorescence and electron microscopy methods to better understand the exact mechanisms and behaviors of the gel itself and the gel-curcumin construct.

C1.00130 PNIPAM: an amphiphilic polymer probing the mean energetic state of water, IRMGARD BISCHOFBERGER, University of Fribourg, Department of Physics, PAOLO DE LOS RIOS, EPF Lausanne, Laboratory of Statistical Biophysics, ILIAN JELEZAROV, University of Zürich, Department of Biochemistry, VERONIQUE TRAPPE, University of Fribourg, Department of Physics — We find that the effect of alcohol on the thermodynamic properties of aqueous solutions of poly-N-isopropyl acrylamide (PNIPAM) directly relates to the mixing enthalpy of the water/alcohol mixture itself. This correlation between solution and solvent thermodynamics indicates that the thermodynamics of aqueous solutions of PNIPAM is primarily determined by the mean energetics of the solvent. Such behavior sheds light on the nature of hydrophobic hydration, which we will discuss in this contribution.

C1.00131 Single molecule discrimination as the sequential hypothesis testing, maximum information gain measurement, ALEXEI GOUN, Postdoctoral researcher — Detection of single molecule and single molecule complexes is used widely in the field of molecular biology, biochemistry, physical chemistry. The task is often to discriminate among several distinct possibilities such as which molecule (A,T,C,G) out of the set is present, is the excitation transfer pair in bound or loose state. At present the approach is to accumulate the sufficient statistics for reliable discrimination among the possible outcomes. We suggest the different approaches that adjust the experimental conditions on every step of the measurement in order to maximize the expected information gain of the experiment. The approach is illustrated on the task of single molecule discrimination. Our simulation shows that approach based on sequential hypothesis testing and sequential experimental planning outperforms traditional maximum likelihood hypothesis testing.

C1.00132 Force extension response of single self-associating polymer chains, CHARLES SING, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — The structure and dynamics of polymeric molecules plays a crucial role in a number of synthetic and biological processes. Great progress has been made in using force spectroscopy methods, such as optical tweezers and atomic force microscopy, to probe these properties of single molecules in novel ways. While there has been significant advances at using analytical theory to model the behavior of, for example, single domain unfolding or multi-domain unfolding of identical domains, we consider for the first time the force-extension behavior of self-associating homopolymers. We use a Brownian dynamics simulation with a Bell-like association model that represents, in a coarse-grained fashion, biological polymers such as von Willebrand Factor that use domain-domain interactions to modulate a larger quaternary structure. We also present a theoretical description of pulling that utilizes a master equation description of the relevant coordinate of the polymer network's "shortest chain." We can accurately reproduce the force-extension features, notably the appearance of a dissipative plateau upon the increase of the association time scale, and provide a clear conceptual description of the appearance of this feature. Qualitative comparison to von Willebrand pulling in experiment is shown.

C1.00133 Modeling the Strength of β -sheet Structures in Silk Crystals and Protein Molecules, DAVID GRUBB, Materials Science & Engineering, Cornell University — The mechanical response of β -sheet structures to a tensile force directed along the axis of one chain can be modeled as an array of elastic springs. The 3-D potential of H-bonds in β -sheets gives a shear stiffness of 4.5Nm^{-1} and the chain repeat stiffness is 60Nm^{-1} . Nanocrystals $>3.5\text{nm}$ long with ≥ 20 H-bonds/chain are the strong component of spider silk. They behave much like macro-scale objects, and two conditions must be met for pull-out failure: (1) the load on the most stressed H-bond exceeds the bond strength. (2) the energy of the system is lower after failure. (1) is the critical condition, and the predicted pull-out load is 3-4 times the H-bond strength. An energetically favorable 'stick-slip' process is kinetically forbidden. Arrays within a single molecule such as titin have fewer bonds and can fail at low loads by the 'stick-slip' process. The logarithmic rate dependence of failure load observed in AFM is 50pN/decade and the stick-slip prediction is 30pN/decade . Simulations at short times and high loads give slopes $>10\times$ higher, matching the prediction for failure at a single bond.

C1.00134 Searching DNA by Brownian Motion of Transcription Factors, ROBIJN BRUINSMA, Department of Physics and Astronomy, UCLA, ALEXANDER GROSBERG, Theoretical Biophysics, New York University — Transcription factor proteins are able to locate their DNA operator binding site by slide-skip motion along DNA without getting trapped by the large binding energy fluctuations associated with partial recognition. Mirny and Slutsky proposed that this can be avoided by assuming that partial recognition involves increased strain energy of the protein. We present an analytical model for such a search in the form of a 2D random walk with DNA arc-length and an internal configurational parameter as coordinates. This leads to a relation between the nature of the DNA randomness and the optimal choice for the internal energy spectrum.

C1.00135 Anomalous Freezing Behavior of Nanoscale Liposomes¹, ERIC SPANGLER, MOHAMED LARADJI, University of Memphis, SUNIL KUMAR, IIT Madras, Chennai, India — Experiments have shown that the melting transition of small liposomes is broadened when compared to large vesicles or planar membranes. Despite their significant biological and biomedical importance, theoretical and computational studies of the phase behavior and structural properties of small liposomes have been limited. Presented here is a systematic computational study of the phase behavior and structural properties of liposomes using a recently developed coarse-grained particle-based model. Great assiduity was given on the effect of liposome diameter on their thermal and structural properties. Below the melting transition, liposomes are faceted with the gel facets separated by “grain” boundaries that are in the fluid phase. In agreement with experiments, we found that the melting transition is significantly broadened as the liposome diameter is decreased and that the heat capacity exhibits two distinct peaks for diameters less than 33 nm, an indication of a decoupling of the melting transition of the two leaflets. This decoupling is clearly demonstrated by the chain order parameters of the two leaflets, which show that the upper leaflet undergoes a melting transition before the inner leaflet.

¹This work is supported by NSF grants (DMR-075547 and EPS-1004083).

C1.00136 Desalination membranes from functional block copolymer via non-solvent induced phase inversion, HYEMIN SUNG, Korea University, JUSTIN POELMA, FRANK LEIBFARTH, CRAIG HAWKER, University of California, Santa Barbara, JOONA BANG, Korea University — Commercially available reverse osmosis (RO) and forward osmosis (FO) membranes are most commonly derived from materials such as polysulfone, polyimide, and cellulose acetate. While these membranes have improved the efficiency of the desalination process, they suffer from mechanical and chemical stability, fouling issues, and low fluxes. In this study, we combine a well-established membrane formation method, non-solvent-induced phase separation, with the self-assembly of a functional amphiphilic block copolymers. An amine and acid functional polystyrene-block-poly(ethylene oxide-co-allyl glycidyl ether) were chosen for the membranes. Membranes were formed by casting a concentrated polymer solution (12 to 25 wt% polymer) on PET fabric followed by immersion in a non-solvent bath. Scanning electron microscopy revealed an asymmetric porous structure consisting of a dense skin layer on top of a highly porous layer. Membrane performance was investigated using an FO test cell under the seawater condition.

C1.00137 Morphological study on a phospholipid mixture and their Dependence of Temperature, Concentration and Chemical Composition, YING LIU, University of Connecticut Chemical Engineering, YONGKUN YANG, University of Connecticut Polymer Program, MU-PING NIEH, University of Connecticut Chemical Engineering/IMS — A variety of morphologies, such as nanodiscs (bicelles), bilayered ribbons, unilamellar vesicles (ULVs), multi-lamellar vesicles (MLVs) and perforated lamellae exist in phospholipid mixtures composed of a long chain phosphatidylcholine (PC), its charged counterpart (i.e., phosphatidylglycerol, PG with the same hydrophobic chain length) and a short-chain PC. Here, we present a comprehensive structural characterization of such mixtures with various combinations of long-chain (e.g., di-14, di-16, di-18 PC) and short-chain (e.g., di-06, di-07 PC) lipids at a constant charged density using small angle neutron scattering (SANS), dynamic light scattering (DLS) and transmission electron microscopy (TEM). A time-resolved DLS study is also carried out to understand the kinetics of the structural transformation as a function of temperature, lipid concentration and composition. The preliminary data indicate that uniform nanodiscs and/or bilayer ribbons generally exist at low temperature, while at high temperature ULVs or MLVs are obtained. Moreover, the nanodiscs coalesce with each other over a period of time. The fundamental understanding of the structural formation mechanism and kinetics can lead to potential application of this system to bionanotechnology, such as drug carrying and therapeutic imaging.

C1.00138 The Effect of Short-Chain Lipid on the Morphology of Bicellar Mixtures¹, MING LI, University of Connecticut, Storrs, CT, USA, HANNAH MORALES, University of Toronto, Toronto, ON, JOHN KATSARAS, Oak Ridge National Laboratory, Oak Ridge, TN, PETER MACDONALD, University of Toronto, Toronto, ON, MU-PING NIEH, University of Connecticut, Storrs, CT, USA — Lipid bicellar mixtures, composed of long-chain phospholipids (usually dimyristoyl phosphatidylcholine (DMPC) and charged lipid dimyristoyl phosphoglycerol (DMPG)) and a short-chain phospholipid (e.g. dihexanoyl phosphocholine (DHPC) or 3-[[3-Cholamidopropyl]dimethylammonio]-2-hydroxy-1-propanesulfonate (CHAPSO)), are ideal substrates for structural characterization of the membrane protein, because they provide the natural lipid bilayer environment and furthermore can be aligned in the magnetic field. Recently, structural phases of zwitterionic DMPC/DHPC and charged DMPC/DMPG/DHPC bicellar mixtures have been studied extensively. However, the effect of the short-chain lipid on the morphology is still unknown. Here we report the phase diagram of DMPC/CHAPSO and DMPC/CHAPSO/DMPG mixtures by SANS and NMR. Compared with DMPC/DHPC and DMPC/DHPC/DMPG, different temperature dependence of morphology is observed in the counterpart of CHAPSO by SANS. Also, The PFG-NMR result shows different diffusion behaviors of polyethylene glycol associated with the membranes composed of DMPC/CHAPSO and DMPC/CHAPSO/DMPG, which are magnetically alignable. Both SANS and NMR results suggest that a bilayered ribbon is formed in the case of DMPC/CHAPSO, DMPC/CHAPSO/DMPG.

¹We gratefully acknowledge the support from National Science Foundation (NSF-CMMI1131589).

C1.00139 Rheology of Vimentin Intermediate Filament Networks¹, HUAYIN WU, Harvard University — A cell's ability to function is highly dependent on its structure and material properties - its capacity to withstand and respond to forces in its environment. The cytoskeleton, which largely determines the cellular mechanical properties, is comprised of biopolymer networks, including filamentous actin, microtubules, and intermediate filaments (IF). Intermediate filaments are much less studied than actin and microtubules. They are much more varied and specialized as well, and have been suggested as being an important platform in mechanotransduction processes in cells. It is thought that they can withstand very high strains and exhibit strain stiffening behavior. We are characterizing vimentin, a type III IF that is found in all vertebrate cells, using rheological techniques. Vimentin elasticity increases upon addition of multivalent cations, which act like molecular crosslinkers. By varying the concentration of cations, we can extract valuable information about how the networks assemble and function.

¹NIH Program Project Grant Intermediate Filaments, Harvard Materials Research and Engineering Center (DMR-0820484)

C1.00140 Force Dependent Changes in Non-Erythroid Spectrin and Ankyrins, ELENI DEGAGA, MARTIN FORSTNER, Syracuse University — Mechanotransduction in cells describes the process by which external physical stimuli are converted into biochemical activity and plays an important role in many biological functions on both the cell and tissue level. However, the specific mechanisms by which mechanical forces lead to particular molecular and cellular responses are much less understood. We investigate the changes in non-erythroid spectrin and ankyrins as a result of equi-biaxial strain application to live cells in culture. Specifically, we focus on the spectrins' role in the ubiquitination process - a vital process in the regulation of protein degradation- of spectrin and ankyrins. We utilize immune-fluorescence staining and fluorescent fusion proteins for quantitative fluorescence imaging as well as biochemical methods to measure changes in of cell's spectrin and ankyrin content. Protein expression levels and localization between cells exposed to mechanical stimuli of different temporal and spatial profiles are compared. In addition, the threshold behavior of cell proliferation - as measured by number densities - of a variety of cell types as a function of mechano-stimulation is investigated.

C1.00141 Dynamics and Structure of Disordered Peptides from Two-Dimensional Infrared Spectroscopy, MIKE REPPERT, JOSHUA LESSING, CHUNTE PENG, KEVIN JONES, CARLOS BAIZ, ANDREI TOKMAKOFF, Department of Chemistry, Massachusetts Institute of Technology — Two-dimensional infrared (IR) spectroscopy is a powerful tool for investigating the ultra-fast dynamics and association of complex biological macromolecules such as proteins and DNA. In addition to the improved spectral discrimination afforded by a two-dimensional spectrum, the ultra-fast time-resolution inherent to the technique provides unique insight (unobtainable by standard linear IR measurements) into the time-scales of macromolecular conformational fluctuations, particularly for intrinsically disordered systems. Here we discuss the use of accurate line shape modeling of peptide amide I vibrations as an advanced method for extracting structural and dynamic information from experimental spectra. The mixed quantum-classical model makes use of standard MD trajectories and a parametrized site energy and coupling map as inputs for excitonic calculations of the delocalized amide I vibrations. We present examples of the application of this method to extract site-specific structural information (such as hydrogen bond number and turn conformation) as well as insight into conformation dynamics and time-scales from experimental data for disordered peptides.

C1.00142 Vibrational Coherence Spectroscopy Investigation of Cytochrome c equilibrium Unfolding¹, YUHAN SUN, KARUNAKARAN VENUGOPAL, PAUL M. CHAMPION, Department of Physics and Center for Interdisciplinary Research on Complex Systems, Northeastern University, Boston, MA 02115 — Using vibrational coherence spectroscopy (VCS) we studied guanidinium hydrochloride (GdHCl) induced equilibrium unfolding of ferric cytochrome c excited at 412 nm. Upon unfolding, we observed that the strong 50cm^{-1} mode, which dominates the VCS spectrum of native cyt c, loses its intensity relative to the 80cm^{-1} mode. The 224cm^{-1} mode (γ_{24}) also shifts to 205cm^{-1} , reflecting the heme configuration change associated with unfolding. We also compared the amplitude of these unfolding sensitive modes at different GdHCl concentrations using a cyt c-imidazole complex as a model system. The peak of the Soret band does not shift when the cyt c- imidazole complex is unfolded. Because the resonance conditions are invariant, the relative intensities are a direct probe of the heme structural changes. Our results show that the 50cm^{-1} mode dramatically loses amplitude, while the 80cm^{-1} mode stays nearly the same. When compared to other Raman studies, which suggest that the heme adopts a more planer structure when cyt c is unfolded, the 50cm^{-1} mode may reflect a similar structural change as the 569cm^{-1} (γ_{21}) mode. We suggest that these modes are diagnostic of a protein-induced ruffling distortion.

¹We acknowledge NSF (MCB-0744738) and NIH (DK-035090) for supporting the work.

C1.00143 Protein Dynamics Studied via a Disclination Network Based Approach¹, RAHMI OZISIK, OSMAN BURAK OKAN, Rensselaer Polytechnic Institute, KERRI SCHULTZ, Hudson Valley Community College, ARAVIND RAMMOHAN, Corning Research Center — Protein dynamical transition at ca. 200 K is an elusive collective process by which the time-scale distribution of different relaxations is strongly altered (Okan, Atilgan, Atilgan, Biophysical J. 2009, 97, 2080; Atilgan, Aykut, Atilgan, Biophysical J. 2008, 94, 79). It is now confirmed that the backbone topology during this dynamic transition remains intact and there is no structural phase transition during such a dynamic transition. However, the dynamics of backbone torsional jumps shows a freezing behavior below the transition temperature (Atilgan et al., 2008). In the current work, we map the heavy atoms of proteins onto a disclination network and probe temperature dependent dynamics on such a construct. Using a series of 40 ns molecular dynamics cooling simulations spanning the temperature range of 320 K to 160 K with 10 K increments, we track the dynamics of orientational defect networks. The size distribution and defect lifetimes in the disclination network are shown to be central for the dynamical transition in proteins.

¹Partial support was provided by NSF Grant No. 1003574 and RPI.

C1.00144 Acoustic Force Microscopy in Aqueous Environments to Determine Protein Folding Dynamics, STEFAN ZAUSCHER, ZEHR PARLAK, JIANMING ZHANG, TERRY OAS, Duke University — Characterizing the dynamic mechanical response of (bio)molecular thin films can give insight into the dynamics of biomolecules on surfaces. Here, acoustic atomic force microscopy (AFM) methods are promising tools since they enable sensitive mapping of the mechanical properties of samples by introducing high frequency modulation while imaging the topography. We are among the first to show that it is possible to utilize acoustic AFM methods in aqueous environments. Accounting for the indentation dependent, off-resonance cantilever dynamics, we are able to obtain spatially resolved elasticity maps of organic thin films in water. Encouraged by these results, we are testing the hypothesis that the rapid unfolding/refolding cycles of the five B domains of SpA-N, a 291 residue protein, composed of five nearly identical 56 to 61 residue domains, confer a unique form of flexibility to the molecule. To this end we employ a non-resonant, acoustic AFM method in a frequency spectroscopy mode, and measure the viscoelastic properties of SpA-N monolayers quantitatively under physiological conditions. We present evidence that the apparent, frequency-dependent stiffness of SpA-N coincides with the kinetics of individual domain folding cycles.

C1.00145 Analysis of Soybean Microtubule Persistence Length; New Evidence on the Correlation between Structural Composition and Mechanical Properties, MITRA SHOJANIA FEIZABADI, CARLY WINTON, JIMMY BARRIENTOS, Seton Hall University — Recent studies on microtubules composed of different β tubulin isotypes indicate their different functionality in terms of their dynamical behavior or the mechanism of their interaction with chemotherapeutic drugs. Along these lines, the result of our recent study measuring the rigidity of neural and non-neural samples of microtubules with different β tubulin isotype compositions suggests that the distinguished mechanical properties of microtubules, such as rigidity, may also be associated with the different distribution of their β tubulin isotypes. In our current study, we have reported the persistence length of a single soybean microtubule. This plant microtubule has a structural composition different from that of mammalian microtubules. Under the same experimental methods of measurement, the soybean microtubules showed a different persistence length as compared to the value of the persistence length that we estimated in the study of both single Bovine Brain and MCF7 microtubules.

C1.00146 Conformational response of a clay binding protein (EGF) by a coarse-grained Monte Carlo simulation¹, BARRY FARMER, LAWRENCE DRUMMY, RAJESH NAIK, Air Force Research Laboratory, MADHAVI KADAKIA, Wright State University, RAS PANDEY, University of Southern Mississippi — Biofunctionalization of montmorillonite (MMT) clay platelets with epidermal growth factor (EGF) appears to play a critical role in tissue regeneration (cell growth and migration) [1]. How the protein (EGF) binds to clay platelet and conforms is very important in its ability to activate the epidermal growth factor receptor. It is however difficult to monitor such structural response systematically in a current laboratory setting. We investigate the structural response of the protein EGF as it binds to the clay platelet with a coarse-grained model already used to investigate binding of short peptides. Both the EGF protein and the clay platelets are described by nodes tethered together by fluctuating covalent bonds. Each residue interacts with a phenomenological interaction (based on its hydrophathy index). Protein and platelet perform their stochastic motion with the Metropolis algorithm. A number of local (e.g. mobility and structural profiles) and global physical quantities such as gyration radius are examined as a function of temperature. We are able to identify the immobilized segments of protein and the variation of its size as a function of temperature. [1] C.A. Vaiana et al Biomacromolecules xxx (2011)

¹This work is supported by the Air Force Research Laboratory.

C1.00147 ABSTRACT HAS BEEN MOVED TO K1.00319 —

C1.00148 Biocompatibility of Titanium, FEREYDOON NAMAVAR, University of Nebraska Medical Center, RENAT SABIRIANOV, University of Nebraska at Omaha, DENES MARTON, UTHSCSA, ALEXANDER RUBINSTEIN, University of Nebraska at Omaha, KEVIN GARVIN, University of Nebraska Medical Center — Titanium is the material of choice for orthopaedic applications because of its known biocompatibility. In order to enhance osteogenic properties of the Ti implants, it is necessary to understand the origin of its biocompatibility. We address the origin of Ti biocompatibility through (1) theoretical modeling, (2) the precise determination of Ti surface chemistry by X-ray photoelectron spectroscopy (XPS), (3) and the study of fibronectin adsorption as a function of Ti (near) surface chemistry by Enzyme-linked immunosorbent assay (ELISA). We compare the protein adsorption on Ti with the native oxide layer and the one coated by TiO₂ in anatase phase using ion beam assisted deposition (IBAD). We show that the thin native sub-stoichiometric titanium oxide layer is crucial for biocompatibility of Ti surface. This is due to the enhancement of the non-specific adsorption of proteins which mediate cell adhesion. Improving the surface oxide quality, i.e. fabricating stoichiometric TiO₂ (using IBAD) as well as nanoengineering the surface topology that matches its dimensions to that of adhesive proteins, is crucial for increased protein adsorption and, as a result, further increases biocompatibility of Ti implant materials.

C1.00149 Partially-Functionalized Isotactic Polystyrene with Blocky Comonomer Segments, ARIEL SIEGEL, WAYNE POWERS, CHANG Y. RYU, Rensselaer Polytechnic Institute, RENSSELAER POLYTECHNIC INSTITUTE COLLABORATION — Isotactic polystyrenes (iPSs) have been functionalized in solution, while the accessibility of functionalizing agent is limited by the formation of crystalline domains at various temperatures. The chemical system used is the borylated isotactic polystyrene system, and we investigated the temperature effects on reaction kinetics to ultimately control the blockiness of borylated segments in the resulting copolymer. The chemical composition of partially borylated iPS reaches a steady state that is dependent on temperature. This synthesis has been performed at many different temperatures, with different steady states being reached at different temperatures. Further analysis by differential scanning calorimetry (DSC) has shown that the higher temperature reactions have greater effect on breaking down the crystal lattice structure of the isotactic polystyrene. As a result, the lower temperature reactions affect the crystalline structure less, and the resulting copolymer has more blockiness.

C1.00150 Rigid amorphous fraction of Nylon 11 determined from TMDSC¹, BIN MAO, PEGGY CEBE, Department of Physics and Astronomy, Tufts University — High precision, high accuracy heat capacity measurements were used to study both neat Nylon 11 and Nylon 11 nanocomposites which had been prepared by different processing procedures. The heat capacity step at the glass transition temperature was characterized from the reversing flow using temperature modulated differential scanning calorimetry, and this allows us to determine the mobile amorphous fraction. Heat fusion was obtained from endotherm area of the total heat flow curve, and was correlated with the degree of crystallinity determined from X-ray diffraction. Based on three phase model of the semicrystalline polymer structure, the rigid amorphous fraction (RAF) in Nylon 11 could be calculated. Studied Nylon 11 samples include solution cast, liquid quenched, and isothermally crystallized films, solution cast films containing multi-walled carbon nanotubes, and electrospun fibers. We observed that a rigid amorphous fraction exists in all Nylon 11 samples, and the amount of RAF is strongly dependent upon the crystalline fraction and the nanofiller content.

¹The authors kindly acknowledge National Science Foundation for financial support through DMR-0602473. X-ray related work was conducted at the Brookhaven National Laboratory, National Synchrotron Light Source, supported by the Department of Energy.

C1.00151 Structure of Oriented PLA/Graphene Nanocomposite Fibers¹, QIAN MA, Tufts University, MAREK PYDA, Poznan University of Medical Sciences, BIN MAO, Tufts University, ERIKA SIMONA COZZA, ORIETTA MONTICELLI, Università di Genova, PEGGY CEBE, Tufts University — Highly-aligned polylactic acid (PLA)/graphene nanocomposite fibers were successfully electrospun. Through a combination of thermal analysis and X-ray scattering, the phase structure, molecular orientation, and fiber shrinkage of the oriented PLA fibers were investigated to evaluate the molecular chain confinement. Calorimetric studies were performed to identify the molecular origin of the post- T_g exothermic peak. We found that the shrinkage of the oriented amorphous polymer serves as a precursor for the cold crystallization revealed by the post- T_g exotherm. Using real-time 2-D wide angle X-ray scattering and molecular retraction tests, we further quantified the orientation level and the oriented amorphous fraction in the as-spun amorphous fibers, and investigated the subsequent formation of oriented crystals during heating under “frozen-in” tension. The preferentially oriented amorphous region that possesses a degree of medium-range order has high similarity with the concept of the rigid amorphous phase that has been widely studied in thermal analysis area, and a new phase structure model was established. Graphene filler has a significant influence on molecular orientation, crystallization behavior, and electrical conductivity of PLA fibers.

¹For support of this research, the authors thank the National Science Foundation, Polymers Program of the Division of Materials Research through DMR-0602473, and the MRI Program under DMR-0520655 for thermal analysis instrumentation.

C1.00152 The Role of Surface Charge of Nucleation Agents on the Crystallization Behavior of Poly(vinylidene fluoride), YING WU, SHAW LING HSU, University of Massachusetts, Amherst — The effect of the surface charge of nucleation agents on the crystallization behavior of poly(vinylidene fluoride) (PVDF) has been investigated. Ion-dipole interaction between the positive surface of nucleation agents and the partially negative CF₂ dipoles of PVDF was considered as a main factor for further lowering free energy barrier for nucleation, and thus increasing significantly the crystallization kinetics. This is in contrast to the behavior observed for nucleation agents possessing either negative surface or neutral charges. Positive nucleation agents led to a remarkable increase in the crystallization temperature (lower supercooling), the melting point and degree of crystallinity of PVDF as compared with that of neat PVDF. The dispersion of each type of nucleation agents is also important. The melting temperature needs to be higher than the melting temperature of PVDF. The detailed crystallization behavior and its kinetics, including the conformational changes of the PVDF chain during the crystallization of neat PVDF and PVDF with specific nucleation agents, have also been investigated. With the addition of positive nucleation agents, the γ and β chain conformations, instead of the α phase, dominate.

C1.00153 Characterization of aging behavior associated with multi-layered polymer laminates

, YING JIN, YING WU, SHAW LING HSU, University of Massachusetts, Amherst — To predict the physical stability of multilayered polymer laminates film, the underlying segmental motion of each layer needs to be characterized as a function of time and temperature. We focused on the dimensional stability of various poly(vinylidene fluoride) (PVDF) and its blends. Because of the significant density difference between the crystals formed and the amorphous phase, dimensional stability or the presence of residual stress is difficult to avoid. We have used a combination of techniques to characterize the effects of various comonomers, nucleation agents or blends on the crystallization behavior, the morphology formed and thus dimensional stability. The stress changes in polymer films were investigated as a function of temperature with the cantilever deflection approach. The volume relaxation with time is observed using density gradient column. The morphological features evolved were also analyzed. The magnitude of the residual stress was quantitatively evaluated. The time evolution reaching a stable structure was also investigated in terms of the local glass transition temperature. We further discussed the changes by adding nuclear agents in order to force the polymer films to reach equilibrium states achieving stability stable in a short time scale.

C1.00154 Optically Fixable and Optically Elastic Photomechanical Responses in Azobenzene Liquid Crystal Polymer Networks

, TIMOTHY WHITE, KYUNG MIN LEE, RICHARD VAIA, TIMOTHY BUNNING, Air Force Research Laboratory, Wright-Patterson AFB — Photoresponsive behaviors in azobenzene functionalized polymers have seen widespread interest for a variety of applications as adaptive materials. In a series of recent works, we have distinguished the photomechanical response of polydomain, monodomain and twisted nematic glassy azobenzene liquid crystal polymer networks (azo-LCNs). Interestingly, these materials primarily exhibit optically fixable shape memory to blue-green irradiation, but in some instances can exhibit “optically elastic” (muscle-like) responses. Towards this end, this contribution will summarize the photomechanical responses of these materials and illustrate some of the underlying contributors that dictate fixable or elastic responses upon removal of the irradiation.

C1.00155 Effect of an external field on nematic order in semiflexible polymers, JUTTA LUETTNER-STRATHMANN, KIRAN KHANAL, Departments of Physics and Chemistry, University of Akron — Semiflexible polymers of sufficient stiffness exhibit liquid crystalline order at sufficient polymer concentrations. In this work, we investigate blends of flexible and semiflexible polymers under a uniform external field with the aid of Monte Carlo simulations of a bond-fluctuation model. The model is an extension of Shaffer's bond-fluctuation model, where chain stiffness is controlled by including different forms of bending penalties, and includes attractive interactions between monomers. From simulations for a range of values of the bending energy, density, and temperature, we determine the effect of an external field on liquid crystalline order and domain formation.

C1.00156 The evaluation of the dynamic data near T_g from a new aspect¹, BEN XU, GREGORY B. MCKENNA, Department of Chemical Engineering, Texas Tech University — In this work, we compare and analyze the G_g obtained by the KWW² and the BSW³ functions for small molecule, polymer and colloidal glass formers in the context of the Dyre shoving model.⁴ The Dyre shoving model relates G_g with temperature by attributing the free-energy barrier for a “flow event” near to T_g to the work done by shoving aside the surrounding molecules; the free-energy barrier is proportional to G_g , which increases as the temperature decreases. Importantly, the model gives a non-singular growth of the relaxation time or viscosity with decreasing temperature and does not invoke ideas related to dynamic heterogeneity and growing length scales, both of which are commonly used in the description of glassy dynamics. To the extent that the material classes investigated seem to be reasonably described by the shoving model, it is suggested that divergence of time scales and length scales may not be essential to the glass transition phenomenon.

¹Acknowledgements: The authors thank the Office of Naval Research under grants N00014-06-1-0922 and N00014-11-1-0424 for support of this work.

²G. Williams and D. C. Watts, Trans. Faraday Soc. 66, 80 (1970); F. Kolrausch, Pogg. Ann. Phys. 12, 393 (1847).

³M. Baumgärtel, A. Schausberger, and H. H. Winter, Rheol. Acta 29, 400 (1990).

⁴J. C. Dyre, N. B. Olsen, and T. Christensen, Phys. Rev. B 53, 2171 (1996).

C1.00157 Formation of Stable Polymer Glasses via Matrix Assisted Pulsed Laser Evaporation

, KIMBERLY SHEPARD, YUNLONG GUO, RODNEY PRIESTLEY, Princeton University — Via Matrix Assisted Pulsed Laser Evaporation (MAPLE), we are able to form amorphous polymer films that exhibit significant changes in material properties and structure. In the MAPLE method, a pulsed laser ablates a target, consisting of a frozen dilute solution of the desired polymer, in order to produce films of the material. By carefully controlling the growth rate of film formation and the substrate temperature during deposition, we are able to form glassy films with structures that are either less or more dense compared to the standard glass. Interestingly, the morphology of the low and high-density amorphous films is significantly different. The low-density glasses are nanostructured and the high-density glasses are not. In this poster, we discuss how MAPLE can be used to tune the morphology and hence, the properties of polymer glasses.

C1.00158 ABSTRACT WITHDRAWN —

C1.00159 A configurational entropy theory for the non-Arrhenius relaxation in disordered systems¹

, YIZHEN WANG, X. FRANK ZHANG, Bioengineering Program and Mechanical Engineering and Mechanics Dept, Lehigh University, JINXIU ZHANG, School of Physics and Engineering, Sun Yat-sen University, China — Here we develop a novel configurational entropy theory to explain the non-Arrhenius slowdown relaxation behavior in disordered systems on approaching the glass transition. The theory explicitly shows that this intriguing slowdown behavior originates from the growth in the configurational entropy loss (and the structural order degree) of the system, associated with the attractive interaction among relaxing units (RUs). A thermodynamic/kinetic equilibrium state with order singularity at the finite temperature T_c due to the attractive interaction among RUs is predicted. An expression is derived for characterizing the average relaxation time of RUs relaxing towards such equilibrium state. The resultant relaxation time expression offers a novel connection between kinetics and thermodynamics, different from that of the $A - G$ entropy equation, and it is shown to be a generalization of several well-known relations in current use. The theory also implies that the diverging relaxation time at finite temperature arises from the existence of an underlying long-range order phase transition at T_c . Our results could provide a novel understanding of the non-Arrhenius slowdown relaxation behavior in disordered systems on approaching the glass transition.

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C1.00160 Purification and Fractionation of PEO-PPO-PEO Triblock Copolymers

, CHANG YEOL RYU, HANJIN PARK, Rensselaer Polytechnic Institute, GYOO YEOL JUNG, Pohang University of Science and Technology — PEO-PPO-PEO triblock copolymers are produced on a commercial scale for nonionic surfactant applications. Anionic polymerization has been employed to produce the block copolymers and it is likely that the triblock copolymer contain low molecular weight contaminants that would interfere with the micellization and gelation in aqueous solution. We have taken advantages of the recent developments on the interaction chromatography (IC) technique to separate the neat triblock copolymers from the as-received triblock copolymers. Because the IC relies on the adsorption of polymers, we were able to purify and fractionate the triblock copolymers on a larger scale than the prep scale SEC. Upon purification of the triblock copolymers, the influence of contaminants in the as-received triblock copolymers will be discussed on the micellization and gelation of the triblock copolymer solution in water.

C1.00161 Size Interplay between Polymer and Nanopores for the Band Broadening of SEC¹, IAN WEISS, POSTECH/Rensselaer Polytechnic Institute, CHANG YEOL RYU, Rensselaer Polytechnic Institute, TAIHYUN CHANG, POSTECH — The size interplay between polymer chains and nanopores plays a key role in governing the retention time of polymer chains in liquid chromatography. These nanopores also contribute to the band broadening of the resulting peaks seen in most liquid chromatography systems including size exclusion chromatography (SEC). We have studied how the relationship between the size of the nanopores and the hydrodynamic radius of the polymers affects the band broadening during SEC. This related to Brown random motion of polymer chains in solution, whose motions are restricted by the presence of nanoporous stationary phase for the SEC. We have prepared model polystyrene samples with extremely narrow polydispersity ($PDI < 1.0001$) using temperature gradient interaction chromatography. Those model samples allow us to directly measure the band broadening of SEC using different size pore columns at various solvent conditions.

¹NSF OISE PIRE 0730243

C1.00162 SANS Mapping of Orientation and Relaxation of Polymer Chains upon Uniaxial Extension¹, HOWARD WANG, LIWEI HUANG, Institute for Material Research and Department of Mechanical Engineering, State University of New York, Binghamton, NY 13902, YANGYANG WANG, Department of Chemistry, University of Tennessee, Knoxville, TN 37996, HAO SUN, SHI-QING WANG, Department of Polymer Science, University of Akron, Akron, Ohio 44325, DAZHI LIU, CARRIE GAO, KE AN, Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831 — Small angle neutron scattering (SANS) has been used to measure entangled chains in polymer melts upon uniaxial stretching. The degree of anisotropy and the coil dimension are discussed in the light of the applicability of the tube model.

¹Supported by NSF CMMI and DMR

C1.00163 X-ray scattering investigation of structural relaxation in an ordered block copolymer melt subjected to uniaxial extensional flow, WESLEY BURGHARDT, ERICA MCCREADY, Northwestern University — The structural dynamics of an ordered styrene-ethylene butylene-styrened triblock copolymer have been studied in uniaxial extensional flow using in situ x-ray scattering. Experiments were performed in a custom instrument consisting of an SER extensional flow fixture housed in a convection oven designed to facilitate x-ray access. Use of synchrotron radiation provided sufficient time resolution to study the structural response during inception of uniaxial flow, and as a function of time following flow cessation. The sample studied here exhibits hexagonally packed cylindrical microdomains of polystyrene embedded in a poly(ethylene butylene) matrix. Application of extensional flow produces multiple structural effects, including deformation of the microphase-separated morphology, and a complex reorientation process in which elongated PS microdomains progressively orient along the stretching axis. A series of experiments was run in which samples were stretching to varying Hencky strains, allowing investigation of the nature of structural relaxation from a variety of flow-induced structural states induced during extensional flow. Significant differences in structural relaxation are found depending on the total applied extensional strain.

C1.00164 Comparative study of polymer chain dynamics in aqueous solutions by FPR and DLS, KIRIL STRELETZKY, RYAN MCDONOUGH, Cleveland State University, RAFAEL CUETO, PAUL RUSSO, Louisiana State University — Self diffusion of tagged polymer chains in aqueous solutions of hydroxypropylcellulose (HPC) was measured by Fluorescence Photo-bleaching Recovery (FPR) and compared to mutual diffusion of scattering species in the same solutions measured by Dynamic Light Scattering (DLS). The effect of the dye presence on thermodynamic concentration fluctuations observed by DLS was also studied. The observed multimodal spectra in DLS and FPR were analyzed with CONTIN and stretched exponential fits. A set of consistent dissimilarities in the modal distributions of FPR and DLS spectra was found. This indicates a comparative limitation or sensitivity in range of detectable diffusive processes between FPR and DLS in this complex system. In addition, it was found that the fluorescent tag and/or tagging process seem to alter the mutual diffusion processes seen by DLS. In particular, a slower mode which is apparent in the non-tagged sample does not appear in the tagged sample. It seems likely that the dye chemically affects the polymer chains keeping them from clustering with each other, altering the solvent environment preventing formation of polymer clusters responsible for the slow mode usually seen in HPC.

C1.00165 Silicone Elastomer Networks with Tunable Modulus for Cell Mobility Studies, JULIE N.L. ALBERT, KIRILL EFIMENKO, JAN GENZER, North Carolina State University — Silicone elastomer networks provide a versatile platform for studying the effects of compliance and surface chemistry on cell movement. One major advantage of these materials over more commonly used poly(acrylamide) surfaces or hydrogel networks is that they do not swell with water; therefore, the physical properties measured in the dry state are representative of those present under aqueous conditions. In this work, we tuned the moduli of poly(dimethylsiloxane) (PDMS) networks by manipulating the cross-link density *in-situ* during network formation. This regulation of cross-link density was accomplished by cross-linking at polymer chain ends with both difunctional and multi-functional cross-linking agents. The difunctional cross-linkers serve as chain extenders whereas the multifunctional cross-linkers facilitate formation of a chemically cross-linked network. Networks with moduli ranging from ≈ 10 kPa to ≈ 1 MPa were fabricated in this fashion by adjusting the polymer molecular weight, the ratio of difunctional to multifunctional cross-linker, and the ratio of total cross-linker to number of polymer chains. The same approach can be applied to fabricate poly(vinylmethylsiloxane) networks, which can be further tailored through side-chain cross-linking or surface functionalization of pendent vinyl groups.

C1.00166 New Insights into Chain Order Dynamics and Structural Development in Sulfur-Vulcanized Natural Rubber Latex using Multiple Quantum NMR and Synchrotron X-Ray Diffraction, JUSTIN CHE, SHIGEYUKI TOKI, Stony Brook University, JUAN VALENTIN, JUSTO BRASERO, Instituto de Ciencia y Tecnología de Polímeros (CSIC), LIXIA RONG, BENJAMIN S. HSIAO, Stony Brook University, STONY BROOK UNIVERSITY TEAM, INSTITUTO DE CIENCIA Y TECNOLOGÍA DE POLÍMEROS (CSIC) COLLABORATION — Network structure, chain dynamics, and structural development in sulfur-vulcanized natural rubber latex were studied by Multiple-Quantum (MQ) NMR and synchrotron x-ray scattering. Three important processes that can influence rubber network structure and its overall mechanical properties were the main focus and analyzed by both of these techniques: pre-vulcanization, drying, and post-vulcanization. MQ NMR experiments can provide quantitative information regarding networks at very small length scales, including network defects, number of cross-links, and spatial distribution of cross-links. Structural development in natural rubber was studied under uniaxial deformation by in-situ synchrotron x-ray diffraction, which can provide information on network structures at much larger length scales. Molecular orientation and strain-induced crystallization was analyzed by both stress-strain relations and wide-angle x-ray diffraction (WAXD). The morphology of the latex rubber particle during deformation was analyzed by small-angle x-ray scattering (SAXS). The combination of these techniques can provide a considerable amount of information regarding rubber network structure.

C1.00167 Chemotaxis of active, self-oscillating polymer gels in solution, PRATYUSH DAYAL, AMITABH BHATTACHARYA, OLGA KUKSENOK, ANNA C. BALAZS, University of Pittsburgh — Fighting, fleeing and feeding are hallmarks of all living things; all these activities require some degree of mobility. Herein, we undertake the first computational study of self-oscillating polymer gels and show that this system can “communicate” to undergo a biomimetic, collective response to small-scale chemical changes. In this study we harness unique properties of polymer gels that undergo oscillatory Belousov-Zhabotinsky (BZ) reaction. The activator for the reaction is generated within these BZ cilia and diffuses between the neighboring gels. In order to simulate the dynamics of the BZ gels in surrounding fluid we have developed a nonlinear hybrid 3D model which captures the elasto-dynamics of polymer gel and diffusive exchange of BZ reagents between the gel and the fluid. We illustrate that multiple BZ gels in solution exhibit a distinct form of chemotaxis, moving towards the highest activator concentration in the solution. Similar ability to sense and move in response to chemical gradients constitutes a vital function in simple organisms, enabling them to find food and flee from poisons.

C1.00168 Effect of Thickness on the Thermal Properties of Hydrogen Bonded Layer by Layer Assemblies, CHOONGHYUN SUNG, AJAY VIDYASAGAR, KATELIN HEARN, JODIE LUTKENHAUS, Texas A&M University — Layer by layer (LbL) assemblies have attracted a lot of attention for their functional versatility and ease of fabrication. However characterizing thermal properties, especially for ultra thin LbL assemblies, has remained a challenging topic. We have investigated the role of the film thickness on the glass transition temperature (T_g) for poly(ethylene oxide)/poly(acrylic acid) (PEO/PAA) and (PEO)/poly(methacrylic acid) (PEO/PMAA) hydrogen bonded LbL assemblies in both bulk as well as in confined thin films using modulated differential scanning calorimetry (MDSC) and temperature-controlled ellipsometry. PEO/PAA LbL assemblies exhibit a well-defined T_g , both in bulk and thin films. For films less than 100 nm thick, the T_g increased slightly as film thickness decreased. On the other hand, PEO/PMAA LbL assemblies displayed clear glass transitions only after thermal treatment, which produces anhydride crosslinks. Also, the thickness dependence on T_g was less pronounced for PEO/PMAA LbL films. It was also seen that the thermal expansion coefficient (α) increased for film thickness below 200nm. We speculate that interactions between the film and substrate likely influence the thickness-dependent T_g .

C1.00169 Layer-by-Layer Assembly of Polyelectrolyte Chains and Nanoparticles on Porous Substrates: Molecular Dynamics Simulations¹, JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, Institute of Materials Science and Department of Physics, University of Connecticut — We performed molecular dynamics simulations of a multilayer assembly of oppositely charged polyelectrolyte chains and nanoparticles on porous substrates with cylindrical pores. The film was constructed by sequential adsorption of oppositely charged species in a layer-by-layer fashion from dilute solutions. The multilayer assembly proceeds through surface overcharging after completion of each deposition step. The substrate overcharging fraction fluctuates around 0.5 for nanoparticles-polyelectrolytes systems and around 0.4 for polyelectrolytes-polyelectrolytes systems. The surface coverage increases linearly with the number of deposition steps. The rate of surface coverage increase as a function of the number of deposition steps changes when the pore is closed. The closing of the pore occurs from the pore entrance for nanoparticles-polyelectrolytes systems. In the case of polyelectrolytes-polyelectrolytes systems the pore plug is formed inside the pore and then spreads towards the pore ends.

¹NSF # DMR-1004576

C1.00170 Interaction between Brush Layers of Bottle-Brush Polyelectrolytes: Molecular Dynamics Simulations¹, DANIEL RUSSANO, Boston University, JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, University of Connecticut — Interactions between tethered layers composed of aggregan (charged bottle-brush) macromolecules are responsible for the molecular origin of the cartilage biomechanical behavior. To elucidate the role of the electrostatic forces in interaction between bottle-brush layers we have performed molecular dynamics simulations of charged and neutral bottle-brush macromolecules tethered to substrates. In the case of charged bottle-brush layers the disjoining pressure P between two brush layers in salt-free solutions increases with decreasing the distance D between substrates as $P \propto D^{-1.8}$. A stronger dependence of the disjoining pressure P on the surface separation D was observed for neutral bottle-brushes, $P \propto D^{-4.6}$, in the same interval of the disjoining pressures. These scaling laws for dependence of the disjoining pressure P on the distance D are due to bending energy of the bottle-brush macromolecules within compressed brush layers. The weaker distance dependence observed in polyelectrolyte bottle-brushes is due to interaction between counterion clouds surrounding the bottle-brush macromolecules preventing strong brush overlap.

¹NSF # DMR-1004576

C1.00171 Synthesis and Physical Behavior of Model Polymer Electrolyte Membranes for Alkaline Fuel Cells, RICK BEYER, SAMUEL PRICE, AARON JACKSON, CHRISTOPHER GOLD, Army Research Laboratory, YUESHENG YE, YOSSEF ELABD, Drexel University — Alkaline fuel cell (AFC) technology holds significant promise for portable power supplies because AFCs are very efficient at temperatures under 200 °C, but also because AFCs can use relatively inexpensive, non-noble metals (Ni, Fe, Co) as the catalyst material. Wide-spread use of the AFC has been prevented by the use of aqueous KOH liquid as the electrolyte, which is easily poisoned by the formation of K_2CO_3 . Development of an semipermeable polymeric alkali anion exchange membrane (AEM) would significantly improve the usefulness of AFCs by eliminating carbonate poisoning and the engineering problems associate with a liquid electrolyte. We have been exploring model copolymers containing phosphonium cations as candidate materials for AEMs. Recent findings on the transport properties and stability of random copolymers of styrene and p-vinylbenzyl-trimethylphosphonium chloride will be presented, as well as ongoing efforts to study the effect of polymer morphology on transport and stability in ionomers based on both phosphonium and ammonium cations.

C1.00172 In-depth Analysis of Proton Mobilities in Sulfonated Block Copolymers, MOON JEONG PARK, SUN JU LEE, SUNG YEON KIM, Department of Chemistry, Division of Advanced Materials Science (WCU), Pohang University of Science and Technology (POSTECH) — Polymer electrolytes are an important component of a wide variety of electrochemical devices such as battery, fuel cell, and chemical sensor owing to their ability to provide a pathway for ion transport between electrodes. Considerable efforts have been devoted to a subject of ion transport mechanisms in polymer electrolytes since the ion mobility in the polymer electrolytes plays a central role in determining the efficiency of the devices. In present study, we carried out an in-depth analysis of proton mobilities in model ionic block copolymers. The system of interests is a series of sulfonated poly(styrene-*b*-methylbutylene) (PSS-*b*-PMB) copolymers. Dilute solutions of PSS-*b*-PMB copolymers in methanol, which indicate highly uniform spherical ionic micelles, were examined yields. In particular, on virtue of the self-assembly nature of block copolymers, the system revealed well-defined ionic PSS domains with different thickness ranging from 3.0 to 7.8 nm. The proton transport in PSS-PMB copolymers was found to be facilitated by the decrease in the ionic domain sizes, which was rationalized by the different proximity of acid groups at the surfaces of ionic domains.

C1.00173 Functionalizing Silica Nanoparticles Designed for Improved Ion Transport, MICHAEL O'REILLY, JAMIE FORD, KAREN WINEY, University of Pennsylvania — Silica nanoparticles have been functionalized with polyethylene oxide and sulfonated polyester to synthesize improved single ion conducting polymer nanocomposites. Our motivation is to minimize ionic aggregation at room temperature by anchoring the sulfonate anion to the surface of a nanoparticle via polymer grafting. The tethered anion's mobility should be restricted, allowing the cation to conduct more easily through the short chain PEO matrix, thereby increasing the free ion content. Secondary benefits of nanoparticle dispersion include suppressed crystallinity and increased viscosity at room temperature in low molecular weight systems where ionic conductivity is elevated.

C1.00174 Effect of water uptake on morphology of polymerized ionic liquid block copolymers and random copolymers, TSEN-SHAN WANG, University of Pennsylvania, YUESHENG YE, YOSSEF ELABD, Drexel University, KAREN WINEY, University of Pennsylvania — Dynamic studies of polymer morphology probe how the physical properties of polymerized ionic liquids are affected by the environment, such as temperature or moisture. For a series of poly(methyl methacrylate-*b*-1-[2-(methacryloyloxy)ethyl]-3-Butylimidazolium X^-) block and random copolymers with hydrophilic counterions ($X^- = Br^-, HCO_3^-, OH^-$), the introduction of water vapor to the system can swell the ionic liquid block, causing enlarged hydrophilic domains and swollen channels for ion conduction. This expected expansion of ionic liquid domains in humid environments can be used to intelligently design these copolymers for use in technological applications. The effect of water vapor exposure in these imidazolium-based acrylate polymers is studied by small-angle X-ray scattering. These morphology results will be discussed alongside complementary studies of water uptake and ion conductivity.

C1.00175 Block Copolymer Exhibiting Simultaneous Electronic and Ionic Conduction, SHRAYESH PATEL, ANNA JAVIER, NITASH BALSARA, University of California, Berkeley and Lawrence Berkeley National Lab — Poly(3-hexylthiophene)-block-Poly(ethylene oxide) (P3HT-PEO) allows for the simultaneous conduction of electronic and ionic charges at the nanometer length scale needed for lithium battery electrodes. In order to study the charge transport properties of P3HT-PEO, we characterized a series of P3HT-PEO block copolymers with and without the addition of lithium bis(trifluoromethanesulfonyl) imide (LiTFSI). We specifically looked at the relationship between morphology and the transport of both electronic and ionic charges. Previously reported work has primarily focused on transport of one charged species. In particular, the results of the study shed light on the effects of LiTFSI on electronic conduction and the intrinsic electronic conduction of the P3HT microphase.

C1.00176 Discontinuous Changes in Ionic Conductivity of a Block Copolymer Electrolyte through the Order-Disorder Transition¹, ALEXANDER TERAN, RODGER YUAN, SCOTT MULLIN, NITASH BALSARA, University of California, Berkeley — Simultaneous small angle X-ray scattering and ionic conductivity measurements of a block copolymer electrolyte as it transitions from an ordered lamellar structure to a disordered phase reveal a discontinuous increase in conductivity at the phase transition. A simple framework for understanding this result is presented, incorporating both morphology factor corrections that account for constraints imposed by the geometry of the conducting phase and 'vehicular' transport of coupled polymer chains and ions.

¹This work was supported by the National Science Foundation

C1.00177 Conformation of polystyrene sulfonate (PSS) and its origin of counterion distribution¹, SHUANGJIANG LUO, QINGBO YANG, JIANG ZHAO, Institute of Chemistry, Chinese Academy of Sciences, LABORATORY OF POLYMER PHYSICS AND CHEMISTRY TEAM — The hydrodynamic radius and electric potential of single chains of polystyrene sulfonate (PSS) is studied, as a function of the molecular weight, by single molecule fluorescence techniques - fluorescence correlation spectroscopy (FCS) and photon count histogram (PCH). The results show different scaling law for low and high molecular weight. When the chain is short ($N < 300$), the scaling power index is about unity, indicating a rod-like conformation, while the index changes to 0.58 when the chain gets longer ($N > 300$), indicating a random coil conformation. The electric potential of the single PSS chains is determined and the results clearly show the decrease of the effective charge density with the increase of molecular weight. The results indicate that the charged chain has increased extent of counterions binding at longer chain length, and therefore takes different conformation.

¹Project supported by National Natural Science Foundation of China (NSFC).

C1.00178 Tuning Thermal Transitions in Dry and Hydrated Polyelectrolyte Layer by Layer Assemblies with Ionic Strength and pH, AJAY VIDYASAGAR, JODIE LUTKENHAUS, Texas A&M University — Layer-by-layer (LbL) assemblies are of significant interest for their potential applications in diverse fields such as energy and drug delivery. However, characterizing their thermal properties has remained a challenge. Here, we present the characterization of dry and of hydrated LbL films containing strong polyelectrolytes poly(diallyldimethylammonium chloride) (PDAC) and poly(styrene sulfonate) (PSS) using modulated differential scanning calorimetry (MDSC) and temperature controlled quartz crystal microbalance with dissipation (QCM-D). Our results suggest that hydrated exponentially growing (assembled from 0.25-1.25 M NaCl solutions) PDAC/PSS LbL films have glass transition temperatures (T_g 's) between 48-51 °C, while linearly growing (assembled from 0 M NaCl) films did not. Other systems explored include poly(allylamine hydrochloride)/poly(acrylic acid) (PAH/PAA) LbL assemblies, which demonstrate linear/exponential growth depending on assembly pH conditions. These results support a standing hypothesis in that linear (or exponential) growth is observed for glassy (or rubbery) LbL films. We have also demonstrated for the first time, thermal transitions in thin PDAC/PSS LbL films using QCM-D by monitoring fluctuations in film hydration and viscoelasticity by probing the film's internal structure as a function of film depth.

C1.00179 Anomalous χ for Polydisperse Polystyrene-*b*-Poly(octyl acrylate)¹, JUMI LEE, Dankook University, HYUNGJU AHN, DU YEOL RYU, Yonsei University, KWANWOO SHIN, Sogang University, JUNHAN CHO, Dankook University — We have performed small-angle neutron scattering (SANS) measurements on a disordered block copolymer from deuterated polystyrene (dPS) and self-adhesive poly(octyl acrylate) (POA) in order to elicit the effective Flory-Huggins χ , which carries the essence of the copolymer phase behavior. The sample for the measurement was prepared by blending two polydisperse dPS-*b*-POAs of different molecular weights for the purpose of adjusting the average size to a proper value. The SANS profiles for the copolymer were fitted to Leibler's scattering function for a polydisperse copolymer system described by Schulz-Zimm distribution. It was shown that the resultant χ as a function of inverse temperature has a strong entropic contribution and a weak enthalpic contribution. By adopting a simple analysis for specific interactions, it was found that the entropically dominated χ for dPS-*b*-POA arises from the steric hindrance of long alkyl side groups of POA.

¹J.C. acknowledges the financial support from Center for Photofunctional Energy Materials at Dankook University.

C1.00180 Thermal Rupture Of Linear Polymer Chains Under Tensile Stress¹, ABHIJIT GHOSH, WON BO LEE, Dept. of Chemical & Biomolecular Engineering, Sogang University — The thermal rupture of a linear alternating copolymer fixed at one end and pulled by a constant force at the other end has been studied using molecular dynamics simulation. The dependence of the first breakage time distribution on the mass ratio of the constituent beads has been studied. The Arrhenian nature of the scission process has been confirmed and an estimate of the effective energy barrier has been made.

¹This work was supported by the Human Resources Development of KETEP grant funded by the Korea government Ministry of Knowledge Economy (No. 20114010203090)

C1.00181 Phase Behavior of Hydrogenated Derivatives of Linear ABC Block-Random Copolymers of Styrene and Isoprene, BRYAN BECKINGHAM, RICHARD REGISTER, Princeton University — The capacity to synthesize block-random copolymers, block copolymers with one or more random copolymer blocks, allows for continuous tuning of the inter-block average segmental interaction parameter, χ , through the composition of the random copolymer without changes to system chemistry. By lithium-initiated anionic polymerization in a mixture of cyclohexane and triethylamine, we synthesized an asymmetric near-monodisperse linear ABC block-random copolymer of styrene and isoprene: $S_{30-I_{12}}-Srl_{12}$, where Srl denotes a random copolymer block with 50 wt. % styrene, and block molecular weights are 30-12-12 kg/mol. Upon complete hydrogenation, the VCH-*hI*-VCH-*hI* triblock exhibits microphase separation into a well-ordered two-domain lamellar structure with an order-disorder transition between 180-185 °C via small-angle x-ray scattering. This two-domain lamellar structure is confirmed using electron density modeling of the SAXS peak intensity and domain spacing arguments. A three-domain lamellar structure is expected in the diene-selective hydrogenated derivative, S-*hI*-S-*hI*, due to increased χ between the middle and end blocks. Additional S-*I*-*Srl* and S-*Srl*-*I* triblock copolymers are being synthesized and the effects of block sequence, end block molecular weight, and hydrogenation (S vs. VCH) on phase behavior are being explored.

C1.00182 Fast field theoretic simulation of block copolymers with the mode Monte Carlo method, YONGJOO KIM, ADAM HANNON, CAROLINE ROSS, ALFREDO ALEXANDER-KATZ, MIT — We explore the self assembly of block copolymers by using a field theoretic simulation method. Former studies on field theoretic simulation methods update the fields by Langevin-like dynamics which is a local update of the fields in real space. Our simulation method updates the mode structure (k-space) of the fields and transfers them to real space. By using a Monte Carlo scheme for updating fields, we decrease simulation time by nearly an order of magnitude. We also consider new self-learning searching strategies using this method. We tested our algorithm by simulating the phase diagram for thin films of diblock copolymers in select graphoepitaxial templates and by simulating the self-assembly of nanoparticles and block copolymers.

C1.00183 Fluctuations/Correlations in Symmetric Diblock Copolymers: Simulations and Theories, JING ZONG, DELIAN YANG, QIANG (DAVID) WANG, Department of Chemical and Biological Engineering Colorado State University — Modeling symmetric diblock copolymers as discrete Gaussian chains with soft, finite-range repulsions as commonly used in dissipative-particle dynamics simulations, we have performed fast off-lattice Monte Carlo (FOMC) simulations¹ in a canonical ensemble with variable box lengths to study the thermodynamic and structural properties of both the disordered and lamellar phases. Our FOMC results for the disordered phase are further compared, without any parameter-fitting, to those from the reference interaction site model (RISM) and the polymer reference interaction site model (PRISM) theories, as well as the Gaussian fluctuation theory, based on the same model system. Such direct comparisons unambiguously and quantitatively reveal the consequences of various theoretical approximations and the validity of these theories in describing the fluctuations/correlations in disordered diblock copolymers.

[1] Q. Wang and Y. Yin, *J. Chem. Phys.*, **130**, 104903 (2009).

C1.00184 Transformation kinetics of BCC sphere morphology of diblock copolymer under electric field, ANDREI ZVELINDOVSKY, DUNG Q. LY, MARCO PINNA, University of Central Lancashire, UK, TAKASHI HONDA, ZEON Corp., Japan, TOSHIHIRO KAWAKATSU, Tohoku University, Japan — We performed Dynamic Self-Consistent Field simulation of BCC sphere morphology of diblock copolymers under an electric field. Several distinct kinetic pathways were determined. Different pathways were found depending on the strength of the applied electric field and orientation of the BCC domain. The fastest growing mode was found in 111 directions. Dynamic critical exponents were deduced from the simulation data. The results are compared with the previous works on different morphologies and on BCC morphology by different techniques.

C1.00185 Genistein Modified Polymer Blends for Hemodialysis Membranes¹, TENG CHANG, THEIN KYU, The University of Akron, LINDA DEFINE, THOMAS ALEXANDER, Summa Health System — A soybean-derived phytochemical called genistein was used as a modifying agent to polyether sulfone/polyvinyl pyrrolidone (PES/PVP) blends to produce multi-functional hemodialysis membranes. With the aid of phase diagrams of PES/PVP/genistein blends, asymmetric porous membranes were fabricated by coagulating in non-solvent. Both unmodified and genistein modified PES/PVP membranes were shown to be non-cytotoxic to the blood cells. Unmodified PES/PVP membranes were found to reduce reactive oxygen species (ROS) levels, whereas the genistein modified membranes exhibited suppression for ~60% of the ROS levels. Also, the genistein modified membranes revealed significant suppression of pro-inflammatory cytokines: IL-1 β , IL-6, and TNF- α . Moreover, addition of PVP to PES showed the reduced trend of platelet adhesion and then leveled off. However, the modified membranes exhibited suppression of platelet adhesion at low genistein loading, but beyond 15 wt%, the platelet adhesion level rose up.

¹Supported by Ohio Soybean Council

C1.00186 Solubilization of Genistein in Poly(Ethylene Glycol) via Eutectic Crystal Melting¹, SASIWIMON BUDDHIRANON, THEIN KYU, The University of Akron — Genistein (5,7,4'-trihydroxyisoflavone) is a phytoestrogen found in soybean. It possesses various biological/pharmacological functions, e.g., tyrosine kinase inhibitory, anticarcinogenic, antioxidant, anti-inflammatory, and anti-microbial activities. However, genistein has poor water solubility and skin permeability, which have seemingly prohibited the progress to preclinical evaluation. Eutectic melting approach has been performed as a means of solubilizing genistein in poly(ethylene glycol) (PEG). Eutectic phase diagrams of blends containing genistein and PEG having three different molecular weights, i.e., 44k, 7k, and 500 g/mol, were established by means of DSC and compared with the theoretical liquidus and solidus lines, calculated self-consistently by taking into consideration all interactions including amorphous-amorphous, crystal-amorphous, amorphous-crystal, and crystal-crystal interactions. The eutectic temperatures were found to decrease with decreasing molecular weight of PEG. Guided by the phase diagram, it was found that genistein can be dissolved in PEG500 up to ~7 wt% at room temperature. More importantly, the solubility of genistein in PEG can be improved to meet the end-use criteria of the PEG/genistein mixtures.

¹Supported by Ohio Soybean Council.

C1.00187 Topographically Uniform but Chemically Heterogeneous Nanostructures by Nanoimprinting Demixed Polymer blends, ZHEN WANG, DAE-UP AHN, YIFU DING, University of Colorado at Boulder — This study examined the coarsening process of phase-separated polymer blends under physical confinement. The physical confinement was realized by nanoimprinting phase-separated PS (polystyrene)/PMMA (polymethylmethacrylate) blend thin films. The influences of the imprint temperature, blend composition and film thickness on the morphological evolutions were systematically investigated. All the patterned PS/PMMA films showed topographically uniform structure after nano-imprinting, regardless of the surface roughness caused by the initial stage of the phase separation. The morphologies, or the phase structures, of the PS/PMMA patterns were found to be dictated by the preferential wetting of PMMA onto silicon oxide surface. The interplay of this preferential wetting and the domain coalescence resulted in a range of complex and unique encapsulated structures. Furthermore, by inhibiting such preferential wetting of a blend component using a neutralized surface, non-capsulated morphology can be achieved.

C1.00188 Properties of PET/PLA Electrospun Blends¹, KEVIN LI, PEGGY CEBE, Tufts University — Electrospun membranes were fabricated from poly(ethylene terephthalate), PET, co-spun with poly(lactic acid), PLA. The PLA contained 2% of the D-isomer, which served to limit the overall degree of crystallinity. Membranes were deposited from blended solutions of PET/PLA in hexafluoroisopropanol. The PET/PLA composition ranged from 0/100, 75/25, 50/50, 25/75, and 100/0. Electrospun membranes were made using either a static flat plate or a rotating wheel as the counter electrode, yielding unoriented mats or highly oriented tapes, respectively. We report on our investigation of the crystallinity, crystal perfection, and mechanical properties of these materials using differential scanning calorimetry, wide and small angle X-ray scattering, and dynamic mechanical analysis. In particular, we study the ability of one blend component (PET) to crystallize in the presence of existing crystals of the second blend component (PLA) which crystallizes first and at a lower temperature than PET.

¹Support from the National Science Foundation, Polymers Program, under DMR-0602473 is acknowledged.

C1.00189 Reactive Poly(Amic Acid)/ Poly(Glycidyl Methacrylate-r-Poly(ethylene Glycol) Methyl Ether Methacrylate) Blends as Gas Permeation Membranes, MICHAEL BEAULIEU, JAMES WATKINS, University of Massachusetts Amherst, Polymer Science and Engineering Department — Polymers containing polar moieties, such as ether groups show an affinity for acidic gases, such as CO₂ due to dipole-quadrupole interactions. Polymer blends in which one of the components is poly(ethylene glycol) (PEG) have been studied extensively in literature as a CO₂/light gas permeation membrane, but due to the crystallization and poor mechanical properties have been difficult to incorporate PEG above 60wt%. In this study, a series of random copolymers containing both glycidyl methacrylate and poly(ethylene glycol) methyl ether methacrylate in different ratios are blended with a poly(amic acid) prepolymer made from 4, 4'-oxydianiline and pyromellitic dianhydride to create gas permeation membranes. By using a reactive blend PEG loadings above 70% have been realized with sufficient mechanical properties, and since the side chain on the PEGMA is short these blends do not suffer from crystallization.

C1.00190 Evaluation of Flame Retardancy, Mechanical Properties, and Bicompatibility of HIPS/PBrS Blends¹, LIUDI ZHANG, SEONGCHAN PACK, Stony Brook University, CORALIE BEAULIEU, Polytech'Nantes, France, MIRIAM RAFAILOVICH, Stony Brook University — Our research focused on thermal and mechanical properties of High Impact Polystyrene (HIPS) system. Brominated Polystyrene (PBrS) was incorporated to replace halogenated Flame Retardant (DB) in HIPS blends. We have previously shown that ditallow functionalized clays could become nearly universal class of compatibilizers [si-2006]. Here we show that a new type of surface with Resorcinol bis (biphenyl phosphate) (RDP) could achieve the same goals. We demonstrate the strong compatibilization on the highly immiscible systems of HIPS/PBrS. Furthermore, we show that this system also works well, when a third component, Antimony Trioxide (AO) is added to provide flame retardant properties. Tensile test, dynamic mechanical analysis, and UL-94 flame test were applied to investigate this system. We found that the amount of AO used in flame retardant formulations could be minimized by addition of RDP clay, which could also increase some mechanical properties that Cloisite 20A clay couldn't. Besides, we evaluated the toxicity of Cloisite 20A and RDP clay. Langmuir-Blodgett trough and atomic force microscopy were used to make and check monolayer clay. Confocal Microscopy was used to assess cell morphology. The results showed RDP clay has potential for biomaterial applications.

¹Supported by NSF-DMR-MRSEC

C1.00191 PVDF/PVIm polymer blend films for fuel cell membranes¹, WENWEN HUANG, Tufts University, MENG ZHAO, FAN YANG, Rochester Institute of Technology, LORNE FAROVITCH, Gallaudet University, PARISA HAGHIGHI, LEONARD MACISCO, TYLER SWOB, THOMAS SMITH, Rochester Institute of Technology, PEGGY CEBE, Tufts University — We report the preparation and characterization of binary blend films of poly(vinylidene fluoride) (PVDF) and poly(1-ethyl-3-vinylimidazolium trifluoromethylsulfonimide) (PVIm+TFSI-). The potential utility of such materials in proton exchange membrane fuel cells is of particular interest. Thin PVDF/ PVIm+TFSI- films were fabricated from solutions of dimethyl formamide by doctor blading. The nature of the PVDF crystalline polymorph and degree of crystallinity was evaluated as a function of the volume fraction of imidazolium polymer and thermal treatment. The morphology, thermal and mechanical characteristics of the blend films was studied by wide angle X-ray diffraction, thermogravimetry, calorimetry, and Fourier transform infrared spectroscopy. In these materials, conditions such as choice of solvent, drying conditions, and thermal treatment affect the crystal phase, crystallite size, and degree of crystallinity of PVDF as well as the distribution of PVIm+TFSI-. The beta phase of PVDF crystals dominates in as-cast films, while the alpha phase is observed after cooling from the melt. PVDF imparts mechanical strength and chemical stability to the composite films, and because of its high crystal melting point ($T_m > 160$ C), serves to improve the high temperature stability of resulting films.

¹Support was provided from the NSF grant DMR 0906455.

C1.00192 Polydispersity Effects on Scaling Behavior of Polymers Grafted on Surfaces of Varying Curvature, PAUL DODD, ARTHI JAYARAMAN, University of Colorado at Boulder — Nanoparticle assembly can be tuned by grafting nanoparticle surface with polymers and in turn manipulating the interactions between the particles and medium. Despite past studies showing the importance of graft molecular weight on effective inter-particle interactions in monodisperse polymer grafted nanoparticles, and evidence of non-trivial polydispersity effects in systems containing polymers grafted on flat surfaces, not much work has been done to explore polydispersity effects in polymer grafted nanoparticles. Using Monte Carlo simulations we elucidate how polydispersity (PDI) in grafted chain lengths affects chain conformations, and in turn the scaling behavior in systems of polymer grafted particles, as a function of grafting density and particle size. With increasing PDI the scaling exponent of the grafted chains at intermediate and high grafting density approaches that of a single chain grafted on the nanoparticle of same size. This is because longer chains in polydisperse systems have to stretch less due to reduced crowding from neighboring shorter chains as compared to monodisperse system. Also, due to reduced crowding effects at high PDI, in densely grafted particles the differences in chain conformations arising from varying curvature becomes negligible.

C1.00193 Size Controlled Polymer Coated Nanoparticles as Efficient Compatibilizers for Polymer Blends, T. KWON, T. KIM, F. ALI, D.J. KANG, B.J. KIM, KAIST, J. BANG, Korea Univ., W.B. LEE, Sogang Univ. — Polymer-coated gold nanoparticles (Au) with controlled size and surface were successfully synthesized and applied to tailor the structures and properties of polytriphenylamine (PTPA) and polystyrene (PS) blends. Two different polymer-coated Au NPs with sizes of 5.9 nm (Au1) and 20.7 nm (Au2) were designed to be thermally stable above 200 °C and neutral to both PS and PTPA phases. Hence, both Au NPs localize at the PS/PTPA interface and function as compatibilizers in the PS/PTPA blend. To show the compatibilizing effect of the particles, the morphological behaviors of PS/PTPA blends containing different particle volume fraction of Au NPs were observed using cross-sectional TEM, and for quantitative analysis, the size distribution of PTPA droplets in the PS matrix was obtained for each sample. The number-average droplet diameter (D_n) of the PTPA domain in the blend was dramatically reduced from 1.4 μ m to 500 nm at a small volume fraction of 1.0 vol% Au1. The same trend of decreasing D_n was also observed with the addition of larger Au2, but a higher volume fraction was required to obtain the same amount of reduction in the PTPA droplet size. To demonstrate the effectiveness of Au NPs as compatibilizers, PS-b-PTPA block copolymers were also synthesized and used as compatibilizers.

C1.00194 Remote fluorescence-based sensing of elastic thin-film elastic moduli, AH YOUNG JEE, University of Illinois at Urbana Champaign, MINYUNG LEE, Ewha Womans University — The fluorescence lifetime of dyes embedded within thin polymer films is sensitive to the local mechanical environment. Here we show that this enables direct measurement of elastic properties of thin films and small samples whose investigation by conventional macroscopic mechanical characterization would not be possible. The specific example of poly(ethylene oxide) (PEO) and its nanocomposite thin films is highlighted. The method is also validated by comparison to a family of other polymers of known macroscopic moduli. Being simple, rapid, and reliable, we propose that this analysis can in principle apply generally to a broad class of soft materials and other polymer multilayer films.

C1.00195 Macroscopic Ordering of CNTs in a Liquid Crystalline Polymer Nano-Composite by Shearing , P. KALAKONDA, S. SARKAR, G.S. IANNACCHIONE, WPI, E. GOMBOS, G.S. HOONJAN, G. GEORGIEV, Assumption College, P. CEBE, Tufts U. — We present a series of complimentary experiments exploring the macroscopic alignment of carbon nanotubes (CNTs) in a liquid crystalline polymer (isotactic polypropylene - *iPP*) nano-composites as a function of temperature, shear, and CNT concentration. The phase behavior of *iPP*+CNT, studied by Modulated Differential Scanning Calorimetry, revealed the evolution of the α -monoclinic transition and its dynamics, which are dependent on CNT content and thermal treatment. These results indicate that the CNT nucleates crystal formation from the melt. Spectroscopic ellipsometry reveals a change in the optical constants that are connected to the ordering of CNTs when the *iPP*+CNT is sheared. This anisotropy is also exhibited in measurements of the electrical and thermal conductivities parallel and perpendicular to the shear direction. The amount of order induced into the dispersed CNTs is relatively low for these low concentration samples (< 5 wt%).

C1.00196 Self-assembly Nano-filled Polymer Blends in a Photovoltaic Thin-film Device , DI XU, JOSEPH ORTIZ, DILIP GERSAPPE, Department of Materials Science and Engineering, Stony Brook University — Engineering heterodyne junction solar cells requires a well-defined morphology of the photoactive polymers and the PCBM conductors such that maximum current reaches the electrodes with minimal resistive scattering. One possible method for accomplishing this may be to use polymer phase segregation in combination with the nanoparticles' natural segregation to the interfaces. In this manner, large-scale devices can be formed using self-assembly methods, rather than fixed methods. We have used Molecular Dynamics simulation to predict the morphology of polymer blends and determine which combination of factors would yield the optimal morphology that would contact the electrodes, while producing the largest number of interfaces. Secondly, we were also able to determine the conditions that would cause the particles to segregate and template along the interfaces, which would provide direct conductivity to the electrodes. Using thin film and bulk structures and by manipulating particle size, the attraction between the particle and the polymer component, and the amount of filler within the material, we can explore the formation of cheaper, more effective and efficient networks.

C1.00197 ABSTRACT WITHDRAWN —

C1.00198 ABSTRACT WITHDRAWN —

C1.00199 ABSTRACT WITHDRAWN —

C1.00200 Transformative Skin: From Anti-biofouling to Reliable Power Cable¹ , XUANHE ZHAO, Soft Active Materials Laboratory, Duke University — This talk will discuss the fundamental physics and potential applications of transformative skin, an electroactive polymer system recently developed at Duke Soft Active Materials Laboratory (SAMs Lab). The working mechanism of the transformative skin is based on the creasing-to-cratering instability in polymers under electrical voltages. The instability can induce failures in power cables and polymer capacitors. By suppressing the instability, one can greatly enhance the reliability and energy density of the cables and capacitors. Surprisingly, the same instability can generate a rich variety of on-demand patterns on polymer surfaces in response to voltages. The feature size of the pattern can be tuned from millimeter to nanometer. The pattern formation and surface deformation can dynamically debond biofilms formed on polymer surfaces, giving extraordinary capability of active antibiofouling.

¹Funding for this research was provided by the NSF's Research Triangle MRSEC (DMR-1121107) and Pratt School of Engineering at Duke University.

C1.00201 Molecular Dynamics Simulation of Diffusivity and Mobility of Ionic Charge Carriers in Model Battery Polymers , SARA WATERS, JON BROWN, New Mexico Institute of Mining and Technology, AMALIE FRISCHKNECHT, Sandia National Labs, JOHN MCCOY, New Mexico Institute of Mining and Technology — Molecular dynamics simulations of poly(ethylene-co-acrylic acid) monomers doped with Lithium ions were conducted using LAMMPS. The drift velocity of the ions resulting from a range of static electric fields were used to compute the ionic mobility. The frequency dependent mobility was also studied by using oscillatory electric fields.

C1.00202 Hypersonic properties of polymer films and multi-layers , JAMES SHARP, PAUL WALKER, ERIC YOUNG, University of Nottingham, VITALI GOUSSEV, Université du Maine, ANDREY AKIMOV, ANTHONY KENT, University of Nottingham — Picosecond acoustic measurements were performed on ultrathin films of polymers and thin film polymer multilayers supported on silicon (Si) substrates using a state of the art THz acoustic technique. In these experiments, a high power laser is used to excite picosecond duration strain pulses in an aluminium film evaporated on the reverse side of the Si substrate. These strain pulses then propagate through the substrate and interact with the polymer film/multi-layer. Vibrations in the film are detected optically using the same (pump-probe) beam which is passed through an optical delay line and reflected from the surface of the polymer film/multi-layer. Ultrathin films of polystyrene and a styrene-butadiene-styrene block copolymer were found to exhibit quantized closed-pipe organ like modes in the 0- 50 GHz regime that were attributed to vibrations of the entire polymer film. Thin film polystyrene/polyvinylpyrrolidone multilayer structures were found to display folded phonon dispersion curves that are characteristic of super-lattice structures. These structures have potential applications in GHz and THz optical switching and biosensing applications.

C1.00203 Local stress in thin polystyrene films , BEKELE GURMESSA, ANDREW CROLL, Department of Physics, North Dakota State University — Thin polymer films have received significant attention due to the deviation of material properties from bulk values. Part of the difficulty in describing the underlying physics is an incomplete understanding of how internal and surface stresses affect thin films. Here we exploit "wrinkling" to create a simple model system in which local stress can be easily tuned. When a thin polymer film bound to an elastic substrate is subjected to a compressive stress the film buckles out of plane. Due to the curvature at each crest and trough of the wrinkles, there arise local stresses in the polymer film. The curvature of the wrinkles is controlled by the modulus of the film and substrate, the film thickness and the applied stress, allowing us to apply an arbitrary local stress. After wrinkling, films are annealed above their glass transition temperature which allows flow and relaxes any stress. The local stress is then transferred to that of a thickness variation in the thin film. Importantly the flow of thin polymer films can be modeled using the well established lubrication theory, resulting in a simple scaling model. Our model allows us to investigate the response of thin films where deviations from bulk behavior are expected, as well as more complex thin diblock polymer films.

C1.00204 Cracking in thin films of colloidal particles on elastomeric substrates , MICHAEL SMITH, JAMES SHARP, University of Nottingham — The drying of thin colloidal films of particles is a common industrial problem (e.g paint drying, ceramic coatings). An often undesirable side effect is the appearance of cracks. As the liquid in a suspension evaporates, particles are forced into contact both with each other and the substrate, forming a fully wetted film. Under carefully controlled conditions the observed cracks grow orthogonal to the drying front, spaced at regular intervals along it. In this work we investigated the role of the substrate in constraining the film. Atomic force microscopy, was used to image the particle arrangements on the top and bottom surfaces of films, dried on liquid and glass substrates. We present convincing evidence that the interface prevents particle rearrangements at the bottom of the film, leading to a mismatch strain between upper and lower surfaces of the film which appears to drive cracking. We show that when the modulus of the substrate becomes comparable to the stresses measured in the films, the crack spacing is significantly altered. We also show that cracks do not form on liquid substrates. These combined experiments highlight the importance of substrate constraint in the crack formation mechanism.

[1] M.I. Smith, J.S. Sharp, Langmuir 27, 8009 (2011)

C1.00205 Reaction Kinetics at the Interface between Immiscible Polymers: Competition between Diffusivity and Reactivity¹, GUANGCUI YUAN, MINGJI WANG, CHARLES C. HAN, Institute of Chemistry, Chinese Academy of Sciences — Reactive blending processes at the interface between deuterated bisphenol-A polycarbonate (*d*PC) and amorphous polyamide (*a*PA) bilayer film were characterized by Fourier transform infrared (FTIR) and neutron reflectivity (NR). It was found that the aminolysis occurred during thermal annealing at 160 – 180 °C, inducing simultaneously scission of *d*PC chains and formation of *d*PC-*a*PA copolymer chains. Two or three stages of reaction kinetics as a function of time were probed by FTIR, depending on the competition between chain diffusivity and chemical reactivity for sample annealing at different temperatures. The late stage was controlled by potential barrier arising from previously formed copolymer, and it appeared earlier when annealing at 160 °C than that at higher temperatures. A phenomenon of transient interfacial instability which origin was ascribed to the mismatching in mobility of the polymer chains on either side of the interface was observed by NR. The copolymer once formed, remains localized at the interface and inhibits the diffusion of other reactive polymer chains still present in the bulk phase toward the interface.

¹ Chinese National Science Foundation (Project 21004069)

C1.00206 Thermal Behaviors of PS Thin Films on Grafted PS Layer with Varied Grafting Density, HOYEON LEE, SUNGMIN PARK, YONGHOON LEE, EUNYOUNG CHOI, DU YEOL RYU¹, Yonsei University, DAVID M. TROMBLY, VENKAT GANESAN², University of Texas — The thermal behavior properties (especially glass transition) are the key parameters for determining the mechanical properties of polymer system. In thin film system, the interfacial interactions at the substrate/polymer and polymer/air influence the transition behavior. In this study, we investigated the inter-relationship between the interfacial interactions arising from grafted polymer layers and the glass transition behavior (T_g) of thin polymer films with same chemical identity. We controlled grafting density of hydroxyl-terminated polystyrene (HO-PS). For polymer chains on the brushes of the same chemical identity with high density, the autophobic dewetting behavior can be attributed to the entropic effects of the polymer and the grafted polymer chains.

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C1.00207 Instability of Surface-initiated ATRP Polyelectrolyte Brushes in Aqueous Environments, CASEY GALVIN, ERICH BAIN, Department of Chemical Engineering, North Carolina State University, Raleigh, NC, EVREN OZCAM, Department of Chemical Engineering, University of California - Berkeley, Berkeley, CA, ADAM HENKE, Department of Chemistry, Columbia University, New York, NY, JIRI SROGL, Institute of Chemistry and Biochemistry, Prague, Czech Republic, JAN GENZER, Department of Chemical Engineering, North Carolina State University, Raleigh, NC — Surface-bound macromolecules have been produced using a number of polymerization schemes, including free-radical polymerization (FRP), reversible addition-fragmentation chain transfer polymerization (RAFT), and atom transfer radical polymerization (ATRP). In order to prove useful in any technology, the tethered polymer chains must remain stable in a variety of environments over relatively long timescales. We have investigated the dependence of the pH and ionic strength of aqueous solutions on the stability of surface-bound polyelectrolyte chains (strong and weak) with varying molecular weights and grafting densities. Our findings suggest that the ester bond in the most common form of ATRP surface initiator (BMPUS) will hydrolyze over a broad pH range, leading to chain degrafting. We further compare the stability of a BMPUS derivative which has had the ester bond replaced with an amide bond, as well as a free-radical initiator containing only aliphatic carbons. Results related to the effect of chain tension on brush stability will also be presented. Finally, we discuss the likely mechanism of degrafting, and ways in which to improve stability.

C1.00208 Lateral phase separation of mixed polymer brushes on planar and spherical surfaces, REID VAN LEHN, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — A mixed polymer brush consists of two (or more) polymer species grafted to a surface at a high density, inducing the polymers to highly stretch to maximize favorable solvent interactions while minimizing polymer overlap. The enthalpic and entropic interactions between the different polymers give rise to lateral phase behavior on the surface. Understanding this phase separation behavior is interesting for applications in nanotemplating and controlled protein adsorption. In this work, we present a novel theoretical model to quickly predict lateral phase separated morphologies of mixed polymer brushes on planar, cylindrical and spherical surfaces. The model combines a Flory-Huggins model for enthalpic interactions between the polymer components with an Alexander-de Gennes model for the entropy of the brush layers. When there is a length difference between the polymer components, these two interactions along with the conformational entropy of the system lead to a range of morphologies including stripes, dimples, mixing, and complete phase separation. The computational efficiency of this model allows for phase diagrams to be generated with great accuracy. The results of our model thus allow for the fast prediction of lateral morphologies on different geometries.

C1.00209 Photonic multilayer sensors from photo-crosslinkable polymer films, MARIA CHIAPPELLI, RYAN C. HAYWARD, University of Massachusetts Amherst — Photo-crosslinkable copolymers containing pendent benzophenone (BP) groups provide a convenient means to fabricate multilayer polymer films. We describe the preparation of alternating multilayers of photo-crosslinkable poly(N-isopropylacrylamide) (PNIPAM), a water-swellaable, temperature sensitive polymer, and poly(para-methylstyrene) (PpMS), a non-swellaable polymer, by sequential spin-coating and photo-crosslinking. This route provides well-defined layered structures with minimal interfacial broadening between layers and uniformity of thickness from layer to layer as determined by dynamic secondary ion mass spectrometry (d-SIMS). Appropriate choices of layer thicknesses yield 1-D photonic gel sensors. The reflectance peak is shifted through the visible spectrum upon swelling or de-swelling of the PNIPAM layers in water, providing an accessible means for colorimetric temperature sensing.

C1.00210 Template polymerization using a controlled reaction scheme, JAN GENZER, PREETA DATTA, NC State University — We employ a Monte Carlo simulation scheme based on the bond fluctuation model to simulate template polymerization via controlled scheme (i.e., termination and chain transfer reactions are neglected) involving co-polymerization of free monomers and monomers bound to a template that consists of four linear substrates with equispaced sites occupied by bound monomers. A new macromolecule is initiated by activation of an initiator; any monomer (free or bound) that is within the reaction distance (nearest neighbors) of the initiator can be incorporated into the chain. As the chain propagates, it adds new monomers to the macromolecule. Those monomers can either be bulk (i.e. free) monomers or those that are placed on the predefined template. We analyze the effect of the number of spacing of the bound monomers on the composition and monomer distribution in the resultant co-polymer. Our results reveal that the larger the total number of bound monomers in the system and the more dense spacing, the greater is the likelihood of those getting incorporated in the growing chains. In addition, a greater number of bound monomers on the linear template promotes polymerization of most/all of the bound monomers to form a linear array attached to the template.

C1.00211 Wrinkling of Inhomogeneously Strained Thin Polymer Films, YU-CHENG CHEN, ALFRED J. CROSBY, University of Massachusetts - Amherst — Surface wrinkles have received much attention recently due to their potential importance in applications. Wrinkles occur due to a mechanical instability when sufficient strain applied to an incompressible thin film. For wrinkles made with a polymer film supported on a soft elastomer, it has been well-established that the amplitude is directly proportional to the wavelength and the square root of the applied strain. Importantly, the wavelength is largely insensitive to the applied strain and defined by the properties of the film and substrate. These dependences have been confirmed with ideal substrates where the global strain is homogeneously distributed, but the influence of strain inhomogeneity has not been considered previously. Will regions that wrinkle first lead to strain localization, or will the system try to homogenize strain globally? We use a recently developed adhesion contact line method to prepare polystyrene thin films with periodic regions of different wrinkle amplitudes, hence strains, on soft substrates. We find that surfaces with multiple wrinkle amplitudes will approach a single amplitude globally upon the application of sufficiently large strains. We derive relationships to describe this process.

C1.00212 Comparison of surface mobility on low and high molecular weight glasses, MARK EDIGER, University of Wisconsin-Madison, KEEWOOK PAENG, Columbia University, LEI ZHU, Merck & Co., LIAN YU, University of Wisconsin-Madison — The glass transition temperature of thin polymer films and the related issue of mobility at glass surfaces have attracted considerable interest in the last twenty years. We have recently conducted experiments on both polymeric and low molecular weight glass formers that provide information about mobility near the free surface. For several polymers, measurements of dye reorientation on freestanding films show a fast population that can be consistently assigned to the near-surface region. For indomethacin (a low molecular weight glass former), we have directly measured surface diffusion by following the decay of imprinted gratings of different periods. For both high and low molecular weight glassformers, we observed enhanced mobility near the free surface (by factors up to 10^4 and 10^7 , respectively) relative to the bulk dynamics. In both cases, surface mobility has a substantially weaker temperature dependence than bulk mobility near the bulk T_g .

C1.00213 Molecular Bottlebrushes as Tensile Machines for Probing Specific Bonds under Tension, YUANCHAO LI, Department of Chemistry, UNC at Chapel Hill, ALPER NESE, Department of Chemistry, Carnegie Mellon University, NATALIA LEBEDEVA, TYLER DAVIS, Department of Chemistry, UNC at Chapel Hill, KRZYSZTOF MATYJASZEWSKI, Department of Chemistry, Carnegie Mellon University, SERGEI SHEIKO, Department of Chemistry, UNC at Chapel Hill — Significant tension on the order of 1 nN is self-generated along the backbone of bottlebrush macromolecules due to steric repulsion between densely grafted side chains. The intrinsic tension is amplified upon adsorption of bottlebrush molecules onto a substrate and increases with grafting density, side chain length, and strength of adhesion of the substrate. This allows us to employ these molecular bottlebrushes as miniature tensile machines to probe the mechanochemistry of specific bonds. For this purpose, bottlebrush macromolecules with a disulfide linker in the middle of the backbone were synthesized by atom transfer radical polymerization (ATRP). Two processes, (i) homolytic cleavage of disulfide and (ii) scission of disulfide due to reduction by dithiothreitol were monitored through molecular imaging by atomic force microscope (AFM). In both cases, the corresponding rate constants increase exponentially with mechanical tension along the disulfide bond. Moreover, the reduction rate at zero force is found to be significantly lower than that in bulk solution, which suggests an acidic composition of the water surface with $\text{pH}=3.7$. This opens a new application of brush-like macromolecules as surface pH sensors.

C1.00214 Simultaneous Vapor Deposition and Phase Separation of Polymer Films, RAN TAO, MITCHELL ANTHAMATTEN, University of Rochester — Initiated chemical vapor deposition (iCVD) is a solventless, free radical technique used predominately to deposit homogeneous films of linear and crosslinked polymers directly from gas phase feeds. The major goal of this research is to force and arrest phase separation of deposited species by co-depositing non-reactive molecules (porogens) with reactive monomers and crosslinkers. We introduce these species during iCVD to force and quench polymer induced phase separation (PIPS) during film growth as a step toward tunable pore-size, density, and morphology. Polymerization, crosslinking and PIPS are intended to occur simultaneously on the substrate, resulting in a vitrified microstructure. Cahn-Hilliard theory predicts that the length scale of phase separation depends on the polymer-porogen interaction energy, the polymerization rate and the species' mobility. A series of films were grown by varying deposition rate, porogen type, and reagent flowrates. Crosslinkers were introduced to limit the growth of phase separated domains and to provide mechanical support during porogen removal. To elucidate how phase separation competes with polymerization and film growth, deposited films were studied using a combination of electron microscopy, profilometry and spectroscopic techniques.

C1.00215 Controlled viscous and viscoelastic instabilities of polystyrene film on topographically patterned poly(methyl methacrylate), ZHENG ZHANG, DAE UP AHN, YIFU DING, University of Colorado at Boulder — We report the spontaneous morphological evolution of polystyrene (PS) films spin-cast on pre-patterned poly(methyl methacrylate) (PMMA) substrates, at annealing temperatures above the glass transition temperatures of both polymers. The influences of the molecular weights and spin-cast volume of PS on the morphological development were systematically examined. Both were found to modulate the instabilities and result in distinctive morphologies. In particular, thick PS films that fully covered the topographically patterned PMMA substrate would dewet through nucleation and growth of randomly formed holes. However, the rupture of thinner PS films were manifested through formation of arrays of non-axisymmetrically confined threads and subsequent capillary instabilities of these threads. Low and high molecular weights of PS gave rise to two different modes of thin-thread instabilities, identified as varicose and peristaltic mode, respectively.

C1.00216 Novel Synthesis of Surface-Grafted Radical Initiator With Improved Stability and Yield, ERICH BAIN, KEITH DAWES, Department of Chemical and Biomolecular Engineering, North Carolina State University, XINFANG HU, CHRISTOPHER GORMAN, Department of Chemistry, North Carolina State University, JIRI SROGL, Institute of Chemistry & Biochemistry, Academy of Sciences of the Czech Republic, JAN GENZER, Department of Chemical and Biomolecular Engineering, North Carolina State University — Polymers grafted at interfaces are attractive for applications including antifouling coatings, biologically functionalized materials, and responsive surfaces. The “grafting from” approach to form densely packed brushes involves functionalizing a substrate with initiating moieties, and carrying out polymerization, e.g., surface-initiated free-radical polymerization (SI-FRP). Azo initiators for SI-FRP are commonly synthesized by a low-yielding route requiring large amounts of potassium cyanide. Those initiators are linked to a substrate by means of an ester group, rendering tethered polymers susceptible to degrafting by hydrolysis. We present a novel synthetic route to an asymmetric azo initiator, whose yield is nearly double that of previous syntheses. Cyanide usage in the new method is reduced by 72 percent. The spacer linking the initiator to a substrate contains only carbon-carbon bonds, resulting in stable brushes. Results are demonstrated for SI-FRP as well as reverse ATRP and RAFT.

C1.00217 Impact of adhesion on thermal boundary conductance at organic-metal interface¹, Y. JIN, C. SHAO, J. KIEFFER, K.P. PIPE, M. SHTEIN, University of Michigan, Ann Arbor — The thermal boundary conductance (TBC) at the interfaces between a small molecular organic semiconductor (copper phthalocyanine CuPc) and several metals (Al, Mg, Au, Ag) has been measured using the 3- ω method at room temperature. The TBC increases with the interfacial bonding strength of the two dissimilar materials. Our measurements of adhesion between the metal and organic films agree qualitatively with the distances between the metal surface and CuPc molecules measured by Stadtmüller et al. [1]. In contrast to the trend observed for organic-metal interfaces, the TBC of organic-organic interfaces (e.g. CuPc/C60) is insensitive to interface bonding due to the large overlap between materials' phonon density of states. Conventional acoustic and diffuse mismatch models fail to describe the observed trend in TBC. Modifying the acoustic mismatch model (AMM) with an effective spring constant describing interfacial bonding, an accurate trend is obtained. To better understand the influence of the molecular structure on TBC, we performed molecular dynamics simulations of interfacial heat transfer and interfacial bonding. These simulations reveal quantitative discrepancies in the simulated TBC relative to that predicted by the modified AMM model in the regime of poor interfacial adhesion, which we attribute to a greater contribution of anharmonicity. The bonding strength for vacuum deposited films is ~ 2 GPa for CuPc/Ag and CuPc/Au, well within the regime in which anharmonic processes play an important role in interface thermal transport. [1] Stadtmüller et al. *PRB* 83 085416

¹We acknowledge the financial support of this work by Air Force Office of Scientific Research MURI program. Grant No. FA9550-08-1-0340

C1.00218 Ion Correlations at an Electrified Liquid/Liquid Interface, NOUAMANE LAANAIT, MIROSLAV MIHAYLOV, BINYANG HOU, HAO YU, University of Illinois at Chicago, PETR VANYSEK, Northern Illinois University, BINHUA LIN, MATI MERON, CARS, University of Chicago, ILAN BENJAMIN, University of California at Santa Cruz, MARK SCHLOSSMAN, University of Illinois at Chicago — Ion correlations have been suggested as the underlying mechanism of a number of counterintuitive phenomena such as like-charge attraction. Here we present the first molecular-level tests of density profiles predicted by an ion correlations model. Synchrotron x-ray reflectivity reveals ion condensation at the liquid/liquid interface, when polarized with an electric field.¹ Tuning the density of this ionic layer allows for a detailed study of ion correlations as a function of the Coulomb coupling strength in the system. We propose a parameter-free density functional theory that describes ion-ion correlations within a weighted density approximation and explicitly treats ion-solvent effects through a solvent interaction potential simulated by molecular dynamics. Agreement with the x-ray reflectivity and the interfacial excess charge is found over the entire experimental range of ion-ion correlation energies up to nearly $4 k_B T$. These results suggest that ion correlations in the electrical double layer can be accurately described by mapping to a simple Coulomb system, in this case a one-component plasma.

¹N. Laanait et al. *J. Chem. Phys.*, **132**, 171101, 2010

C1.00219 Fluctuations of one-dimensional interface in the directed polymer formulation: role of a finite interface width¹, ELISABETH AGORITSAS, DPMC-MaNEP, University of Geneva (Switzerland), VIVIEN LECOMTE, Laboratoire Probabilités et Modèles Aléatoires, Universités Paris VI and Paris VII (France), THIERRY GIAMARCHI, DPMC-MaNEP, University of Geneva (Switzerland) — An elastic interface living in a disordered medium always exhibits geometrical fluctuations, characterized in particular by the distribution of its relative displacements as a function of the lengthscale r , whose variance defines the interface roughness $B(r)$. Those fluctuations are the manifestation of the probability and associated effective free-energy of the different configurations of the interface, in presence of disorder and at finite temperature. Focusing specifically on the one-dimensional interface, we use the exact mapping of the static interface on the directed polymer in random medium in order to explore both analytically and numerically the role of a finite interface width $\xi > 0$, assuming a short-range elasticity and a random-bond quenched disorder. Confirming the existence of a low-temperature regime where the finite microscopic width plays a crucial role, as predicted by previous Gaussian-Variational-Method predictions [*Phys.Rev.B* 82, 184207 (2010)], we propose a coherent picture of the physics at stake, compatible both with numerical computations and generic scaling arguments.

¹This work was supported in part by the Swiss SNF under MaNEP and Division II.

C1.00220 Wang-Landau simulations of polymer adsorption on diluted surfaces¹, PAULO MARTINS², Instituto de Física, Universidade Federal de Mato Grosso, Cuiabá, MT, Brazil, THOMAS VOGEL, DAVID LANDAU, Center for Simulation Physics, University of Georgia, Athens, GA, USA — We consider a single linear lattice homopolymer in three dimensions that interacts with a diluted planar surface. A fraction p of the total number of the sites on the substrate is attractive, while the remaining $1 - p$ remains neutral. Our focus is on the conformational transitions the polymer can experience under different environmental conditions, for instance, the surface dilution and the strength of the substrate attraction, compared to the intensity of the monomer-monomer interactions. To get insights on the phase diagram we have performed extensive Monte Carlo simulations, by using the Wang-Landau sampling, for different values of the surface attraction ϵ and the concentration of attractive sites p , specially near the surface percolation threshold p_c .

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C1.00221 The Behavior of Water at the Interface with Polystyrene¹, SELEMON BEKELE, Tennessee Tech University, MESFIN TSIGE, The University of Akron — Solid-aqueous interfaces are of great importance in many industrial applications ranging from oil recovery to biotechnology. The behavior of interfacial water differs drastically from that of the bulk liquid and strongly depends on the atomistic details of the surface itself. Molecular dynamics simulations have been used extensively to study the structure and dynamics of the interface between a polymeric thin film and water. Using a fully atomistic molecular dynamics simulation, we have examined the structure and dynamics of water and atactic polystyrene (aPS) chains near the aPS-water interface. In this talk, we present results for the contact angle of water and the interfacial surface tension at the aPS-water interface.

¹This work is supported by the NSF (DMR0847580).

C1.00222 MD study of polymer melts confined in thin films and nanopores, HENDRIK MEYER, Institut Charles Sadron, CNRS Strasbourg, France — The structure of chains is strongly affected if they are confined to films or pores smaller than the radius of gyration [1,2]. We report new molecular dynamics simulations of polymer melts confined between structureless walls comparing the thin film and pore confinement. It is shown that the form factor which is measured in scattering experiments is affected in a subtle way by the corrections to ideality [2]. The strong confinement reduces the number of overlapping chains and thus reduces entanglements. This leads to a clear acceleration in thin film confinement. For pore confinement, an acceleration is also found for intermediate pore diameters, but for extreme confinement, chains are segregated and they will block each other. [1] H. Meyer et al *Eur. Phys. J. Sp.Top.* 141 (2007) 167. [2] N. Lee et al *EPL* 93 (2011) 48002.

C1.00223 Adsorption of Derivatized Dextran Polyelectrolytes onto Nanocrystalline Cellulose¹, ALAN ESKER, JOSHUA KITTLE, XIAOSONG DU, Virginia Tech, Department of Chemistry (0212), Blacksburg, VA 24061, FENG JIANG, MAREN ROMAN, Virginia Tech, Department of Wood Science and Forest Products (0323), Blacksburg, VA 24061, HOLGER WONDRAKZEK, ANDREAS KOSCHELLA, THOMAS HEINZE, Center of Excellence for Polysaccharide Research, Friedrich Schiller University of Jena, Humboldtstrasse 10, Jena, 07743 Germany — The adsorption of a series of cationically derivatized dextran polyelectrolytes onto anionic nanocrystalline cellulose (ANC) has been studied using quartz crystal microbalance with dissipation monitoring (QCM-D) and surface plasmon resonance (SPR). Samples of dimethylaminoethyl-dextran (DMAE-Dex), diethylaminoethyl-dextran (DEAE-Dex), and diisopropylaminoethyl-dextran (DIAE-Dex) had degrees of substitution (DS) ranging from 0.06-0.90. DMAE-Dex, DEAE-Dex, and DIAE-Dex all showed decreasing adsorption onto ANC and decreasing water content of the adsorbed film with increasing DS. Additionally, DEAE-Dex films adsorbed onto ANC had lower water contents than DMAE-Dex films with the same DS. Interestingly, QCM-D results for DIAE-Dex with high DS revealed mass loss, while SPR results clearly showed DIAE-Dex adsorbed onto ANC. These observations were consistent with dehydration of the ANC substrate. This study indicates that by controlling the DS and hydrophobic content of the polyelectrolyte, the water content of the film can be tailored.

¹National Science Foundation (CHE-0724126)

C1.00224 ABSTRACT WITHDRAWN —

C1.00225 Engineering Novel Thermoreversible Hydrogels with Applications in Regenerative Medicine and Delivery Systems, DIVYA BHATNAGAR, State University of New York at Stony Brook, NIKHIL MEHANDRU, Harvard University, JAPBANI NANDA, W. Tresper Clarke High School, YICHENG SUN, Mission San Jose High School, MIRIAM RAFAILOVCH, State University of New York at Stony Brook — A major concern in regenerative medicine is the increasing need for effective biomaterials for scaffolds, cell delivery vehicles, and drug delivery systems. In this study, we engineered a thermo reversible composite hydrogel of hard, medium and soft stiffness by blending Pluronic F127 (F127) with biocompatible hyaluronic acid (HA) and bioadhesive gelatin. Rheological analysis demonstrated that hard gel produced the highest elastic modulus in both HA-F127 and Gelatin-F127 hydrogels. It was found that increasing the concentration of HA and gelatin increased the critical solution temperature (CST) at which the solution gels. Glucose and sodium chloride, additives commonly found within the body, were analyzed to have minimal effect on the mechanical properties but caused a decrease in CST. Adult human dermal fibroblasts were plated on the composite hydrogels to demonstrate scaffolding and cell delivery. The highest growth was observed in hard Gelatin-F127 hydrogels. Cells also showed the best response to hard Gelatin-F127 gels in shear modulation force microscopy and were found to be homogeneously distributed in the three-dimensional matrix of the gels. Our novel composite hydrogel displayed synergistic properties of its individual components and had the necessary characteristics for effective use in the medical setting: mechanical strength, cell adhesion and viability.

C1.00226 Synchrotron SAXS and WAXD Studies of Cellulose Nascent Crystals: Experiment and Structure Analysis, YING SU, CHRISTIAN BURGER, BENJAMIN S. HSIAO, BENJAMIN CHU, Stony Brook University, STONY BROOK UNIVERSITY TEAM — Cellulose nascent crystals extracted from biomass (wood pulp, jute and cotton) by combined chemical and mechanical treatments are low cost, environmentally friendly and high performance materials to form the barrier layer in ultrafiltration membranes. This research project is aimed at using the synchrotron X-ray scattering methods to characterize the nascent crystalline nanofibers in different formats. The SAXS (Small Angle X-ray Scattering) data of cellulose nanofiber suspensions was analyzed and the polydisperse ribbon model with rectangular cross section fit the data well. The 2D and 3D simulations of WAXD (Wide Angle X-ray Diffraction) pattern of jute cellulose fibers solved the contents ratio of cellulose I-alpha and I-beta and Hermans' orientation parameter P2.

C1.00227 Friction between Brush Layers of Charged and Neutral Bottle-Brush Macromolecules. Molecular Dynamics Simulations¹, DANIEL RUSSANO, Boston University, JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, University of Connecticut — We used MD simulations to study lubricating properties of neutral and charged bottle-brush coatings as a function of the compression and shear stresses, and brush grafting density. Our simulations have shown that in charged systems under shear there is a layer with excess of counterions found in between brush bearing surfaces. The main deformation mode of the charged layers is associated with the backbone deformation resulting in the backbone deformation ratio, α , and shear viscosity, η , being universal functions of the Weissenberg number, W . In the case of neutral systems in addition to the backbone deformation there is also side chain deformation. The coupling between backbone and side chain deformation violates universality in α dependence on W and results in scaling exponents varying with compression stress and brush grafting density. Existence of different length scales controlling deformation of neutral bottle-brushes manifests itself in shear viscosity, η , dependence on the shear rate, $\dot{\gamma}$. Shear viscosity, η , as a function of the shear rate, $\dot{\gamma}$, has two plateaus and shear thinning regimes. The low shear rate plateau and shear thinning regime correspond to the backbone deformation while the second plateau and shear thinning regime at moderate shear rates is due to side chain deformation. For both systems the value of the friction coefficient increases with increasing the shear rate.

¹NSF # DMR-1004576

C1.00228 Dynamics of Nanoparticle Adhesion¹, ANDREY DOBRYNIN, JAN-MICHAEL CARRILLO, University of Connecticut, ELIE RAPHAEL, ESPCI — We have performed molecular dynamics simulations of peeling of nanoparticles from substrate to understand the dynamics of nanoparticle adhesion. In our simulations we have calculated the potential of mean force characterizing the strength of the nanoparticle interaction with the substrate as a function of the particle-substrate separation. These simulations have shown that the detachment of the nanoparticle from substrate occurs through neck formation. The neck height decreases with increasing nanoparticle shear modulus (crosslinking density). Furthermore our simulations have established that the detachment time t_R scales with the applied force as f^{-5} . This strong force dependence is a result of the fine interplay between nanoparticle surface energy, elastic energy and its adhesion to the substrate that controls the shape of the nanoparticle.

¹ACS: PRF No. 49866-ND7

C1.00229 Measuring Adhesion of Freestanding Polymer Nano-fibers, XIN WANG, Northeastern University, JOHNNY NAJEM, SHING-CHUNG WONG, University of Akron, KAI-TAK WAN, Northeastern University — A novel method is used to measure directly adhesion between two freestanding polymer nano-fibers. A single fiber is attached to two microspheres readily glued to an atomic force microscope (AFM) cantilever. Another freestanding fiber is similarly prepared on a mica substrate. The fibers are arranged in orthogonal crossed-cylinder geometry. External load is applied to deform the two fibers into complementary V-shapes, and the force response allows determination of elastic modulus. At a critical tensile load, "pull-off" occurs and the adhering fibers spontaneously detach from each other, yielding the interfacial adhesion energy. Loading-unloading cycles are performed to investigate fiber degradation and repeated adhesion-detachment.

C1.00230 Differential AC chip calorimeter for in situ investigation of vapor deposited thin films, MATHIAS AHRENBURG, CHRISTOPH SCHICK, HEIKO HUTH, EVGENI SCHOIFET, University of Rostock, MARK EDIGER, KATIE WHITAKER, University of Wisconsin - Madison, Wisconsin, USA — Physical vapor deposition (PVD) can be used to produce thin films with particular material properties like extraordinarily stable glasses of organic molecules. We describe an AC chip calorimeter for in-situ heat capacity measurements of as-deposited nanometer thin films of organic glass formers. The calorimetric system is based on a differential AC chip calorimeter which is placed in the vacuum chamber for physical vapor deposition. The sample is directly deposited onto one calorimetric chip sensor while the other sensor is protected against deposition. The device and the temperature calibration procedure are described. The latter makes use of the phase transitions of cyclopentane and the frequency dependence of the dynamic glass transition of toluene and ethylbenzene. Sample thickness determination is based on a finite element modeling (FEM) of the sensor sample arrangement. A layer of toluene was added to the sample sensor and its thickness was varied in an iterative way until the model fits the experimental data.

C1.00231 Effective Temperature: from Red-Blood-Cell Membrane Fluctuations to trapped active particles, EYAL ISAAC BEN ISAAC, NIR GOV, None — Biologically driven nonequilibrium fluctuations are often characterized by their non-Gaussianity or by an “effective temperature”, which is frequency dependent and higher than the ambient temperature. We address these two measures theoretically by examining a randomly kicked particle, with a variable number of kicking motors, and show how these two indicators of nonequilibrium behavior can contradict. Our results are compared with new experiments on shape fluctuations of red-blood cell membranes, and demonstrate how the physical nature of the motors in this system can be revealed using these global measures of nonequilibrium. Furthermore, our concept of The concept of the effective temperature is extended to active particles trapped in a potential well. We calculated the average escape time and find that Kramers’ reaction-rate theory is found to quite hold in this system. Using this calculated escape time, together with the exact calculation of the active diffusion coefficient for the escaped (free) active particle; one can attempt to fully describe the long-time random-walk of the tracer particle in the active gel.

C1.00232 Structural and phase transitions of one and two polymer mushrooms, DELIAN YANG, QIANG (DAVID) WANG, Colorado State University — A polymer mushroom here refers to a group of n homopolymer chains end-grafted at the same point on a flat, impenetrable and homogeneous substrate. Using lattice self-consistent field (LSCF) calculations with the Kronecker δ -function interactions (instead of the commonly used nearest-neighbor interactions), we have studied the structures of one and two polymer mushrooms in an explicit solvent as a function of the polymer volume fraction, the solvent quality characterized by the Flory-Huggins χ parameter, and the distance between the two mushrooms. We have constructed phase diagrams of these systems showing the coil-globule transition (CGT) of one mushroom and how it is coupled with the fused-separated transition (FST) of two mushrooms. Since LSCF results are exact only in the limit of $n \rightarrow \infty$, we also use the newly proposed fast lattice Monte Carlo (FLMC) simulations¹ with the same Hamiltonian as in LSCF theory to examine how this limit is approached with increasing n . Direct comparisons between LSCF and FLMC results without any parameter-fitting quantify the fluctuation/correlation effects neglected in LSCF theory. We also find a second-order symmetric-asymmetric transition (SAT) for one-mushroom system in the globule state, and examine its coupling with CGT and FST. [1] Q. Wang, *Soft Matter*, **5**, 4564 (2009); **6**, 6206 (2010).

C1.00233 Quantification of Complex Topologies in Macromolecular and Nanoscale Structures using Small-Angle Scattering, SIDDHARTH PRADHAN, RAMANTH RAMACHANDRAN, DURGESH RAI, GREGORY BEAUCAGE, University of Cincinnati — Polymers are characterized by molecular weight distribution, tacticity, block copolymer content and branch content and chain topology. The branch structure and particularly the topology of branched chains has remained a difficult characterization problem. Recently we have developed a scaling model that can be coupled with small-angle scattering to measure the average branch length, number of branches and branch-on-branch structure in macromolecules of complex topology. This method has been extended to understand the structure of two dimensional structures and crumpling in these macromolecular systems. We have explored a wide range of materials in this regard. This poster will give an overview of the current uses for the scaling model for macromolecular topology. References pertaining to this poster can be found at <http://www.eng.uc.edu/~gbeaucag/BranchingPapers.html>.

C1.00234 SOFT CONDENSED MATTER —

C1.00235 Microfluidic Insights into Filter Design, SORELL MASSENBURG, DAVID WEITZ, Harvard University — Nearly every application involving fluid relies heavily upon filtration, yet filter design is not well understood. Previous studies show that hard sphere clogging in microfluidic channels is well described by a probabilistic model that also reveals information about the clogging material's proclivity to aggregation. Design features, such as pore size distribution, can be modeled in two dimensions using soft lithographic techniques to fabricate microscale pores. We then test the efficacy of variations in pore design by clogging these pores with polystyrene microparticles. The clogging behavior of these fabricated pores is then compared to the aforementioned probabilistic model to elucidate the function of various features of filter design.

C1.00236 Photoelastic study of sound waves in grain packings, XAVIER NOBLIN, GUILLAUME HUILLARD, JEAN RAJCHENBACH, LPMC, UMR 6622 CNRS-UNS, Parc Valrose, 06108 Nice Cedex 2, France — By means of photoelasticity, we success in visualizing in real time the propagation of acoustic waves in a granular packing of cylinders. Our experimental procedure allows an access to the local state of stress of individual grains as a function of time with a good accuracy. We first present results on 1d chains of cylinders that are constrained by a static confinement force. Both linear and nonlinear regimes are presented. We emphasize the role of the grains roughness on the propagation properties, and also of the solid friction with the walls. Our results concerning the wave velocity as a function of the amplitude, and of the confinement force, are compared to the theory and to the spherical beads case. We then present experimental results on 2d pilings, in particular for the wave speed.

C1.00237 Dense granular flow around a rigid or flexible intruder, EVELYNE KOLB¹, PMMH, ESPCI, MOKHTAR ADDA-BEDIA², LPS, ENS, ANNETTE HOSOI COLLABORATION³, KO OKUMURA COLLABORATION⁴ — We experimentally studied the flow of a dense granular material around an obstacle (rigid cylinder or flexible plate) placed in a 2 dimensional confined cell at a packing fraction near the 2D jamming threshold. In the case of the rigid obstacle, the displacement field of grains as well as the drag force experienced by the obstacle were simultaneously recorded and a parametric study was done by changing the cell size, the intruder diameter or the packing fraction. The drag force experienced by the intruder and the formation of a wake behind the obstacle were very sensitive to the approach to jamming. The same experimental set-up was adapted to a flexible intruder and coupling between the granular flow and fibre deflexion were imaged. The deformation of the fibre could be compared with theoretical predictions from elastica.

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C1.00238 Mechanisms of defect motion in hexagonal systems on sinusoidal substrates, NICOLAS GARCIA, LEOPOLDO GOMEZ, DANIEL VEGA, Depto. de Fisica-IFISUR-Univ. Nac. del Sur. ANPCyT y Conicet., Argentina — In this work we have studied through a Landau's free energy functional approach the dynamic and equilibrium configurations of two-dimensional hexagonal systems constrained to lie on a substrate with sinusoidal topography. Similarly to previous studies, we have found a strong coupling between defects and geometry, where the regions with the highest local Gaussian curvature act as sink for disclinations. We have studied the influence of the local curvature of the substrate on the diffusional dynamics of dislocations and disclinations. We have found a novel mechanism of defect diffusion where linearly correlated arrays of dislocations (scars) move according to the gradient of curvature.

C1.00239 Colloidal cluster array formation by weak ac electric fields¹, WENCESLAO GONZÁLEZ-VIÑAS, RAHEEMA ASLAM, MOORTHY PICHUMANI, University of Navarra — We study experimentally the influence of weak alternating electric fields on dilute colloids with a free surface open to the air. When the experimental conditions minimize the evaporation of the solvent, a well-defined one-dimensional cluster array is formed along the straight contact line. The cluster array evolves due to a hydrodynamical instability which can be controlled by the applied field [1]. Once the clusters are formed, if the evaporation is favored, the contact line recedes. Under these conditions, the capillary flows towards the clusters strengthen. As a consequence, elongated columns of particles are deposited on the substrate. The characteristic length between these columns is controlled during the initial stages of the cluster formation [2]. To shed light on the cluster formation mechanisms, further work is currently carried out for identifying similar phenomena without the existence of a free surface.

[1] M. Pichumani et al. Phys. Rev. E 83 (2011), 047301

[2] R. Aslam et al. In preparation

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C1.00240 Melting of Colloidal Crystals¹, YI PENG, ZIREN WANG, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China, AHMED ALSAYED, Complex Assemblies of Soft Matter, CNRS/UPENN/Rhodia UMI 3254, Bristol, Pennsylvania 19007, USA, ARJUN YODH, Department of Physics and Astronomy, University of Pennsylvania, 209 South 33rd Street, Philadelphia, Pennsylvania 19104, USA, YILONG HAN, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China — We experimentally studied the melting and freezing behaviors of colloidal crystals composed of diameter tunable poly-N-isopropylacrylamide (NIPA or pNIPAM) microgel spheres by bright-field and confocal video microscopies. The melting behaviors of three-dimensional (3D), two-dimensional (2D) and multilayer thin films of both single crystals and polycrystals were systematically studied with single-particle dynamics. Thick films (>4 layers) melt heterogeneously, while thin films (<5 layers) melt homogeneously even in polycrystals. A novel heterogeneous melting at dislocation is discovered in 5- to 12-layer films. The equilibrium phase behaviors are different in three thickness regimes: thick films have a liquid-solid coexistence regime which decreases with the film thickness and vanishes at 4 layers, thin films melt into the liquid phase in one step, while monolayers melt in two steps with an intermediate hexatic phase. These results provide new challenges in theory.

¹GRF grants 601208 and 601911

C1.00241 Formation of Uniform Hollow Silica microcapsules, HUAN YAN, CHANJOONG KIM, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, Kent, OH44242, USA — Microcapsules are small containers with diameters in the range of 0.1 – 100 μm . Mesoporous microcapsules with hollow morphologies possess unique properties such as low-density and high encapsulation capacity, while allowing controlled release by permeating substances with a specific size and chemistry. Our process is a one-step fabrication of monodisperse hollow silica capsules with a hierarchical pore structure and high size uniformity using double emulsion templates obtained by the glass-capillary microfluidic technique to encapsulate various active ingredients. These hollow silica microcapsules can be used as biomedical applications such as drug delivery and controlled release.

C1.00242 Multiblock Janus particles with tunable patch size, JIE ZHANG, QIAN CHEN, SUNG CHUL BAE, STEVE GRANICK, University of Illinois at Urbana-Champaign — Micro-printing methods are used to systematically tune the size, position and number of functionalized patches on colloidal particles with excellent monodispersity. This study introduces two new members of the Janus particle family: triblock particles with two small poles, and eyeball Janus particles. Without the intervention of any external field, the former form chain, ring, coil and knot structures. In principle, dynamic and reconfigurable colloidal bilayers can be built from eyeball Janus particles.

C1.00243 Effective static and high-frequency viscosities of concentrated suspensions of soft particles, CARLOS I. MENDOZA, Instituto de Investigaciones en Materiales, UNAM — We obtain an analytic expression that allows determining the static and high-frequency viscosities as function of the volume fraction of a concentrated suspension of soft spherical particles. The particles consist of a hard core of radius a covered by a porous layer of thickness d . The proposed expression incorporates the results for the intrinsic viscosity obtained on the basis of a cell model into a recently obtained relation for the effective viscosity of concentrated colloidal suspensions [J. Chem. Phys. 130, 044904 (2009)]. In this model, the correlations between the particles due to crowding effects are introduced through an effective volume fraction which is then used as integration variable in a differential effective medium procedure. The final expression is simple, accurate, and allows collapsing all the data in a universal master curve. The only difference between the static and high-frequency cases is that in the last case the effective volume fraction also incorporates hydrodynamic interactions arising from the so-called relaxation term. We have tested the accuracy of our model with experiments and simulations. In all cases the agreement with the data is extremely good.

C1.00244 Nanoparticle adsorption from a crowded solution at a solid/liquid interface, INDERMEET KOHLI, SHARMINE ALAM, ASHIS MUKHOPADHYAY, Wayne State University — Adsorption of nanoparticles at solid-liquid interface is of great importance in the field of colloidal science and biophysics. Protein adsorption is one of the most significant processes and can be mimicked by colloidal systems. We will present results of our studies of the kinetics of adsorption of gold nanoparticles from a crowded polyvinyl alcohol (PVA) polymer solution on a solid/liquid interface using phase-modulated ellipsometry. The experimental system mimics many biological processes, where the adsorption of particles or proteins takes place in the presence of many other components.

C1.00245 Responsive Poly (ϵ -carbobenzyloxy-L-lysine)-based Colloidal Particles: Exploring and Characterizing the Inverse α -Helix to Random Coil Transition in m-Cresol¹, CORNELIA ROSU, Louisiana State University, SIBEL TURKSEN-SELÇUK, ERIC SOTO-CANTU, None, PAUL S. RUSSO, Louisiana State University — Like other synthetic polypeptides, poly (ϵ -carbobenzyloxy-L-lysine), PCBL, exhibits unique properties that make it a good candidate for a broad range of applications and fundamental investigations. This work explores one particular feature found in PCBL in the single solvent, m-cresol: a sharp, reversible coil-to-helix transition at 27°C. In nature, such polypeptides undergo similar transitions while attached to living cells. Tethering PCBL polymers to spherical silica particles enables the study of effects such as polypeptide chain length, grafting density and core particle curvature in a fundamental way. This can be accomplished in a single, organic solvent without interference from strong pH and salt effects. This presentation will concern steps taken to make such studies a reality. Methods to characterize grafting density have been established, good control has been exerted over the core size and, by some synthetic routes, also the molecular weight of the PCBL chains in the shell. The coil-to-helix transition is observed for some particles but not all.

¹Supported by NSF Polymers Program, DMR 1005707.

C1.00246 Evidence for localized surface plasmon polaritons in a liquid crystal containing gold nanoparticles¹, KUNAL TIWARI, ANKIT SINGH, SURESH SHARMA, University of Texas at Arlington — We report an observation of the localized surface plasmon polaritons (SPPs) in a nematic liquid crystal containing 14 nm diameter gold nanoparticles (Au NPs). We observe attenuated total reflection (ATR) of p-polarized laser beam incident upon a high-index prism/liquid-crystal-Au-NPs/glass structure used in the Kretschmann configuration.¹ Unlike the ubiquitous ATR configuration, in which the prism base is coated with a noble metal thin film, our experimental set up does not utilize any such coating. The ATR observed at a specific incident angle and only for p-polarized laser reflects the excitation of localized SPPs at NP/liquid-crystal interface. We discuss possible SPPs related effects, which can significantly change the electro-optical properties of polymer-dispersed liquid crystals.²

¹1. E. Kretschmann, Z. Phys. 241, 313 (1971); 2. A. Hinojosa and S. C. Sharma, Appl. Phys. Letts., 97, 081114 (2010)

C1.00247 Novel Ordering of Soft Matter Using Chromonic Lyotropic Liquid Crystals¹, MATTHEW LOHR, DANIEL BELLER, MARCELLO CAVALLARO, University of Pennsylvania, SEVDE ARPACI, Bogazici University, JOHN NAPP, California Institute of Technology, KATHLEEN STEBE, RANDALL KAMIEN, University of Pennsylvania, PETER COLLINGS, Swarthmore College, ARJUN YODH, University of Pennsylvania — Chromonic lyotropic liquid crystals (CLLCs) are a unique and powerful system for governing self-organization in soft materials due to their temperature- and concentration-dependent ability to form nematics in (bio-compatible) aqueous suspensions. We present preliminary observations on several novel soft matter phases governed by the ordering of CLLCs. We first examine the phase behavior of low-concentration chromonic aggregates in surfactant-based lyotropic lamellar, hexagonal and nematic phases, and observe phase separation and mutual ordering. We also discuss the placement of colloidal particles at the interface of a thermotropic nematic liquid crystal and a chromonic nematic liquid crystal, and present initial results on defect coupling across the interface and colloidal self-organization from elastic interactions. We also present additional preliminary work examining the structure of CLLCs in confinement and their interactions with biologically inspired materials.

¹This work was supported by the National Science Foundation through DMR-0804881, the PENN MRSEC DMR11-20901, and NASA NNX08AO0G.

C1.00248 Segregation by Complementarity of nanoDNA based on Liquid Crystal Ordering and Centrifugation¹, GREGORY SMITH, ETHAN TSAI, T. ROBINS, ARMOND KHODAGHLYAN, Liquid Crystal Materials Research Center, University of Colorado, Boulder (CO) U.S.A., GIULIANO ZANCHETTA, TOMMASO FRACCIA, TOMMASO BELLINI, Dipartimento di Chimica, Biochimica e Biotecnologie per la Medicina, Università degli Studi di Milano, Italy, DAVID WALBA, NOEL CLARK, Liquid Crystal Materials Research Center, University of Colorado, Boulder (CO) U.S.A., LIQUID CRYSTAL MATERIALS RESEARCH CENTER, UNIVERSITY OF COLORADO, BOULDER (CO) U.S.A. COLLABORATION, DIPARTIMENTO DI CHIMICA, BIOCHIMICA E BIOTECNOLOGIE PER LA MEDICINA, UNIVERSITÀ DEGLI STUDI DI MILANO COLLABORATION — Nanometer length DNA segments (<20 base pair long) that are complementary can duplex and condense to make liquid crystal phases at concentrations >~500 mg/mL. This nanoDNA duplexing combined with order-disorder phase separation offers a means of sequestering molecules in mixtures of different DNA sequences based on their degree of complementarity. Here we show that isotropic and liquid crystalline phases, comprising respectively single strands and duplexes in multi-component nanoDNA solutions, can be physically separated by liquid crystal condensation followed by centrifugation.

¹This work was supported by NSF MRSEC Grant DMR-0820579.

C1.00249 Ferromagnetic viscoelastic liquid crystalline materials, CRISTINA SCHLESIER, PETR SHIBAEV, SCOTT MCDONALD, Fordham University, Dept of Physics — Novel ferromagnetic liquid crystalline materials were designed by mixing ferromagnetic nanoparticles with glass forming oligomers and low molar mass liquid crystals. The matrix in which nanoparticles are embedded is highly viscous that reduces aggregation of nanoparticles and stabilizes the whole composition. Mechanical and optical properties of the composite material are studied in the broad range of nanoparticle concentrations. The mechanical properties of the viscoelastic composite material resemble those of chemically crosslinked elastomers (elasticity and reversibility of deformations). The optical properties of ferromagnetic cholesteric materials are discussed in detail. It is shown that application of magnetic field leads to the shift of the selective reflection band of the cholesteric material and dramatically change its color. Theoretical model is suggested to account for the observed effects; physical properties of the novel materials and liquid crystalline elastomers are compared and discussed. [1] P.V. Shibaev, C. Schlesier, R. Uhrlass, S. Woodward, E. Hanelt, Liquid Crystals, 37, 1601 (2010) [2] P.V. Shibaev, R. Uhrlass, S. Woodward, C. Schlesier, Md R. Ali, E. Hanelt, Liquid Crystals, 37, 587 (2010)

C1.00250 Modeling Mechanotunable Transmembrane Transport in Lipid Vesicles, ISAAC G. SALIB, OLGA KUKSENOK, ANNA C. BALAZS, University of Pittsburgh, Pittsburgh, PA 15261, USA — Using Dissipative Particle Dynamics approach, we study the effects of applied stress on transmembrane transport in lipid vesicles. The lipids comprising the vesicle are composed of a hydrophilic head group and two hydrophobic tails. The vesicle is immersed into the hydrophilic solution and initially contains a number of amphiphilic species inside its cavity. We show that such enclosed species can be released “on demand” by vesicle’s stretching. We find that the magnitude of the external force required to release the vesicle’s content depends on the chemical nature and volume fraction of the enclosed species. Furthermore, we isolate the scenarios where the stretching of the lipid vesicle depleted of the enclosed species results in its “refilling” with the fresh species from the outer solution. Our results illustrate that applied mechanical stress provides an effective means to fine tune the transmembrane transport in lipid vesicles.

C1.00251 ABSTRACT WITHDRAWN —

C1.00252 Simulations of buckling of gel-phase lipid bilayers , JAMES KINDT, Emory University, Department of Chemistry — The structure of lipid bilayer vesicles below the main chain transition temperature is believed to be approximately polygonal, based on evidence of faceting from electron microscopy. The structure and mechanics of the interfaces between facets, (ridges) are issues that may be pertinent to the rate of trans-bilayer permeability as well as vesicle melting. Here we present evidence from atomistic molecular dynamics simulations that the preferred angle between facets is strongly dependent on the tilt orientation of lipid tails with respect to the ridge vector.

C1.00253 Investigation of the Physics of Flocculation in Algal Systems¹ , FLINT PIERCE, JEREMY LECHMAN, JOHN HEWSON, Sandia National Laboratories — Algae biofuel production has gained a great deal of interest in recent years due to the high photosynthetic efficiency of various algae strains and the ability of stressed algae populations to produce large quantities of lipids within their cells. Separation of the algae from the background aqueous medium engenders large energetic costs for standard separation techniques including filtration, centrifugation, and dissolved air flotation since algae cells are small (microns to 10s of microns), have densities similar to the surrounding fluid, and normally occur at low volume fractions ($1E-4$ -> $1E-3$). Flocculation is one possible route to reducing the cost of collecting the algae biomass, since large algae flocs can easily be removed from the aqueous environment through either differential settling or standard filtration. To this end, We model flocculating systems of algae cells using discrete particle dynamics techniques which incorporate a recently developed adhesive granular potential to govern the cell interactions. This potential is shown to reproduce morphological characteristics, kinetics, and size distributions that agree well with known results for flocculation in the diffusive regime (DLCA). We further investigate flocculation under steady shear and compare our results to both experiment and predictions from various orthokinetic models.

¹Support provided by LDRD office at Sandia National Laboratories

C1.00254 Nonlinear Dynamic Heat Capacity of a Simple Chain Polymer , JONATHAN BROWN, JOHN MCCOY, New Mexico Tech — Molecular dynamics simulations were run on a simple bead-spring polymer system, known to be a glass former, with varying amplitude sinusoidal temperature oscillations. Small amplitude sinusoidal temperature produces a small amplitude sinusoidal energy, and dynamic heat capacity is the complex-valued transfer function between the two. For large amplitude temperature oscillations, the energy is no longer sinusoidal, and linear response theory breaks down. Instead, the resulting energy is can be written as a Fourier series. From the Fourier coefficients, we derived the entropy generated per cycle, which is related to the imaginary part of the dynamic heat capacity in the linear limit. Using this, we formulated a nonlinear extension of the dynamic heat capacity.

C1.00255 High-Pressure Dynamic Light Scattering Implemented in a Diamond Anvil Cell¹ , KEVIN LYON, WILLIAM OLIVER, University of Arkansas — In recent years full-spectrum analysis in light-scattering has been utilized to explore the liquid-glass transition at variable temperatures and ambient pressure. Our lab is currently working on developing dynamic light scattering in a diamond anvil cell to extend this characterization method to high pressures. There are many inherent complications in the implementation of dynamic light scattering in a diamond anvil cell such as distinguishing between self-beating and homodyne contributions to the signal. However, if successful, it would give rise to a several decade window for analysis of glass-forming dynamics not attainable through Brillouin or Raman alone. Progress toward an effective method for obtaining DLS in a diamond anvil cell for the purposes of such analyses will be presented.

¹We gratefully acknowledge support from NSF under grant NO.: DMR-0552944

C1.00256 Wet granular walkers and climbers , ZEINA S. KHAN, Chemical Engineering Department, Texas Tech University, AUDREY STEINBERGER, Laboratoire de Physique, Ecole Normale Supérieure de Lyon, RALF SEEMANN, Experimental Physics, Saarland University, STEPHAN HERMINGHAUS, Max Planck Institute for Dynamics and Self-Organization — We have observed that when a bidisperse mixture of glass beads is moistened by a fluid and shaken sinusoidally in a vertical container, small clusters of beads take off from the surface of the pile and rapidly climb up the container walls against gravity. These self-organized clusters are held together and against the wall by liquid capillary bridges, and are led by one large grain with one or more small grains trailing behind. When similar clusters are placed on a horizontally vibrating substrate they self-align and travel horizontally along the axis of vibration with a ratchet-like motion. We report a detailed experimental study performed for the simplest walker system consisting of one large and one small bead, and present a simple model that accounts for the observed behavior. Reference: Z.S. Khan *et al.*, *New J. Phys* **13**, 053041 (2011).

C1.00257 Surface melting of wet granular matter in two dimensions , CHRISTOPHER MAY, KAI HUANG, INGO REHBERG, Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany — The transition from the solidlike to the liquidlike state of a monolayer of wet glass beads under horizontally swirling motion is investigated experimentally. Due to the cohesion arising from the formation of capillary bridges, the wet particles initially form a crystal like structure at moderate driving. As the driving frequency increases, this structure is found to melt with two steps: A rearrangement into a hexagonal packing sheltered by a premelted layer, followed by a melting from the surface. This process is characterized by means of Voronoi tessellation and bond orientational order parameters, and discussed within the scenario of KTHNY theory that accounts for crystal melting in two dimensions.

C1.00258 Coefficient of restitution for wet impacts , FRANK GOLLWITZER, KAI HUANG, Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany, CHRISTOF A. KRÜLLE, Maschinenbau und Mechatronik, Hochschule Karlsruhe - Technik und Wirtschaft, D-76133 Karlsruhe, Germany, INGO REHBERG, Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany — As the experience of playing football in the rain may tell, wetting could influence the coefficient of restitution (COR) dramatically. This is due to the extra energy dissipation from the wetting liquid, for instance viscous damping. To unveil the underlying mechanisms accounting for the influence, we study experimentally the COR by tracing free falling particles bouncing on a wet surface. The dependence of the COR on the impact velocity, various particle and liquid properties will be presented and discussed in terms of dimensionless Stokes' and capillary numbers.

C1.00259 Characterizing the movement of grains in a 2D rotating drum with imposed vibrations , NORA SWISHER, BRIAN UTTER, James Madison University — We study particle trajectories and surface behavior of photoelastic grains in a 2D circular rotating drum subjected to imposed vertical vibrations. Granular materials are ubiquitous, from industrial processing and pharmaceutical powder mixing to avalanches and sinkholes, yet general equations of flow are not known for these materials. For granular materials, flow is characterized by sudden avalanches, large shear gradients, and history dependence and these characteristics make it difficult to form general equations of flow. This jamming transition is general, occurring in foams, emulsions, and traffic, and can vary significantly with vibration (the "granular temperature"). To quantitatively measure the flow, jamming, and mixing properties of the grains, we analyze images to determine each particle's position and velocity for each frame. External vibration leads to increased compaction of the grains, larger rearrangements, and a narrower shear band. Particle tracking allows us to closely analyze the velocity profiles, trajectories of individual grains, and separation and diffusion of originally neighboring grains. We will present results on the stability of the pile as well as the effects on mixing as external vibration is varied.

C1.00260 Simulating Topological Defects in Twisted Fiber Bundles¹, ISAAC R. BRUSS, GREGORY M. GRASON, Department of Polymer Science and Engineering, University of Massachusetts, Amherst — Twisted bundles are a common motif found in naturally occurring structures of self-assembled fibers, such as collagen and fibrin. By understanding the general principles governing such organizations, new synthetic materials—from the nano to the macroscale—may also be realized. Recently, continuum elasticity theory has been applied to describe generic twisted fiber bundles. This has revealed a relation between a bundle's twist and the presence of topological defects in the cross-sectional packing of the fibers. Here we employ numerical simulations to examine this interdependence. We model a bundle's cross-section as beads confined to a plane. The interactions between beads is governed by a modified Lennard-Jones potential that accounts for the effects of twist. We observe configurations that range from perfect hexagonal packing for cases of no twist, to defect populated structures above a critical amount of twist. For small bundles of less than ~ 100 beads, there exists a discrete spectrum of energy ground states corresponding to integer numbers of five-fold disclinations. For larger bundles, we hope to uncover what types of defect arrangements effectively screen the stresses caused by twist, and compare these to current predictions of the internal organization of collagen fibrils.

¹Center for Hierarchical Manufacturing (CMMI-1025020)

C1.00261 Molecular Adhesion of Curved Filaments: Self-Assembly of Bacterial Flagellar Bundles¹, LUIS CAJAMARCA, University of Massachusetts Amherst, Physics Department, GREGORY GRASON, University of Massachusetts Amherst, PSE Department — The self-assembly of chiral filaments, such as filamentous proteins, introduces an unavoidable frustration between inter-filament and intra-filament geometries. We study the self-assembly of bacterial flagella with a model that focuses on three geometric features: a preferred distance of closest approach; a preferred relatively-parallel orientation; and a mechanical cost for changes of helical shape. As a result, intrinsically curved filaments cannot simultaneously minimize all three driving forces, even in the limiting case of 2-filament contacts. Using a model of depletion-driven and electrostatically-stabilized interactions we present a phase diagram for two filament bundles depicting the complex thermodynamic behavior of adhesive contact using three ratios: one describes the shape of the filaments, and the other two capture the competition of the modulus associated with mechanical deformations and with the cost of having a non-zero twist vs the modulus associated to changes in inter-filament spacing. Finally, we describe the dependence of these ratios on experimentally-adjustable variables and predict critical concentrations of depletant molecules for known polymorphic configurations which may favor the filaments to undergo a transition from non-adhesive to adhesive state.

¹NSF CMMI 10-68852

C1.00262 Self-assembly of Janus Ellipsoids¹, YA LIU, University of Pittsburgh, WEI LI, Lehigh University, TONI PEREZ, Newcastle University, GENEVIEVE BRETT, Skidmore University, JAMES GUNTON, Lehigh University — The self-assembly of particles into a desired mesoscopic structure and function are considered as a bottom-up strategy to obtain new bulk materials that have potential applications in broad fields including drug delivery, photonic crystals, biomaterials and electronics. We propose a primitive model of Janus ellipsoids that represent particles with an ellipsoidal core and two semi-surfaces coded with dissimilar properties, for example, hydrophobicity and hydrophilicity, respectively. We investigate the effects of the aspect ratio on the self-assembly morphology and dynamical aggregation processes using Monte Carlo simulations. We find that the size and structure of the aggregates can be controlled by the aspect ratio, which should be an interesting result from a design viewpoint.

¹We thank the support from Mathers Foundation, NSF, NSF REU grant and NSF Teragrid resources.

C1.00263 Electron Shock Waves with a Significant Current behind the Shock Front¹, MOSTAFA HEMMATI, Arkansas Tech University — Electrical breakdown of a gas in a strong electric field is carried out by a wave with a strong discontinuity at the wave front, traveling with speed comparable to speed of light. For theoretical investigation of electrical breakdown of a gas, we apply a one-dimensional, steady profile, constant velocity, three component fluid model. For current bearing breakdown waves, in addition to the set of electron fluid dynamical equations, the shock conditions on electron velocity and temperature need to be modified as well. For breakdown waves, considering a significant current behind the shock front, we will derive the boundary conditions on electron velocity and temperature at the shock front. The modified set of boundary conditions has made the integration of the set of electron fluid dynamical equations through the dynamical transition region of the wave possible. The wave profile for electric field and electron velocity, temperature and number density will be presented.

¹The author would like to acknowledge the Arkansas Space Grant Consortium's financial support of this research project.

C1.00264 X-ray Studies of Rapidly Evolving Interfacial Nanostructures, YELING DAI, Department of Physics, UC San Diego, BINHUA LIN, MATI MERON, KYUNGIL KIM, BRIAN LEAHY, Center for Advanced Radiation Sources(CARS), University of Chicago, OLEG SHPYRKO, Department of Physics, UC San Diego — Interfacial nanostructures represent a class of systems that is of great interest for studies of quasi-2D systems, chemical self-assembly, surfactant behavior and biologically relevant membranes. During the compression process, the self-assembled nanoparticle films at the air-liquid interface exhibit rich mechanical behavior, undergoing a rapid structural evolution which is marked by the transition from monolayer to multilayer and/or the formation of periodic wrinkles and folds. Due to the compression rate of the barrier, the timescale of this evolution is typically several minutes, which is much shorter than the time the conventional X-ray Reflectivity (XR) takes for a liquid surface measurement. Therefore we explore the ability of Grazing Incidence X-ray Off-Specular (GIXOS) scattering to capture the elastic properties, structures and surface fluctuating modes of Au nanoparticle films during the rapid structural evolution. We present here the detailed analysis of GIXOS data from the self-assembled Au nanoparticle films and show how we obtain quantitative, Angstrom-resolution details of electron density profile normal to the surface with a temporal resolution that allows us to study in-situ the rapid evolution of Au nanoparticle films structure in response to the compression.

C1.00265 STATISTICAL AND NONLINEAR PHYSICS —

C1.00266 Frequency Enhancement in Coupled Noisy Excitable Elements: The effect of excitability, system size and topology¹, WEI-YIN CHIANG, PIK-YIN LAI, Dept. of Physics and Center for Complex Systems, National Central University, Chungli, Taiwan 320, R.O.C., C.K. CHAN, Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan 115, R.O.C. — The oscillatory dynamics of coupled noisy excitable FitzHugh-Nagumo elements is investigated as a function of the coupling strength g . For a system consists of coupled noisy excitable elements, the synchronize frequency will be higher than the uncoupled frequencies of each element. As g increases, there is an unexpected peak in the mean of frequency distribution before reaching synchronization at the optimal coupling strength. This enhancement level is investigated systematically on depending on hypercubic lattices in different dimensions, Erdos-Renyi random graphs and random networks with fixed coordination numbers. It is found that the maximal enhancement coupling and enhancement level depend on the connection topology and spatial dimensions, the enhancement level and the frequency distribution widths follow scaling laws as verified by different lattices(honeycomb, square, and hexagonal) in two-dimensions, suggesting some sort of universality in frequency enhancement.

¹National Science Council of Taiwan under grant nos. 98-2112-M-008-023-MY3, 97-2112-M-001-003

C1.00267 Phase Diagram of the mixed spin-2 and spin-5/2 Ising system with two different single-ion anisotropies¹ , JOSÉ CRUZ FILHO, MAURICIO GODOY, ALBERTO ARRUDA, Instituto de Física, Universidade Federal de Mato Grosso, 78060-900, Cuiabá, MT, Brazil — In the last five decades the Ising model has been one of the most largely used to describe critical behavior of several systems in the nature. In particular, in the physics of the condensed matter it is important to describe critical behavior and other thermodynamics properties of a variety of physic systems (disordered system, spins glass, random field Ising model, etc.). Recently, several extensions have been made in the spin-1/2 Ising model to describe a wide variety of physic systems. For example, the models consisting of mixed spins of different magnitudes are interesting extensions, which are so-called mixed-spin Ising models. In this work we present a study of the effects of two single-ion anisotropies in the phase diagram and in the compensation temperatures of the mixed spin-2 and spin-5/2 Ising ferrimagnetic system. We employ the mean-field theory based on the Bogoliubov inequality for the Gibbs free energy, and the Landau expansion of the free energy in the order parameter to describe the phase diagrams. In the plane critical temperature versus single-ion anisotropie the phase diagram display behavior tricritical (second-order transition separated of the first-order transition lines by a tricritical point).

¹Financial support from the Brazilian Agencies FAPEMAT, CAPES, and CNPq is gratefully acknowledged

C1.00268 Monte Carlo Study of a Mixed Spin-1 and Spin-3/2 Ising Ferrimagnet with Random Anisotropies¹ , JOAO PEREIRA, ALBERTO ARRUDA, MAURICIO GODOY, Instituto de Física, Universidade Federal de Mato Grosso, 78060-900, Cuiaba, Mato Grosso, Brazil — The interest in studying magnetic properties of systems of mixed spin Ising has been grown in last years. This is due to such systems have less translational symmetry than their single-spin counterparts. This property is very important to study some type of ferrimagnetism, which are of current interest. One of the most interesting features of the ferrimagnetism is that they can exhibit compensation temperature. Spin systems mixed with spins in the two sublattices and with random anisotropies are not commonly studied. Monte Carlo method have been proven to be reliable and relatively simple technique to analyze mixed Ising model. In this work, we performed Monte Carlo simulations to study a mixed system ferrimagnetism on a square lattice. The model system consists of two interpenetrating sublattices with spins spin-1 and spin-3/2 in the presence of random anisotropies. The magnetic properties such as magnetization, susceptibility and Binder cumulant, were determined to obtain the critical temperature of the system in various situations. We also determined the phase diagram in the plane temperature versus anisotropy strength for several values of the randomness anisotropy probability.

¹Financial support from the Brazilian Agencies FAPEMAT, CAPES and CNPq is gratefully acknowledged.

C1.00269 Measurement of organization in complex and co-evolving networks¹ , GEORGI GEORGIEV, Assumption College and Tufts University — We apply a new method for measurement of organization of complex and co-evolving networks using the quantity of physical action. We consider simple arrangements of elements in a network and constraints to their motion along paths and calculate the amount of organization in each system using the following measure: organization is the inverse of the average sum of physical actions of all elements in a system per unit motion multiplied by the Planck's constant. The meaning of quantity of organization here is the number of quanta of action per one unit motion along a path of an element. A unit motion along a path for a network, such as internet, is the transmission of one bit of information. The calculation can be expanded to systems consisting of many elements and constraints and also can be followed as a function of time with improvement of the organization of a system or connected systems and networks. Thus, the principle of least action becomes the driving force, and the least action state of the system, the attractor for all of the paths of its elements and states of its constraints. We consider also the rate of constraint minimization, or decrease of action per element and motion, as a function of the number of elements i.e. quality as a function of quantity. Increase of quantity, within specified limits, leads to increase of level of organization and vice versa.

¹The author thanks Assumption College for research support.

C1.00270 Direct Method in Determining the Direction of Action in the Coupling Map Ring , WANG-CHUANG KUO, DI LUO, Department of Physics, Natl. Sun Yat-Sen University, Kaohsiung, Taiwan, ROC — Recently, Hung and Hu provided a genuine way to carry binary data on a coupling map ring (CMR) for the chaotic communication (Phys. Rev. Lett., 101, 244102 (2008)). They use the temporal transfer entropy (TTE) to determine the direction of action, which tells bit 1 or 0, between two neighboring chaotic maps of the CMR. A direct method based on the correlation between the changes of two chaotic data is not only capable to resolve the carried bits but more efficient than the scheme of TTE.

C1.00271 Jamming in complex networks with degree correlation , ANA PASTORE Y PIONTTI, IFIMAR Universidad Nacional de Mar del Plata- CONICET, Funes 3350 (7600) Mar del Plata, Argentina, LIDIA BRAUNSTEIN, IFIMAR Universidad Nacional de Mar del Plata- CONICET and Center for polymer studies, Boston University, Boston, MA 02215, USA, PABLO MACRI, IFIMAR Universidad Nacional de Mar del Plata- CONICET, Funes 3350 (7600) Mar del Plata, Argentina — We study the effects of the degree-degree correlations on the pressure congestion J for a diffusive transport process on scale free complex networks. Using the gradient network approach we find that the pressure congestion for disassortative (assortative) networks is lower (bigger) than the one for uncorrelated networks which allow us to affirm that disassortative networks enhance transport through them. This result agrees with the fact that many real world transportation networks naturally evolve to this kind of correlation. We explain our results showing that for the disassortative case the clusters in the gradient network turn out to be as much elongated as possible, reducing the pressure congestion J and observing the opposite behavior for the assortative case. Finally, we apply our transportation process to real world networks, and the results agree with our findings for model networks.

C1.00272 Stretch-induced stress patterns and wrinkles in hyperelastic thin sheets , RUI HUANG, VISHAL NAYYAR, K RAVI-CHANDAR, University of Texas at Austin — Wrinkles are commonly observed in stretched thin sheets and membranes. This paper presents a numerical/experimental study on stretch-induced wrinkling of hyperelastic thin sheets. The model problem is set up for uniaxial stretching of a rectangular sheet with two clamped ends and two free edges. A two-dimensional stress analysis is performed first under the plane-stress condition to determine stretch-induced stress distribution patterns in the elastic sheets, assuming no wrinkles. As a prerequisite for wrinkling, development of compressive stresses in the transverse direction is found to depend on both the length-to-width aspect ratio of the sheet and the applied tensile strain. Next, an eigenvalue analysis is performed to find the potential buckling modes of the elastic sheet under the prescribed boundary conditions. A nonlinear post-buckling analysis is performed to show evolution of stretch-induced wrinkles. The wrinkle wavelength decreases with increasing strain, in good agreement with the prediction by a scaling analysis. However, as the tensile strain increases, the wrinkle amplitude first increases and then decreases, eventually flattened beyond a moderately large strain, in contrast to the scaling analysis. Finally, experimental measurements with polyethylene sheets will be presented in comparison with the numerical results.

C1.00273 Random fields at an absorbing state transition , HATEM BARGHATHI, THOMAS VOJTA, Department of Physics, Missouri University of Science and Technology, Rolla, MO 65409 — We investigate a nonequilibrium phase transition in the presence of disorder that locally breaks the symmetry between two equivalent absorbing states. Such "random-field" disorder is known to have dramatic effects on equilibrium phase transitions; in low dimensions it can completely destroy the phase transition. In contrast, we demonstrate that the absorbing state transition of the one-dimensional generalized contact process persists in the presence of random fields. However, the dynamics in the inactive phase becomes ultraslow. We illustrate our theory by means of large-scale Monte-Carlo simulations.

C1.00274 Fluctuation-driven Turing patterns in predator-prey dynamics, THOMAS BUTLER, Massachusetts Institute of Technology, NIGEL GOLDENFELD, University of Illinois at Urbana-Champaign — Models of diffusion-driven pattern formation that rely on the Turing mechanism are utilized in many areas of science. However, many such models suffer from the defect of requiring fine tuning of parameters or an unrealistic separation of scales in the diffusivities of the constituents of the system in order to predict the formation of spatial patterns. In the context of a generic model of predator-prey population dynamics, we show that the inclusion of intrinsic noise in Turing models leads to the formation of “quasipatterns” that form in generic regions of parameter space and are experimentally distinguishable from standard Turing patterns. The existence of quasipatterns removes the need for unphysical fine tuning or separation of scales in the application of Turing models to real systems. We also exhibit numerical simulations of the formation of quasi-patterns deep in the quasi-pattern phase.

C1.00275 The Explanation of the Photon’s Electric and Magnetic Fields; and its Particle and Wave Characteristics, RUSSELL MOON, Dr, VICTOR VASILIEV, Pr — Using the principles of the Vortex Theory, the creation of the photon’s electric and magnetic components are explained: the condensed region of space is responsible for creating the photon’s electric component and its particle effect; its expansion and contraction is responsible for its frequency; its motion through three dimensional space creates a wave in the surrounding space. This wave is responsible for the photon’s magnetic component and wave characteristics. The simultaneous expansion and contraction of both the dense region of space that is the photon and the surrounding space it passes through explains why the electric and magnetic effects are at right angles to each other. Also the photon’s particle and wave characteristics are explained.

C1.00276 Pure Quantum Gravity Simulation in 1+1 Dimensions using Causal Dynamical Triangulation, NORMAN ISRAEL, JOHN LINDNER, The College of Wooster — Causal Dynamical Triangulation (CDT) is a conservative approach to quantizing gravity. It involves decomposing spacetime into “triangular” building blocks. In computer simulations, we implement CDT in 1+1 dimensions without matter. We compute the ratio of the corresponding universe’s mean size to its spread and compare with analytical results.

C1.00277 Contesting the paradigm of chirality, EFI EFRATI, University of Chicago — In 1893 Lord Kelvin coined the term chirality, and stated what is to become the elementary paradigm of chirality: ‘I call any geometrical figure, or any group of points, chiral, and say it has chirality, if its image in a plane mirror, ideally realized cannot be brought to coincide with itself’. While the notion of chirality has greatly advanced our understanding of the structures of molecules and crystals, it has been shown to be inconsistent with every pseudo-scalar quantification. In this talk I will present a tabletop demonstration of a chiral structure which is constructed through the achiral summation of identical elementary units which are symmetric under reflection. The seeming contradiction to the definition of chirality is reconciled by proposing an alternative definition, relying on the physicist interpretation of the right hand rule.

C1.00278 Phase-Space Networks of Frustrated Spin Models, YILONG HAN, Hong Kong University of Science and Technology — We propose a complex-network approach to study phase-space structures of frustrated spin models and lattice gas models. Their highly degenerated ground states are mapped as discrete networks such that the quantitative network analysis can be applied to phase-space studies. The resulting phase spaces share some common features and establish a class of complex networks with unique Gaussian spectral densities. A one-to-one correspondence is discovered between the six-vertex model (jigsaw puzzle) and sphere stack.

C1.00279 Common features in phase-space networks of frustrated spin models and lattice-gas models, FENG WANG, YI PENG, YILONG HAN, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China, SOFT MATTER AND VIDEO MICROSCOPY LAB TEAM — We mapped the phase spaces of the following four models into networks: (1a) the Ising antiferromagnet on triangular lattice at the ground state and (1b) above the ground state, (2) the six-vertex model (i.e. square ice or spin ice), (3) 1D lattice gas and (4) 2D lattice gas. Their phase-space networks share some common features including the Gaussian degree distribution, the Gaussian spectral density, and the small-world properties. Models 1a, 2 and 3 with long-range correlations in real space exhibit fractal phase spaces, while models 1b and 4 with short-range correlations in real space exhibit non-fractal phase spaces. This result supports one of the untested assumptions in Tsallis’s non-extensive statistics.

C1.00280 Simple Design Rules for Spike Neural Network Based General Purpose Networks, ARNAB ROY, J. DAVID SCHAFFER, CRAIG LARAMEE, Binghamton University — It has been much lamented over the past decade that, although spiking neural networks (SNNs) have exciting proven computational properties, there are no design rules for assembling networks for specific purposes. Here we offer design approaches for creating three general purpose networks namely, a temporal pattern (serial channel) detector, sequence detector (parallel channel), and any specific mapping of input to output spike patterns on a serial channel. Central pattern generators are instances of this last design. These design rules are based on synchrony detection which SNNs do so well. Here we also introduce a modification to the basic SRM0 model which not only reduces the computational cost, but also enables us to develop these design rules. We discuss how these designs may be combined into fairly general spatio-temporal pattern detectors. Finally, by adding a capability for feature discovery/extraction, we envision an approach to learning spatio-temporal pattern classifiers.

C1.00281 Vulnerability and Vaccination Strategies on realistic complex network, THIERRY PLATINI, Virginia Bioinformatics Institute, ANDREA APOLLONI, Laboratoire de Physique ENS-Lyon — The general understanding of non-equilibrium stochastic processes evolving on complex networks become an important challenge. In the framework of epidemiology, one of the key challenges is the identification and the understanding of the role of critical and vulnerable nodes in the diffusion process. Considering the SIER model evolving on a large realistic complex networks, we present a study of the vulnerability for different viral strength. Our result are used to evaluate the possible vaccination strategies.

C1.00282 Transitions in Physiologic Coupling: Sleep Stage and Age Dependence of Cardio-respiratory Phase Synchronization¹, RONNY P. BARTSCH, PLAMEN CH. IVANOV, Harvard Medical School and Division of Sleep Medicine, Brigham and Womens Hospital, Boston, MA 02115, USA — Recent studies have focused on various features of cardiac and respiratory dynamics with the aim to better understand key aspects of the underlying neural control of these systems. We investigate how sleep influences cardio-respiratory coupling, and how the degree of this coupling changes with transitions across sleep stages in healthy young and elderly subjects. We analyze full night polysomnographic recordings of 189 healthy subjects (age range: 20 to 90 years). To probe cardio-respiratory coupling, we apply a novel phase synchronization analysis method to quantify the adjustment of rhythms between heartbeat and breathing signals. We investigate how cardio-respiratory synchronization changes with sleep-stage transitions and under healthy aging. We find a statistically significant difference in the degree of cardio-respiratory synchronization during different sleep stages for both young and elderly subjects and a significant decline of synchronization with age. This is a first evidence of how sleep regulation and aging influence a key nonlinear mechanism of physiologic coupling as quantified by the degree of phase synchronization between the cardiac and respiratory systems, which is of importance to develop adequate modeling approaches.

¹Supported by: NIH Grant 1R01HL098437-01A1, Office of Naval Research Grant 000141010078, Brigham and Womens Hospital BRI Fund and the German Academic Exchange Service (DAAD).

C1.00283 Levels of complexity in scale-invariant neural signals¹, PLAMEN CH. IVANOV, Harvard Medical School and Division of Sleep Medicine, Brigham and Womens Hospital, Boston, MA 02115, USA, QIANLI D.Y. MA, Nanjing University of Posts and Telecommunications, Nanjing 210003, China, RONNY P. BARTSCH, Harvard Medical School and Division of Sleep Medicine, Brigham and Womens Hospital, Boston, MA 02115, USA — Many physiological systems exhibit complex scale-invariant and nonlinear features characterized long-range power-law correlations, indicating a possibly common control mechanism. It has been suggested that dynamical processes, influenced by inputs and feedback on multiple time scales, may be sufficient to give rise to this complexity. Two examples of physiologic signals that are the output of hierarchical multiscale physiologic systems under neural control are the human heartbeat and human gait. We show that while both cardiac interbeat interval and gait interstride interval time series under healthy conditions have comparable scale-invariant behavior, they still belong to different complexity classes. We compare results from empirical findings and stochastic feedback modeling approaches to cardiac and locomotor dynamics, which provide new insights into the multicomponent neural mechanisms regulating these complex systems.

¹Supported by: NIH Grant 1R01HL098437-01A1, Office of Naval Research Grant 000141010078, Brigham and Womens Hospital BRI Fund and the German Academic Exchange Service (DAAD).

C1.00284 Characteristics of group networks in the KOSPI and the KOSDAQ, KYUNGSIK KIM, JEUNG-SU KO, Department of Physics, Pukyong National University, Busan 608-737, Korea, MYUNGGI YI, Department of Biomedical Engineering, Pukyong National University, Busan 608-737, Korea — We investigate the main feature of group networks in the KOSPI and KOSDAQ of Korean financial markets and analyze daily cross-correlations between price fluctuations for the 5-year time period from 2006 to 2010. We discuss the stabilities by undressing the market-wide effect using the Markowitz multi-factor model and the network-based approach. In particular we ascertain the explicit list of significant firms in the few largest eigenvectors from the undressed correlation matrix. Finally, we show the structure of group correlation by applying a network-based approach. In addition, the relation between market capitalizations and businesses is examined.

C1.00285 Multifractal Analysis of Asian Foreign Exchange Markets and Financial Crisis, GABJIN OH, Chosun University, OKYU KWON, National Institute for Mathematical Sciences, WOO-SUNG JUNG, POSTECH — We analyze the multifractal spectra of daily foreign exchange rates for Japan, Hong-Kong, Korea, and Thailand with respect to the United States Dollar from 1991 to 2005. We find that the return time series show multifractal spectrum features for all four cases. To observe the effect of the Asian currency crisis, we also estimate the multifractal spectra of limited series before and after the crisis. We find that the Korean and Thai foreign exchange markets experienced a significant increase in multifractality compared to Hong-Kong and Japan. We also show that the multifractality is strongly related to the presence of high values of returns in the series.

C1.00286 Rural-urban migration including formal and informal workers in the urban sector: an agent-based numerical simulation study, NILTON BRANCO, THARNIER OLIVEIRA, Departamento de Física, Universidade Federal de Santa Catarina, Florianopolis SC, Brazil, JAYLSON SILVEIRA, Departamento de Economia, Universidade Federal de Santa Catarina, Florianopolis SC, Brazil — The goal of this work is to study rural-urban migration in the early stages of industrialization. We use an agent-based model and take into account the existence of informal and formal workers on the urban sector and possible migration movements, dependent on the agents' social and private utilities. Our agents are placed on vertices of a square lattice, such that each vertex has only one agent. Rural, urban informal and urban formal workers are represented by different states of a three-state Ising model. At every step, a fraction a of the agents may change sectors or migrate. The total utility of a given agent is then calculated and compared to a random utility, in order to check if this agent turns into an actual migrant or changes sector. The dynamics is carried out until an equilibrium state is reached and equilibrium variables are then calculated and compared to available data. We find that a generalized Harris-Todaro condition is satisfied [1] on these equilibrium regimes, i.e, the ratio between expected wages between any pair of sectors reach a constant value.

[1] J. J. Silveira, A. L. Espíndola and T. J. Penna, *Physica A*, **364**, 445 (2006).

C1.00287 Non-equilibrium vortex relaxation in disordered type-II superconductors¹, ULRICH DOBRAMYSL, MICHEL PLEIMLING, UWE C. TAUBER, Department of Physics, Virginia Tech — We study the non-equilibrium steady states and relaxation properties of driven vortex lines in the presence of both randomly distributed point and columnar pinning centers. We model the vortices as interacting elastic lines and employ a Langevin molecular dynamics algorithm to extract steady-state and non-stationary time-dependent behavior. In order to characterize the relaxation properties towards thermal equilibrium, we investigate transient two-time correlation functions. In particular we compare results obtained for systems with randomly distributed point pins and parallel columnar defects.

¹Research supported by DOE-BES, Grant No. DE-FG02-09ER46613.

C1.00288 Dynamics of Sheared Polydisperse Emulsions, XIN DU, KENNETH DESMOND, DANDAN CHEN, KAZEM EDMOND, ERIC WEEKS, Physics Dept., Emory University, WEEKS' LAB TEAM — Polydispersity is an important parameter in the jamming transition of soft materials which has not been well understood yet. In our work, we study the elastic response of a high volume fraction polydisperse emulsion to a periodic shear stress. The droplets' dynamics is imaged by confocal microscopy. Our results reveal that most of the droplets in the emulsion exhibit an elastic and periodic motion under the shear stress. However, the smaller droplets often move with anomalously large or small amplitudes compared to the mean motion. Some droplets also move nearly perpendicular to the mean flow field. The broad distribution of the amplitudes and phases of the smaller droplets' motions can be attributed to the motion of the larger droplets and the distribution of the droplet sizes.

C1.00289 The rigidity (unjamming) transition of disordered solids is caused by non-affinity, ALESSIO ZACCONE, Cavendish Laboratory, University of Cambridge — I will present a theoretical framework which allows one to account for the non-affinity of particle displacements due to disorder within a statistical mechanical description of the elasticity of disordered solids (1). A few important results can be derived analytically from first principles for disordered harmonic packings/lattices. First of all, the theory successfully recovers the unjamming or rigidity transition $G(z-2d)$, where G is the shear modulus and z the coordination number, in excellent quantitative agreement with the numerical simulations of Ref. (2). Secondly, the theory explains this scaling law, which was hitherto enigmatic, in terms of the competition between the elastic (bonding) energy of the solid and the non-affine relaxations which are a consequence of structural disorder and contribute a dissipative term to the free energy of the solid. Potential applications to unsolved issues related to transport and vibrational properties of disordered solids will be briefly discussed. References (1) A. Zaccane and E. Scossa-Romano, *Phys. Rev. B* **83**, 184205 (2011) (2) C.S. O'Hern, et al. *Phys. Rev. E* **68**, 011306 (2003).

C1.00290 Amended tunneling model to explain the anisotropy of the glassy properties of crystals and quasicrystals¹, DRAGOS-VICTOR ANGHEL, Horia Hulubei National Institute of Physics and Nuclear Engineering, DMITRY CHUROCHKIN, University of Chile — The low temperature acoustic and thermal properties of amorphous, glassy materials are remarkably similar and they can be explained to a large extent by assuming that the material contains a large number of dynamic defects. These dynamic defects are tunneling systems and are modeled by an ensemble of two-level systems (TLS). Crystals with defects—with a large enough amount of disorder—exhibit also glass-like properties, but these properties are not so universal and, even more, they are not isotropic. In Phys. Rev. B **75**, 064202 (2007) we proposed an amended model for the description of the interaction of two-level systems with arbitrary strain fields. Here we show how this model explains the anisotropy of the glass-like properties of disordered crystals and quasicrystals.

¹Financial support from the ANCS grant 114/05.10.2011 and JINR-IFIN grants N4063 and Titeica-Markov are gratefully acknowledged

C1.00291 Dynamical Mechanism of Superdiffusive Processes and Multifractals, KYUNGSIK KIM, Department of Physics, Pukyong National University, Busan 608-737, Korea, JAE-WON JUNG, National Institute of Meteorological Research, KMA, Seoul 156-720, Korea, SEUNG-KYU SEO, Department of Physics, Pukyong National University, Busan 608-737, Korea — The diffusive process and the multifractal property are investigated in the Baduk. We ascertain that the difference of position between black and white stones undergoes the superdiffusion. In our study, we mainly estimate and analyze the generalized Hurst exponent, singularity spectrum, and multifractal strength in the tipping points of the Baduk. We also discuss the multifractal property of three segments, after analyzing the multifractality. In multifractal structures, it is found that segment 5 has shown a stronger multifractal behavior than the other segments for the tipping points of the Baduk.

C1.00292 On the metal-insulator-transition in vanadium dioxide, AZITA JOVAINI, SHIGEJI FUJITA, University at Buffalo, SALVADOR GODOY, UNAM, AKIRA SUZUKI, Tokyo University of Science — Vanadium dioxide (VO₂) undergoes a metal-insulator transition (MIT) at 340 K with the structural change from tetragonal to monoclinic crystal. The conductivity σ drops at MIT by four orders of magnitude. The low temperature monoclinic phase is known to have a lower ground-state energy. The existence of the k -vector $\mathbf{k}$ is prerequisite for the conduction since the $\mathbf{k}$ appears in the semiclassical equation of motion for the conduction electron (wave packet). The tetragonal (VO₂)₃ unit is periodic along the crystal's x -, y -, and z -axes, and hence there is a three-dimensional k -vector. There is a one-dimensional $\mathbf{k}$ for a monoclinic crystal. We believe this difference in the dimensionality of the k -vector is the cause of the conductivity drop.

C1.00293 On Van Hove Singularities in Pure Cubic Crystals, AZITA JOVAINI, JAMES PIENKA, SHIGEJI FUJITA, University at Buffalo, SALVADOR GODOY, UNAM, AKIRA SUZUKI, Tokyo University of Science — Pure elements form crystals of various lattices, cubic, tetragonal and others. At very low temperatures the lattice heat capacities in three dimensional crystals obey Debye's T^3 -law, where T is the absolute temperature. X-ray scattering experiments and lattice dynamics calculations reveal van Hove singularities when the density of states is plotted as a function of the phonon frequency. A physical origin of the singularities, jumps in the derivative of the density of states, is clarified. The singularities occur in three and two dimensions when the constant-frequency plane touches the Brillouin zone boundary *and* undergoes a curvature inversion. The face-centered cubic lattice is composed of two simple cubic sublattices and one tetragonal sublattice. The first (second) major peaks in the observed density of states in aluminum (Al) are shown to arise from the transverse phonons associated with the cubic (tetragonal) sublattices. We predict that the density of states has one major peak with a shoulder (two peaks with shoulders) for a body-centered cubic (face-centered cubic) crystal.

C1.00294 Aging processes in reversible reaction-diffusion systems¹, NASRIN AFZAL, Virginia Tech, JUSTIN WAUGH, University of Colorado Boulder, MICHEL PLEIMLING, Virginia Tech — Reaction-diffusion systems with reversible reactions generically display power-law relaxation toward chemical equilibrium. In this work we investigate, through numerical simulations, aging processes that characterize the non-equilibrium relaxation. Studying a model which excludes multiple occupancy of a site, we find that the scaling behaviors of the two-time correlation and response functions are similar to that discovered previously in an exactly solvable version with no restrictions on the occupation numbers. In particular, we find that the scaling of the response depends on whether the perturbation conserves a certain quantity or not. Our results point to a high degree of universality in relaxation processes taking place in diffusion-limited systems with reversible reactions.

[1] N. Afzal, J. Waugh, and M. Pleimling, J. Stat. Mech. P06006 (2011).

¹Supported in part by the US National Science Foundation through Grant DMR-0904999.

C1.00295 Numerical master equation approach for complex transport processes¹, JANNE KAUTTONEN, JUHA MERIKOSKI, University of Jyväskylä — Applicability of the numerical master equation analysis in studies of complex non-equilibrium systems is discussed. For small systems (up to $\sim 10^6$ states), solving of master equations directly is found very useful especially when studying parameter sensitive and elusive properties, such as drifts caused by the ratchet effect. Also various types of optimization methods can be applied. Efficient numerical methods for solving large master equation systems are discussed. Properties that can be readily computed include mean values and fluctuations of trajectory and state dependent observables, such as velocity, diffusion coefficient and shape deformations of the object. To further study the microscopic mechanisms of complex transport processes, we apply a graph optimization method to master equation sets. This allows one to identify the dominating processes that are responsible for the transport. We present detailed case studies for reptating polymers and metal-on-metal atomic islands in non-homogeneous potentials. These models represent complex many-particle systems with rich nonlinear behavior, such as inversions and increasing of velocity and large shape deformations in external potentials.

¹Supported by the Finnish Academy of Science and Letters and the Magnus Ehrnrooth foundation

C1.00296 String Theory (Knot Really), KARL SMITH, JOHN LINDNER, The College of Wooster — Knots can make one string out of two, without adhesive, simply by entanglement. We present a computer simulation of knots untying. A series of spherical masses connected by spring forces and excluded by normal forces approximate the strings. We tie the simulated strings into knots and tug on their ends with constant forces. Plotting time to untie versus a static coefficient of friction reveals critical frictions above which the knots hold. The critical frictions depend on the knot type (including square, thief, and surgeon's thief knots) and might be used to classify practical knots.

C1.00297 Metal Insulator transition in Vanadium Dioxide, AZITA JOVAINI, SHIGEJI FUJITA, AKIRA SUZUKI, SALVADOR GODOY, None, FUJITA AND ALL COLLABORATION, SUZUKI AND ALL COLLABORATION — MAR12-2011-000262 Abstract Submitted for the MAR12 Meeting of The American Physical Society Sorting Category: 03.9 (T) On the metal-insulator-transition in vanadium dioxide AZITA JOVAINI, SHIGEJI FUJITA, University at Buffalo, SALVADOR GODOY, UNAM, AKIRA SUZUKI, Tokyo University of Science — Vanadium dioxide (VO₂) undergoes a metal-insulator transition (MIT) at 340 K with the structural change from tetragonal to monoclinic crystal. The conductivity σ drops at MIT by four orders of magnitude. The low temperature monoclinic phase is known to have a lower ground-state energy. The existence of the k -vector $\mathbf{k}$ is prerequisite for the conduction since the $\mathbf{k}$ appears in the semiclassical equation of motion for the conduction electron (wave packet). The tetragonal (VO₂)₃ unit is periodic along the crystal's x -, y -, and z -axes, and hence there is a three-dimensional k -vector. There is a one-dimensional $\mathbf{k}$ for a monoclinic crystal. We believe this difference in the dimensionality of the k -vector is the cause of the conductivity drop. Prefer Oral Session X Prefer .

C1.00298 GENERAL PHYSICS —

C1.00299 Neutrosophic Physics as a new field of research

FLORENTIN SMARANDACHE, University of New Mexico — Neutrosophic Physics describes collections of objects or states that are individually characterized by opposite properties, or are characterized neither by a property nor by the opposite of that property. Neutrosophic Physics means a mixture of physical concepts/ideas/spaces/laws/theories $\langle A \rangle$ with their opposite $\langle \text{anti}A \rangle$ or with their neutral $\langle \text{neut}A \rangle$ {where $\langle \text{neut}A \rangle$ means neither $\langle A \rangle$ nor $\langle \text{anti}A \rangle$, but in between, i.e. the neutral part}, and it is a combination of heterogeneous contradictory things which hold together. There are many cases in scientific fields (and in humanistic fields) that an item $\langle A \rangle$ and its opposite $\langle \text{anti}A \rangle$ or their neutral $\langle \text{neut}A \rangle$ are simultaneously valid. - Several examples of neutrosophic physics: (1) unmatter, which is formed by matter and antimatter that bind together (Smarandache, 2004); (2) neutral Kaon, which is a pion & anti-pion composite (Santilli, 1978) and therefore a form of unmatter; (3) neutrosophic cosmological model (Rabounski-Borissova, 2011); (4) among possible Dark Matter candidates there may be exotic particles that are neither Dirac nor Majorana fermions; (5) mercury (Hg) is a state that is neither liquid nor solid under normal conditions at room temperature; (6) non-magnetic materials are neither ferromagnetic nor anti-ferromagnetic; (7) quark gluon plasma (QGP) is a phase formed by quasi-free quarks and gluons that behaves neither like a conventional plasma nor as an ordinary liquid; (8) neutrosophic methods in General Relativity (Rabounski-Smarandache-Borissova, 2005); (9) neutrosophic cosmological model (Rabounski-Borissova, 2011); etc.

C1.00300 Superconductors (*History & Advanced Research*)

MONA KHORRAMI, Sanofi-Aventis Group Co. — *Superconductors* are materials that have no resistance to electricity's flow; they are one of the last great frontiers of scientific discovery. In 1911 superconductivity was first observed in mercury by Dutch physicist Heike Kamerlingh Onnes When he cooled it to the temperature of liquid helium, 4 degrees Kelvin (-452F, -269C), its resistance suddenly disappeared. It was necessary for Onnes to come within 4 degrees of the coldest temperature that is theoretically attainable to witness the phenomenon of superconductivity. The next great milestone in understanding how matter behaves at extreme cold temperatures occurred in 1933. German researchers Walther Meissner and Robert Ochsenfeld discovered that a superconducting material will repel a magnetic field. A magnet moving by a conductor induces currents in the conductor. This is the principle on which the electric generator operates. But, in a superconductor the induced currents exactly mirror the field that would have otherwise penetrated the superconducting material - causing the magnet to be repulsed. This phenomenon is known as strong diamagnetism and is today often referred to as the "Meissner effect" (an eponym). In 1941 niobium-nitride was found to superconduct at 16 K. In 1953 vanadium-silicon displayed superconductive properties at 17.5 K. And, in 1962 scientists at Westinghouse developed the first commercial superconducting wire, an alloy of niobium and titanium (NbTi).

C1.00301 Teaching: the Wave Mechanics of McLeods' Stringy Electron, Explicit Nucleons, and Through-the-Earth Projections of Constellations' Stick Figures

ROGER DAVID MCLEOD, Univ. Massachusetts Lowell. Naturoptics for Safe Recovery of Vision., DAVID MATTHEW MCLEOD¹, Naturoptics for Safe Recovery of Vision. Bastyr Univ — This shows how Hooke's law, for electron, proton and neutron, 2D and 3D, strings, builds electromagnetic string-waves, extending, and pleasing, Schrödinger. These are composed of spirally linked, parallel, north-pole oriented, neutrino and antineutrino strings, stable by magnetic repulsions. Their Dumbo Proton is antineutrino-scissor cut, and compressed in the vicinity of a neutron star, where electrostatic marriage occurs with a neutrino-scissor cut, and compressed, electron, so a Mickey Neutron emerges. Strings predict: electron charge is $-1/3 e$, Dumbo P is 25 % longer than Mickey N, and Hooke says relaxing springs fuel three, separate, non-eternal, inflations, after Big Bangs. Gravity is strings, longitudinally linked. Einstein says Herman Grid's black diagonals prove human vision reads its information from algebraically-signed electromagnetic field distributions, (diffraction) patterns, easily known by ray-tracing, not requiring difficult Spatial Fourier Transformation. High-schoolers understand its application to Wave Mechanics, agreeing that positive-numbered probabilities do not enter, to possibly displease God. Detected stick-figure forms of constellations: like Phoenix, Leo, Canis Major, and especially Orion, fool some observers into false beliefs in things like UFHumanoids, or Kokopelli, Pele and Pamola!

¹Deceased

C1.00302 Properties of Neutrinos and Leptonic Processes

SAMINA MASOOD, University of Houston Clear Lake — We study the effect of the modifications in the properties of neutrinos to the scattering crosssections of purely leptonic processes. Neutrinos change their behavior in the hot and dense media and the properties like mass, induced magnetic moment, number density and the refractive energy are also modified as a result. We investigate that how these properties affect the leptonic decays and scattering processes. Some of the important applications of these results are also indicated in this study.

C1.00303 POST-DEADLINE ABSTRACTS —

C1.00304 Measurement Setup for Characterizing Thermoelectric Materials at High Pressure¹

MATTHEW JACOBSEN, WEI LIU, BAOSHENG LI, Mineral Physics Institute, Stony Brook University — Several investigations have recently resulted in the development of methods for studying thermoelectric materials at high pressure. However, these investigations have focused primarily on probing the electrical resistivity and Seebeck coefficient. While these are important to the effective operation of thermoelectric materials, they are only part of the whole picture. In an effort to address this on a bulk materials scale, facilities have been developed in the High Pressure Laboratory of the Mineral Physics Institute to investigate these properties, along with investigations of the thermal conductivity and ultrasonic sound velocity. With these facilities, it is likely that further studies of these materials will help advance the theoretical understanding of thermoelectrics and further the development of new, more effective thermoelectric materials.

¹This work was supported by DoE/NNSA (DEFG5209NA29458 to BL).

C1.00305 X-ray imaging of electrospinning polymer solutions¹

ISRAEL GREENFELD, ARKADII ARINSTEIN, Technion, KAMEL FEZZAA, Argonne National Laboratory, MIRIAM H. RAFILOVICH, State University of New York, Stony Brook, EYAL ZUSSMAN, Technion — The study of electrospinning polymer solution jets, and the evolution of the polymer entangled network during electrospinning, is of interest in clarifying nanofibers microstructure. We used fast X-ray phase-contrast imaging to investigate the flow of electrospinning PEO and PMMA semidilute solutions. The jet profile, velocity and absorbance were measured at high resolution ($< 1 \mu\text{m}/\text{pixel}$) for the first 10 mm of jet length, at various electrospinning conditions. Jet radius measurements demonstrate a viscosity-dominated flow, with common power-dependence on the distance from the orifice. The flow field was analyzed by imaging solutions with micron-size silica particles, revealing axial velocities of 0.5-1 m/s and strain rates of 200-300 1/s, as well as radial and rotational velocity components. The measured axial velocity provides a direct indication for rapid solvent evaporation as early as 2-3 mm from the jet start. X-ray absorption measurements reveal substantial polymer concentration rise along the jet and at the jet boundaries, evidence for rapid evaporation. Additionally, at high stretching conditions, the polymer concentration rises at the jet center, implying polymer network lateral contraction as predicted by theory.

¹We acknowledge the support of the United States-Israel Binational Science Foundation. Use of the Advanced Photon Source at Argonne National Laboratory was supported by the U.S. DOE.

C1.00306 Nano-indentation experiments: from viruses to cells, WOUTER ROOS, DAAN VORSELEN, Department of Physics and Astronomy, VU University, Amsterdam, The Netherlands, JACK VAN LOON, DESC, Department of Oral Cell Biology, ACTA-VU University, Amsterdam, The Netherlands, GJJS WUITE, Department of Physics and Astronomy, VU University, Amsterdam, The Netherlands — Over the last years AFM imaging and nanoindentation have become an indispensable tool for biophysical studies in liquid at the nano- and micro-scale. We look at both these length scales, at the cellular as well as the sub-cellular level. In particular, we perform combined imaging and force spectroscopy experiments on viral particles to elucidate their structure and mechanics [1]. These studies revealed that Noro virus has found an intriguing way to increase its mechanical strength. These self-assembling, natural nanoparticles incorporate a pre-stress during assembly, consolidating the structure of its protein shell that protects the genome [2]. Next, we studied whole cells. Mechanical loading is increasingly recognized as an important stimulus to cells. Establishing the local viscoelastic properties within a cell is vital to the understanding of the underlying mechanisms of cytoskeletal changes in response to these stimuli. We study the mechanical response of mammalian bone forming (osteoblast-like) cells on a substrate of physiological stiffness using spherical, μm -sized probes and we compare these results to the properties of bone forming cells originating from fish (teleosts).

[1] Roos et al. Nature Physics (2010), 6:733

[2] Baclayon et al. Nano Letters (2011), 11:4865

C1.00307 Study of the interactions of magnetosomes inside magnetotactic bacteria (MTB) through modeling and experimentation¹, JIAJIA DONG, Hamline University, ANDRÉ KÖRNIG, Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, STEFAN KLUMPP, Max Planck Institute of Colloids and Interfaces, Department of Theory & Biosystems, DAMIEN FAIVRE, Max Planck Institute of Colloids and Interfaces, Department of Biomaterials — Since the discovery in 1970s, magnetotactic bacteria (MTB) have enjoyed great interest to biomimetic and biophysical research, due to their fine-tuned synthesis of magnetosomes (magnetic nanocrystals enclosed in organelles) and challenges in understanding the precise mechanism of magnetotaxis via aligning the magnetosomes. We investigate magnetosomes inside an MTB cell as a chain of magnetic crystals and explore their internal interactions as well as the influence from an external magnetic field. Applying both analytical and simulation approaches, we are able to identify the threshold external magnetic field for effective magnetosome alignment depending on crystal configurations. The results agree well with high resolution X-ray diffraction data. They also provide a simple and quantitative model for elucidating the mechanical stability of the magnetosome chain, thus the energetically favorable states of MTB in the presence of an external magnetic field.

¹Study of the interactions of magnetosomes inside magnetotactic bacteria (MTB) through modeling and experimentation

C1.00308 Tailoring the localelectronic and structural properties of colloidal nanocrystals, MARIA LONGOBARDI, University of California, Berkeley, LBNL and University of Salerno, Italia, MATT SHELDON, TOMOYA ARAI, University of California, Berkeley and LBNL, ALESSANDRO SCARFATO, University of Salerno, Italia, A. PAUL ALIVISATOS, MICHAEL F. CROMMIE, University of California, Berkeley and LBNL — Recent advances in wet-chemical synthesis techniques allow unprecedented control of the composition, size, shape, and surface chemistry of colloidal nanocrystals. The structural, opto-electronic and magnetic properties of these materials can be tailored to enable new quantum phenomena with applications in biology, energy harvesting, and fundamental physical studies. Moreover, sophisticated understanding of colloidal nanocrystals requires local probes of individual particles, such as scanning tunneling microscopy (STM) and spectroscopy (STS), that can measure the local density of states (LDOS) and particle wave-functions in real space with atomic resolution. Here, we present our STM/STS studies of the structural and electronic properties of individual CdS, Cu₂S and binary CdS/Cu₂S heterostructure nanocrystals. Detailed local study of electronic properties of the nanocrystals could bridge the existing knowledge gap between bulk and nanoscale. Such understanding is crucial for the design of novel materials based on colloidal nanocrystals.

C1.00309 Non-uniform forcing of a magnetic soap film, RANDY BACK, REGAN BECKHAM, The University of Texas at Tyler — The effects of a non-uniform magnetic field on a suspension of magnetic nanoparticles in a soap film are investigated. Experiments show that a strong non-uniform field will form a two-dimensional structure of magnetic nanoparticles within the soap film. A model is developed to compare with experimental results for several different magnetic field configurations. The system is modeled with a two-dimensional thin film equation with no-flux boundary conditions. We show qualitative agreement between the model and experiments.

C1.00310 The cryogenics magnetocaloric effect in the blocking state superparamagnetic nanocapsules¹, SONG MA, XIANGUO LIU, TENG YANG, ZHIDONG ZHANG, Institute of Metal Research, Chinese Academy of Sciences — The large cryogenics magnetocaloric effect was obtained in superparamagnetic nanocapsules when they are in blocking state. Interestingly, the entropy change of superparamagnetic nanocapsules (Lanthanide-transition metal intermetallic compound), including GdAl₂/Al₂O₃, TbAl₂/Al₂O₃, DyAl₂/Al₂O₃ nanocapsules, shows an unusual sharp increase, when the nanocapsules go into their blocking state. Combining the structural and magnetic analysis, we find the high moment density and low anisotropy energy play crucial role in exciting and hindering the rotation of the moment process, which finally decide the magnitude of the entropy change. The entropy change dependence of the temperature change and applied magnetic field was obtained according to the Langevin theory.

¹National Natural Science Foundation of China with Grant number 50901078

C1.00311 ABSTRACT WITHDRAWN —

C1.00312 ABSTRACT WITHDRAWN —

C1.00313 Following the Dynamics of DNA in Living Cells, JOSHUA MILSTEIN, Department of Physics, University of Toronto, KRISHNAN RAGHUNATHAN, MIKE CHU, JENS-CHRISTIAN MEINERS, Department of Biophysics, University of Michigan — Cells are brimming with molecular activity, but the cellular interior is much more than a test tube for biochemical reactions. The intracellular environment imposes a variety of mechanical constraints and engenders interactions from molecular crowding to a range of motor-driven activity responsible for transcription, replication, cargo transport, cytoskeletal rearrangement, chromosomal remodeling, and so on. We have developed a two-color correlational microscopy technique to follow the dynamics of DNA interacting with the *in vivo* cellular environment. Substantial differences between live cells and dead, yet structurally intact, cells point to a strong coupling of active, motor-driven fluctuations in the cell. This suggests that the motion of native, cellular DNA may similarly be driven by active processes, instead of relying on purely thermal, passive fluctuations. We also note that the correlations provide a sensitive measure for the effective length of the DNA probe on a length scale around one persistence length (~ 50 nm). This paves the way for experiments with more complex DNA probes that can bind transcription factors to form protein-mediated DNA loops, the dynamics of which could be observed through this method.

C1.00314 Enhanced resonant magnetoelectric coupling in frequency-tunable composite multiferroic bimorph structures, PETER FINKEL, NUWC, SAM LOFLAND, Rowan University, DWIGHT VIEHLAND, Virginia Tech — We report on the enhanced resonant magnetoelectric (ME) coupling in composite multiferroic magnetostrictive/piezoelectric composites bimorph structures. The approach was shown to provide more than ten-fold gain in ME coefficient and broad-band range magnetic and electric field assisted stress-configurable resonance frequency tuning up to 100% in these ME structures. The ME structures were investigated using optical spectroscopy. It was shown that this principle of continuously tuned resonance could be used to improve selectivity, signal to noise ratio and universality and sensitivity of ME magnetic sensors.

C1.00315 Strongly interacting lattice bosons in disorder potential: a strong coupling approach¹, CHIEN-HUNG LIN, RAJDEEP SENSARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742, USA, KRISHNENDU SENGUPTA, Theoretical Physics Department, Indian Association for the Cultivation of Science, Kolkata-700032, India, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742, USA — We use a strong coupling canonical transformation to study the phase diagram of strongly interacting bosons in an optical lattice in the presence of one-body disorder potential. Our strong coupling approach treats the disorder potential non-perturbatively and can be applied to moderately high disorder potentials as long as the on site repulsion energy scale for the bosons (U) is larger than the scale of the disorder potential (V). Within the strong coupling approach, we systematically derive the low energy effective Hamiltonian, and, using variational Gutzwiller type wavefunctions, study the phase diagram of the disordered Hubbard model, identifying the Mott insulator, superfluid and Bose glass phases.

¹This work is supported by ARO-DARPA-OLE and UMD-CNAM.

C1.00316 Imaging of nearby NV centers beyond diffraction limit, FANG-WEN SUN, JIN-MING CUI, GUANG-CAN GUO, Key Lab of Quantum Information, University of Science and Technology of China, MICRO-CAVITY TEAM — Nitrogen-Vacancy (NV) centers in diamond have been widely applied in physical and biological study. Single NV center has shown its good quality as a single-photon source. More importantly, when two NV centers are close to each other within tens of nanometers, the strong dipole-dipole interaction can be applied in quantum information techniques. Diamond nanocrystal with NV center has been applied for imaging biological processes. Therefore, to image and distinguish two nearby NV centers is becoming more and more important. In experiment, NV centers are usually detected with scanning confocal optical fluorescence microscopy where the single-photon counts of spontaneous emission are measured to describe their optical imaging. Also, the method of stimulated emission depletion fluorescence microscopy was used to distinguish two nearby NV centers. Here, we proposed a new technique based on our home-built confocal scanning microscopy to image two nearby single NV centers. With the new imaging technique, we have experimentally imaged and distinguished two NV centers with the distance about 40nm, which is well beyond the diffraction limit. This imaging technique can, in principle, distinguish particles with any overlapping.

C1.00317 Phase transition kinetics and critical phenomena of the site dilute Ising model with long range interactions¹, KANG LIU, CHRISTOPHER SERINO, WILLIAM KLEIN, Boston University, HARVEY GOULD, Clark University — We consider the effect of quenched site dilution on the phase transition kinetics and critical phenomena of the Ising model with long range interactions. First, we generalize the Harris criterion to mean-field and near mean-field systems with long range interactions and show that the critical exponents of both the critical point and spinodal do not change regardless of the dimensionality. This is supported by measurements of the isothermal susceptibility near the spinodal line from Monte-Carlo simulations. We also generalize the Coniglio-Klein method by mapping the dilute Ising critical point onto an equivalent site-bond percolation problem. In addition, using the Hubbard-Stratanovich transformation, we are able to write down a coarse-grained field theory for a specific dilution realization and use it to interpret simulations of the defect density dependent local growth of the stable phase after an instantaneous quench.

¹The authors wish to thank the DOE for support.

C1.00318 Computation of Shock Waves in Binary Inert Gas Mixtures of Diatomic Gases Using the Generalized Boltzmann Equation, RAMESH AGARWAL, GENG QIAN, Washington University in St. Louis — This paper describes the methodology for computing non-equilibrium shock waves in a binary inert mixture of monoatomic and diatomic gases using the Generalized Boltzmann Equation (GBE). For solving the classical Boltzmann equation for a mixture of monoatomic gases or the Generalized Boltzmann equation for a mixture of diatomic gases, these equations are formulated in impulse space, instead of velocity space. A binary mixture of two inert gases results in four coupled GBEs. The computational framework available for the classical Boltzmann equation is extended by including the rotational and vibrational degrees of freedom in the GBE for a mixture of diatomic gases in impulse space. The problem including both rotational - translational (RT) and vibrational - translational (VT) energy transfers is solved by applying a two-stage splitting procedure to the four coupled GBEs. The two stages consist of free molecular transport and RT -VT relaxations. Computations are presented for the shock structure in a binary mixture of N_2 and Ar, and N_2 and O_2 with 1:1 density ratio at Mach 5. This is the first time, such complex computations are being reported in the literature. The methodology can be easily applied to an inert mixture containing an arbitrary number of species.

C1.00319 Optomechanically Induced Transparency and Slow Microwaves in Circuit Nano-electromechanics, XIAOQING ZHOU, École Polytechnique Fédérale de Lausanne, Switzerland/Max-Planck-Institut für Quantenoptik, Germany, FREDRIK HOCKE, Walther-Meißner-Institut, Germany, ALBERT SCHLIESSER, École Polytechnique Fédérale de Lausanne, Switzerland, ACHIM MARX, HANS HUEBL, Walther-Meißner-Institut, Germany, RUDOLF GROSS, Walther-Meißner-Institut, Germany/Technische Universität München, Germany, TOBIAS J. KIPPENBERG, École Polytechnique Fédérale de Lausanne, Switzerland/Max-Planck-Institut für Quantenoptik, Germany — Using a low-mass (~ 15 pg), high-Q ($> 100\,000$) nanomechanical oscillator coupled to a Nb superconducting quarter wave cavity, we realize a circuit nano-electromechanical system coupling microwaves to mechanical motion oscillating at 1.45 MHz. By exciting the system on the lower motional sideband with a strong drive tone, a transparency window for a probe field is created originating from the effect of optomechanically induced transparency (OMIT). This phenomenon, analogous to electromagnetically induced transparency in Atomic Physics, arises from the interference of different excitation pathways for an intracavity probe field. We utilize the transparency window to demonstrate slow microwave propagation. A tunable delay up to 4 ms is demonstrated experimentally for a microwave pulse on resonance with the cavity. Furthermore, we systematically investigate the temporal dynamics of this transparency window when the drive tone is modulated, and the effect of the oscillator's Duffing nonlinearity on the OMIT window.

C1.00320 Performance of Multi Walled Carbon Nanotubes Grown on Conductive Substrates as Supercapacitors Electrodes using Organic and Ionic liquid electrolytes, ANDREW WINCHESTER, SUJOY GHOSH, BEN TURNER, Southern Illinois University Carbondale Department of Physics, X.F. ZHANG, Northeastern University Boston, SAIKAT TALAPATRA, Southern Illinois University Carbondale Department of Physics — In this work we will present the use of Multi Walled Carbon Nanotubes (MWNT) directly grown on inconel substrates via chemical vapor deposition, as electrode materials for electrochemical double layer capacitors (EDLC). The performance of the MWNT EDLC electrodes were investigated using two electrolytes, an organic electrolyte, tetraethylammonium tetrafluoroborate in propylene carbonate (Et_4NBF_4 in PC), and a room temperature ionic liquid, 1-butyl-3-methylimidazolium hexafluorophosphate (BMIM- PF_6). Cyclic voltammetry, galvanostatic charge-discharge, and electrochemical impedance spectroscopy measurements to obtain values for the capacitance and internal resistance of these devices will be presented and compared.

C1.00321 Measure of nonclassical correlation in coherence vector representation, TAO ZHOU, JINXIN CUI, GUI LU LONG¹, Department of Physics, Tsinghua University, Beijing 100084 — We consider the coherence vector representation (CVR) of a bipartite state and obtain a necessary and sufficient condition for a zero-discord state. Based on this, a measure of quantum, classical and total amount of correlations in bipartite states is proposed in this representation. Analytical expressions for this measure are available for any bipartite states. Our measure of nonclassical correlation coincides with the geometric measure of quantum discord for some particular states. References: T Zhou, J. Cui and G L Long, PRA A84, 062105 (2011)

¹presenter

C1.00322 Law of Universal Repulsion, YONGQUAN HAN, None — All objects in the universe repel each other. Repulsion between two objects is directly proportional to the external energy (mv^2) of their relative motion and indirectly proportional to their relative motion radius (one object is in relative rest, while the other one is in relative motion). **Application examples** Suppose a man whose mass is 100 kg, runs on the earth at a speed of 10 meters per second. The radius of the earth is 637100 meters. The repulsion between the earth and the man is: $F=mv^2/r=0.00157N$; if his speed reaches the first cosmic speed (7.9 km per second), then calculate: $F=mv^2/r=980N$, just overcome the gravity of the earth. A car with a certain velocity running in a straight highway (actually with some slight curves) can't fly up. However, if it encounters an arched bridge, it is possible for the car to fly. That is the consequence of the arch bridge has changed its movement radius, and the repulsion is increased. A aircraft's taking off and flying are not only because of the fluid - air, but also because of the change of its motion radius (forming virtual arched bridge in the air), which increases the repulsion.

C1.00323 Supersymmetry approach to delocalization transition in the network model of weak field quantum Hall effect and related models, VAGHARSH MKHITARYAN, Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112, USA, SHANTHANU BHARDWAJ, ILYA GRUZBERG, James Franck Institute, University of Chicago, Chicago IL 60637, USA — Recently, a two-channel random network model was proposed for quantum Hall effect in a weak (non-quantizing) magnetic field. For the anisotropic variant of this network, we analytically average over the randomness using the supersymmetry method, and map the network onto a model of interacting $u(1,1|2)$ superspins. We analyze the resulting superspin model by relating it to a nonlinear sigma-model. We argue that the phase diagram of the superspin model does not change qualitatively if we identify $u(1,1|2)$ superspins with ordinary $su(2)$ spin-1/2's. This allows us to develop a deeper insight and extend the phase diagram into the regions inaccessible to a sigma-model approach. We further extend our approach to a related two-channel network models and discuss their physical implications.

C1.00324 Giant Electro-Mechanical Energy Conversion in [011] cut Relaxor Ferroelectric Single Crystals, PETER FINKEL, NUWC, WEN DONG, CHRIS LYNCH, UCLA, AHMED AMIN, NUWC — Giant electro-mechanical energy conversion is demonstrated under a ferroelectric/ferroelectric phase transformation in [011] cut and poled lead titanate-based relaxor perovskite morphotropic single crystals. It is found that under mechanical pre-stress, a relatively small oscillatory stress drives the material reversibly between rhombohedral and orthorhombic phases with a remarkably high polarization and strain jumps induced at zero bias electric field and room temperature. The measured electrical output per cycle is more than an order of magnitude larger than that reported for linear piezoelectric materials. Ideal thermodynamic cycles are presented for this electro-mechanical energy conversion followed by a presentation and discussion of the experimental data.

C1.00325 Direct and Indirect Two-color Coherent Control in Bulk Silicon, JINLUO CHENG, JULIEN RIOUX¹, JOHN SIPE, Department of Physics, University of Toronto, 60 St. George Street, Toronto, Ontario, Canada M5S 1A7 — Using an empirical pseudopotential model for electron states and an adiabatic bond charge model for phonon states, we investigate the two-color direct and indirect coherent current injection with an incident optical field composed of a fundamental frequency and its second harmonic, and calculate the response tensors of the electron (hole) charge and spin currents. We show the current control for three different polarization scenarios: For co-circularly polarized beams, the direction of the charge current and the polarization direction of the spin current can be controlled by a relative-phase parameter; for the co-linearly and cross-linearly polarized beams, the current amplitude can be controlled by that parameter. For the indirect gap injection, the spectral dependence of the maximum swarm velocity shows that the direction of charge current reverses under an increase in photon energy.

¹Currently at Department of Physics, University of Konstanz, D-78457 Konstanz, Germany.

C1.00326 C-Axis Properties of DyNi₂B₂C System, W.C. LEE, Dept. of Physics, Sookmyung Women's Univ. Seoul 140-742, Korea — We have measured the electrical resistivity along c-axis $\rho_c(T, H)$ of the DyNi₂B₂C single crystal with the magnetic fields perpendicular to the c-axis and the magnetization isotherms $M(H)$ of the DyNi₂B₂C single crystal with magnetic fields perpendicular and parallel to the c-axis. We confirmed that Neel temperature T_N is 10.3K from the $\rho_c(T)$ result which is consistent with that from previous $\rho_{ab}(T)$ result. In addition, the constructed critical fields $H_{c2}(T)$ curve and magnetic transitions diagram of DyNi₂B₂C from $\rho_c(T)$ magnetic fields perpendicular to c-axis is similar to that of $\rho_{ab}(T)$ result, which is thought to arise that 3 D magnetic structure of DyNi₂B₂C.

C1.00327 Topological insulators on a Mobius Strip¹, LANG-TAO HUANG, Department of Physics, Tsinghua University, Beijing 100084, China, DUNG-HAI LEE², Department of Physics, University of California at Berkeley, Berkeley, CA 94720, USA — We study the two dimensional Chern insulator and spin Hall insulator on a non-orientable Riemann surface, the Mobius strip, where the usual bandstructure topological invariant is not defined. We show that while the flow pattern of edge currents can detect the twist of the Mobius strip in the case of Chern insulator, it can not do so in spin Hall insulator [1].

[1] Lang-Tao Huang and Dung-Hai Lee, Phys. Rev. B **84**, 193106 (2011)

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²Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA.

C1.00328 Extension of the Non-Hermitian Quantum Walk Model into a 2D Hexagonal Lattice¹

, LANG-TAO HUANG, Department of Physics, Tsinghua University, Beijing 100084, China — We generalize the 1D non-Hermitian quantum walk model of M. S. Rudner, and L. S. Levitov [1] to three different cases: 1D model with next nearest hopping, 2D model with and without next nearest hopping on hexagonal lattice respectively. We find that the quantization of the average decay length is always robust to next nearest hopping with real hopping parameter in 1D, but in the case of 2D, this quantization is only present in some special circumstances. We also find the 2D model is compatible to the 1D one by setting one of the hopping terms to zero. As to the Haldane model, quantization of this type exists only in 0 or π magnetic flux phases.

[1] M. S. Rudner and L. S. Levitov, Phys. Rev. Lett. **102**, 065703 (2009).

¹We acknowledge the supports by (i) NSFC Grant No. 11074143, and (ii) the Program of Basic Research Development of China Grant No. 2011CB921901.

C1.00329 The Pirouette effect in turbulent flows

, ALAIN PUMIR, Ecole Normale Supérieure de Lyon and CNRS, HAITAO XU, EBERHARD BODENSCHATZ, Max-Planck Institute for Dynamics and Self Organisation, Goettingen, Germany — The dynamics of the velocity gradient tensor plays a crucial role for our understanding of turbulent flows. I will discuss recent numerical and experimental results concerning the “perceived velocity gradient tensor,” constructed with the help of 4 points (a tetrad). This tensor depends on the overall size of the tetrad, thus permitting to study the properties of the flow as a function of scale. I will in particular consider the statistical properties, as well as the dynamical properties of the velocity gradient tensor, in relation to the dynamics of the shape of the tetrad. These properties shed some new light on the intriguing preferential alignment between vorticity and the eigenvector, corresponding to the intermediate eigenvalue of the strain.

C1.00330 Spintronic Oscillator based on feed-back mechanism

, ASHWIN TULAPURKAR, Department of Electrical Engineering, Indian Institute of Technology-Bombay, Mumbai, India, DINESH DIXIT, Department of Physics, Indian Institute of Technology-Bombay, Mumbai, India, KATSUNORI KONISHI, Graduate School of Engineering Science, Osaka University, Osaka, Japan, C. TOMY, Department of Physics, Indian Institute of Technology-Bombay, Mumbai, India, YOSHISHIGE SUZUKI, Graduate School of Engineering Science, Osaka University, Osaka, Japan — Nano-scale rf oscillators based on the magnetic tunnel junctions is an active area of research. These oscillators are based on the spin-transfer torque effect, in which a dc current drives the magnetization into precessional motion. Here we present a novel design of a spintronic oscillator which is not based on spin-transfer torque effect. This new oscillator is comprised of a magnetic tunnel junction whose top and bottom contacts are connected to a bias-T. A dc current is passed through the low frequency port of the bias-T and the high frequency port is connected to a “feed-back” wire which runs below the MTJ. Any fluctuation in the magnetization direction of the free layer of MTJ, drives ac current through the feed-back wire, which in turn exerts ac magnetic field on the free layer. The feedback wire is oriented such that the ac magnetic field amplifies the magnetization fluctuations for positive value of dc current. For negative value of dc current, the feedback loop suppresses the fluctuations. We find that if the positive dc current passing through the MTJ is more than a critical value, continuous precessing states of the magnetization are possible. Oscillators with better quality factors are possible using the feedback scheme.

C1.00331 Stability and collapse of a dipolar condensate in a 1D optical lattice¹

, MATTIA JONASINIO, LUIS SANTOS, Leibniz University of Hannover, STEFAN MÜLLER, JULIETTE BILLY, EMANUEL HENN, HOLGER KADAU, AXEL GRIESMAIER, TILMAN PFAU, 5 Institute of Physics, University of Stuttgart — The stability properties of a dipolar condensate are strongly affected by the external confining potential, as a consequence of the long range and anisotropic character of the dipole-dipole interaction. In contrast to a contact interacting gas, the presence of a 1D lattice induces a crossover from a dipolar destabilized to a dipolar stabilized regime for increasing lattice depth. In the deep lattice regime, a dipolar condensate can be stabilized at large negative scattering length in the interaction-dominated regime. As a consequence of the dipolar potential shape, the condensate collapse in the deep lattice regime features a *local* character (as opposed to the global character of the usual contact interacting gas): the condensate develops a surface density modulation resulting in several isolated local collapses. Finally, the stabilizing effect of the external potential plays an important role during the time-of-flight expansion. A dipolar condensate can be stable as long as it is trapped but can immediately collapse as soon as the external potential is removed. This makes the mapping of the time of flight expansion onto the momentum distribution highly non trivial.

¹Funded through the QUEST excellence program and the DFG research grant

C1.00332 Spin wave excitation by spin-transfer torque in a magnetic insulator

, JIANG XIAO, Department of Physics, Fudan University, GERRIT BAUER, IMR, Tohoku University — We study the excitation of spin waves in magnetic insulators by the current-induced spin-transfer torque. We predict preferential excitation of surface spin waves induced by an easy-axis surface anisotropy. The critical excitation current for the surface spin wave is inversely proportional to the penetration depth and surface anisotropy. Compared to the bulk modes, the critical current and excitation power of such surface spin wave are greatly reduced and enhanced, respectively.

C1.00333 Calculating the density of states in disordered systems using free probability¹

, JIAHAO CHEN, ERIC HONTZ, MATTHEW WELBORN, JEREMY MOIX, TROY VAN VOORHIS, Department of Chemistry, Massachusetts Institute of Technology, ALBERTO SUÁREZ, Departamento de Ingeniería Informática, Escuela Politécnica Superior, Universidad Autónoma de Madrid, Ciudad Universitaria de Cantoblanco, RAMIS MOVASSAGH, ALAN EDELMAN, Department of Mathematics, Massachusetts Institute of Technology — We approximate the density of states in disordered systems by decomposing the Hamiltonian into two random matrices and constructing their free convolution. The error in this approximation is determined using asymptotic moment expansions. Each moment can be decomposed into contributions from specific joint moments of the random matrices; each of which has a combinatorial interpretation as the weighted sum of returning trajectories. We show how the error, like the free convolution itself, can be calculated without explicit diagonalization of the Hamiltonian. We apply our theory to Hamiltonians for one-dimensional tight binding models with Gaussian and semicircular site disorder. We find that the particular choice of decomposition crucially determines the accuracy of the resultant density of states. From a partitioning of the Hamiltonian into diagonal and off-diagonal components, free convolution produces an approximate density of states which is correct to the eighth moment. This allows us to explain the accuracy of mean field theories such as the coherent potential approximation, as well as the results of isotropic entanglement theory.

¹Funded by NSF SOLAR NSF Grant No. 1035400

C1.00334 Transport Coefficients of a Normal Fermi Gas at Unitarity

, HUA LI, KEVIN BEDELL, Boston College, JASON JACKIEWICZ, New Mexico State University — We studied the transport properties of a two component Fermi gas in the unitary limit. Transport coefficients of the Fermi gas are calculated in the extreme low-temperature limit. To calculate the transport coefficients we need the scattering amplitudes. The scattering amplitudes are calculated from the Landau parameters. These parameters are obtained from the local version of the induced interaction model for computing Landau parameters [1]. The leading order finite temperature corrections to the transport coefficients are also calculated [2]. The calculated temperature dependent spin diffusivity is compared with the experimental measurement. A minimum of the spin diffusivity with a value of order $\hbar/m$ is observed at some finite temperature below the Fermi temperature.

C1.00335 Thermally-induced resonance in folding-unfolding transition of a stretched RNA, WON KYU KIM, Department of Physics and PCTP, Pohang University of Science and Technology, Pohang 790-784, South Korea, CHANGBONG HYEON, School of Computational Sciences, Korea Institute for Advanced Study, Seoul 130-722, South Korea, WOKYUNG SUNG, Department of Physics and PCTP, Pohang University of Science and Technology, Pohang 790-784, South Korea — The biopolymers are often situated in constrained, thermally fluctuating environment in the cell. To understand how they respond to a minute but temporally varying signal, we study folding-unfolding dynamics of a stretched RNA under a small oscillatory force. We find via numerical simulations that the small oscillation enhances the folding (unfolding) dynamics, even at a high (low) stretching condition where the folding (unfolding) is improbable, leading to a minimum mean transition time at an optimal frequency, a phenomenon dubbed as Resonant Activation (RA). In addition, the folding-unfolding transition can be maximally synchronous to the oscillation at another optimal frequency, characteristics of the Stochastic Resonance (SR). These noise-assisted resonance phenomena, RA and SR, which can also be largely modulated by the polymer parameters, provide a glimpse of how a biopolymer self-organizes in response to the environmental fluctuation in the cell.

C1.00336 Effect of inter-layer single-electron hopping and pair-hopping on superconductivity in multi-layered cuprates, KAZUTAKA NISHIGUCHI, Department of Physics, The University of Tokyo, KAZUHIKO KUROKI, Department of Applied Physics and Chemistry, The University of Electro-Communications, RYOTARO ARITA, Department of Applied Physics, The University of Tokyo, TAKASHI OKA, HIDEO AOKI, Department of Physics, The University of Tokyo — The multi-layered cuprates, which remain the highest- T_c material to date, still harbor unsolved problems. Specifically, the reason why T_c increases as we go from the single-layer system to trilayer has not been microscopically understood. Here we have studied the superconductivity in the n -layered Hg-series cuprate $\text{HgBa}_2\text{Ca}_{n-1}\text{Cu}_n\text{O}_{2+2n+\delta}$ by solving the Eliashberg equation for a multi-orbital Hubbard model with the random phase approximation (RPA) as well as with the fluctuation exchange approximation (FLEX). The hopping parameters are obtained by downfolding from first principles calculations based on the density functional theory (DFT) for the Hg-series cuprates with $n=1, 2, 3$. The result indicates that the enhancement of T_c with n is not explained in terms of the band structure alone. We then consider the possible ingredients in multi-layered cuprates that may affect T_c for different numbers of CuO_2 planes, specifically, the inter-layer single-electron hopping and inter-layer Cooper-pair hopping originating from the inter-layer Coulomb interaction, which we vary to probe the superconducting nature.

C1.00337 Superfluid correlations of ladder-type Hubbard model with trapping potential, SUSUMU YAMADA, MASAHIKO OKUMURA, RYO IGARASHI, ATSUSHI YAMAMOTO, MASAHIKO MACHIDA, Japan Atomic Energy Agency — In this study, we investigate possibility of superfluidity derived from repulsive interactions in optical lattice systems using the DMRG method. We calculate superfluid correlations in 2-leg ladder-type Hubbard models with varying the repulsive parameter U and the trapping one V , and then clarify dependences of the superfluid correlations on the parameters. The calculation results show that there are two hotspots, whose superfluid correlations are remarkably high, in the space spanned by U and V for suitable fillings. In this presentation, we present the results, compare them with those in more than 2-leg Hubbard models, and reveal the best situation in which the superfluidity correlation develops.

C1.00338 Critical Lamellar Thickness of Polymer Crystal Growth Studied by Dynamic Monte Carlo Simulations¹, XIAOMING JIANG, WENBING HU, State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, China — We set up a parallel-oriented slit to block lamellar crystal growth of chain molecules, and found a critical spacing of the slit gate, which reflected the critical lamellar thickness (L_{min}) for crystal growth. The values of L_{min} measured at various temperatures provided useful information about the role of lamellar crystal thickness in the kinetics of polymer crystal growth. More interesting, we found that the excess lamellar thicknesses decreased with the increase of temperatures, in contradictory to the prediction of Lauritzen-Hoffman theory.

¹This work is supported by National Natural Science Foundation of China (Grant No. 20825415) and National Key Basic Research Program of China (Grant No. 2011CB606100).

C1.00339 Strain-induced transition from intramolecular to intermolecular crystal nucleation¹, YIJING NIE, WENBING HU, State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, China — We performed dynamic Monte Carlo simulations of strain-induced crystallization of bulk polymer chains. We observed that for small crystallites grown at relatively high temperatures, the probabilities of adjacent chain-folding jump down at a critical strain. The result implies that polymer chains prefer to choose intramolecular crystal nucleation at small strains, and the intermolecular crystal nucleation becomes dominant only when the strain is higher than the critical value. In addition, the critical strains appear as almost constant to temperatures.

¹This work is supported by National Natural Science Foundation of China (Grant No. 20825415) and National Key Basic Research Program of China (Grant No. 2011CB606100).

C1.00340 Single Crystalline TiO_2 Nanorod grown on Transparent Conducting Substrates for Dye-Sensitized Solar Cells, XIAOYAN PENG, University of Puerto Rico, BOQIAN YANG, University of Massachusetts Amherst, PETER FENG, University of Puerto Rico — Single crystalline TiO_2 nanorods have been synthesized by pulse laser deposition technique on indium tin oxide glass substrates. During the deposition, oxygen pressures were kept under 100, 200 and 500 mTorr, respectively. Scanning Electron Microscopy images show vertical nanorod arrays with the same diameters of 200-300 nm were obtained under different oxygen pressures, but with various density of the arrays. The TiO_2 nanorods growth under 200 mTorr oxygen pressures were pure highly crystalline anatase according to X-ray diffraction measurement. The highly crystalline and vertical TiO_2 nanorod arrays contributed to the achievement of the high conversion efficiency of light-to-electricity. High conversion efficiency was obtained with the vertically aligned TiO_2 single crystalline nanorod cell.

C1.00341 Transitions between multiple attractors in a granular mixing experiment, RALF STANNARIUS, FRANK RIETZ, University of Magdeburg — We report on a granular experiment that produces multiple quasi-periodic patterns in a rotating flat container filled with a bidisperse mixture (0.3 mm and 0.9 mm diameter) of spherical grains. The cell depth is fixed to 0.5 cm (of the order of 10 bead layers), the height is 8 cm. Cell widths are either 17 cm or 50 cm. After an initial transient period, the system develops a lateral band texture of size-segregated grains. These bands show a pronounced spatio-temporally periodic drift in axial direction, sometimes with reflection at the cell ends. In the course of long durations of the experiment, the system switches between different states that appear to be marginally stable oscillatory solutions over many periods. Ageing of the particles as well as external influences on the experiment can be excluded as explanations. In the long term limit, the system does not tend towards a stationary state, neither to a complete segregation, nor to stable bands or uniformly mixed states. The results complement and extend previous observations in cylindrical geometries, and represent a challenge for modeling and theoretical description.

C1.00342 Ultra high resolution neutron scattering: Neutron Resonance Spin-Echo and Larmor Diffraction, ANDREW WALTERS, THOMAS KELLER, BERNHARD KEIMER, Max Planck Institute for Solid State Research — The TRISP spectrometer at the FRM II neutron source near Munich, Germany, is a unique world-leading neutron scattering instrument which employs the Neutron Resonance Spin-Echo technique (NRSE). Linewidths of dispersive excitations with energy transfers up to 50 meV can be measured with an energy resolution in the μeV range without the restrictive flux limitations that normally apply to high resolution neutron triple-axis spectrometers. Pioneering studies on the electron-phonon interaction in elemental superconductors¹ and the lifetimes of magnetic excitations in archetypal magnetic systems will be reviewed.² The instrument can also be used as a Larmor diffractometer, enabling d-spacings to be measured with a resolution of $\frac{\Delta d}{d} \sim 10^{-6}$, i.e. more than one order of magnitude more sensitive than conventional diffraction techniques.³ Ongoing and future NRSE and Larmor diffraction projects will be outlined, especially in regard to prospective studies which will take full advantage of the new low temperature and high pressure sample environment capabilities now available at TRISP.

¹P. Aynajian et al., *Science* **319** 1509 (2008)

²S. Bayrakci et al., *Science* **312** 1928 (2006)

³C. Pfeleiderer et al., *Science* **316** 1871 (2007)

C1.00343 ABSTRACT WITHDRAWN —

C1.00344 Quantum Diffraction Without de Broglie Waves, A.M. KADIN, Princeton Junction, NJ, S.B. KAPLAN, Yorktown Heights, NY — It is well established that composite particles, from neutrons to atoms to large molecules, sometimes behave as de Broglie waves, with wavelength $\lambda = h/p$, where p is the total momentum of the given composite particle. The primary evidence of these de Broglie waves is the observation of diffraction patterns from diffracting objects such as crystal lattices or one or more orifices. Indeed, it is generally believed that such de Broglie waves are universal quantum aspects of all matter. It is argued here (see also [1]) that only primary quantum fields such as electrons are truly de Broglie waves. In contrast, composite particles are small confined quantum waves that follow essentially classical particle trajectories, without extended wavelike behavior given by the de Broglie relation. For example, a neutron is properly a particle on the fm scale, not an extended wave on the nm scale. The momentum change of such a quasiclassical particle during a collision is constrained by quantum transition rules of the crystal lattice or other extended object. In particular, for elastic scattering from a crystal lattice with reciprocal lattice vectors $\mathbf{G}_i$, the allowable momentum changes are $\Delta\mathbf{p} = \hbar\mathbf{G}_i/2\pi$, which reproduces the standard crystal diffraction pattern. This corresponds to emission of a degenerate phonon with zero energy. This provides a logically consistent picture of the microworld, avoiding most of the paradoxes associated with the orthodox interpretation of quantum mechanics. [1] A.M. Kadin, "Waves, Particles, and Quantized Transitions: A New Realistic Model of the Microworld", <http://arxiv.org/abs/1107.5794> (2011).

Monday, February 27, 2012 2:30PM - 5:18PM —

Session D1 GIMS GMAG: Focus Session: High Magnetic Fields, THz Spectroscopy, MRI 203

2:30PM D1.00001 Novel magnetic textures in $\text{SrCu}_2(\text{BO}_3)_2$ from magnetostriction up to 97.4 tesla¹, MARCELO JAIME, Marcelo Jaime, National High Magnetic Field Laboratory (NHMFL), Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — Quantum magnets are model systems wherein strongly frustrated spin interactions generate a variety of exotic magnetic phases of current interest, including quantum spin ices, spin liquids, spin supersolids and complex magnetic superstructures. $\text{SrCu}_2(\text{BO}_3)_2$, the only classic realization of the spin-1/2 Heisenberg antiferromagnet in the Shastry-Sutherland (orthogonal spin dimer) lattice is known to exhibit numerous magnetization plateaus due formation of stripe-like magnetic textures in high fields. However, the fine structure of these plateaus remains controversial on both experimental and theoretical fronts due to the existing limits for achievable magnetic fields in the laboratory, the sensitivity of current magnetization techniques, and the uncontrolled nature of available theoretical approaches for highly frustrated magnetic lattices. This talk will describe how we probe magnetic textures in $\text{SrCu}_2(\text{BO}_3)_2$ via a recently-developed *magnetostriction* technique based on optical fiber Bragg gratings [1]. We achieve microstrain (nm-resolution) sensitivity in ultrahigh pulsed fields to 97.4 T using the NHMFL 100 tesla multi-pulse magnet system [2]. The magnetostriction data reveal fine structure corresponding to all magnetization plateaus, and a significant lattice response to the long-predicted 1/2-saturation plateau at 82 T, as well as a new feature at 73.6 T that we attribute to a never before observed structure corresponding to 2/5 of magnetization saturation [3]. These data are complemented by simultaneous magnetocaloric-effect measurements, and are supported by numerical results obtained using a controlled density matrix renormalization group method.

[1] Daou R. et al., *Rev. Sci. Instrum.* **81**, 033909 (2010).

[2] Sims J.R., et al. *IEEE Trans. Appl. Supercond.* **18**, 587-591 (2008).

[3] M. Jaime et al., submitted. In collaboration with R. Daou, S.A. Crooker, F. Weickert, A. Uchida, A. Feiguin, C.D. Batista, H. Dabkowska, and B. Gaulin.

¹Supported by the National Science Foundation, the US DOE, and the State of Florida.

3:06PM D1.00002 Superconducting critical current measurements in pulsed magnets, FEDOR F. BALAKIREV, Los Alamos National Laboratory, Los Alamos, NM, USA, PHILIP J.W. MOLL, NIKOLAI D. ZHIGADLO, JANUSZ KARPINSKI, BERTRAM BATLOGG, Laboratory for Solid State Physics, ETH Zurich, Switzerland — Measurements of critical current in single crystals of high temperature superconductor using pulsed magnetic fields are tricky due to short time scale, fast field sweep rate and sheer absolute current values in restricted sample space. We will present a measurement system design that addresses the challenges via a combination of Field Programmable Gate Array (FPGA) fast-response signal generation and detection architecture and Focused Ion Beam crystal shaping.

3:18PM D1.00003 Development of a high-field electron paramagnetic resonance spectrometer, EKATERINA E. ROMANOVA, FRANKLIN H. CHO, VIKTOR STEPANOV, SUSUMU TAKAHASHI, University of Southern California — Electron paramagnetic resonance (EPR) spectroscopy is a powerful and versatile technique to study structure and dynamics of biomolecules. Structural investigations of biological molecules begin with site-directed spin labeling (SDSL). Using SDSL, a nitroxide spin label containing a stable unpaired electron is covalently attached at a specific site within a bio-macromolecule. The time resolution and the sensitivity of EPR spectrometer become higher when the system is operated at higher frequencies and magnetic fields. In addition, a fine spectral resolution obtained with a high-field EPR (HFEP) enables us to study details of the conformation in biological molecule by determining the orientation of a spin-label or the relative orientation of two spin-labels embedded in the molecule. In this presentation, we will report the development of a 115/230 GHz continuous wave (cw) and pulsed EPR spectrometer at USC. The spectrometer is based on a 700/100 mW solid-state source at 115/230 GHz respectively, a 12-Tesla magnet and a superheterodyne detection system. The system also has the 2nd synthesizer for double electron-electron resonance (DEER) spectroscopy. HFEP measurements with spin-labeled CS DNA will be discussed.

3:30PM D1.00004 Sensitivity of charge transport measurements to local inhomogeneities, DANIEL KOON, St. Lawrence University, FEI WANG, DIRCH HJORTH PETERSEN, OLE HANSEN, Department of Micro- and Nanotechnology, Technical University of Denmark — We derive analytic expressions for the sensitivity of resistive and Hall measurements to local variations in a specimen's material properties in the combined linear limit of both small magnetic fields and small perturbations, presenting exact, algebraic expressions both for four-point probe measurements on an infinite plane and for symmetric, circular van der Pauw discs. We then generalize the results to obtain corrections to the sensitivities both for finite magnetic fields and for finite perturbations. Calculated functions match published results and computer simulations, and provide an intuitive, visual explanation for experimental misassignment of carrier type in n-type ZnO and agree with published experimental results for holes in a uniform material. These results simplify calculation and plotting of the sensitivities on an $N \times N$ grid from a problem of order N^5 to one of order N^3 in the arbitrary case and of order N^2 in the handful of cases that can be solved exactly, putting a powerful tool for inhomogeneity analysis in the hands of the researcher: calculation of the sensitivities requires little more than the solution of Laplace's equation on the specimen geometry.

3:42PM D1.00005 Polarization Modulation THz TDS of Topological Insulators¹, DEEPU GEORGE, CHASE ELLIS, Dept of Physics, SUNY Buffalo, TOBIAS KIESSLING, Universitat Wurzburg, JOHN CERNE, ANDREA MARKELZ, Dept of Physics, SUNY Buffalo, MARKELZ GROUP COLLABORATION, CERNE GROUP COLLABORATION — Optical hall conductivity measurements are powerful alternatives to DC transport measurements in samples in which the latter are challenging. They provide a deeper understanding of interactions in correlated systems and also serve as a measure of disorder in such systems. Aoki et al[1] has studied Quantum Hall Effect in graphene theoretically and has predicted that Optical Hall Conductivity should be measurable with an accurate detection of the Hall angle in the THz regime. Shimano et al [2] has reported evidence for Quantum Hall Plateau in the longitudinal conductivity σ_{xx} in the THz region in a 2DEG system. In this work, we have developed a new broadband technique which rapidly measures complex Faraday and Kerr angles. Our technique is capable of measuring the entire complex conductivity tensor with a single scan, with an accuracy of 5mRad in the frequency range 0.2 to 2.5THz. We have employed this to study topological insulators and have observed a magnetic field dependent absorption around 0.5THz. 1. Morimoto, T., Jour. of Phys: Conference Series, 2009. 150(2). 2. Ikebe, Y., et al., PRL, 2010. 104(25): p. 256802.

¹NSF MRI-R2 DBI2959989 NSF-DMR1006078

3:54PM D1.00006 Analysis of complex mixtures using a new, high resolution Trapped Ion Mobility Spectrometer – Mass Spectrometer¹, FRANCISCO FERNANDEZ-LIMA, Texas A&M University, CHRISTOPHER THOMPSON, DESMOND KAPLAN, MELVIN PARK, Bruker Daltonics — Over the last decade, a variety of new types of Ion Mobility Spectrometry (IMS) analyzers have been developed (e.g., periodic focusing DC ion guide, segmented quadrupole drift cell, multistage IMS, field asymmetric IMS and transient wave ion guide). High resolution IMS ($R > 50$) has been mainly restricted to long IMS cells (1-2 m), where ions are separated based on size-to-charge ratio as they are pushed by an electric field through a stationary bath gas. In the present work we describe a Trapped Ion Mobility Spectrometer (TIMS) and its applications. In as much as TIMS uses an electric field to hold ions stationary in a moving bath gas, it represents a paradigm shift in mobility analysis. This results in an analyzer capable of high resolution mobility separations ($R > 80$) in a compact (< 10 cm), low voltage (< 300 V) design. Hybridization with a mass analyser (TIMS-MS) provides versatility for the analysis, separation and structural characterization of a variety of chemical compounds with increasing complexity. In particular, examples of TIMS – MS separation for complex biological and heteroatom hydrocarbons will be shown.

¹This work was supported by the National Institute of Health (Grant No. 1K99RR030188-01) and a 2010 & 2011 Bruker Daltonics, Inc. Fellowship.

4:06PM D1.00007 Measurement of statistical nuclear spin polarization in a nanoscale GaAs sample, FEI XUE, DENNIS WEBER, PHANI PEDDIBHOTLA, MARTINO POGGIO, Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — We measure the statistical polarization of quadrupolar nuclear spins in a sub-micrometer ($0.6 \mu\text{m}^3$) particle of GaAs using magnetic resonance force microscopy. The crystalline sample is cut out of a GaAs wafer and attached to a micro-mechanical cantilever force sensor using a focused ion beam technique. Nuclear magnetic resonance is demonstrated on ensembles containing less than 5×10^8 nuclear spins and occupying a volume of around $(300 \text{ nm})^3$ in GaAs with reduced volumes possible in future experiments. We discuss how the further reduction of this detection volume will bring the spin ensemble into a regime where random spin fluctuations, rather than Boltzmann polarization, dominate its dynamics. The detection of statistical polarization in GaAs therefore represents an important first step toward 3D magnetic resonance imaging of III-V materials on the nanometer-scale.

4:18PM D1.00008 Carbon nanotube quantum dots as highly sensitive THz spectrometers¹, MOHAMED RINZAN, Physics department, Georgetown university, GREG JENKINS, DENNIS DREW, Physics department, University of Maryland, SERHIL SHAFRANJUK, Department of physics and astronomy, Northwestern university, PAOLA BARBARA, Physics department, Georgetown university — We show that carbon nanotube quantum dots (CNT-Dots) coupled to antennas are extremely sensitive, broad-band, terahertz quantum detectors. Their response is due to photon-assisted single-electron tunneling (PASET)[1], but cannot be fully understood with orthodox PASET models[2]. We consider intra-dot excitations and non-equilibrium cooling to explain the anomalous response. REFERENCES: [1] Y. Kawano, S. Toyokawa, T. Uchida and K. Ishibashi, THz photon assisted tunneling in carbon-nanotube quantum dots, Journal of Applied Physics 103, 034307 (2008). [2] P. K. Tien and J. P. Gordon, Multiphoton Process Observed in the Interaction of Microwave Fields with the Tunneling between Superconductor Films, Phys. Rev. 129, 647 (1963).

¹Funded by Airforce office of scientific research, Grant #. FA9550-09-1-0697

4:30PM D1.00009 Ultrafast electro-optic modulation for Terahertz upconversion spectroscopy, MATTHEW DECAMP, ZHIYUAN CHEN, University of Delaware — Traditional time-domain terahertz (THz) spectroscopy techniques require the combination of sub-picosecond laser systems and time-delay stages for spectral analysis, making the design of a portable THz spectrometer challenging. In this work, we demonstrate an alternative method of spectrally resolving coherent THz radiation using narrow band optical light and passive optical spectrum analyzers. This method utilizes THz induced electro-optic modulation of a narrow band laser to upconvert the spectral content of the THz radiation to the visible portion of the electro-magnetic spectrum. This device does not require any movable parts and is well suited for spectrally analyzing both broadband and narrowband THz radiation. The spectral resolution of this technique is limited by the bandwidth of the optical radiation and the non-linear medium. Further advancements will include the development of a portable THz spectrometer, suitable for either research or clinical applications.

4:42PM D1.00010 Detection of internal molecular structural motions using anisotropic spectroscopy¹, ROHIT SINGH, DEEPU GEORGE, Department of Physics, University at Buffalo, SUNY, TIMOTHY KORTER, Department of Chemistry, Syracuse University, ANDREA MARKELZ, Department of Physics, University at Buffalo, SUNY — The far infrared spectroscopy of molecular crystals reveals both intra and inter molecular vibrational modes [1,2]. With the significant increase in complexity of structures, one finds increasing overlap in the internal modes. As an overall strategy to measure the correlated structural motions in protein, we use anisotropic and birefringent behavior of molecular crystals to develop a new technique called MOSTS (Modulated Orientation Sensitive THz Spectroscopy). We achieve high sensitivity and mode separation by using single molecular crystal such as sucrose and rapid modulation of the relative alignment of the terahertz polarization and the crystal axes by rotating the sample. By locking into the signal at the rotation frequency we determine the polarization sensitive signal and map out the optically active vibrational resonances. To illustrate the technique we compare our measured spectra with the calculated and find a close agreement.

[1] D.G. Allis, J.A. Zeidler, P.F. Taday and T.M. Korter, *Chem. Phys. Lett.*, 463, 84 (2008).

[2] P.U. Jepsen and J.C. Stewart, *Chem. Phys. Lett.*, 442, 275 (2007).

¹NSF MRI² grant DBI2959989.

4:54PM D1.00011 Ultra-Low Frequency MRI: Novel Imaging Sequences¹, MATTHEW NICHOLS, PAUL SANGIORGIO, JOHN CLARKE, Department of Physics, University of California, Berkeley — Our ultra-low field MRI system operates at a field of 0.132 mT with the signal detected by a Superconducting QUantum Interference Device (SQUID) coupled to an untuned, superconducting, second-derivative gradiometer. Operation at such low fields requires that we prepolarize the protons of our specimen in a field of about 150 mT prior to imaging to increase the sample magnetization. With the ultimate goal of *in vivo* imaging of prostate tissue by taking advantage of the enhanced longitudinal-relaxation-time at low fields, we seek to decrease the imaging time and optimize the signal-to-noise ratio of our imaging pulse sequences to make *in vivo* imaging viable in a clinical setting. To achieve this, we begin with standard imaging sequences used in other frequency domains and adapt them to our specific purposes and requirements, in particular the need to prepolarize. We describe modified inversion recovery and multiple echo imaging sequences, specifically Carr-Purcell-Meiboom-Gill (CPMG) pulse train and fully balanced Steady-State Free Precession (SSFP) sequences. We present the results of applying these sequences to imaging agarose gel phantoms.

¹Work supported by NIH

5:06PM D1.00012 Millimeter-wave and terahertz spectroscopy for the detection of ionized air and chemical vapor, BENJAMIN GRABER, US. Naval Research Laboratory/Temple University, RONGJIA TAO, Temple University, DONG HO WU, US. Naval Research Laboratory — Our previous work has demonstrated that the time domain terahertz spectroscopy (TDTS) of chemical vapor or ionized air produces characteristic spectrum from which one can identify chemicals or an ionization source, such as nuclear isotopes. While the average power of TDTS is only less than micro-Watts, the peak power of terahertz pulse can exceed kilo-Watts. When terahertz pulse is concentrated within a small area this large peak power produces a very large electric field, exceeding several kV/m. We investigate the field strength dependence of TDTS to see how it affects the detection capability of TDTS for chemical vapor and ionized air when the peak power is varied over the range from a few mW to kW. At the same time we performed similar experiments using a CW millimeter-wave spectroscopy over the frequency range from 75 GHz to 110 GHz and the power strength range from a few micro-Watts to several mW. We will present the details of our experimental results and discuss the merits of both systems for accuracy and long range detection of vapors. We will also examine some theory to understand the data.

Monday, February 27, 2012 2:30PM - 5:30PM –
Session D2 GMAG: Invited Session: Harnessing Local Atomic Structure to Control Magnetic Interactions in Complex Oxides 204AB

2:30PM D2.00001 Interface engineering in manganites: from diodes to transistors, HAROLD HWANG, Stanford University and SLAC National Accelerator Laboratory — Perovskite manganites show strong coupling between charge, spin, and lattice degrees of freedom as exemplified by 'colossal magnetoresistance'. The recent advances in thin film growth techniques have enabled the generation of novel phases at oxide heterointerfaces, the atomic control of their interface electronic structure, and their incorporation in novel device platforms. We apply these techniques to manganite thin films, first emphasizing the subtleties in optimizing the growth kinetics and stoichiometry [1,2], which has enabled us to create atomically precise heterostructures exhibiting room temperature metallic ferromagnetism in superlattices composed of just 5 unit cell layers [3]. The interface electronic structure was examined using Schottky junctions formed between $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ and Nb-doped SrTiO_3 , where the band offset (Schottky barrier height) can be controlled by the termination layer at the interface [4]. This band engineering technique was applied in making a metal-base transistor [5], which takes advantage of the strong internal electric field at interfaces. An analysis of many devices enables the quantitative understanding of the evolution from a hot-electron transistor to a permeable base transistor. This structure provides a platform for developing devices incorporating the exotic ground states of perovskite oxides and their interfaces.

[1] J. H. Song, T. Susaki, and H. Y. Hwang, *Adv. Mater.* **20**, 2528 (2008).

[2] D. A. Muller, L. Fitting Kourkoutis, M. Murfitt, J. H. Song, H. Y. Hwang, J. Silcox, N. Delby, and O. L. Krivanek, *Science* **319**, 1073 (2008).

[3] L. Fitting Kourkoutis, J. H. Song, H. Y. Hwang, and D. A. Muller, *PNAS* **107**, 11682 (2010).

[4] Y. Hikita, M. Nishikawa, T. Yajima, and H. Y. Hwang, *Phys. Rev. B* **79**, 073101 (2009).

[5] T. Yajima, Y. Hikita, and H. Y. Hwang, *Nature Mater.* **10**, 198 (2011).

3:06PM D2.00002 New material design strategies to realize strong coupling in multiferroics and beyond¹, CRAIG FENNIE, Cornell University, School of Applied & Eng. Physics — Perovskite ABO_3 oxides display an amazing variety of phenomena that can be altered by subtle changes in the chemistry and internal structure, making them a favorite class of materials to explore the rational design of novel properties. In this talk I will review a recent advance in which rotations and tilts of the BO_6 octahedra give rise to a novel form of ferroelectricity. Octahedral rotations strongly influence other structural, magnetic, orbital, and electronic degrees of freedom in perovskites and related materials. Thus, I want to discuss the idea that octahedral rotation-driven ferroelectricity has the potential to robustly control emergent phenomena with an applied electric field. As one example, I will show from first principles how these "functional" octahedral rotations simultaneously induce ferroelectricity, magnetoelectricity, and weak ferromagnetism in a class of naturally occurring Ruddlesden-Popper (RP) $(\text{ABO}_3)_2(\text{AO})$ layered perovskites and discuss the challenges to realize electric field switching of magnetism in these RP and in $(\text{ABO}_3)/(\text{A}'\text{BO}_3)$ perovskite superlattice novel multiferroics.

N. A. Benedek and C. J. Fennie, *Phys. Rev. Lett* **106**, 107204, 2011;

J. M. Rondinelli and C. J. Fennie, arXiv 2011; N. A. Benedek and C. J. Fennie, arXiv 2011.

¹CJF was supported by the DOE-BES under Award Number DE-SC0002334.

3:42PM D2.00003 Reversal of Magnetic Interactions by Electric field, PHILIP RYAN, Argonne National Laboratory — Direct magneto-electric coupling describes the interaction between magnetic and electric polarization through an intrinsic microscopic phenomenon in a single phase material. Systems which exhibit such coupling are potential candidates for use in a multistate logic memory storage device whereupon magnetic control with electric fields or ferroelectric control with magnetic fields could be used to alter memory bits. I will present x-ray resonant magnetic scattering results providing direct evidence of a magneto-electric cross field effect mediated through strong spin-lattice coupling in a single phase rare earth titanate film. Compressively strained EuTiO_3 is, as in bulk, an antiferromagnetic-paraelectric material, however through strain the balance of the magnetic interactions, both antiferromagnetic and ferromagnetic, shifts whereby the two approach energetic degeneracy. By applying an electric field *in-situ* one can tip the delicate equilibrium and suppress the long range antiferromagnetic order. This is accompanied by the emergence of short range ferromagnetic order. In addition we have qualitatively replicated the microscopic preferential shift from antiferromagnetic to ferromagnetic order with electric field using first principles density functional calculations.

4:18PM D2.00004 Strain-induced oxygen defect formation and interfacial magnetic phase separation in $\text{SrTiO}_3(001)/\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ ¹, CHRIS LEIGHTON, University of Minnesota — The remarkable functionality and epitaxial compatibility of complex oxides provides many opportunities for new physics and applications in oxide heterostructures. Perovskite manganites and cobaltites provide excellent examples, being of interest for solid oxide fuel cells, catalysis, ferroelectric RAM, gas sensing, resistive switching memory, and oxide spintronics. However, the same delicate balance between phases that provides this diverse functionality also leads to a serious problem - the difficulty of maintaining desired properties close to the interface with other oxides. Although this problem is widespread, manifests itself in several ways, and could present a significant roadblock to the development of heterostructured devices for oxide electronics, there is no consensus as to its origin, or even whether it is driven by electronic or chemical effects. In this work, using $\text{SrTiO}_3(001)/\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ as a model system, we have combined epitaxial growth via high pressure oxygen sputtering with high resolution x-ray diffraction, atomic resolution electron microscopy and spectroscopy, and detailed magnetic, transport, and neutron scattering measurements to determine the fundamental origin of the deterioration in interfacial transport and magnetism. The effect is found to be due to nanoscopic magnetic phase separation in the near-interface region driven by a significant depletion in interfacial hole doping due to accumulation of O vacancies. This occurs due to a novel mechanism for accommodation of lattice mismatch with the substrate based on formation and long-range ordering of O vacancies, thus providing a fundamental link between strain state and O vacancy density. Further impacts of the O vacancy ordering and interfacial magnetic phase separation, such as formation of a spin-state superlattice and an extraordinary coercivity enhancement, will also be discussed. Work in collaboration with M. Sharma, M. Torija, J. Schmitt, C. He, S. El-Khatib, J. Gazquez, M. Varela, M. Laver and J. Borchers.

¹Work supported by NSF and DOE (neutron scattering).

4:54PM D2.00005 Directly probing the effect of strain on magnetic exchange interactions, KATHRIN DORR, Institute for Physics, MLU Halle-Wittenberg — Thin films of transition metal oxides of the perovskite type ABO_3 ($B = 3d$ or $4d$ metal) have revealed abundant examples for strain-driven changes of magnetic ordering. One most popular is the strain-induced ferromagnetic ferroelectric state of otherwise antiferromagnetic paraelectric EuTiO_3 . Another promising example is the strain control of orbital occupation and magnetic coupling at oxide interfaces of SrRuO_3 with manganites. In spite of strong efforts, the theoretical treatment of magnetic exchange in complex oxides has remained a challenge, and experiments continue to show unpredicted / unexplained large effects of the epitaxial strains in films. In order to provide meaningful experimental data on strain dependences, epitaxial thin films should be grown in various coherent strain states on different substrates without changing anything but the strain. This is inherently difficult: possible problems may arise from a strain-dependent oxidation level or microstructure. As a complementary approach, the in-plane strain of epitaxial oxide films can be controlled reversibly using a piezoelectric substrate, even though the accessible reversible strain of 0.1 – 0.2% is an order of magnitude smaller. In my talk, I will address reversible-strain studies on $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$, $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ ($x = 0, 0.2, 0.3$) and SrRuO_3 films, showing the strain response of the magnetic Curie temperature, the magnetization and the electrical resistance and discussing the current understanding of the strain effects on magnetic ordering. In $\text{La}_{0.8}\text{Sr}_{0.2}\text{CoO}_3$, a strain-driven phase transition between ferromagnetic and spin-glass-like could be established by combining the piezoelectric substrate with a tuned buffer system providing varied as-grown strain states. In SrRuO_3 , a tetragonal tensile strain state shows a suppression of the ordered magnetic moment. Lattice parameters and symmetries of the films were determined by x-ray diffraction. It is noted that the atomic displacements (bond lengths and angles) under strain in these compounds are yet essentially unknown and subject to present research.

Monday, February 27, 2012 2:30PM - 5:30PM –
Session D3 DCMP: Invited Session: Stripe Order and Fermi-Surface Reconstruction in Cuprate Superconductors 205AB

2:30PM D3.00001 Fermi-surface reconstruction by stripe order in cuprate superconductors, FRANCIS LALIBERTÉ, University of Sherbrooke — The origin of pairing in a superconductor resides in the underlying normal state. In the cuprate high-temperature superconductor YBCO, application of a magnetic field to suppress superconductivity reveals a ground state that appears to break the translational symmetry of the lattice, pointing to some density-wave order [1,2,3]. In another cuprate, Eu-LSCO, the onset of stripe order - a modulation of spin and charge densities - at low temperature is well established [4]. By a comparative study of thermoelectric transport in the cuprates YBCO and Eu-LSCO, we show that the two materials exhibit a very similar process of Fermi-surface reconstruction as a function of temperature and doping [5,6]. This strongly suggests that Fermi-surface reconstruction is caused by stripe order in both cases, compelling evidence that stripe order is a generic tendency of hole-doped cuprates.

Work done in collaboration with J. Chang, N. Doiron-Leyraud, E. Hassinger, R. Daou, D. LeBoeuf, M. Rondeau, B. J. Ramshaw, R. Liang, D. A. Bonn, W. N. Hardy, S. Pyon, T. Takayama, H. Takagi, I. Sheikin, L. Malone, C. Proust, K. Behnia and L. Taillefer.

- [1] N. Doiron-Leyraud *et al.*, Nature **447**, 565 (2007).
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- [3] D. LeBoeuf *et al.*, Phys. Rev. B **83**, 054506 (2011).
- [4] J. Fink *et al.*, Phys. Rev. B **83**, 092503 (2011).
- [5] J. Chang *et al.*, Phys. Rev. Lett. **104**, 057005 (2010).
- [6] F. Laliberté *et al.*, Nat. Commun. **2**, 432 (2011).

3:06PM D3.00002 Competition between charge and superconducting orders in underdoped YBCO , MARC-HENRI JULIEN, Laboratoire National des Champs Magnétiques Intenses - Grenoble — We report nuclear magnetic resonance measurements (NMR) showing that high magnetic fields induce a static, unidirectional, modulation of the charge density in the CuO_2 planes of underdoped $\text{YBa}_2\text{Cu}_3\text{O}_y$ [T. Wu et al., Nature 477, 191 (2011)]. The appearance of the charge order coincides with the Fermi surface reconstruction inferred from quantum oscillation and other transport measurements. This charge order appears to be most probably the same $4a$ -periodic stripe modulation as in La-214 cuprates. That it develops only when superconductivity fades away (no charge order is observed under strong fields parallel to the planes) and near the same $1/8$ hole doping as in La-214 suggests that charge order, although visibly pinned by CuO chains in $\text{YBa}_2\text{Cu}_3\text{O}_y$, is an intrinsic propensity of the superconducting planes of high- T_c copper oxides. Since field induced stripe order is also compatible with neutron scattering data in La-214 and with STM data in Bi-2212, charge order could be a generic competitor of high T_c superconductivity.

Work performed with T. Wu, H. Mayaffre, S. Krämer, M. Horvatic, C. Berthier (LNCMI Grenoble), W.N. Hardy, R. Liang, D.A. Bonn (University of British Columbia, Vancouver)

3:42PM D3.00003 The electronic state of underdoped YBCO at high magnetic fields and low temperatures: evidence from quantum oscillatory phenomena¹ , GIL LONZARICH, University of Cambridge — Quantum oscillations in bulk and transport properties have been observed in underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ via a range of techniques and by independent researchers in applied magnetic fields above 20T and temperatures below 10K. The consensus is that the oscillations are periodic in the reciprocal of the magnetic field and consist of a number of components with frequencies (fundamental or otherwise) of below 2kT, nearly an order of magnitude lower than that observed in the overdoped state of $\text{Ti}_2\text{Ba}_2\text{CuO}_{6+x}$. Moreover, the temperature dependence of the amplitude of the strongest oscillatory components that can be measured accurately follows closely that expected for elementary excitations of fermionic character. I will discuss a model of the Fermi surface that can potentially account for each of the periodic components observed, and that appears to be consistent with a number of other known properties in the high-field low-temperature state.

¹Work performed in collaboration with S. E. Sebastian, N. Harrison, R. Liang, D. A. Bonn, and W. N. Hardy.

4:18PM D3.00004 Evidence for competing orders in underdoped $\text{YBa}_2\text{Cu}_3\text{O}_y$, CYRIL PROUST, Laboratoire National des Champs Magnétiques Intenses (CNRS) — 25 years after the discovery of high temperature cuprate superconductors, the observation of quantum oscillations has deeply changed the theoretical landscape relevant to these materials. The measurements of quantum oscillations on both sides of the phase diagram of cuprates confirm the existence of a Fermi surface with sharply defined excitations on the overdoped side and also show that the Fermi surface has suffered a drastic modification on the other side. The small Fermi pockets inferred from quantum oscillations in the underdoped regime combined with the negative Hall and Seebeck coefficients pointing to electrons as dominant charge carriers, greatly strengthen the case that the Fermi surface of underdoped $\text{YBa}_2\text{Cu}_3\text{O}_y$ undergoes a reconstruction because the translational symmetry of its lattice is broken at low temperature. Many studies, such as those of the Hall and Seebeck effects, point to a reconstruction of the Fermi surface due to stripe order. More recently, NMR measurements discover a static, unidirectional, modulation of the charge density in the CuO_2 planes that has the $4a$ -periodic stripe modulation. In this talk, I will show the impact of this charge order on some transport properties, in particular c -axis transport. A crossover to a coherent regime of metallic behavior of the c -axis resistivity at low temperature coincides with the emergence of the charge order. I will also address the topical question of competition between the charge order and superconductivity in high fields.

4:54PM D3.00005 Fermi-surface reconstruction by charge-stripe order in a cuprate superconductor , STEVE KIVELSON, Stanford University — No abstract available.

Monday, February 27, 2012 2:30PM - 5:30PM — Session D4 DAMOP: Long-range Interacting Rydberg and Dipolar Gases 205C

2:30PM D4.00001 Rydberg-Rydberg interactions in ultracold atomic gases , SEBASTIAN HOFFERBERTH, JONATHAN BALEWSKI, STÉPHAN JENNEWEIN, ALEXANDER KRUPP, HUAN NGUYEN, JOHANNES NIPPER, MICHAEL SCHLAGMUELLER, CHRISTOPH TRESP, ROBERT LOEW, TILMAN PFAU, University of Stuttgart — The giant size and large polarizability of Rydberg-atoms make them ideal to study many-body collective effects. We present recent results from the ultra-cold Rydberg experiments in our group. Firstly, we discuss studies of Förster resonances, which appear when two-body-states are tuned into resonance. The resulting strong dipolar interatomic interactions vary in strength and angular dependency based on the magnetic substates involved. We study these interactions in a Ramsey atom interferometer, where the two interferometer arms are atoms in the ground and in the Rydberg state. Using this phase sensitive tool, Förster resonances are studied with unprecedented accuracy. The coherent technique enables to resolve several resonances and study their coherence properties. Secondly, we present our new setup for studying single Rydberg-excitations in optical traps smaller than the Rydberg-blockade sphere. Such ensembles, where all trapped atoms coherently share a single Rydberg-excitation, form a two-level “superatom” whose Rabi-oscillation is collectively enhanced. Our new apparatus combines single ion-detection, sub-micron optical resolution, and highly flexible optical trapping potentials to study coherent dynamics of individual superatoms as well as interactions between superatoms.

2:42PM D4.00002 Towards single-photon optical nonlinearities using cold Rydberg atoms , THIBAUT PEYRONEL, MIT, OFER FIRSTENBERG, Harvard, QIYU LIANG, VLADAN VULETIC, MIT, MIKHAIL LUKIN, Harvard — Effects of the Rydberg blockade in cold atomic clouds have been intensively explored over the last few years. Optical fields can be coherently mapped onto atomic states with a Rydberg component using EIT techniques thanks to the long lifetime of the Rydberg states. As the dipole-dipole interaction between Rydberg atoms prevents several polaritons from propagating simultaneously within a Rydberg volume, it gives rise to strong non-linearities which are mapped back on the probe optical field. We aim at bringing the Rydberg-EIT into the single-photon regime in order to produce non-classical highly correlated states of light. Rubidium atoms are loaded in a far off-resonant (1064nm) optical dipole trap, where densities are typically large enough to reach high optical depths within a single blockade volume. In this regime, the outgoing photon-photon correlation function is expected to exhibit highly non-classical behavior, corresponding to trains of spatially separated single-photons. Moreover, EIT techniques together with a high-resolution imaging system allow the observation of Rydberg excitations in the quasi-1D configuration, and should pave the way to in-situ monitoring of strongly correlated many-body states such as the crystallisation of Rydberg atoms.

2:54PM D4.00003 Altering Photon Statistics using Strong Rydberg Interactions, JOHANNES OTTERBACH, Physics Department, Harvard University, Cambridge, MA, USA, DAVID PETROSYAN, Institute of Electronic Structure and Laser, FORTH, Crete, Greece, ALEXEY V. GORSHKOV, Institute for Quantum Information, California Institute of Technology, Pasadena, CA, USA, THOMAS POHL, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, MICHAEL FLEISCHHAUER, Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany, MIKHAIL D. LUKIN, Physics Department, Harvard University, Cambridge, MA, USA — The recent advance in coherently controlling and manipulating strong, long-range Rydberg interactions has triggered extensive research in studying interesting many-body effects as, e.g. the use of Rydberg blockade effects for quantum information processing and crystal formation. In this talk I show that Rydberg interactions can be used to alter the photon statistics of a weak probe field after propagating in a coherently prepared atomic Rydberg gas under conditions of Electromagnetically Induced Transparency (EIT). The Rydberg blockade mechanism leads to an effective two-level physics when two photons are separated less than the blockade radius resulting in a strong anti-correlation of two photons separated by an avoided volume. Implications of the formation of such hard-sphere photons for the recent experiment of Pritchard et al. [Phys. Rev. Lett. 105, 193603 (2010)] and the observation of such correlation in future experiments will be discussed.

3:06PM D4.00004 Collective quantum jumps of Rydberg atoms, TONY LEE, California Institute of Technology, HARTMUT HAEFFNER, University of California, Berkeley, MICHAEL CROSS, California Institute of Technology — A quantum system under constant observation may occasionally switch between two metastable states. These quantum jumps are usually observed in a single object, like an atom, electron, or superconducting qubit. We report on a collective type of quantum jump in a group of atoms with long-range Rydberg interaction, laser driving, and spontaneous emission. Over time, the system occasionally jumps between a state of low Rydberg population and a state of high Rydberg population. The jumps are inherently collective and in fact exist only for a large number of atoms. We explain how entanglement and quantum measurement enable the jumps, which are otherwise classically forbidden.

3:18PM D4.00005 Quantum crystals in a trapped Rydberg-dressed Bose-Einstein condensate¹, C.-H. HSUEH, Department of Physics, National Taiwan Normal University, T.-C. LIN, Department of Mathematics, National Taiwan University, T.-L. HORNG, Department of Applied Mathematics, Feng Chia University, W.C. WU, Department of Physics, National Taiwan Normal University — Spontaneously crystalline ground states, called quantum crystals, of a trapped Rydberg-dressed Bose-Einstein condensate are numerically investigated. As a result described by a mean-field order parameter, such states simultaneously possess crystalline and superfluid properties. A hexagonal droplet lattice is observed in a quasi-two-dimensional system when dressing interaction is sufficiently strong. Onset of these states is characterized by a drastic drop of the non-classical rotational inertia proposed by Leggett [Phys. Rev. Lett. 25, 1543 (1970)]. In addition, an AB stacking bilayer lattice can also be attained. Due to an anisotropic interaction possibly induced by an external electric field, transition from a hexagonal to a nearly square droplet lattice is also observed.

¹We acknowledge financial support from NSC, Taiwan.

3:30PM D4.00006 Quantum Magnetism with Polar Molecules: Tunable Generalized t - J Model, ALEXEY GORSHKOV, California Institute of Technology, SALVATORE MANMANA, University of Colorado, Boulder, KEVIN KUNS, California Institute of Technology, KADEN HAZZARD, GANG CHEN, JUN YE, University of Colorado, Boulder, EUGENE DEMLER, MIKHAIL LUKIN, Harvard University, ANA MARIA REY, University of Colorado, Boulder — We show that dipolar interactions between ultracold polar molecules in optical lattices can be used to realize a highly tunable generalization of the t - J model, which we refer to as the t - J - V - W model. The “spin” is encoded in the rotational degree of freedom of the molecules, while the interactions are controlled by applied static electric and continuous-wave microwave fields. We show that the tunability and the long-range nature of the interactions in the t - J - V - W model enable enhanced superfluidity in one dimension and controllable preparation of robust d-wave superfluids in two dimensions. The latter may provide fundamental insights into high-temperature superconductivity. [References: Phys. Rev. Lett. 107, 115301 (2011); Phys. Rev. A 84, 033619 (2011); arXiv:1110.5330]

3:42PM D4.00007 Tunable Superfluidity with Ultracold Polar Molecules on quasi-1D Optical Lattices, SALVATORE R. MANMANA, JILA & CU Boulder, 440 UCB, Boulder, CO 80309, ALEXEY V. GORSHKOV, KEVIN A. KUNS, IQI, CalTech, Pasadena, CA 91125, GANG CHEN, JUN YE, JILA & CU Boulder, 440 UCB, Boulder, CO 80309, EUGENE DEMLER, MIKHAIL D. LUKIN, Physics Department, Harvard University, Cambridge MA 02138, ANA MARIA REY, JILA & CU Boulder, 440 UCB, Boulder, CO 80309 — By selecting two dressed rotational states of ultracold polar molecules on an optical lattice, strong electric dipole-dipole interactions allow to directly emulate spin Hamiltonians and a highly tunable generalization of the t - J model, the t - J - V - W model. We present the phase diagram of the simplest experimentally realizable case, the t - $J_{\perp}$ model with long-range dipolar spin-exchange interactions, on (quasi) one-dimensional chain and ladder systems as obtained from extensive density matrix renormalization group (DMRG) calculations. For the chain, we discuss the possible realization of unconventional quasi-long-range-order caused by the dipolar interactions. While the phase diagram of the dipolar t - $J_{\perp}$ chain is similar at low filling to that of the standard t - J chain, the superconducting region is strongly enhanced. We approach the ladder systems by coupling square plaquettes and comparing the numerical results to a mean-field description. We discuss the possibility to enhance superconductivity in these ladder systems by the presence of the dipolar interactions.

3:54PM D4.00008 Dynamical generation and detection of entangled quantum magnetic states in ultracold polar molecules, KADEN HAZZARD, SALVATORE MANMANA, UC Boulder, JILA, NIST, ALEXEY GORSHKOV, Institute for Quantum Information, California Institute of Technology, ANA MARIA REY, UC Boulder, JILA, NIST — We show that *existing* ultracold polar molecule experiments in optical lattices may generate strongly correlated many-body states by mimicking far-from-equilibrium dynamics of models of quantum magnetism. Recent theory shows that molecules’ rotational states can emulate quantum spins with strong (100-10,000Hz) “spin-spin” interactions. Applying external fields generates a zoo of models: spin-1/2 and larger Heisenberg and XXZ models, and well beyond. We consider the dynamics of the easily prepared fully polarized initial state for the XXZ case predicted to be realized in current experiments. Our analytic and DMRG calculations show that the dynamics can: (i) verify and characterize the spin model (XXZ) description of the system, (ii) generate interesting, entangled states (e.g., cat states, GHZ), and (iii) explore behavior where no quantitative theory is presently possible.

4:06PM D4.00009 Interactions of polar molecules dressed by far-off-resonant light: Entangled dipoles up- or down-holding each other, MIKHAIL LEMESHKO, ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138, USA, BRETISLAV FRIEDRICH, Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, D-14195 Berlin, Germany, FRIEDRICH TEAM — We show that the electric dipole-dipole interaction between a pair of polar molecules undergoes an all-out transformation when superimposed by a far-off resonant optical field. The combined interaction potential becomes tunable by variation of wavelength, polarization and intensity of the optical field and its dependence on the intermolecular separation exhibits a crossover from an inverse-power to an oscillating behavior. The ability thereby offered to control molecular interactions opens up avenues toward the creation and manipulation of novel phases of ultracold polar gases among whose characteristics is a long-range entanglement of the dipoles’ mutual orientation. We devised an accurate analytic model of such optical-field-dressed dipole-dipole interaction potentials, which enables a straightforward access to the optical-field parameters required for the design of intermolecular interactions in the laboratory.

4:18PM D4.00010 Clustering of cold polar molecules in arrays of one-dimensional tubes, MICHAEL KNAP, Graz University of Technology, EREZ BERG, EUGENE DEMLER, Harvard University — Cold polar molecules allow to study exciting new phenomena which arise from the long-range and anisotropic nature of their mutual interactions. Here, we demonstrate that a Wigner crystal of polar molecules confined in planar arrays of one-dimensional tubes can be made unstable with respect to the formation of clusters of particles. By controlling the orientation of the external electric field which aligns the dipolar moments, increasingly complex structures with a varying number of particles per cluster and thus varying periodicity are formed. The spatial agglomeration of multiple polar molecules results from the interaction and can be described classically. However, we show that the effect survives when quantum fluctuations are present. For systems of a finite number of tubes, the result is a sequence of "clustered" Luttinger liquid states. Finally, we determine the ratio between the interaction and the kinetic energy which is necessary for the spatial agglomeration of polar molecules. We find that the requirements for clustering are reachable in current experiments with cold polar molecules.

4:30PM D4.00011 A dielectric superfluid of polar molecules¹, SETH RITTENHOUSE, ITAMP, Harvard-Smithsonian Center for Astrophysics, RYAN WILSON, JOHN BOHN, JILA and the Department of Physics, University of Colorado — We consider a Bose-Einstein condensate of heteronuclear molecules in an applied electric field. In the strong field regime, the molecules are fully polarized and produce fields that tend to be weak compared to the applied field. However, in weaker applied fields the internal fields due to the polarization of the molecules can become comparable to the applied field, and the system develops a dielectric character. We derive a set of self-consistent mean-field equations that couple the condensate density to its polarization field, leading to the emergence of polarization modes that are coupled to the quasiparticle spectrum of the condensate. While the roton instability is suppressed in this system, the coupling gives rise to a phonon-like instability that is characteristic of a dielectric material with a negative static dielectric function.

¹This work was supported by funding from the NSF and the DOE

4:42PM D4.00012 Dipolar gases in two coupled one-dimensional lattices, MARIANNE BAUER, Cambridge University, MEERA PARISH, University College London — We consider dipolar bosons in two tubes of one-dimensional lattices, where the boson filling fraction is the same in each tube and the dipoles are aligned to be maximally repulsive. In the classical limit of zero inter-site hopping, the bosons arrange themselves into an ordered crystal for any rational filling fraction, forming a complete devil's staircase like in the single tube case [1]. When we turn on hopping within each tube, we obtain a competition between the crystalline Mott phases and a superfluid of defects or solitons. However, in contrast to the single tube case [2], we find that solitons in different tubes can bind into pairs for certain topologies of the filling fraction. This provides an intriguing example of pairing that is purely driven by correlations close to a Mott insulator.

[1] P. Bak and P. Bruinsma, Phys. Rev. Lett. 49, 249 (1982)

[2] F. J. Burnell, M. M. Parish, N. R. Cooper and S. L. Sondhi, Phys. Rev. B, 80, 174519 (2009)

4:54PM D4.00013 Paired Phases of Dipoles in a Bilayer System, ARGHAVAN SAFAVI-NAINI, MIT, SEBNEM GUNES SOYLER, ICTP Trieste, GUIDO PUPILLO, ISIS and IPCMS, Universite de Strasbourg and CNRS, HOSSEIN SADEGHPOUR, ITAMP, BARBARA CAPOGROSSO-SANSONE, University of Oklahoma — By means of large scale quantum Monte Carlo simulations we study a system of dipolar lattice bosons in bilayers geometries and with no hopping between layers. We investigate under which conditions pairing (e.g. paired superfluidity, paired supersolidity) is stabilized and make estimates for current experimental setups. We also study temperature effects and possible experimental signatures of such phases.

5:06PM D4.00014 Bond Order Solid of Two-Dimensional Dipolar Fermions, SATYAN BHONGALE, George Mason University, LUDWIG MATHEY, University of Hamburg, SHAN-WEN TSAI, University of California, Riverside, CHARLES CLARK, NIST, JQI, ERHAI ZHAO, George Mason University — Cold atoms provide a promising platform to solve problems that, although computationally infeasible, are of immense importance to condensed matter physics and material science. Ultra-cold bosonic atoms have been quite successful in emulating the Bose-Hubbard model. Experiments are now underway towards mapping out the unknown phase diagram of the Fermi-Hubbard model. Recent experimental advances in cooling dipolar gases to quantum degeneracy provide an unprecedented opportunity to engineer Hubbard-like models with long range interactions. Here, with the aid of functional renormalization group technique, we show that two new and exotic types of order emerge generically in dipolar fermion systems: bond order solids of p- and d-wave symmetry. Similar, but manifestly different, phases of two-dimensional correlated electronic systems have previously only been hypothesized. Our results suggest that these phases can be constructed flexibly with dipolar fermions, using currently available experimental techniques, providing detectable experimental signatures.

5:18PM D4.00015 Re-entrant first-order phase transitions and anomalous hysteresis of dipolar Bose gases in a triangular optical lattice, DAISUKE YAMAMOTO, Condensed Matter Theory Laboratory, RIKEN, Wako, Saitama 351-0198, Japan, IPPEI DANSHITA, Computational Condensed Matter Physics Laboratory, RIKEN, Wako, Saitama 351-0198, Japan, CARLOS SÁ DE MELO, School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332, USA — We study the hysteresis behavior of dipolar Bose gases loaded into a triangular optical lattice. A large-size cluster mean-field approximation is applied to the corresponding extended Bose-Hubbard model to take into account metastable states. We find that the phase transition between supersolid (or solid) and superfluid states is always first-order except for the particle-hole symmetric point. In the phase diagram, the supersolid and solid phases are sandwiched in between the superfluid phase, and the system exhibits a re-entrant behavior from superfluid to solid (to supersolid), and back to superfluid with varying the chemical potential. Our most remarkable finding is that in the hysteresis accompanying this "re-entrant" first-order phase transition, the quantum melting transition from supersolid or solid to superfluid can occur while the reverse process is impossible since the superfluid phase remains locally stable for any value of the chemical potential. Moreover, the hysteresis curve of density versus chemical potential does not form a "hysteresis-loop" structure unlike the case of the conventional first-order transition. We show that this anomalous behavior of the hysteresis is a common property of systems exhibiting a re-entrant first-order phase transition.

Monday, February 27, 2012 2:30PM - 5:30PM — Session D5 DCMP: Vanadium Oxides; Metal-insulator Transitions 206A

2:30PM D5.00001 Metal-Insulator Transition in ultrathin CaVO_3 Films, MAN GU, JIWEI LU, STUART WOLF, University of Virginia — Bulk CaVO_3 (CVO) with a $3d^1$ electronic configuration has been found to exhibit metallic and Pauli paramagnetic behavior. We have synthesized epitaxial ultrathin films of CVO on single crystal (100) SrTiO_3 substrates by pulsed electron deposition. The CVO films were capped with 2.5nm SrTiO_3 layer. Compared with single crystal CVO, thin film CVO demonstrated very large resistance ratios (RR), e.g., $R(300\text{K})/R(2\text{K})$ more than 3000. The temperature dependent Hall measurement showed mostly that the large RR determined by the change in mobility, we observed the metal-insulator transition at $\sim 100\text{K}$ in CVO ultrathin films with thickness below 4nm, which was not observed in either thick CVO films or STO films. Above 100K, ultrathin CVO exhibited the metallic behavior, and below 100 K, it became an insulator. The emergence of MIT could be attributed to a pseudogap that appeared at Fermi surface with decreasing film thickness, indicating a transition from 3D metal to 2D insulator transition in ultrathin CVO films at temperatures lower than 100K. A metal-insulator transition was further characterized by I-V measurements, the insulator phase was only observed with driven current below 100K and $2 \times 10^{-6}\text{A}$.

2:42PM D5.00002 Thermoelectric response in the incoherent transport region near Mott transition: the case study of $\text{La}_{1-x}\text{Sr}_x\text{VO}_3$, MASAKI UCHIDA, K. OISHI, Y. ONOSE, J. FUJIOKA, Y. TOKURA, University of Tokyo, M. MATSUO, M. MORI, S. MAEKAWA, JAEA, W. KOSHIBAE, RIKEN ASI, S. MIYASAKA, Osaka University — We report a systematic investigation on the high-temperature thermoelectric response in a typical filling-control Mott transition system $\text{La}_{1-x}\text{Sr}_x\text{VO}_3$. In the vicinity of the Mott transition, incoherent charge transport appears with increasing temperature and the thermopower undergoes two essential crossovers, asymptotically approaching the limit values expected from the entropy consideration, as known as Heikes formula. By comparison with the results of the dynamical mean field theory, we show that the thermopower in the Mott critical state mainly measures the entropy per charge carrier that depends on electronic degrees of freedom available at the measurement temperature. Our findings verify that the Heikes formula is indeed applicable to the real correlated electron systems at practical temperatures ($T > 200$ K).

2:54PM D5.00003 First-principles calculations of phonons in VO_2 ¹, ERIC J. WALTER, HENRY KRAKAUER, TYLER HUFFMAN, M.M. QAZILBASH, College of William and Mary — Vanadium dioxide (VO_2) undergoes a metal-insulator transition at 340K. This is accompanied by a structural transition from a metallic, high-temperature rutile phase to a low-temperature monoclinic insulating phase. Recently, it has become possible to produce single crystal platelets of VO_2 deposited on a oxidized silicon substrate. These micro-crystals are under strain which can potentially alter their properties compared to bulk samples. Infrared micro-spectroscopy on these samples permits accurate measurements of their electronic and phonon properties as the micro-crystals are driven reversibly across the temperature-driven insulator-to-metal transition (IMT). We present *ab-initio* calculations of phonons in the rutile and monoclinic phases of VO_2 . These calculations were performed using first-principles density functional theory using both LDA and LDA+U. The effect of the Hubbard parameters and strain on both phases is discussed. We compare our results to the single crystal measurements and previous experimental results.

¹Supported by ONR

3:06PM D5.00004 Infrared micro-spectroscopy of strained VO_2 micro-crystals, M.M. QAZILBASH, T. HUFFMAN, E.J. WALTER, H. KRAKAUER, Department of Physics, College of William and Mary, JIANG WEI, D.H. COBDEN, Department of Physics, University of Washington, Seattle, H.A. BECHTEL, M.C. MARTIN, Advanced Light Source, Lawrence Berkeley National Laboratory, G.L. CARR, National Synchrotron Light Source, Brookhaven National Laboratory, D.N. BASOV, Department of Physics, University of California, San Diego — The temperature-driven insulator-to-metal transition (IMT) in vanadium dioxide (VO_2) is accompanied by a structural instability (SI). The IMT and SI lead to a drastic change in the electronic properties, crystal structure, and lattice dynamics. We performed infrared micro-spectroscopy on single crystal platelets of VO_2 deposited on oxidized silicon substrate by physical vapor deposition. The firm attachment of these micro-crystals to the substrate causes strain which can alter their properties compared to bulk samples. We report infrared data on these micro-crystals and demonstrate both their electronic and phonon properties in the monoclinic M1 phase and the rutile phase. We also compare their infrared conductivity to that of bulk single crystals and thin films. Finally, we compare infrared-active phonon features to first-principles density functional theory calculations.

3:18PM D5.00005 Ultrafast Pump Probe Transmission Spectroscopy of VO_2 , NATHANIEL BRADY, University of Alabama at Birmingham, KANNATASSEN APPAVOO, Vanderbilt University, MINAH SEO, PRASHANTH UPADHYA, Los Alamos National Laboratory, JOYEETA NAG, RICHARD HAGLUND, Vanderbilt University, ROHIT PRASANKUMAR, Los Alamos National Laboratory, DAVID HILTON, University of Alabama at Birmingham — We have performed nondegenerate pump-probe transmission spectroscopy, pumping with an above the band gap (1.5 eV) 50 fs pulse and probing with a 0.4 eV (below the band gap) pulse to monitor the dynamics of the formation of the metallic phase in vanadium dioxide (VO_2). Below the percolation threshold (< 330 K), we find an initial drop in transmission consistent with electron-hole generation across the band gap, while in the fully metallic phase (< 365 K), we see an initial rise in transmission due to transient heating of electrons at the Fermi surface. In the transitional region, the data show complex time dependence consistent with the nucleation and growth of metallic domains in the semiconducting phase and ultrafast heating of metallic precursors in the insulating phase.

3:30PM D5.00006 Ultrafast Spectroscopy and Optically-Induced Phase Transitions of Single Crystal VO_2 ¹, AARON JONES, JAE PARK, JIM COY, DAVID COBDEN, XIAODONG XU, University of Washington — We investigate the metal-insulator phase transition (MIT) of single crystal VO_2 platelets using non-degenerate optical pump-probe spectroscopy. The pump pulse is at 800 nm and the probe pulse varies between 1.3 μm and 2.4 μm , covering the optical gap (~ 2 μm) of VO_2 . We observe ultrafast carrier relaxation on the timescale of 0.5 ps or less in the insulating phase. Higher pump powers induce coherent acoustic phonon oscillations which we explore by adjusting probe wavelength and pump fluence. At temperatures just below the transition, we observe optically induced MIT at a time scale less than 300 fs (pulse width limited), and we investigate the dependence on crystal size, wavelength, and temperature. The properties of the insulator do not seem consistent with a conventional band semiconductor.

¹Work supported by DoE Grant BES DE-SC0002197 and NSF Grant DGE-0718124

3:42PM D5.00007 THz induced insulator to metal transition in VO_2 metamaterial, MENGKUN LIU, Boston University, HAROLD HWANG, Massachusetts Institute of Technology, HU TAO, Tufts University, ANDREW STRIKWERDA, KEBIN FAN, GEORGE KEISER, AARON STERNBACH, Boston University, KEVIN WEST, SALINPORN KITTIWATANAKUL, JIWEI LU, STUART WOLF, University of Virginia, FIORENZO OMENETTO, Tufts University, XIN ZHANG, Boston University, KEITH NELSON, Massachusetts Institute of Technology, RICHARD AVERITT, Boston University — We use metamaterial enhanced high field terahertz (THz) pulses (up to $\sim 4\text{MV/cm}$) to induce the insulator-to-metal transition in vanadium dioxide (VO_2) thin films at 320K. Ultrafast THz field enhancement in the gaps of metamaterial split ring resonators releases free electrons in VO_2 by the Poole-Frenkel effect. The accelerated hot electrons transfer energy to the lattice via electron phonon coupling inducing the persistent metallic phase. A large nonlinear signature is observed in VO_2 as modulations of the metamaterial resonance on a picosecond time scale. Our results provide insight into electric field induced phase transitions in VO_2 and paves the way for studying nonlinear high THz field effects in many other strongly correlated materials.

3:54PM D5.00008 Optical control of structural evolution of ultrathin VO₂ film following a photoinduced metal-insulator phase transition¹, HAIDAN WEN, X-ray Science Division, Argonne National Laboratory, EFTIHIA BARNES, Department of Materials Science and Engineering, Pennsylvania State University, JUNE H. LEE, YUELIN LI, DONALD A. WALKO, ERIC M. DUFRESNE, X-ray Science Division, Argonne National Laboratory, MARTIN HOLT, Center for Nanoscale Materials, Argonne National Laboratory, DARRELL G. SCHLOM, Department of Materials Science and Engineering, Cornell University, VENKATRAMAN GOPALAN, Department of Materials Science and Engineering, Pennsylvania State University, JOHN W. FREELAND, X-ray Science Division, Argonne National Laboratory, — Using ultrafast x-ray diffraction technique, we have demonstrated that the structural symmetry in VO₂ thin film across the metal-insulator transition (MIT) can be controlled by the optical pump fluence. After an 800 nm, 50 fs laser excitation, the structural evolution of a 13nm-thick, MBE-grown VO₂ film on TiO₂ substrate was monitored by a synchrotron based x-ray diffraction with 100 picosecond (ps) time resolution. By adjusting the pump fluence, the VO₂ film can be prepared in selected structural state 100 ps after excitation, and transits through the known structural phases (tetragonal, monoclinic M2, monoclinic M1) in tens of nanoseconds time scale. When pumping at high fluence (28 mJ/cm²), a new transient state that exhibits lower symmetry than the thermal equilibrium tetragonal phase has been identified and its evolution pathway has been measured.

¹Work at Argonne is supported by the U.S. Department of Energy under Contract No. DE-AC02-06CH11357.

4:06PM D5.00009 In-situ measurements of Stress Relaxation across Metal Insulator Transition in Correlated Oxide Thin Films, VISWANATH BALAKRISHNAN, SHRIRAM RAMANATHAN, Harvard School of Engineering and Applied Sciences — Stress relaxation across the metal-insulator transition in correlated oxide thin films such as VO₂ and SmNiO₃ is of great importance since it could be directly related to the symmetry breaking structural component of the transition and also affects the properties and performance of the electronic devices significantly. We present in-situ stress relaxation measurements across the thermally triggered metal insulator transition and its impact on the transition characteristics and stability. Mesoscopic size effects, micro-patterning and geometrical confinement effects on the metal insulator transition and associated stress relaxation will be addressed. Correspondence between onset of the electrical transition with stress relaxation leads to several interesting observations regarding the transition dynamics and will be discussed.

4:18PM D5.00010 In-Plane Impedance Spectroscopy measurements in Vanadium Dioxide thin films¹, JUAN RAMIREZ, University of California, San Diego, EDGAR PATINO, Universidad de los Andres, RAINER SCHMIDT, Universidad Complutense de Madrid, AMOS SHARONI, Bar-Ilan University, MARIA GOMEZ, Universidad del Valle, IVAN SCHULLER, University of California, San Diego — In plane Impedance Spectroscopy measurements have been done in Vanadium Dioxide thin films in the range of 100 Hz to 1 MHz. Our measurements allows distinguishing between the resistive and capacitive response of the Vanadium Dioxide films across the metal-insulator transition. A non ideal RC behavior was found in our thin films from room temperature up to 334 K. Around the MIT, an increase of the total capacitance is observed. A capacitor-network model is able to reproduce the capacitance changes across the MIT. Above the MIT, the system behaves like a metal as expected, and a modified equivalent circuit is necessary to describe the impedance data adequately.

¹This work has been supported by AFOSR, COLCIENCIAS, CENM and Ramon y Cajal Fellowship.

4:30PM D5.00011 Photoemission Study of VO₂ Above and Below the Transition Temperature¹, LUCA MORESCHINI, Advanced Light Source, YOUNG JUN CHANG, Advanced Light Source and Fritz-Haber Institut, DAVIDE INNOCENTI, Advanced Light Source and Università di Tor Vergata, ANDREW L. WALTER, Advanced Light Source and Fritz-Haber Institut, JONATHAN DENLINGER, AARON BOSTWICK, ELI ROTENBERG, Advanced Light Source — Angle-resolved photoemission (ARPES) experiments on VO₂ have traditionally been hindered by the quality of cleaved single crystals. The lack of a clear metal-insulator transition (MIT) in low photon energy measurements has even lead to the assumption of a surface region with a different electronic structure. With the *in situ* pulsed-laser-deposition (PLD) system available on beamline 7.0.1 at the Advanced Light Source we have grown VO₂(001) films on a TiO₂ substrate and measured the band structure above and below the transition temperature. We discuss our results in comparison with the available calculations, and we show that the MIT is clearly visible for photon energies within the UV range.

¹Work supported by U.S. DOE (DE-AC02-05CH11231 for ALS), the Max Planck Society, and the Swiss National Science Foundation (PBELP2- 125484)

4:42PM D5.00012 Photoemission measurements of strained VO₂¹, JUDE LAVEROCK, ANDREW PRESTON, DAVE NEWBY, KEVIN SMITH, Boston University, SALINPORN KITTIWATANAKUL, JIWEI LU, STUART WOLF, University of Virginia, MATS LEANDERSSON, BALASUBRAMANIAN THIAGARAJAN, MAX-lab, Lund University — The metal-insulator transition of VO₂ has been a textbook example for many years, despite a clear understanding of its microscopic origins proving elusive. Recently, the promise towards novel applications of high-quality thin films, in which the properties of the transition can be tailored by applied strain, has thrust VO₂ back into focus. Here, we report photoemission measurements of strained VO₂ thin films epitaxially grown on TiO₂(110) and TiO₂(100) substrates. The applied strain for these two films lead to moderate and large compressive rutile c-axis strains, respectively. By making use of the incident photon polarization, we observe the changes in polarization anisotropy both across the transition and as a function of applied strain, and demonstrate how we can use this to learn more about the origin of the MIT in VO₂.

¹BU program supported in part by DoE Grant No. DE-FG02-98ER45680.

4:54PM D5.00013 Correlations of local electronic properties in vanadium dioxide thin films¹, ADAM PIVONKA, KEVIN O'CONNOR, ALEX FRENZEL, CHANGHYUN KO, SHRIRAM RAMANATHAN, Harvard University, ERIC HUDSON, Penn State University, JENNIFER HOFFMAN, Harvard University — We probe the local electronic properties of a vanadium dioxide thin film using scanning force microscopy. We scan a conductive cantilever in contact mode across the surface of the sample. At each point, we sweep the voltage applied to the sample, obtaining current versus voltage curves with nanoscale resolution while inducing a transition from the insulating to metallic state. We identify individual grains of ~50-100 nm, and extract the electronic properties of each grain, such as transition voltage, hysteresis, dielectric constant, and metallic state resistance. We discuss the correlations between these properties.

¹This work is supported by the NSF NSEC (PHY 01-17795). Adam Pivonka acknowledges the support of the NSF GRFP and Hertz Foundation.

5:06PM D5.00014 Correlation of Valence State and Transport Properties in VO₂ Films¹, SALINPORN KITTIWATANAKUL, Physics Department, University of Virginia, JUDE LAVEROCK, Physics Department, Boston University, STUART WOLF, Physics Department, University of Virginia, JIWEI LU, Materials Science and Engineering Department, University of Virginia — Vanadium dioxide (VO₂) exhibits a metal semiconductor transition (MST) that is accompanied by the abrupt change in the electrical conductivity, optical transmittance and reflectance in infrared region, which can be used in electronic devices such as temperature sensors and electric switches. VO₂ thin films were grown on c-plane Al₂O₃ substrates with different O₂ flow rates. The XRD scans have been performed to confirm the single phase and highly textured VO₂ films despite the change in the growth parameter, i.e. the oxygen partial pressure. The valence state of vanadium on different films was investigated by soft x-ray spectroscopy. The Hall bars were fabricated for electrical transport and Hall measurements. As the O₂ flow rate increases, the XRD results show decreasing lattice parameter, hence increasing compressive strain along b-axis of monoclinic VO₂; the transport measurements also show the increasing transition temperature (T_{MST}) and the increasing change in resistivity associated with the strain and valence state of vanadium. Hall measurements reveal a sudden increase in carrier concentration from 10²⁰ to 10²⁴ cm⁻³ around T_{MST} , while the mobility remains constant before and after MST. The correlation among the valence state, the strain and MST in VO₂ will be discussed.

¹Authors are thankful to financial supports from VMEC and NRI.

5:18PM D5.00015 Metal-insulator transition in VO₂ macro single domain crystals due to phase boundary motion, HONGLYOU JU, Physics Dept., Yonsei Univ., BONGJIN MUN, Applied Physics Dept., Hanyang Univ., KAI CHEN, Advanced Light Source, LBNL & CAMP-Nano, Xi'an Jiaotong Univ., CATHERINE DEJOIE, NOBUMICHI TAMURA, MARTIN KUNZ, ZHI LIU, SUNG-KWAN MO, Advanced Light Source, LBNL, JOONSEOK YOON, Physics Dept., Yonsei Univ., CHANGWOO PARK, Hanbat National Univ. & Advanced Nano Products — Metal insulator transition (MIT) characteristics of macro-size VO₂ single domain crystals, exhibiting a high resistance ratio of $\sim 10^5$ within as small as 10^{-3} °C in the vicinity of MIT temperature, were investigated by temperature-dependent electrical transport, optical microscopy, and synchrotron-based polychromatic x-ray micro-diffraction measurements. Our results clearly show that MIT initiated via inhomogeneous nucleation, proceeds with the propagation of sharp phase boundary between the metallic (R) and insulating (M1) phases, along the rutile c axis. In this talk, we will present evidences of MIT of single domain VO₂ crystals with sharp phase boundary motion and discuss the implications of our findings on to the origin of MIT and related phenomena.

Monday, February 27, 2012 2:30PM - 5:30PM – Session D6 DMP: Focus Session: Graphene Devices - Bolometers and Optical Response 206B

2:30PM D6.00001 Probing Dirac electron transport in graphene by far-infrared spectroscopy, JIE SHAN, KELIANG HE, LIANG ZHAO, Case Western Reserve University, KIN FAI MAK, NICK PETRONE, JIM HONE, TONY HEINZ, Columbia University — The transport properties of Dirac fermions in graphene are a subject of intense interest. While various scattering mechanisms including impurities, graphene phonons and substrate phonons have been examined by dc transport measurements,¹ direct determination of the scattering rates under different experimental conditions remains challenging.² In this paper we report on the far-infrared optical conductivity spectrum of monolayer graphene samples obtained by Fourier transform infrared spectroscopy. From the frequency dependence of the optical conductivity we determine both the Drude weight and the carrier scattering rate. The dependence of these transport parameters on temperature and electrostatic doping will be presented, and the importance of many-body Coulomb interactions between Dirac electrons will be discussed.

¹Das Sarma, S., Adam, S., Hwang, E. H. & Rossi, E. Rev. Mod. Phys. 83, 407-470, (2011).

²Horng, J. et al. Phys. Rev. B 83, 165113, (2011).

2:42PM D6.00002 Ultrathin dual-gated graphene p-n junction photodetectors, NITYAN NAIR, NATHANIEL GABOR, QIONG MA, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, WENJING FANG, JING KONG, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — Optoelectronic devices composed of atomically thin graphene and boron nitride membranes yield great promise for next-generation photonics and optoelectronic research, yet numerous fabrication challenges remain. We use chemical vapor deposited (CVD) graphene to produce atomically thin, local bottom-gates for high-quality exfoliated graphene optoelectronic devices. By incorporating CVD graphene instead of the more conventional silicon bottom-gate electrodes, we create very low-profile dual-gated field effect p-n junction devices with hexagonal boron nitride as the insulating gate dielectric layer. Combining electron-beam and photolithography techniques, we can shape the bottom-gates to locally modulate the carrier density in the active graphene layer. In addition to avoiding optical transmission through thick top-gate electrodes, our approach allows us to perform temperature dependent photoresponse measurements over various device length scales and with direct control of local electronic carrier densities.

2:54PM D6.00003 Graphene-based Optical Modulator, MING LIU, XIANG ZHANG, UC Berkeley — Data communications have been growing at a speed even faster than Moore's Law, with a 44-fold increase expected within the next 10 years. Data Transfer on such scale would have to recruit optical communication technology and inspire new designs of light sources, modulators, and photodetectors. The past decade has seen the flourish of researches in silicon-based optical modulators. However, their performance is limited by the weak refractive index changes in silicon, and consequently large footprint and stringent fabrication tolerance are required. Here we raise a totally new mechanism for optical modulation. Instead of changing the refractive index in silicon, we use graphene as an active layer and change its absorption coefficient by turning on/off the interband transitions. This turning is realized through shifting the Fermi level by simply a back gate. In this way, we can operate the optical modulator at a relatively high speed (1.2 GHz) over a broad range (1.3 to 1.6 μm), while keep the smallest footprint ($\sim 25 \mu\text{m}^2$). More details of the device will be discussed in the talk.

3:06PM D6.00004 Tunable optical properties of graphene¹, FENG WANG, UC Berkeley — Graphene, a single layer of carbon atoms, exhibits novel two-dimensional electronic behavior. Optical spectroscopy provides a powerful toolkit study graphene physics. In this talk, I will show how we can use infrared spectroscopy to probe gate-dependent interband transitions as well as intraband transitions. I will also discuss how we can use electrical gating to control inelastic light scattering processes in graphene.

¹DOE, ONR, NSF, Packard foundation

3:42PM D6.00005 Photoconductivity of electro-oxidized epitaxial graphene¹, FEIHU WANG, MIKHAIL ITKIS, ELENA BEKYAROVA, ROBERT HADDON, University of California, Riverside, HADDON RESEARCH GROUP TEAM — We report the enhanced photosensitivity of epitaxial graphene (EG) after electrochemical oxidation in nitric acid. The onset of photoconductivity appears at a photon energy of ~ 1.7 eV while the responsivity reaches 200 A/W in the UV spectral range (3.5 eV, 350 nm). The observed photoresponse is attributed to the formation of deep traps at the electro-oxidized EG interface, which release charge carriers under illumination and a significantly prolonged life time of photoexcitations due to the effect of the traps on the recombination dynamics. The enhanced photosensitivity and high selectivity in the UV spectral range make electro-oxidized EG an interesting alternative to the less spectrally selective Si for UV detection, although further optimization of the chemistry is required to shorten the photoresponse time while preserving the high sensitivity.

¹This study was supported by DOD/DMEA under contract H94003-10-2-1003 and NSF-MRSEC through contract DMR-0820382.

3:54PM D6.00006 Photo-controlling electrical properties of graphene-based field-effect transistor with photo-reactive copolymer, CHI-YUAN LIN, Department of Photonics and Institute of Electro-Optical Engineering, National Chiao Tung University, Taiwan, FOREST SHIH-SEN CHIEN, Department of Physics, Tunghai University, Taiwan, CHEN-SHIUNG CHANG, Department of Photonics and Institute of Electro-Optical Engineering, National Chiao Tung University, CHIA-CHEN HSU, Department of Physics, National Chung-Cheng University, Taiwan — Here, we presented a photo-controlling graphene-based FET device. The tri-stable current of graphene device can be achieved in room temperature using the photo-assisted poling (PAP) and photo bleaching (PB) on photo-reactive copolymer PMMA-DR1. PMMA-DR1 was used as a dielectric film between graphene and top gate, where the top gate was the ITO film for applied voltage and excited laser passing. PAP operation created a polarization of PMMA-DR1 film, while the current of graphene FET device was varied due to Fermi energy of graphene was directly influenced by the polarization. The strength of polarization was associated with the gate voltage and laser power during the process of PAP operation. In contrast to the PAP operation, the PB operation was able to destroy the polarization of PMMA-DR1 film, while the current of graphene FET device returned to the initial value. Combining with PAP and PB operations, three current states identified as 1, 0 and -1 states can be achieved in room temperature. The current change ratios were 150% and 50% for 1 state and -1 state, comparing with initial state 0.

4:06PM D6.00007 Imaging of Polarization-dependent Photocurrent in Graphene Photodevices, MINJUNG KIM, DUHEE YOON, Department of Physics, Sogang University, Seoul 121-742, Korea, HO ANG YOON, SANG WOOK LEE, Division of Quantum Phases and Devices, School of physics, Konkuk University, Seoul 143-701, Korea, HYEONSIK CHEONG, Department of Physics, Sogang University, Seoul 121-742, Korea — Recently, a metal-graphene-metal photodetector for high-speed optical communications was reported. In addition, a graphene-based photodetector was reported to be able to absorb broadband light owing to the unique band structure of graphene [Mueller et al., Nature Photonics 4, 297 (2010)]. We investigated the polarization dependence of the photocurrent generated in metal-graphene-metal junctions. The graphene photodevice was fabricated by depositing Pd/Au and Ti/Au electrodes on single-layer graphene samples. When the polarization of incident laser beam is rotated with respect to the metal-graphene-metal junction, the photocurrent is significantly modulated. In addition, we measured the exact positions where the photocurrent is generated by measuring the photocurrent and Raman images of the graphene photodevices simultaneously.

4:18PM D6.00008 Supercollisions and Electron-Lattice Cooling in Graphene, JUSTIN SONG, School of Engineering and Applied Sciences, Harvard and Department of Physics, MIT, MICHAEL REIZER, None, LEONID LEVITOV, Department of Physics, MIT — Hot carrier proliferation is dependent on slow cooling between electron and lattice systems. In graphene, these cooling rates can be slow due to a small Fermi surface size and the momentum-conserving character of electron-phonon scattering. This in concert with the small ratio between the sound velocity, s , and the Fermi velocity, v_F , such that $s/v_F = 1/100$ produces a phase space constrained by the Fermi wavevector, k_F . In each of these first order scattering events, the energy exchanged between electronic and lattice systems is of the order $T_{BG} = \hbar k_F$ which at typical doping densities can be many times smaller than $k_B T$; non-thermal phonons are the dominant contributors to scattering dramatically suppressing cooling power. This constraint can be lifted by considering "supercollisions" that utilize the full thermal distribution of phonons. While the frequency of supercollisions may be lower than the first order process, energy transfer for supercollisions is now on the order of $k_B T$ which is many times larger than the first order process. We will show that this large exchange of energy allows supercollisions to give a dramatic boost to the cooling rate dominating over the first order process.

4:30PM D6.00009 Hot Carrier-Assisted Intrinsic Photoresponse in Graphene, NATHANIEL GABOR, Massachusetts Institute of Technology Physics, JUSTIN SONG, SEAS Harvard University, QIONG MA, NITYAN NAIR, Massachusetts Institute of Technology Physics, THITI TAYCHATANAPAT, Harvard University Physics, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science Japan, LEONID LEVITOV, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology Physics — Graphene is considered an excellent candidate for photodetection and energy harvesting applications due to its broadband optical response and high internal quantum efficiency, yet measurements have not clearly determined the photocurrent generation mechanism. Here, we report on the intrinsic photoresponse of dual-gated monolayer and bilayer graphene p-n junction devices. Local laser excitation of wavelength 850 nm at the p-n interface leads to striking six-fold photovoltage patterns as a function of bottom- and top-gate voltages. These patterns, together with the measured spatial and density dependence of the photoresponse, provide strong evidence that non-local hot carrier transport, rather than the photovoltaic effect, dominates the intrinsic photoresponse in graphene [1,2] The hot carrier regime manifests as a strong photo-thermoelectric effect in which the photogenerated carrier population remains hot while the lattice stays cool. [1] Science v. 334, p. 648-652 (2011). [2] Nano Lett. ASAP 10.1021/nl202318u (2011).

4:42PM D6.00010 Graphene Terahertz Photodetector¹, XINGHAN CAI, GREG JENKINS, ANDREI SUSHKOV, JUN YAN, H.D. DREW, MICHAEL S. FUHRER, Center for Nanophysics and Advanced Materials, University of Maryland, College Park — A graphene photodetector device is fabricated using mechanically exfoliated single layer graphene on SiO₂/Si substrate contacted by two dissimilar metal electrodes (chromium and gold) using standard electron beam lithography. The graphene is etched into a strip shape with specific width and coupled to a bow tie antenna structure to improve coupling to long-wavelength radiation and enhance the electric field in the center of the device. We have observed the response of the graphene photodetector to optical (632.8nm) and infrared laser (118um) radiation as a function of gate voltage and device width. Experimental results and comparison to a model of graphene plasmon-enhanced photodetection will be discussed.

¹This work is supported by CNAM, IARPA, the ONR MURI program, and NSF grants DMR-0804976 and DMR-1105224.

4:54PM D6.00011 Bolometric photo response of dual-gated bilayer graphene¹, JUN YAN, M.-H. KIM, Center for Nanophysics and Advanced Materials and Department of Physics, University of Maryland, College Park, J.A. ELLE, Institute for Research in Electronics and Applied Physics, and Department of Physics, University of Maryland, College Park, A.B. SUSHKOV, G.S. JENKINS, Center for Nanophysics and Advanced Materials and Department of Physics, University of Maryland, College Park, H.M. MILCHBERG, Institute for Research in Electronics and Applied Physics and Department of Physics, University of Maryland, College Park, H.D. DREW, M.S. FUHRER, Center for Nanophysics and Advanced Materials and Department of Physics, University of Maryland, College Park — We study the photo response of dual-gated bilayer graphene devices under infrared radiation. By comparison to Joule heating measurements using a second harmonic transport technique, we determine that the photo response is bolometric instead of photoconductive. The measured large electron-phonon heat resistance of our device is in good agreement with theoretical estimates in magnitude and temperature dependence, and enables our graphene bolometer operating at a temperature of 5 K to have a low noise equivalent power ($33 \text{ fW/Hz}^{1/2}$) and fast response time (sub nanosecond).

¹This work is supported by IARPA, the ONR MURI program, and NSF grants DMR-0804976 and DMR-1105224. J.A.E. and H.M.M. acknowledge the support of NSF.

5:06PM D6.00012 GHz response of bilayer graphene hot electron bolometer, M.-H. KIM, J. YAN, J.A. ELLE, A.B. SUSHKOV, G.S. JENKINS, H.M. MILCHBERG, M.S. FUHRER, H.D. DREW, Center for Nanophysics and Advanced Materials and Department of Physics, University of Maryland, College Park, MD 20742 — An intrinsic GHz speed of a hot-electron bolometer (HEB) based on dual-gated bilayer graphene (BLG) was recently reported (J. Yan, arXiv:1111.1202). The thermal response time is governed by the weak electron acoustic phonon scattering which also results in a high thermal resistance for the lattice cooling of the hot electrons. The time response of BLG HEB was measured as a function of temperature, bias current, and laser power using two time delayed pulses from a $1.03 \mu\text{m}$ pulsed laser. In addition, we probed the energy gap dependence of the time response revealing information about the electron density in gapped BLG. We report the temperature dependence of the heat capacity and thermal resistance obtained from these measurements. This work is supported by IARPA grant #W911NF1010443

5:18PM D6.00013 Non-linear plasma transport in graphene channels and application to the detection of terahertz signals, SERGEY RUDIN, GREG RUPPER, U.S. Army Research Laboratory, Adelphi, Maryland 20783 — The non-linear electron plasma response to electromagnetic signal applied to a gated graphene conduction channel can be used to make a graphene based Dyakonov-Shur terahertz detector. The hydrodynamic model predicts a resonance response to electromagnetic radiation at the plasma oscillation frequency. With less damping and higher mobility, the graphene conduction channels may provide higher quality plasma response than possible with semiconductor channels. Our analysis of plasma oscillations in a graphene channel is based on the hydrodynamic equations which we derive from the Boltzmann equation accounting for both electrons and holes, and including the effects of viscosity and finite mobility.

Monday, February 27, 2012 2:30PM - 5:30PM –

Session D7 DCMP: Quantum Hall Effect in Mono-, Bi- and Trilayer Graphene 207

2:30PM D7.00001 Correlated random hopping disorder in graphene at high magnetic fields: Landau level broadening and localization properties, ANA L.C. PEREIRA, Universidade Estadual de Campinas, CAIO H. LEWENKOPF, Universidade Federal Fluminense, EDUARDO R. MUCCIOLO, University of Central Florida — Disorder is key to understand the electronic transport properties in graphene, particularly in the quantum Hall regime. There is still some debate on the most relevant disorder mechanisms for transport in graphene. Among those, ripple disorder is believed to play an important role. Static ripples give rise to random correlated hopping disorder, which is the disorder mechanism analyzed in this work. We study the density of states and localization properties of the lowest Landau levels of graphene at high magnetic fields, focusing on the effects caused by correlated long-range hopping disorder. We find that the broadening of the lowest Landau level shrinks exponentially with increasing disorder correlation length. The broadening also grows linearly with magnetic field and with disorder amplitudes. More importantly, we observe that the ratio between the $n=1$ and $n=0$ Landau level widths depends only on the correlation length and is rather insensitive to the disorder strength and to the magnitude of the magnetic field. This allows a closer contact of our results with experiments. In addition, the lowest Landau level peak shows a robust splitting (inferred from the analysis of the participation ratio), whose origin we identify as the breaking of the sublattice (valley) degeneracy.

2:42PM D7.00002 Electrically tunable quantum anomalous Hall effect in graphene decorated by 5d transition-metal adatoms, HONGBIN ZHANG, Forschungszentrum Juelich, Germany, CESAR LAZO, University of Kiel, Germany, STEFAN BLÜGEL, Forschungszentrum Juelich, Germany, STEFAN HEINZE, University of Kiel, Germany, YURIY MOKROUSOV, Forschungszentrum Juelich, Germany — Based on first-principles calculations, we predict that 5d transition-metals on graphene present a unique class of hybrid systems exhibiting topological transport effects that can be manipulated effectively by external electric fields [1]. The origin of this phenomenon lies in the exceptional magnetic properties and the large spin-orbit interaction of the 5d metals leading to significant magnetic moments accompanied with colossal magnetocrystalline anisotropy energies. A strong magneto-electric response is predicted that offers the possibility to switch the spontaneous magnetization direction by moderate electric fields, enabling an electrically tunable quantum anomalous Hall effect.

[1] preprint: <http://arxiv.org/abs/1108.5915>

2:54PM D7.00003 Scanning gate microscopy on graphene in the quantum Hall regime, JAMES HEDBERG, YOICHI MIYAHARA, MICHAEL HILKE, GUILLAUME GERVAIS, PETER GRÜTTER, McGill University, JULIEN RENARD, JOSHUA FOLK, University of British Columbia — Scanning Gate Microscopy was performed on monolayer graphene devices in the quantum hall regime. The devices studied consisted of exfoliated graphene deposited on SiO₂, etched in a Hall Bar configuration, and electrically contacted by standard lithographic techniques. Using a custom built scanning probe microscope (SPM), operating at liquid Helium temperatures and below, in magnetic fields up to 16 T, we spatially mapped the position dependent effects of a movable gate, i.e. the charged tip of the SPM, on the conductivity of the graphene device. Using a global backgate to modulate the carrier density, we can visually observe the transitions between filling factors. Striking features are observed in the resistance versus position maps, offering insights into the microscopic properties of graphene in the quantum Hall regime.

3:06PM D7.00004 Confining potential and Landau level edge states in graphene¹, GUOHONG LI, ADINA LUCAN-MAYER, EVA Y. ANDREI, Department of Physics and Astronomy, Rutgers University — Two-dimensional electron systems in the Quantum-Hall (QH) regime host gapless one-dimensional chiral edge states which are responsible for the quantization of the Hall conductivity. In the regime of the fractional QH effect the edge states form a chiral Luttinger liquid which presents unusual quantum properties such as fractionally charged excitations and interference patterns that could serve as building blocks for QH qubits. Observing and exploiting these properties requires precise control of the edges, but in semiconductor-based 2DES were edge states were studied thus far, achieving the necessary control was difficult. This is because the smooth confinement potential in these systems imposes a length scale which is much larger than the magnetic length leading to incompressible strips and to non-universal behavior. We will show that this limitation is not present in graphene. Using scanning-tunneling-microscopy and spectroscopy to follow the spatial evolution of Landau levels toward an edge, we demonstrated that in graphene it is possible to control the edge states by varying the distance to the screening plane and by controlling the confinement geometry.

¹This work was supported by DOE under DE-FG02-99ER45742, by the Lucent-Alcatel foundation and by NSF under NSF-DMR-0906711

3:18PM D7.00005 Unconventional Sequence of Fractional Quantum Hall States in Suspended Graphene, BENJAMIN FELDMAN, Harvard University, BENJAMIN KRAUSS, JURGEN SMET, Max-Planck-Institut für Festkörperforschung, AMIR YACOBY, Harvard University — Graphene provides a unique platform to study many-body correlations due to the relativistic nature of its charge carriers and their fourfold degeneracy. We report local electronic compressibility measurements of a suspended graphene flake performed using a scanning single-electron transistor. Between filling factors $\nu = 0$ and 1, our measurements reveal incompressible fractional quantum Hall states at $\nu = 1/3, 2/3, 2/5, 3/5, 3/7, 4/7$ and $4/9$, which clearly follow the standard composite fermion sequence. In contrast, between $\nu = 1$ and 2, incompressible states occur only at $\nu = 4/3, 8/5, 10/7$ and $14/9$. These fractions correspond to a subset of the composite fermion sequence involving only even numerators, suggesting a robust underlying symmetry. We extract the energy gaps of each fractional quantum Hall state as a function of magnetic field and find that $\nu = 1/3, 2/3, 4/3$, and $8/5$ are strongest at low field, persisting below 1.5 T. Our results provide insight into the interplay between electronic correlations and SU(4) symmetry in graphene.

3:30PM D7.00006 Quantum Hall effect on centimeter scale chemical vapor deposited graphene films, TIAN SHEN, Department of Physics, Purdue University/National Institute of Standards and Technology, WEI WU, QINGKAI YU, Center for Advanced Materials and ECE, University of Houston, CURT RICHTER, RANDOLPH ELMQUIST, DAVID NEWELL, National Institute of Standards and Technology, YONG CHEN, Department of Physics, Purdue University — We report observations of well developed half integer quantum Hall effect on mono layer graphene films of 7 mm by 7 mm in size. The graphene films are grown by chemical vapor deposition on copper, then transferred to SiO₂/Si substrates, with typical carrier mobilities $\approx 4000 \text{ cm}^2/\text{Vs}$. The large size graphene with excellent quality and electronic homogeneity demonstrated in this work is promising for graphene-based quantum Hall resistance standards, and can also facilitate a wide range of experiments on quantum Hall physics of graphene and practical applications exploiting the exceptional properties of graphene.

3:42PM D7.00007 Spin-skyrmion in graphene, WENCHEN LUO, RENÉ CÔTÉ, University of Sherbrooke — In the presence of a magnetic field, the band structure of the two-dimensional electron gas in graphene consists in a series of Landau levels with energy $E_n = \pm \sqrt{2} v_F \sqrt{|n|} \ell$. Each Landau level is 4-fold degenerate including valley and spin degrees of freedom. Working in the Hartree-Fock approximation and a finite Zeeman coupling, we compute the energy required to excite a spin-skyrmion (or antiskyrmion) in Landau levels $n = 1, 2$ at filling factors $\nu = 4, 8$. We show that a skyrmion-antiskyrmion pair has lower energy than an electron-hole pair at these two filling factors. We compare our results with a field-theoretical calculation [1] and with a recent experimental measurement of the transport activation gap in this system.

[1] Kun Yang, S. Das Sarma and A. H. MacDonald, Phys. Rev. B **74**, 075423 (2006).

3:54PM D7.00008 Coulomb impurity under magnetic field in graphene: a semiclassical approach, YUHUI ZHANG, National High Magnetic Field Laboratory and Department of Physics, Florida State University, YAFIS BARLAS, National High Magnetic Field Laboratory, Florida State University, KUN YANG, National High Magnetic Field Laboratory and Department of Physics, Florida State University — We address the problem of a Coulomb impurity in graphene in the presence of a perpendicular uniform magnetic field. We show that the problem can be solved below the supercritical impurity magnitude within the WKB approximation. Without impurity the semiclassical energy correctly reproduces the Landau level spectrum. For values below the supercritical impurity magnitude the energy spectrum still evolves as square root B with a renormalized fine structure constant. For a given Landau level the WKB energy depends on the absolute value of angular momentum in a way which is consistent with the exact diagonalization result. Below the supercritical impurity magnitude, the WKB solution can be expanded as a convergent series in powers of the effective fine structure constant. Relevance of our results to validity of the widely used Landau level projection approximation is discussed.

4:06PM D7.00009 Chern-Simons theory of an anomalous metallic state in half-filled monolayer graphene¹, PALLAB GOSWAMI, BITAN ROY, KUN YANG, National High Magnetic Field Laboratory and Florida State University — The ground state of half-filled monolayer graphene undergoes a novel metal-insulator transition with increasing strength of applied magnetic field. In a weak magnetic field the ground state at half-filling corresponds to a critical metallic state, that governs the $\nu = -2$ to $\nu = 2$ quantum Hall plateau transition. In the strong magnetic field regime this critical state gives way to an interaction driven quantum Hall insulator state. Currently there is no satisfactory theoretical explanation of the insulating phase and the phase transition. Motivated by this issue, we investigate the nature of the ground state in clean half-filled monolayer graphene, using a lattice Chern-Simons theory. In contrast to the results obtained previously by mean-field calculations in the Landau level basis, our analysis in the unpolarized regime shows the existence of an anomalous semimetallic state up to a critical strength of magnetic field, and the critical strength is determined by non-universal details of interaction strength. In the polarized regime the dynamics of the relevant metallic state changes dramatically, and new insulating phases do emerge.

¹NSF

4:18PM D7.00010 ABSTRACT WITHDRAWN —

4:30PM D7.00011 Bilayer graphene as a helical quantum Hall ferromagnet¹, RENE COTE, JEREMIE P. FOUQUET, WENCHEN LUO, Université de Sherbrooke — The two-dimensional electron gas (2DEG) in a graphene bilayer supports a variety of uniform broken-symmetry ground states in Landau level $N = 0$ and at integer filling factors $\nu \in [-3, 4]$. When a bias is applied between the layers at filling factors $\nu = 1, 3$, the ground state evolves from an interlayer coherent state at small bias to a state with orbital coherence at higher bias where *electric* dipoles associated with the orbital pseudospins order spontaneously in the plane of the layers. We show that by further increasing the bias the 2DEG goes first through an electron crystal with an orbital pseudospin texture at each site and then into a helical state where the pseudospins rotate in space. The pseudospin textures in the crystal and the helical states are due to the presence of a Dzyaloshinsky-Moriya interaction in the effective pseudospin Hamiltonian when orbital coherence is present in the ground state. We study in detail the electronic structure these nonuniform states as well as their collective excitations and compute their electromagnetic absorption.

¹This work has been supported by a grant from NSERC

4:42PM D7.00012 Theory of integer quantum Hall effect in bi-layer graphene, BITAN ROY, OSKAR VAFEK, National High Magnetic Field Laboratory and Department of Physics, Florida State University, Tallahassee, Florida 32306, USA — Bi-layer graphene in a quantizing external magnetic field exhibits plateaus of Hall conductivity at various integer fillings. Moreover, electron-electron interactions in suspended doubly gated bi-layer graphene appear sufficiently strong (and short-ranged) to result in a finite gap persisting down to zero magnetic field. In this talk we will demonstrate the competition of various orders within the zeroth Landau level and how their interplay is influenced by the filled Landau levels lying below the Fermi energy. Scaling behavior of the gap at the neutrality point will be discussed. Besides the splitting of the zeroth Landau level, degeneracy lifting of the rest of the Landau levels will be discussed.

4:54PM D7.00013 Electronic transport in ABA trilayer graphene, E.A. HENRIKSEN, D. NANDI, J.P. EISENSTEIN, California Institute of Technology — We present measurements of the electronic transport in ABA trilayer graphene field-effect devices fabricated with both a back and top gate, at zero, low and high magnetic fields. While the zero field resistivity exhibits a saddle point as a function of the two gate voltages that is similar to bilayer graphene, the low-field Hall data are consistent with a two-band system having a band overlap characteristic of semimetals. At high magnetic fields the quantum Hall effect is clearly observed, and displays features which can be traced to the underlying band overlap, as well as a lifting of the lattice mirror symmetry. Overall the transport in ABA trilayers is that of a semimetal in which the band structure can be strongly modified via the electric field effect. This work is supported by the DOE under grant No. DE-FG03-99ER45766 and the Gordon and Betty Moore Foundation.

5:06PM D7.00014 Quantum Hall liquid to Charge density wave phase transitions in ABC-trilayer graphene, YAFIS BARLAS, University of California at Riverside, RENE COTE, MAXINE RONDEAU, University of Sherbrooke, Quebec, Canada — We study interaction driven states within ABC-stacked trilayer graphene's 12-fold degenerate Landau level which appear near the neutral system Fermi level. The 12-fold degeneracy of the zero-energy LL is due to spin and valley degeneracy along with a degenerate set of triplet ($n = 0, 1, 2$) LL orbitals. We predict that at filling factors $\nu = -5, -2, 1, 4$ a quantum phase transition from a quantum Hall liquid state to a triangular charge density wave occurs as a function of the single-particle induced LL orbital splitting. This transition is preceded by a softening of the magneto-roton minima of the quantum Hall liquid which appears at $q l_B \sim 2.4$. The charge density wave is a manifestation of the LL orbital pseudospin textures with nonzero winding numbers. The phase diagrams at other filling factors along with the experimental consequences of our theoretical predictions will also be addressed.

5:18PM D7.00015 ABSTRACT WITHDRAWN —

Monday, February 27, 2012 2:30PM - 5:18PM —
Session D8 GMAG: Organo-metallics: Magnetic and other Properties 208

2:30PM D8.00001 Polymorphism in Low-dimensional Molecule-based Materials: Synthetic Control of Magnetic and Electronic Structure¹, ADORA BALDWIN, JAMIE MANSON, Eastern Washington University, JOHN SCHLUETER, Argonne National Laboratory — Competition for hydrogen bonds in molecule-based materials frequently leads to the stabilization of polymorphic structures with similar energies. Herein, we report that among magnetic coordination polymers selective crystallization of the $[\text{Cu}(\text{HF}_2)(\text{pyrazine})_2]\text{SbF}_6$ and $[\text{Cu}_2\text{F}(\text{HF})(\text{HF}_2)(\text{pyrazine})_4](\text{SbF}_6)_2$ polymorphs can be achieved through control of pressure and temperature during the crystallization process. Through this manner, orbital order and magnetic dimensionality (2D vs. 1D) can be controlled in this system. Similarly, in the analogous $[\text{Co}(\text{HF}_2)(\text{pyrazine})_2]\text{SbF}_6$ system, selective crystallization of the $[\text{CoF}_2(\text{pyrazine})_2]\text{SbF}_6(\text{H}_2\text{O})_3(\text{H}_3\text{O})$ polymorph has been achieved. While these cobalt materials exhibit a 2D magnetic structure, the interlayer coupling is diminished in the hydrated material. Among cation radical salts, five polymorphic phases in the $[\text{bis}(\text{ethylenedithio})\text{tetrathiafulvalene}]_2\text{Ag}(\text{CF}_3)_4(1,1,2\text{-trichloroethane})$ system have been crystallized, four of which have superconducting ground states. Among the superconducting salts, the ones with intercalated charge ordered layers exhibit a five-fold enhancement of T_c .

¹Supported by Argonne, a U.S. Department of Energy Office of Science laboratory, operated under Contract No. DE-AC02-06CH11357.

2:42PM D8.00002 Ground-state properties of $\text{EtMe}_3\text{Sb}[\text{Pd}(\text{dmit})_2]_2$ by many-variable variational Monte Carlo method, SATOSHI MORITA, RYUI KANEKO, MASATOSHI IMADA, Department of Applied Physics, University of Tokyo — The organic Mott insulator $\text{EtMe}_3\text{Sb}[\text{Pd}(\text{dmit})_2]_2$ is a strongly correlated electron system on a nearly-regular triangular lattice and regarded as a spin liquid material. We investigate its effective low-energy model derived from first principles calculations and band+dimensional downfolding. The *ab initio* effective Hamiltonian is given in the form of the two-dimensional single-band extended Hubbard model on an anisotropic triangular lattice with short-ranged Coulomb and exchange interactions. Its ground state is calculated by the many-variable variational Monte Carlo method with quantum-number projection and multi-variable optimization. We draw the ground-state phase diagram as a function of scaling parameters for the interactions and the geometrical frustration by extending the *ab initio* model. We discuss Mott transitions and magnetic properties.

2:54PM D8.00003 Reduced Influence of Electronic Correlations in a Half-Filled System: Metallic Properties and Charge Order Transition in κ -(ET)₂Hg(SCN)₂Cl¹, NATALIA DRICHKO, Johns Hopkins University, REBECCA BEYER, MARTIN DRESSEL, University Stuttgart, Germany, HARALD JESCHKE, University Frankfurt, Germany, JOHN SCHLUETER, Argonne National Laboratory, ELENA ZHILYAEVA, RIMMA LYUBOVSKAYA, Institute of Problems of Chemical Physics, Russia — The family of κ -(ET)₂Hg(SCN)_xCl_{2-x} can be described within a model of a metal with a half-filled conductance band. Our calculations indicate that the value of the on-site Coulomb repulsion U is relatively small in these system. We investigate the effects of lower U on the optical properties of κ -(ET)₂Hg(SCN)₂Cl in the metallic state and below the metal-insulator transition. Optical conductivity spectra in the metallic state above 35 K show a behavior already observed for half-filled metals on the edge of the Mott insulating state: an optical transition between Hubbard bands at frequencies equal to U is present in spectra at all temperatures, being a precursor of a Mott transition, while a coherent carriers response develops below $T^*=150$ K. We note an influence of the lower U value both on the position of the “U-band” and on a relatively high T^* . Untypically for a half-filled system, a metal-insulator transition at 35 K is found that is of a charge-order nature. A possibility of a charge-order ground state in a half-filled system in case of low U and relatively high nearest-neighbor Coulomb repulsion V is discussed.

¹Supported by H. Blewett fellowship

3:06PM D8.00004 Non-monotonic magnetic field dependence of the staggered-moment in two-dimensional frustrated antiferromagnets, MOHAMMAD SIAHATGAR, BURKHARD SCHMIDT, PETER THALMEIER, Max Planck Institute for Chemical Physics of Solids — We present an efficient method to identify the degree of frustration in quasi-two-dimensional (2D) antiferromagnets described by the J_1 - J_2 quantum Heisenberg model. The frustration ratio J_2/J_1 is commonly obtained from the analysis of magnetic susceptibility, specific heat, and saturation field. We show that the field-induced suppression of quantum fluctuations causes a nonlinear and non-monotonic magnetic field dependence of the staggered moment which depends strongly on the frustration ratio. This serves as a powerful criterion to determine J_2/J_1 using a combination of the exact diagonalization method on finite clusters and the spin-wave analysis. We apply this method to the quasi-2D compound Cu(pz)₂(ClO₄)₂ obtaining an intermediate ratio of $J_2/J_1 \simeq 0.2$ for the frustration.

3:18PM D8.00005 Effects of Pressure on the Magnetic Properties of Prussian Blue Analogues¹, M.K. PEPPRAH, E.S. KNOWLES, M.F. DUMONT, J.S. XIA, M.W. MEISEL, Dept. Physics and NHMFL, Univ. Florida, C.H. LI, D.R. TALHAM, Dept. Chemistry, Univ. Florida — Prussian blue analogues (PBAs) have been shown to exhibit interesting magnetic characteristics under various external stimuli: charge transfer induced spin transition (CTIST),² a temperature effect; persistent photo-induced magnetism (PPIM),³ an optical effect; and pressure induced electron transfer (PIET).⁴ Our research has established that photocontrol of the magnetic response of CoFe-PBA, can be extended to higher temperatures, accompanied by a decrease in magnetization, using heterostructured PBA particles composed of Rb_aCo_b[Fe(CN)₆]_c· m H₂O cores surrounded by shells of K_jNi_k[Cr(CN)₆]_l· n H₂O.⁵ This effect is attributed to strain in the shell, induced by a lattice expansion in the core during illumination. We report a similar effect in the core-shells accompanied by PIET under application of external pressure and probe the similarities between optical and pressure effects.

¹Supported by NSF DMR-0701400 (MWM), DMR-1005581 (DRT), and DMR-0654118 (NHMFL).

²N. Shimamoto *et al.* Chem. Lett. **31**, (2002) 486.

³O. Sato *et al.* Science **272** (1996), 704-705.

⁴V. Ksenofontov *et al.* Phys. Rev. B **68** (2003) 024415.

⁵M. F. Dumont *et al.* Inorg. Chem. **50** (2011) 4295.

3:30PM D8.00006 Effect of hydrostatic pressure on a low dimensional S=1/2 gapped quantum antiferromagnet by inelastic neutron scattering¹, TAO HONG, Oak Ridge National Laboratory, C. STOCK, NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA., I. CABRERA, C. BROHOLM, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, Maryland 21218, USA, Y. QIU, J.B. LEO, S.J. POULTON, J.R.D. COPLEY, NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA. — We report an inelastic neutron scattering study of a quasi-two-dimensional $S=1/2$ dimer system piperazinium hexachlorodipicrate (PHCC) under hydrostatic pressure up to $P=9.0$ kbar. The spin gap Δ decreases with increasing pressure. The observation of three fold degenerate triplet excitation at $P=6.0$ kbar is consistent with the theoretical prediction and the bandwidth of the dispersion relation is unaffected within the experimental uncertainty. At $P=9.0$ kbar the spin gap is reduced to $\Delta=0.55$ meV from $\Delta=1.0$ meV at ambient pressure [1].

[1] T. Hong *et. al.*, Physical Review B **82**, 184424 (2010)

¹The work at ORNL was partially funded by the Division of Scientific User Facilities, Office of BES, DOE. The work at JHU was supported by the NSF through Grants No. DMR- 0306940 and No. DMR-0706553.

3:42PM D8.00007 Density functional theory study of alkali doped picene, MILAN TOMIC, HUNPYO LEE, ROSER VALENTI, HARALD O. JESCHKE, Institut fuer Theoretische Physik, Goethe-Universitaet Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — We employ density functional theory methods to determine the equilibrium structures of A_x picene where $A = \text{Na, K, Rb, Cs}$ and $x = 1, 2, 3$. We find that alkali doping with one, two and three alkali ions per picene molecule leads to subsequent filling of the LUMO and LUMO+1 derived bands of picene, leading to quarter, half and three quarter filled systems. We analyse the electronic structures using tight binding methods to derive the kinetic energy part of the underlying Hubbard Hamiltonian. As the interaction strength U on the picene molecules is expected to be large compared to the band width, we also employ manybody methods on the resulting Hamiltonian. We compare our results to photoemission experiments.

3:54PM D8.00008 First principles investigation of the Fabre salts, ANTHONY JACKO, ROSER VALENTI, HARALD O. JESCHKE, Institut fuer Theoretische Physik, Goethe-Universitaet Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — The Fabre salts (TMTTF)₂X are one dimensional charge transfer salts with a very rich phase diagram including charge ordered, Mott insulating, antiferromagnetic and spin Peierls phases. The structure involves stacks of TMTTF molecules with varying degree of dimerization. Open questions involve the role of the anions in the phase transitions. We investigate the electronic structure of compounds with a number of different anions like $X = \text{AsF}_6, \text{PF}_6$ and Br. We discuss the properties of the underlying Hubbard Hamiltonian for these materials.

4:06PM D8.00009 Scaling Theory of the Mott Transition and Breakdown of the Grüneisen Scaling Near a Finite-Temperature Critical End Point, LORENZ BARTOSCH, University of Frankfurt — We discuss a scaling theory of the lattice response in the vicinity of a finite-temperature critical end point. The thermal expansivity is shown to be more singular than the specific heat such that the Grüneisen ratio diverges as the critical point is approached, except for its immediate vicinity. More generally, we express the thermal expansivity in terms of a scaling function which we explicitly evaluate for the two-dimensional Ising universality class. Recent thermal expansivity measurements on the layered organic conductor κ -(BEDT-TTF) $_2X$ close to the Mott transition are well described by our theory.

[1] Lorenz Bartosch, Mariano de Souza, and Michael Lang, *Physical Review Letters* **104**, 245701 (2010).

4:18PM D8.00010 Tuning the magnetic dimensionality by charge ordering in the molecular TMTTF salts, KAZUYOSHI YOSHIMI, Department of Physics, University of Tokyo, Nanosystem Research Institute "RICS", AIST, HITOSHI SEO, Condensed Matter Theory Laboratory, RIKEN, SHOJI ISHIBASHI, Nanosystem Research Institute "RICS", AIST, STUART BROWN, Department of Physics and Astronomy, UCLA — Low-dimensional (D) organic conductors TMTTF $_2X$ are considered as a prototypical system for investigations of D-crossover phenomena, since the transfer integrals connecting the conduction chains are readily controlled by applied pressure [1]. In addition, recent NMR experiments in TMTTF salts imply the existence of another type of D-crossover which accompanies a multiferroic property; decreasing the ferroelectric-type charge ordering (FCO) by pressure is associated with the suppression of the antiferromagnetic (AF) transition temperature [2]. In this work, we theoretically investigate the interplay between FCO and magnetic states in TMTTF salts [3], and show that FCO increases 2-D AF spin correlation, whereas in the 1-D regime two different spin-Peierls states are stabilized. By performing first-principles band calculations for different salts and comparing our results with experiments, we identify the controlling parameters in the experimental phase diagram to be not only the inter-chain transfer integrals but also the amplitude of the FCO. [1] D. Jerome, *Science* **252**, 1509 (1991). [2] W. Yu *et al.*, *Phys. Rev. B* **70** 121101 (2004). [3] K. Yoshimi, H. Seo, S. Ishibashi, and S. E. Brown, arXiv:1110.3573 and arXiv:1110.3575.

4:30PM D8.00011 Charge dynamics in Mott-insulating and charge-ordered organic crystals: a possibility of the Berezinskii-Kosterlitz-Thouless transition, YAMAGUCHI TAKAHIDE, TOHRU WATANABE, YOSHIHIKO TAKANO, KOUTA KODAMA, SHINYA UJI, National Institute for Materials Science, HIROSHI M. YAMAMOTO, RIKEN — The organic Mott insulator κ -(BEDT-TTF) $_2Cu[N(CN)_2]Cl$ exhibits power-law current-voltage characteristics in a low current range at temperatures below ≈ 10 K. The power-law current-voltage characteristics are similar to those observed in the charge-ordered organic crystals θ -(BEDT-TTF) $_2MzN(SCN)_2$ ($M = Cs$ and Rb) and are accounted for in the same way in terms of exciton excitations: The electric field assists the thermal unbinding of pairs of a doublon and a holon that attract each other due to the two-dimensional long-range Coulomb interaction. The two-dimensional Coulomb interaction arises from the layered structure of the organic crystals and their large dielectric anisotropy. The in-plane dielectric constant can be understood within the context of the same model in terms of polarization of the bound pairs. We discuss a possibility of the Berezinskii-Kosterlitz-Thouless transition in these layered organic crystals. κ -(BEDT-TTF) $_2Cu[N(CN)_2]Cl$ has a much smaller magnetoresistance (25 % in 10 T at 0.3 K) than θ -(BEDT-TTF) $_2CsZn(SCN)_4$ (≈ 10000 % in 10 T at 0.1 K), which probably reflects different spin states of the excitations for the Mott and charge-ordered states. Yamaguchi Takahide *et al.* *PRB* **84**, 035129 (2011)

4:42PM D8.00012 ^1H NMR study on X-ray irradiated κ -(BEDT-TTF) $_2Cu[N(CN)_2]Br$, KAZUYA MIYAGAWA, University of Tokyo, TAKAHIKO SASAKI, Tohoku University, NAOKI YONEYAMA, Yamanashi University, NORIO KOBAYASHI, Tohoku University, KAZUSHI KANODA, University of Tokyo — The κ -(BEDT-TTF) $_2Cu[N(CN)_2]Br$ (κ -Br) is a quasi-two dimensional superconductor with T_c of 12 K. By substituting Cl for Br in the insulating layer, the system becomes a Mott insulator, κ -(BEDT-TTF) $_2Cu[N(CN)_2]Cl$ (κ -Cl), with the Neel temperature of 25 K. So, κ -Br salt is situated close to the Mott transition. Recently, Sasaki *et al.*, have reported the transformation from a metallic (superconducting) state to an insulating state by the x-ray irradiation. The 500h-irradiated thin sample shows insulating behavior in the temperature dependence of resistivity. We report the ^1H NMR studies on the 500h-irradiated κ -Br salt. Below 150 K, where the nuclear relaxation is dominated by electron spins, $1/T_1$ of the irradiated sample increases from that of the non-irradiated sample and is even larger than the value of κ -Cl. Nevertheless, there is no manifestation of magnetic ordering; that is, neither a line broadening nor a divergent peak in $1/T_1$ down to 1.5 K. We will discuss the electronic state of irradiated κ -Br salt based on experimental results.

4:54PM D8.00013 TCP, a new quasi-one-dimensional conducting platinate: DC and NMR studies¹, J.A. ALEXANDER, R.I. LEATHERBURY, O. GAFAROV, A.A. GAPUD, A.P. WEBER, L. PHAM, R.E. SYKORA, A. KHAN, University of South Alabama, A.P. REYES, P. KUHN, National High Magnetic Field Laboratory — $Cs_4[Pt(CN)_4](CF_3SO_3)_2$, or TCP, is the newest member of the family of quasi-one-dimensional conducting platinites that includes the widely studied $K_2[Pt(CN)_4]Br_{0.303}(H_2O)$ (KCP) – best-known for its metal-insulator transition consistent with a Peierls instability. Unlike KCP, however, we have found properties unique to TCP. X-ray diffraction shows longer Pt-Pt separations, and undergoes subtle change with cooling. DC resistivity measurements presented technical challenges that had to be resolved, but in the end revealed a more highly insulating phase at room temperature, and the temperature dependence of resistivity has an anomalous “peak” at around 150 K. NMR also presented a technical challenge in that the ^{195}Pt nucleus, which had been successfully used for NMR studies on KCP, did not produce a usable signal in TCP, wherein we utilized the peripheral ^{133}Cs nuclei instead. Quadrupole splitting of spin states of ^{133}Cs measured as a function of orientation showed consistency with the angular dependence expected of the known symmetry axes of ^{133}Cs . Preliminary measurements of longitudinal relaxation time T_1 also reveal an anomalous temperature dependence in the vicinity of 150 K. All these considerations point to a possible structural transformation, as will be discussed.

¹Funded by an NSF-RUI grant.

5:06PM D8.00014 Experimental and theoretical study of the temperature dependent structural and electronic properties of the spin liquid candidate κ -(BEDT-TTF) $_2Cu_2(CN)_3$, JOHN A. SCHLUETER, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, United States, MARIANO DE SOUZA, RUDRA SEKHAR MANNA, MICHAEL LANG, Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt, Germany, ROSER VALENTI, HARALD O. JESCHKE, Institut fuer Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt, Germany — The organic charge transfer salt κ -(BEDT-TTF) $_2Cu_2(CN)_3$ is of great experimental as well as theoretical interest due to the interplay of the effects of electronic correlations, low dimensionality and spin frustration. Besides the spin liquid property at very low temperatures, the material has interesting anomalies at 6K, 60K and 150K. Even though the structure of the material has been determined several times over the past 20 years, complete structural data are only available at room temperature. In our work, we fill this gap by precisely determining the structure at 300K, 250K, 200K, 150K, 100K and 20K. We analyze the structures using density functional theory and tight binding methods. We show that the triangular lattice Hubbard Hamiltonian parameters are temperature dependent, with the interaction strength increasing with decreasing temperature and with the frustration going through a minimum at 150 K. Our results point to the fact that even in the absence of structural phase transitions, experimental determination of structures at various temperatures may be important as a starting point for realistic many-body theoretical investigation of complex materials.

**Monday, February 27, 2012 2:30PM - 5:30PM –
Session D9 GMAG: Magnetic Devices and Applications 209**

2:30PM D9.00001 Dual microbead-labeled DNA manipulation with magnetic traps in a microfluidic device, M. HOWDYSHELL, M. SIMON, M. POIRIER, R. SOORYAKUMAR, The Ohio State University — Biomolecular responses to mechanical force underlie many critical functions in the context of cellular physiology. In order to develop the technology to apply forces on individual biomolecules, we utilize an array of ferromagnetic disks on a silicon surface to trap and manipulate tethered DNA molecules. The force activation is achieved through remotely controlled programmable weak external magnetic fields that do not damage the biological entity. Moreover, to exploit both hydrodynamic and magnetic forces, the magnetic disks are imprinted within microfluidic channels, while a tethered microbead attached on each end of the DNA strand provides convenient force transmitting handles. Two separate approaches that are utilized involve use of two superparamagnetic beads or a superparamagnetic and nonmagnetic bead pair. The independently controlled hydrodynamic and magnetic forces allow for manipulation of the DNA in all directions within a horizontal plane. Hundreds of magnetic traps are readily patterned onto a single channel, providing the potential to multiplex an ensemble of individual molecules within the device.

2:42PM D9.00002 Testing of a Helmholtz Microcoil in a Diamond Anvil Cell NMR, CHING LIN¹, SAM WEIR², University of California, Davis, SAMUEL WEIR³, Lawrence Livermore National Laboratory, NICHOLAS CURRO⁴, University of California, Davis, LAWRENCE LIVERMORE NATIONAL LABORATORY COLLABORATION — A new designed, multi-turn tungsten Helmholtz micro-coil has been constructed and tested on the solid-state bulk NMR experiment. A Helmholtz micro-coil with diameter 950 μm is embedded on diamond culet and produces a nearly uniform AC magnetic field inside a sample space. A Fluorine polycrystal will be used to test our Helmholtz micro-coil, and the measured NMR data will be compared with the ones produced by other type of diamond anvil cell coils. The Helmholtz micro-coil will be used for high pressure NMR and future investigation of magnetic properties of heavy fermion superconductors.

¹A Condensed Matter Experiment Graduate Student in UCD Physics Department

²A Condensed Matter specialist in UCD Physics Department

³A staff & specialist in LLNL

⁴A Condensed Matter Associate Professor in UCD Physics Department

2:54PM D9.00003 Magneto-mechanical resonant detection of superparamagnetic microbeads trapped by magnetic domain walls¹, ELIZABETH RAPOPORT, DANIEL MONTANA, GEOFFREY BEACH, Massachusetts Institute of Technology — Manipulation of superparamagnetic (SPM) beads with magnetic domain walls (DWs) is of interest for lab-on-chip applications. DWs can trap SPM beads and tagged entities, enabling remote manipulation with nanoscale precision [1, 2]. Previously, we have demonstrated DW driven capture and transport of single microbeads at speeds approaching 1000 $\mu\text{m/s}$ [3]. Here, we demonstrate that the strong magnetostatic bead-DW binding leads to a unique magneto-mechanical resonance [4]. We show experimentally that this resonance can be used to distinguish bead populations based on their size, presenting a new mechanism for bead metrology. Moreover, the bead-DW interaction can be used to sense and characterize magnetic beads without the need for sensor surface functionalization. Exploiting the dual functionality of DWs as both bead carriers and sensors, we present an integrated device capable of high-speed transport and electrical sensing of the magneto-mechanical resonance of individual trapped beads.

[1] G. Vieira et al., Phys. Rev. Lett. 103, 128101 (2009).

[2] M. Donolato et al., Adv. Mater. 22, 2706 (2010).

[3] E. Rapoport, G.S.D. Beach, Appl. Phys. Lett. in press.

[4] E. Rapoport, G.S.D. Beach, J. Appl. Phys. in press.

¹Supported by the MIT CMSE under NSF-DMR-0819762 and by the MIT Deshpande Center.

3:06PM D9.00004 Cascaded Magneto-Optical Ring Resonator Structures for Tunable Faraday Rotation and Reduced Isolator Footprint, MEHMET CENGIZ ONBASLI, Massachusetts Institute of Technology, JUEJUN HU, University of Delaware, LEI BI, Micron Technology, GERALD F. DIONNE, Massachusetts Institute of Technology Lincoln Laboratory, CAROLINE A. ROSS, Massachusetts Institute of Technology — On-chip optical isolators are indispensable components of integrated optics, and can be modified to enable four-port and multi-port circulators and modulators. We have implemented an on-chip optical isolator by placing a racetrack resonator next to a single mode waveguide and coating half of the resonator with a uniformly magnetized magneto-optical film, which breaks the time-reversal symmetry of light propagation and provides different refractive indices and phase shifts for forward and backward propagating waves. At every pass, the optical mode inside the resonator accumulates Faraday rotation in addition to phase shift due to propagation. The transmission from the output port of the waveguide has a Lorentzian dip due to the resonance peak of the resonator. Light can only propagate in the clockwise direction inside the resonator. Here we model how cascading multiple ring resonators can increase the overall quality factor of the isolator and narrow the resonance linewidth, due to the longer photon lifetime inside the cavity. As a result of better control of Faraday rotation, the isolation ratio is enhanced and the device footprint is reduced with respect to Mach-Zehnder waveguide isolators.

3:18PM D9.00005 On the Energy Transfer Performance of Mechanical Nanoresonators Coupled with Electromagnetic Fields: Applications with magnetic nanoparticles, H. JAVAHERI, B. BARBIELLINI, G. NOUBIR, Northeastern University — The energy transfer performance in electrically and magnetically coupled mechanical nanoresonators is studied [1]. Using the resonant scattering theory, we show that magnetically coupled resonators can achieve the same energy transfer performance as for their electrically coupled counterparts, or even outperform them within the scale of interest. Magnetic and electric coupling are compared in the *Nanotube Radio*, a realistic example of a nano-scale mechanical resonator. The energy transfer performance is discussed for magnetic coupling in magnetite (Fe_3O_4) nanoparticles.

[1] H. Javaheri, B. Barbiellini, G. Noubir, arXiv:1108.0633.

3:30PM D9.00006 Increased Sensitivity of Magnetoelectric Sensors at Low Frequencies Using Magnetic Field Modulation, JONATHAN PETRIE, Army Research Laboratory, DWIGHT VIEHLAND, DAVID GRAY, Virginia Tech University, SANJAY MANDAL, GOLLAPUDI SREENIVASULU, GOPALAN SRINIVASAN, ALAN EDELSTEIN, Oakland University — Magnetoelectric (ME) laminate sensors are vector magnetometers that can detect pT magnetic fields at 1 kHz, although sensitivity may be reduced at lower frequencies. These passive sensors consist of alternating layers of magnetostrictive and piezoelectric materials. A magnetic field causes the magnetostrictive layer to strain the piezoelectric material and create measurable charge. We have shown¹ that since the strain response is a nonlinear function of the bias field, sweeping the magnetic bias on the magnetostrictive layer can modulate the ME response and increase the operating frequency of the sensor. This upward shift lowers the $1/f$ noise and increases the signal amplitude if the new operating frequency is near a mechanical resonance mode of the sensor. Using this modulation technique, the low frequency sensitivity has been improved by more than an order of magnitude and we have achieved a detectivity of 7 pT/ $\sqrt{\text{Hz}}$ at 1 Hz. In addition to increasing the magnetic signal frequency, we can use magnetic modulation to increase the operating frequency of acoustic signals detected by these sensors. This occurs because the ME sensors are nonlinear devices. In these cases using magnetic field modulation, the signal appears as sidebands around the modulation frequency.

¹To be published in Journal of Applied Physics.

3:42PM D9.00007 Bipolar exchange bias modulation in $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{BiFeO}_3$ heterostructure based field effect devices, STEPHEN WU, SHANE CYBART, JAMES PARKER, PU YU, R. RAMESH, R.C. DYNES, University of California, Berkeley / Lawrence Berkeley National Lab — We have fabricated and performed electrical transport measurements on a multiferroic field effect device with a BiFeO_3 (antiferromagnetic/ferroelectric) gate dielectric and a $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (ferromagnetic) channel to investigate the effect of BiFeO_3 (BFO) polarization on interfacial magnetism by using exchange bias as a diagnostic tool. A reversible static shift in exchange bias through zero applied magnetic field is observed by electrically poling BFO. This bipolar exchange bias modulation behavior strongly suggests that interfacial magnetization is being reversed through the application of electric field. To investigate this phenomenon further we have measured temperature dependent exchange bias, temperature dependent resistivity, and Hall Effect coefficients on multiple devices. Also a comparison to an identical control device using a $\text{Pb}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{O}_3$ (ferroelectric) gate dielectric and $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (LSMO) channel is offered, which provides insight into the interfacial magnetic interactions uniquely occurring in the BFO/LSMO system. We analyze these results in the context of proposed models, which suggest that we are modulating both carrier density and interfacial magnetic coupling strengths; both of which have a strong effect on the bipolar modulation of exchange bias.

3:54PM D9.00008 Effect of the exchange bias field on the magnetoimpedance response in multilayered FeNi-IrMn films and CoFeSiB-IrMn ribbons, KERIM TURE, MEHMET YUMAK, GULEN AKTAS, Bogazici University, Department of Physics, JUAN MANUEL FLOREZ, Department of Materials Science and Engineering, MIT, PATRICIO VARGAS, Departamento de Fisica, Universidad Técnica Federico Santa Mara, CAROLINE A. ROSS, Department of Materials Science and Engineering, MIT, CARLOS GARCIA, Bogazici University, Department of Physics — The magnetoimpedance effect (MI) has been widely used in sensitive magnetic field (MF) sensors, but its intrinsic nonlinear properties are disadvantageous for sensor applications near zero field. The combination of ferromagnetic (FM) and antiferromagnetic (AFM) layers produce an asymmetrical MI (AMI) peak positions which are shifted to higher MF as the probe frequency increases, so linear MI behavior can be obtained around zero external field by tuning the frequency. Here, AMI was extensively studied in multilayer strips of exchange-coupled FeNi-IrMn . The effect of the thickness of the FM layer and the angle dependence in three stripe samples with EB induced; parallel, perpendicular and forming an angle of 45 with the direction of the wire were studied. MI ratio raise with increasing thickness of the FM layer is attributed to the stronger pinning of the FM adjacent to the IrMn. Also, a combination of the EB angle affects and direction of the applied MF can tune; the number of peaks in the MI response, the asymmetry between peaks and the shift of the MI response. Besides, an antiferromagnetic layer was deposited on the top of CoFeSiB amorphous ribbons enhancing the MI effect at low frequencies and shifting the MI response at higher frequencies.

4:06PM D9.00009 Tailoring Giant Magneto-impedance Effect in Ultrasoft Ferromagnetic Microwires¹, A. CHATURVEDI, A. RUIZ, P. MUKHERJEE, H. SRIKANTH, M.H. PHAN, Department of Physics, University of South Florida Tampa FL 33620, V.S. LARIN, Microfir Thenologii Industriale, Moldavia — Research on soft ferromagnetic microwires exhibiting giant magneto-impedance (GMI) effect, which is a large change of the ac impedance of a ferromagnetic conductor in a static magnetic field, for advanced magnetic sensor applications is an area of topical interest. In this study we show how the GMI effect and its field sensitivity are optimized in Co-B-Si-Mn microwires by varying the magnetic core to glass shell diameter ratio (d). The microwires have been fabricated by the glass-coated melt spinning method. The largest values of GMI (245%) and its field sensitivity 25%/Oe are achieved at $f = 13\text{MHz}$ for the microwires with $d = 0.86$. The d dependence of the magneto-impedance has been analyzed based on those of the magneto-resistance and magneto-reactance. Our studies indicate that the microwires with optimized GMI response are attractive candidate materials for structural health self-monitoring and magnetic biosensing applications.

¹CIFM and FCASST

4:18PM D9.00010 Soft ferromagnetic microribbons with enhanced GMI effect for advanced magnetic sensor applications¹, A. RUIZ, A. CHATURVEDI, P. MUKHERJEE, H. SRIKANTH, M.H. PHAN, Department of Physics, University of South Florida — Soft ferromagnetic ribbons with giant magneto-impedance (GMI) effect are attractive candidate materials for high-performance magnetic sensor applications. GMI is a large change in the ac impedance of a ferromagnetic conductor subject to a dc magnetic field. There is a need for further improving GMI response of existing materials, as well as reducing the size of a GMI-based sensor for use in micro-sensing systems. In this work, we report the enhancement of GMI in soft ferromagnetic ribbons (Metglas® 2714A) at high frequencies by reducing the width of the ribbon to the micrometer scale. This finding is of practical importance, as sensors with enhanced field sensitivity and reduced size find wider ranging applications. The origin of the enhanced GMI effect in the microribbon is explained in terms of the skin and demagnetization effects. The relative contributions to the magneto-impedance from the magneto-resistance and magneto-reactance have been analyzed and discussed in detail.

¹CIFM and FCASST

4:30PM D9.00011 Designing New Metal-Semiconductor Hybrid Structures With Large Geometric Magnetoresistance¹, LISA PUGSLEY, L.R. RAM-MOHAN, Worcester Polytechnic Institute, S.A. SOLIN, Washington University, St. Louis — The extraordinary magnetoresistance (EMR) in metal-semiconductor hybrid structures was first demonstrated using a four-contact configuration for a circular semiconductor wafer with a concentric metallic inclusion in it. The EMR effect, which is observed at room temperature, is very suitable for use in read heads in magnetic data storage devices. This effect depends on the orbital motion of carriers in an external magnetic field, and the remarkably high magnetoresistance response (the change in resistance with a magnetic field) observed suggests that the geometry of the metallic inclusion can be optimized to significantly enhance the EMR. The theory and simulations to achieve this goal are considered by comparing various 2D structures in an external magnetic field to evaluate the EMR in them using finite element analysis and geometric optimization. For a $10\text{ }\mu\text{m}$ square semiconductor wafer with a square metallic inclusion we see a range in resistance from -400 to $400\text{ }\Omega$ for $-1\text{ T} \leq B \leq 1\text{ T}$. This response can be optimized by changes in contact orientation and the size and shape of the metallic region. Extension to 3D is being investigated at present, which would allow for modeling of magnetic field sensors that also provide the direction of the field.

¹This work was supported by the NSF under grants ECS-0725427 and ECCS-0725538. SAS has a financial interest in PixelEXX, a start-up company whose mission is to market imaging arrays.

4:42PM D9.00012 Ultra wideband, high sensitivity magneto-optic field sensor¹, DONG HO WU, ANTHONY GARZARELLA, Naval Research Laboratory, VINCE FRATELLO, Integrated Photonics Inc. — Using the bismuth rare-earth iron garnet thick films we have demonstrated a magneto-optic (MO) field sensor. The sensor made of all dielectric materials is nearly noninvasive, and is operated at room temperature. The sensor's sensitivity is scalable; the same sensor design can be used for a low-field sensor to measure fields below nano-Tesla or for a high-field sensor to measure several hundred Tesla. The highest sensitivity that we have achieved with the sensor is about $30\text{ pT}/(\text{Hz})^{1/2}$. Presently its frequency range is limited from DC to 2 GHz. We have carried out several different experiments with this sensor to explore a few interesting applications, such as electromagnetic signal interception tests over a very broad frequency range. In this presentation we will report our experimental results obtained from this MO field sensor.

¹This work is supported by DARPA

4:54PM D9.00013 Diamagnetic repulsion, the method of magnetic images & suitability of the solenoid and dipole models¹, MING YIN, Benedict College, Columbia, SC29204, HUAIZHOU ZHANG, TIMIR DATTA, University of South Carolina, Columbia, SC29208 — The repulsion of a permanent magnet from a diamagnetic region was investigated. A magnet of moment m can be described by two models (i) solenoid - a circulating current of appropriate value; second (ii) a magnetic dipole comprising of a pair of north and south poles of separated by a distance. The magnetic field (B) of a permanent magnet was measured. The magnet was modeled as a solenoid with a circulating surface current. The Biot-Savart law field (B) was computed in Matlab. The experimental data of was in excellent agreement with the Matlab results. However, for computing the repulsion force (F) between the magnet and its diamagnetic image by the direct integration of the current-current interaction require detailed knowledge of the two current densities. However such knowledge is not essential if image is modeled as a dipole. When the magnet is a distance z above the diamagnetic interface then the image current I_2 gives rise to a image dipole m_2 and the $F \sim m_2 \text{div } B$, where the div of the holding field is computed at the distance $2z$ below the magnet. In this model F is directly proportional to both m' and the derivative of the field and a negative slope indicates repulsion, all three were confirmed.

¹Supported at Benedict College by DOD award #60177-Rt-H.

5:06PM D9.00014 ABSTRACT WITHDRAWN —

5:18PM D9.00015 Magnetic Field Assisted assembly using programmable array of solenoids - A Manufacturing Approach, VIJAY KASISOMAYAJULA, ANTHONY FIORY, MICHAEL BOOTY, NUGGEHALLI RAVINDRA, New Jersey Institute of Technology — The use of an array of programmable solenoids to implement a magnetic field driven assembly of heterogeneous micro-components onto a substrate is studied. A lower limit of component size, the upper limit of the rate of assembly and the efficiency of the assembly from various perspectives is presented. Various statistical tests are performed on the assembly process to determine its feasibility. A comparison is made between this method of assembly and established assembly techniques in the literature.

Monday, February 27, 2012 2:30PM - 5:30PM —
Session D10 DCOMP: Invited Session: Advancements in Computational Physics using NSF's TeraGrid/XSEDE Resources 210A

2:30PM D10.00001 Benchmark Calculations of Atomic Collision Processes¹, KLAUS BARTSCHAT, Drake University — The rapid development of computational resources has resulted in enormous improvements in the accuracy of numerical calculations of atomic collision processes. This talk will concentrate on recent advances in the computational treatment of charged-particle and intense short-pulse laser interactions with atoms, ions, and small molecules. Examples include electron collisions with heavy complex targets that are of significant importance in many modelling applications in plasma and astrophysics, fundamental studies of highly correlated 4-body Coulomb processes such as simultaneous ionization with excitation, and the accurate solution of the time-dependent Schrödinger equation in the presence of intense femto/attosecond laser fields, which paves the way for quantum dynamic imaging and coherent control.

¹Work supported by the NSF under PHY-0903818 and PHY-1068140, and the TeraGrid/XSEDE allocation TG-PHY090031.

3:06PM D10.00002 Prediction and Design of Materials from Crystal Structures to Nanocrystal Morphology and Assembly¹, RICHARD HENNIG, Materials Science and Engineering, Cornell University — Predictions of structure formation by computational methods have the potential to accelerate materials discovery and design. Here we present two computational approaches for the prediction of crystal structures and the morphology of nanoparticles. Many materials properties are controlled by composition and crystal structure. We show that evolutionary algorithms coupled to ab-initio relaxations can accurately predict the crystal structure and composition of compounds without any prior information about the system. We will discuss results for various systems including the prediction of unexpected quasi-1D and 2D electronic structures in Li-Be compounds under pressure [1] and of the crystal structure of the superconducting high-pressure phase of Eu [2]. The self-assembly of nanocrystals into mesoscale superlattices provides a path to the design of materials with tunable electronic, physical and chemical properties for various applications. The self-assembly is controlled by the nanocrystal shape and by ligand-mediated interactions between them. To understand this, it is necessary to know the effect of the ligands on the surface energies (which tune the nanocrystal shape), as well as the relative coverage of the different facets (which control the interactions). Density functional calculations for the binding energy of oleic acid-based ligands on PbSe nanocrystals determine the surface energies as a function of ligand coverage. The Wulff construction predicts the thermodynamic equilibrium shape of the PbSe nanocrystals as a function of the ligand coverage. We show that the different ligand binding energies on the 100 and 111 facets results in different ligand coverages on the facets and predict a transition in the equilibrium shape from octahedral to cubic when increasing the ligand concentration during synthesis. Our results furthermore suggest that the experimentally observed transformation of the nanocrystal superlattice structure from fcc to bcc is caused by the preferential detachment of ligands from particular facets, leading to anisotropic ligand coverage [3].

[1] J. Feng, R. G. Hennig, N. W. Ashcroft and Roald Hoffmann. Nature 451, 445 (2008).

[2] W. Bi, Y. Meng, R. S. Kumar, A. L. Cornelius, W. W. Tipton, R. G. Hennig, Y. Zhang, C. Chen, and J. S. Schilling. Phys. Rev. B 83, 104106 (2011).

[3] J. J. Choi, C. R. Bealing, K. Bian, K. J. Hughes, W. Zhang, D.-M. Smilgies, R. G. Hennig, James R. Engstrom, and Tobias Hanrath. J. Am. Chem. Soc. 133, 3131 (2011).

¹Supported in part by the National Science Foundation through TeraGrid computational resources under Grant No. DMR050036

3:42PM D10.00003 Scalable DAG-Based PDE Frameworks for Multi-Scale Multi-Physics Problems¹, MARTIN BERZINS, SCI Institute University of Utah, Salt Lake City, Utah — The task-based approach to software and parallelism is well-known and has been proposed as a potential candidate, named the silver model, for exascale software. This approach is not yet widely used in the large-scale multi-core parallel computing of complex systems of partial differential equations. The central idea is to use a Directed Acyclic Graph (DAG) based approach to express the structure of the underlying software. The aim of this talk is to explore the usefulness of DAG based approaches, using recent developments in the parallel Uintah software framework for partial differential equations to assess how well the DAG type approach works on present-day large-scale architectures for complex multi-physics multiscale applications up to 200K cores. As a result of these investigations, a preliminary and tentative evaluation of the DAG type approach for PDE software infrastructures will be given. The conclusion is that these approaches show great promise for petascale but that considerable algorithmic challenges remain.

¹Support from NSF PetaApps and DOE NETL and INCITE is acknowledged

4:18PM D10.00004 Simulations of Strongly Correlated Systems¹, JUANA MORENO, Louisiana State University

— The field of strongly correlated systems is one of the most active areas in condensed matter physics. This interest is motivated, in part, by a variety of complex emergent phenomena, including high-temperature superconductivity, quantum criticality and complex phases induced by electron-phonon couplings. The recent very rapid development of high performance heterogeneous computer platforms together with a similar emergence of highly accurate many-body algorithms allow the treatment and modeling of complex correlated material systems which were intractable just a few years ago. Important progress has been made by the development of finite size methods, including exact diagonalization and Quantum Monte Carlo techniques. However, due to the minus sign problem, these methods are limited to small lattice sizes. Another successful approach is the dynamical mean field approximation and its cluster extensions, which treat the local or short-ranged dynamical correlations exactly and non-local or long-ranged correlations in a mean field approximation. Due to the effective medium, the Fermion minus sign problem is much milder than that found in finite sized simulations. However, it is still the primary limitation of these methods. To address this problem, multiscale approaches are used which treat only the correlations at the shortest length scales with exact cluster solvers, intermediate length scales are treated using a diagrammatic approach, such as the parquet equations or the dual-fermion formalism and, the longest length scales are captured by the mean field. I will discuss how these new algorithms impact a few model systems including our understanding of quantum criticality in the Hubbard and Anderson model, new phases in ultracold quantum gases, spintronics materials and the role of electron-phonon interaction. I will conclude discussing recent algorithm redesign motivated by the evolution towards hybrid multicore architectures employing graphical processing unit (GPU).

¹This research is supported by DOE SciDAC DE-FC02-06ER25792, NSF OISE-0952300 and EPS-1003897, and by XSEDE TG-DMR100007.

4:54PM D10.00005 Accessing correlated electron motion on the attosecond timescale, JOHANNES FEIST, ITAMP, Harvard-Smithsonian Center for Astrophysics

— In the last decade, there have been tremendous advances in the production of coherent ultrashort light pulses as short as 80 attoseconds ($1 \text{ as} = 10^{-18} \text{ s}$). The availability of these pulses has led to the development of the field of attosecond physics, which aims to follow and control electron motion on its natural timescale (1 atomic unit of time is about 24 attoseconds). One of the major goals of attosecond physics is to access correlated electron dynamics. This requires a description of the target system that goes beyond the commonly used single-active-electron approximation. The large bandwidth of ultrashort pulses and many-photon absorption in strong infrared fields make such a description extremely challenging. I will discuss our work on the full numerical solution of the two-electron Schrödinger equation for helium, which already displays rich correlation effects. I will focus on two applications: The first is attosecond streaking, in which temporal information about the photoionization process in an attosecond pulse is mapped into a momentum shift by a synchronized infrared pulse. This promises to give access to the Eisenbud-Wigner-Smith time delay of photoionization. I will discuss the additional effects that are induced by the infrared field, and how these have to be taken into account for attosecond streaking to fulfill its promise. I will then discuss the possibility of accessing two-electron wave packet dynamics in doubly excited states of helium by an attosecond pump-attosecond probe setup. Such experiments have been called the “holy grail” of attosecond physics and should come within reach in the near future. I will discuss our recent proposal of using two-photon absorption from a single pulse as a coherent reference wave, which can be used to increase the experimental signal by almost two orders of magnitude. This provides direct access to time-dependent observables (e.g., the distance between the two electrons) of the two-electron wave packet.

Monday, February 27, 2012 2:30PM - 5:30PM –

Session D11 DMP: Focus Session: Graphene Structure, Stacking, Interactions: Mesoscopics

210B

2:30PM D11.00001 Electronic localization in rotated graphene multi-layer, GUY TRAMBLÉ DE LAIS-

SARDIERE, Cergy-Pontoise University, OMID FAIZY NAMARVAR, DIDIER MAYOU, LAURENCE MAGAUD, Institut Néel CNRS — Rotated graphene bilayers show an interesting electronic structure with a tendency to layer decoupling at large rotation angles and a stronger electronic mixing at small angles, associated with a strong decrease of the velocity ([1] and Refs. therein). These inter-layer mixed states allow us [2] to address the long lasting problem of the origin of the Moiré pattern observed on STM images. For large and intermediate rotation angles, we present analytical and numerical studies of the local density of states in the Moiré that compare well to STM spectra. For very small angles, the inter-layer mixed states ultimately lead to electronic confinement in AA stacking regions in an energy range close to the Dirac point. In graphene multi-layer (up to 10 layers) containing twisted intercalated layers [3], we found both bands with a strong velocity reduction, and bands without velocity reduction. This could explain [2] why velocity renormalization is not observed experimentally in rotated multi-layers on SiC [3,4].

[1] G. Trambly de Laissardière et al., Nano Lett. 10, 804 (2010).

[2] G. Trambly de Laissardière et al., in preparation.

[3] M. Sprinkle et al., J. Phys. D: Appl. Phys. 43, 374006 (2010).

[4] M. Sprinkle et al., Phys. Rev. Lett. 103, 226803 (2009).

2:42PM D11.00002 Interferences and Fabry-Perot Oscillations in ABA Trilayer Graphene,

LEONARDO CRISTIANO CAMPOS, KAWIN SURAKITBOVORN, Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139 USA, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Namiki 1-1, Tsukuba, Ibaraki 305-0044, Japan, PABLO JARILLO-HERRERO, Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139 USA, DEPARTMENT OF PHYSICS, MASSACHUSETTS INSTITUTE OF TECHNOLOGY/NATIONAL INSTITUTE FOR MATERIALS SCIENCE TEAM — ABA trilayer graphene (TLG) is a 2D system with multiple sub-bands which can be divided into one monolayer graphene-like sub-band and one bilayer graphene-like sub-band, therefore comprising a system wherein massive and massless bands coexist. Here, we study electronic transmission in the ballistic regime through a 70nm-wide tunable electrostatic potential barrier on exfoliated ABA trilayer graphene encapsulated by hexagonal Boron Nitride. We report Fabry-Perot oscillations of the conductance caused by multiple reflections of the charges in the potential barrier, and we also present a study of their magneto dependence.

2:54PM D11.00003 Quantum Pumping in Graphene Nanoribbons¹, TEJINDER KAUR, Dept. of Physics and

Astronomy, Ohio University, LILIANA ARRACHEA, Dept. de Física, Universidad de Buenos Aires, Argentina, NANCY SANDLER, Dept. of Physics and Astronomy, Ohio University — The interest in the development of devices at the nanoscale has intensified the search for mechanisms that provide control of transport properties while reducing effects of heat dissipation and contact resistance. Charge pumping, in which dc currents are generated in open-quantum systems by applying local de-phased time-dependent potentials, may achieve these goals. We analyze the properties of non-equilibrium zero-bias currents through nano-ribbons using a tight-binding Hamiltonian and the Keldysh formalism beyond the adiabatic and perturbative regimes. Using a numerical implementation with two local single-harmonic time-dependent potentials, we first contrast results for 1d and 2d metallic systems (square lattice). Next, we focus on quasi-1d systems and graphene ribbons, and discuss the role of reservoirs. We analyze the dependence of the dc pumped current as a function of different parameters such as chemical potential, pumping amplitude, and frequency. We observe a considerable increase of pumped current with the dimensionality of the system. Furthermore, we show that lattice mismatch with reservoirs favors the pumping mechanism for graphene ribbons.

¹Supported by NSF-PIRE and NSF-MWN/CIAM

3:06PM D11.00004 Conductance fluctuations in graphene as a probe of broken-symmetry and fractional quantum Hall states, JURGEN SMET, Max Planck Institute for Solid State Research — The observation in macroscopic transport studies of the interaction induced broken symmetry and fractional quantum Hall states in graphene normally requires very clean samples and/or strong magnetic fields. Here we report that even when these fragile states are not developed well enough to produce any of the quantum Hall signatures, they are strongly visible in differential conductance fluctuations that appear as a result of charge carrier localization when the system breaks up into compressible islands with incompressible areas in between when the corresponding integer or fractional filling factor is approached. The conductance fluctuations give access to local information even though a macroscopic measurement is performed. The existence of a landscape of compressible islands is unambiguously proved in Coulomb blockade phenomena in the quantum Hall insulating regime where all other conduction channels are switched off. This work has been carried in collaboration with D.S. Lee, V. Skakalova, R.T. Weitz, K. von Klitzing.

3:42PM D11.00005 Interference of electronic states between the two misoriented crossed graphene nanoribbons¹, K.M. MASUM HABIB, ROGER LAKE, Dept of Electrical Engineering, Univ of California Riverside — In a twisted bilayer graphene, where one layer is rotated with respect to the other one, for rotation angles more than 20 degrees each layer remains electronically decoupled even though they are vertically separated by only a fraction of a nanometer. A relative rotation between two graphene nanoribbons (GNRs), with one place on top of the other, creates a crossed GNR (xGNR) with an overlap region that is neither AA nor AB stacking. The geometry of the overlap region of the xGNR is that of a twisted bilayer graphene. Calculations, based on the extended Huckel theory and the non-equilibrium Green's function formalism, show that the electronic states of the individual GNRs of an unbiased xGNR are decoupled from each other similar to the decoupling that occurs in a twisted bilayer graphene. The decoupling occurs due to the quantum mechanical interference between the electronic states of the individual GNRs. This results in a strong suppression of inter-GNR transmission over a large energy of window. The transmission is, however, a strong function of the potential difference between the GNRs and the atomistic geometry of the overlap region which depends on relative translation and rotation angle between the GNRs. Thus, a bias can be used to control the inter-GNR current.

¹This work is supported by the Microelectronics Advanced Research Corporation Focus Center on Nano Materials (FENA).

3:54PM D11.00006 Gap opening in graphene by 1D and 2D periodic corrugations, IVAN NAUMOV, ALEXANDER BRATKOVSKY, Hewlett-Packard Laboratories, 1501 Page Mill Road, Palo Alto, California 94304, USA — Using first-principles methods and symmetry arguments, we show that a graphene monolayer, which is periodically corrugated in one or two direction(s), can be either semimetal or semiconductor, depending on how strong corrugation is or how the initial symmetry is broken. In the case of 1D periodic ripples, a gap at the Dirac points opens up only due to (i) breaking of the inversion symmetry or equivalence between A and B sublattices and/or (ii) merging of two inequivalent Dirac points, **D** and **-D**. Since breaking the inversion symmetry has only relatively modest effect, a tangible gap can be mainly induced by mutual annihilation of the Dirac points, which requires large corrugations, close to mechanical breaking point. In contrast to 1D, the 2D ripples can additionally induce a semiconducting gap via mixing of electronic states belonging to two different **K**, **K'** valleys. In this case, a gap on the order of 0.5 eV can be opened up at strains safely lower than the graphene failure strain [1].

[1] I.I. Naumov, A.M. Bratkovsky, arXiv:1104.0314v1.

4:06PM D11.00007 Electronic structure and energetics of graphene antidot lattice, MASAHIRO SAKURAI, Institute for Solid State Physics, University of Tokyo, SUSUMU SAITO, Department of Physics, Tokyo Institute of Technology, YASUTAMI TAKADA, Institute for Solid State Physics, University of Tokyo — We have made a systematic study of the electronic structure and the energetics of graphene with periodic array of vacancy clusters (graphene antidot lattice) in the framework of the density-functional theory (DFT). We find that the electronic property of the system is well controlled by its lattice periodicity. More specifically, this system can be either metallic or semiconducting, depending on its lattice geometry. Interestingly, some of them are predicted to be direct-gap semiconductors. For example, graphene sheet with high-symmetry arrangements of periodic circle-shape vacancies always has a direct fundamental gap [1]. The DFT total-energy calculations indicate that the geometry of hole edges plays an important role in determining its stability. [1] "Electronic properties of graphene and boron-nitride based nanostructured materials" M. Sakurai, Y. Sakai, and S. Saito, J. Phys.: Conf. Ser. 302 (2011) 012018.

4:18PM D11.00008 ABSTRACT WITHDRAWN —

4:30PM D11.00009 Localization and Conductivity of Graphene with Adsorbates, DIDIER MAYOU, Institut Néel, CNRS, GUY TRAMBLAY DE LAISSARDIERE, Cergy-Pontoise University — We compute the conductivity of graphene for two models of resonant and non resonant adsorbates. Away from the Dirac point the conductivity is well given by the semi-classical Drude formula and localization lengths are exponentially large. For some energies, near the Dirac point, the conductivity is well represented by $\sigma \simeq 4e^2/\pi h - \alpha \text{Log}(L_i/L_e)$ as a function of the inelastic scattering length L_i and the elastic mean free path $L_e < L_i$. This implies a magneto-conductivity that varies also linearly with $\text{Log}(B)$ where B is the magnetic field. Our results suggest that the divergence of the localization length which is expected close to the Dirac point affects only a narrow energy region.

4:42PM D11.00010 Effects of disorder on recombination and relaxation processes via acoustic phonons in graphene, FEDIR VASKO, VLADIMIR MITIN, ANDREI SERGEEV, SUNY at Buffalo — Recombination and relaxation processes via acoustic phonons are allowed in a disordered graphene because of violation of the energy-momentum conservation requirements. These processes are analyzed taking into account the interference of electron-phonon and electron-impurity scattering mechanisms. The recombination and relaxation rates are calculated for the cases of intrinsic and heavily-doped graphene. The transient evolution of nonequilibrium carriers is described by the exponential fit dependent on doping conditions and disorder level. The obtained electron recombination and relaxation rates are compared with available experimental data. [1] F. Vasko et al., Phys. Rev. B 84, 155445 (2011).

4:54PM D11.00011 Phase coherent states in graphene heterostructure with chiral asymmetry¹, JUNHUA ZHANG, ENRICO ROSSI, Department of Physics, College of William and Mary — The chiral nature of the fermionic excitations in graphene, bilayer graphene, and topological insulators, induces unique electronic properties in these materials. In bilayer heterostructures the interlayer interaction can induce the formation of an interlayer phase coherent state. An interesting class of heterostructures is constituted by bilayers in which the electrons in the two layers have different chirality. An example of such a system that can be realized experimentally is the heterostructure formed by single layer graphene and bilayer graphene. In this talk I will discuss the conditions for the realization of an interlayer phase-coherent state in chiral-asymmetric heterostructures. In particular I will show how the voltage difference between the two layers affects the conditions for the realization of the phase coherent state, and its properties. I will then discuss the relevance for experiments of our results.

¹Work supported in part by the Jeffress Memorial Trust, Grant No. J-1033

5:06PM D11.00012 Visualizing Electronic Chirality and Berry's Phases in Graphene Systems Using Photoemission with Circularly Polarized Light, YANG LIU, GUANG BIAN, TOM MILLER, TAI-CHANG CHIANG, University of Illinois, Urbana-Champaign — Electronic chirality near the Dirac point is a key property of graphene systems, which is revealed by the spectral intensity patterns as measured by angle-resolved photoemission spectroscopy under various polarization conditions. Specifically, the strongly modulated circular patterns for monolayer (bilayer) graphene rotate by ± 90 degrees (± 45 degrees) in changing from linearly to circularly polarized light; these angles are directly related to the phases of the wave functions and thus visually confirm the Berry's phase of π (2π) around the Dirac point. The details are verified by calculations.

5:18PM D11.00013 Electronic Properties of Curved Graphene-Ring Structures¹, DAIARA FARIA, Ohio University / Universidade Federal Fluminense, Brazil, ANDREA LATGÉ, Universidade Federal Fluminense, Brazil, SERGIO ULLOA, NANCY SANDLER, Ohio University — Recently, deformed graphene in the form of bubbles have been produced on different substrates in a variety of controllable shapes [1]. These findings raise the possibility of changing the electronic properties of these structures allowing for band-structure engineering. We have undertaken a study of the electronic properties of graphene-ring systems with circularly symmetric Gaussian curvature in the Dirac approximation. We obtain energy spectra and wave functions using perturbation theory on the gauge field amplitude describing the curvature. We further analyze the competition between curvature-induced magnetic field and real external fields and the resulting persistent currents generated in their presence. As expected, the results depend on the boundary conditions describing the confined ring edges. In addition, we discuss the effects of the angular asymmetry in the probability density due to the curvature [2] on single rings and more complex confined annular geometries.

[1] T. Georgiou et al., APL 99

[2] Wakker et al., PRB 84.

¹Supported by Capes and NSF - MWN/CIAM

Monday, February 27, 2012 2:30PM - 5:30PM – Session D12 DMP: Graphene Transport: Disorder Scattering 210C

2:30PM D12.00001 Theory of 2D Transport in Graphene for Correlated Disorder¹, QIUZI LI, EUYHEON HWANG, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742, USA, ENRICO ROSSI, Department of Physics, College of William and Mary, Williamsburg, Virginia 23187, USA, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742, USA — We theoretically revisit graphene transport properties as a function of carrier density, taking into account possible correlations in the spatial distribution of the Coulomb impurity disorder in the environment. We find that the charged impurity correlations give rise to a density-dependent graphene conductivity, which agrees well qualitatively with the existing experimental data. We also find, quite unexpectedly, that the conductivity could increase with increasing impurity density if there is sufficient interimpurity correlation present in the system. In particular, the linearity (sublinearity) of graphene conductivity at lower (higher) gate voltage is naturally explained as arising solely from impurity correlation effects in the Coulomb disorder.

¹Work supported by ONR-MURI, NRI-SWAN and CNAM

2:42PM D12.00002 Simultaneous Raman and electrical transport measurements of disordered graphene in situ in ultra-high vacuum¹, JACOB TOSADO, University of Maryland, VINCE BALLAROTTO, Laboratory for Physical Sciences, WILLIAM G. CULLEN, MICHAEL S. FUHRER, University of Maryland — Resonant Raman scattering in graphene gives unique information about disorder, as the D peak is observed only in the presence of disorder which produces intervalley scattering of the electrons. The nature of disorder in graphene prepared by various techniques and on various substrates of the subject of significant research, with significant attention being paid to scattering by charged impurities; resonant scatterers due to vacancies, chemisorbed impurities, etc.; and non-resonant short-range impurities. In order to study the effect of these types of disorder on graphene's electronic properties and Raman spectra simultaneously, we have developed a facility combining thermal deposition, ion bombardment, electrical transport and micro-Raman measurements in an ultra high vacuum environment. We will discuss the capabilities of this facility and present the results of Raman and electrical transport measurements on controllably disordered graphene.

¹This work was supported by the Laboratory for Physical Sciences, and an NRI supplement to the UMD-NSF-MRSEC grant DMR 0520471

2:54PM D12.00003 Creating Vacancies in Supported and Suspended Graphene Field Effect Transistors, SHUREN HU, A.K.M. NEWAZ, ANTHONY HMELO, KIRILL BOLOTIN, Vanderbilt University — We have studied the creation of vacancy defects in both graphene samples supported on SiO₂ substrate and suspended graphene devices. The defects were created by irradiating graphene with a 30KeV Ga⁺ ion beam in UHV; the effect of these defects on electrical transport in graphene was measured *in situ*. We find that the number of defects created in supported devices is dramatically higher in comparison with suspended devices. Using Monte-Carlo and SRIM simulations, we identify the formation of defects by secondary ions in the case of supported devices as a likely explanation of these results. We have also observed that the transport quality degrades drastically with respect to vacancy defect density and follows the same general trend for both supported and suspended graphene. These results may be important in designing devices for high radiation working environments, such as space electronics.

3:06PM D12.00004 Scattering mechanisms in graphene suspended in liquids. II. Flexural phonons (Theory)¹, YEVGENIY PUZYREV, A.K.M. NEWAZ, BIN WANG, KIRILL BOLOTIN, SOKRATES PANTELIDES, Physics and Astronomy Department, VANDERBILT UNIVERSITY COLLABORATION — Recent experiments reported strong scattering of charge carriers by flexural phonons in suspended graphene in vacuum.² Our experimental data (previous talk) show that the carrier mobility observed for devices immersed in non-polar liquids, namely toluene and hexane, are significantly larger than the mobility limitation due to scattering by flexural phonons. We performed molecular dynamics simulations of graphene sheets suspended in hexane, toluene, and in vacuum at room temperature. We find that the interaction of molecules of the liquid with graphene suppresses the amplitude of the phonons by $\sim 50\%$. We show computationally that this suppression is equivalent to an effective increase of the bending rigidity³ of graphene from a free-space value ~ 1.3 eV in vacuum to ~ 3.6 eV in liquids. Therefore, we demonstrated that scattering by out-of-plane flexural phonons is reduced by the presence of liquids.

¹NSF CAREER DMR-1056859 and DTRA grant HDTRA1-10-0047.

²Castro E. V., *et al.*, "Limits on Charge Carrier Mobility in Suspended Graphene due to Flexural Phonons," Phys. Rev. Lett. 105, 266601, 2010.

³Fasolino A., Los J. H., Katsnelson M. I., "Intrinsic ripples in graphene," Nature Mat. 6, 858, 2007.

3:18PM D12.00005 Scattering mechanisms in graphene suspended in liquids. I. Coulomb scattering (Experiment), A.K.M. NEWAZ, YEVGENIY PUZYREV, BIN WANG, SOKRATES PANTELIDES, KIRILL BOLOTIN, Vanderbilt University — Enhanced dielectric screening of charged impurities by high- κ environment of graphene is predicted to improve the electronic quality of graphene devices by suppressing Coulomb scattering. However, experiments reported so far demonstrate that electronic transport in graphene is only modestly modified by a high- κ environment. Here we fabricate large area multiterminal graphene devices suspended in liquids and study electronic transport in graphene as a function of liquid's dielectric constant. We observe a rapid increase of mobility μ with κ due to dielectric screening in non-polar solvents ($\kappa \leq 5$). We also find that charged ions present in polar solvents ($\kappa \geq 18$) cause a drastic drop in mobility counteracting the gains by dielectric screening in polar high- κ liquids. Furthermore, molecular dynamics simulations establish that scattering by out-of-plane flexural phonons is suppressed by the presence of liquids (next talk). We expect that our findings may provide avenues to control and reduce carrier scattering in future graphene-based electronic devices.

3:30PM D12.00006 Short range disorder in Graphene: A Green's function based approach¹, SANKALPA GHOSH², Physics Department, IIT Delhi, New Delhi-110016, India, NEETU AGGARWAL (GARG), MANISH SHARMA, Center for Applied Research in Electronics, IIT Delhi, New Delhi-110016, India — Electrons at the Fermi level in graphene monolayer behave like massless Dirac fermions. Using Green's function based technique we study the transport of such electrons in the presence of randomly located electrostatic impurities in different geometries and compare such transport in graphene with the transport in conventional semiconductors. This study would eventually be used to mimic short range disorder that would be superimposed on a regular structure. Comparison with the optical phenomena will be used to understand such transport. We further extend this technique to study the transport in the presence of magnetic scatterers.

¹SG and MS are supported by SERC division, Department of Science and Technology, Govt. of India, NA is supported by CSIR, India

²The first author is an Assistant professor, the second author is a graduate student, the third author is an Associate Professor

3:42PM D12.00007 Universal conductance fluctuations in Dirac materials in the presence of long-range disorder¹, E. ROSSI, Department of Physics, College of William and Mary, Williamsburg, VA 23187, USA, J.H. BARDARSON, Department of Physics, University of California, Berkeley, CA 94720, USA; Materials Sciences Division, LBNL, Berkeley, M.S. FUHRER, CNAM, Department of Physics, University of Maryland, College Park, MD 20742-4111, USA, S. DAS SARMA, CMTC, Department of Physics, University of Maryland, College Park, MD 20742-4111, USA — We study quantum transport in Dirac materials with a single fermionic Dirac cone (strong topological insulators and graphene in the absence of intervalley coupling) in the presence of long-range disorder [1]. We show, by calculating the conductance fluctuations, that in the limit of very large system size and disorder strength, quantum transport becomes universal. However, a systematic deviation away from universality is obtained for realistic system parameters. By comparing our results to existing experimental data on $1/f$ noise, we suggest that many of the graphene samples studied to date are in a non-universal crossover regime of conductance fluctuations, and provide an explanation for the origin of the $1/f$ noise in Dirac materials and in graphene in particular.

[1] E. Rossi, J. H. Bardarson, M. S. Fuhrer, S. Das Sarma, *Universal conductance fluctuations in Dirac materials in the presence of long-range disorder*. arXiv:1110.5652v1 (2011)

¹Work supported by the Jeffress Memorial Trust, Grant No. J-1033 (ER), DOE DE-AC02-05CH11231 (JHB), ONR-MURI (SDS, MSF), and NRI-SWAN (SDS).

3:54PM D12.00008 Diamagnetism of Graphene with Long-Range Scatterers, MASAKI NORO, Department of Physics, Tokyo Institute of Technology, MIKITO KOSHINO, Department of Physics, Tohoku University, TSUNEYA ANDO, Department of Physics, Tokyo Institute of Technology — We study weak-field orbital susceptibility of graphene containing scatterers with long-ranged potential. The effects of scattering from such impurities are taken up self-consistently by using Green's function technique within a self-consistent Born approximation. To see dependence on the potential range, we consider scatterers with a Gaussian potential and screened charged impurities. Because Green's function or self-energy for long-range impurities strongly depends on wave vector, we have to numerically calculate Green's function and vertex functions. In graphene, the susceptibility diverges at the Dirac point as a delta function of the Fermi energy. For the Gaussian potential, results show that the delta function in the ideal graphene is broadened by disorder, due to the mixing between the states at the Dirac point and other states. The susceptibility as a function of the Fermi energy rapidly decreases away from the Dirac point, with effective width determined by the potential range. As the scattering strength increases, the peak at the Dirac point is less prominent and the susceptibility has a long tail, corresponding to the strong mixing among states due to scattering. These behaviors are obtained only when the vertex corrections are properly taken into account. For charged impurities, the susceptibility shows a double-peak structure caused by the strong variation of the effective scattering strength as a function of the Fermi energy.

4:06PM D12.00009 Current decay rate due to electron-electron scattering in graphene, BEN YU-KUANG HU, The University of Akron — Electron-electron scattering in graphene does not conserve electrical current, because of the linear dispersion of the bands in graphene near the Dirac point. In graphene, when two electrons with initial momenta $\mathbf{k}_1$ and $\mathbf{k}_2$ undergo electron-electron scattering to final states $\mathbf{k}'_1$ and $\mathbf{k}'_2$, in general the total current $\mathbf{v}(\mathbf{k}_1) + \mathbf{v}(\mathbf{k}_2) \neq \mathbf{v}(\mathbf{k}'_1) + \mathbf{v}(\mathbf{k}'_2)$ [see e.g., Li *et al.*, Appl. Phys. Lett. **97**, 082101 (2010)]. We calculate the electric current relaxation rate due to the electron-electron scattering of an electron that is injected into extrinsic graphene at low temperature. When the energy of injected electron relative to the Fermi energy is small compared to the Fermi energy, the current decay rate is small due to phase-space restrictions. The current decay rate grows monotonically as the energy of the injected electron increases.

4:18PM D12.00010 Electron energy relaxation in disordered graphene via e-phonon interaction, WEI CHEN, AASHISH CLERK, McGill University — Motivated by recent experiments, we study theoretically the energy relaxation of hot electrons in disordered graphene via electron-phonon interactions. In contrast to previous treatments [1], we explicitly treat the effects of electronic disorder. Using the Keldysh diagram technique, and including vertex corrections, we identify various mechanisms through which disorder can significantly change the magnitude and temperature dependence of the electronic energy relaxation rate. [1]Felix Von Oppen, Francisco Guinea, Eros Mariani, Phys. Rev.B **80**, 075420 (2009)

4:30PM D12.00011 Electron scattering at graphene edges, S.-J. CHOI, SUNGHUN PARK, H.-S. SIM, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea, QUANTUM ELECTRON TRANSPORT THEORY GROUP TEAM — We theoretically study the reflection of electrons at edges in monolayer graphene in a low-energy limit. We consider both of zigzag and armchair edge cases. We find that in the case of zigzag edge, the reflection phase is determined by the rotation of electron pseudospin during the reflection, which is attributed to the chirality between the pseudospin and the electron momentum. On the other hand, in the case of armchair edge, the reflection phase does not contain the information of pseudospin rotation, because of intervalley mixing. The pseudospin rotation can be detected via the measurement of reflection phase in an interferometry setup in graphene with zigzag edge.

4:42PM D12.00012 Highly Defective Graphene: The thinnest insulating membrane¹, AURELIEN LHERBIER², UCL/IMCN/NAPS, STEPHAN ROCHE³, CIN2/ICN-CSIC and Universitat Autònoma de Barcelona, OSCAR A. RESTREPO, UCL/IMCN/BSMA, YANN-MICHEL NIQUET, CEA-UJF/INAC/SP2M/L-Sim, ARNAUD DELCORTE, UCL/IMCN/BSMA, JEAN-CHRISTOPHE CHARLIER, UCL/IMCN/NAPS — The electronic structure and transport properties of two-dimensional highly defective sp² graphene are investigated theoretically. Using classical molecular dynamics, large planes of highly defective graphene-based sheets are first generated. An accurate empirical tight-binding Hamiltonian is then elaborated, allowing the prediction of elastic mean free paths, conductivities, and charge mobilities using a real-space order-N Kubo-Greenwood method. In sharp contrast to pristine graphene, the highly defective sp² carbon sheet displays high density of states close to the Dirac energy. However, the dynamics of the corresponding electronic wavepackets reveals extremely short mean free paths (below 1 nanometer) and quantum interferences, both yielding to particularly strong localization phenomena. Consequently, these highly defective graphene-based sheets, although exhibiting a metallic character through the density of states, are from an electronic transport perspective among the most insulating two-dimensional one-atom-thick membrane ever made.

¹Belgium FNRS, PAI6, ARC 11/16-037, ETSF e-I3 211956, ANR 09-NANO-016-01

²Université catholique de Louvain, Institute of Condensed Matter and Nanoscience. ETSF-European Theoretical Spectroscopy Facility

³Catalan Institute of Nanotechnology, campus UAB ICREA, Barcelona

4:54PM D12.00013 Boundary scattering in quasi-ballistic graphene/hexagonal boron nitride mesoscopic wires, KAZUYUKI IGUCHI, Institute of Industrial Science, University of Tokyo, SATORU MASUBUCHI, IIS and Institute for Nano Quantum Information Electronics, University of Tokyo, TAKEHIRO YAMAGUCHI, MASAHIRO OHNUKI, Institute of Industrial Science, University of Tokyo, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, TOMOKI MACHIDA, IIS and INQIE, University of Tokyo, and PRESTO-JST — In a quasi-ballistic transport regime where the mean free path is larger than the width of conduction channel, diffusive boundary scattering results in an anomalous positive magnetoresistance due to a magnetic commensurability effect between cyclotron motion and sample width. In this work, we fabricate a high-mobility two terminal graphene mesoscopic wire on hexagonal boron nitride with a mean free path comparable to sample width $\sim 1 \mu\text{m}$. Magnetoresistance of the graphene mesoscopic wire shows a peak structure at a magnetic field which scales with the ratio of the cyclotron radius R_c to the wire width w . The peak field increases with back-gate voltage as a consequence that the ratio w/R_c is modified due to the change in R_c . These results indicate the quasi-ballistic transport and diffusive boundary scattering in graphene on hexagonal boron nitride.

5:06PM D12.00014 Effects of disorder induced scattering in chemical vapor deposited Graphene., MING-YANG LI, CHIU-CHUN TANG, Dep. Of Physics, National Tsing Hua University, Taiwan, LAIN-JONG LI, Research Center for Applied Sciences, Academia Sinica, CHENG-CHUNG CHI, JENG-CHUNG CHEN, Dep. Of Physics, National Tsing Hua University, Taiwan — The effect of the short-range scatters in chemical vapor deposited (CVD) graphene on the quantum interference effect of carrier scattering remains to be an interesting question. We study the magneto-resistance and low-frequencies noise of our CVD graphene by varying carrier density and temperature. Unlike previous studies of exfoliated clean graphene flakes, we have found in the vicinity of the Dirac-point (DP) WL signal cannot be fully described in terms of breaking the valley symmetry due to trigonal warping of the bands and atomically sharp disorder [1,2]. The discrepancy regime is coincident with the suppression of noise figures and the vanishing of Hall coefficient. Our data suggest that in low mobility CVD graphene an extra inter-valley elastic scattering process should be considered under the theoretical basis in Ref.1. More detailed experimental results and theoretical analysis will be presented and discussed. Ref[1]: E. McCann, et al., Phys. Rev. Lett. 97 146805(2006) Ref[2]: J.Phys. : Condens. Matter 22 205301 (2010)

5:18PM D12.00015 Efros-Shklovskii Variable Range Hopping in Reduced Graphene Oxide Sheets, DAEHA JOUNG, Nanoscience Technology Center and Department of Physics, University of Central Florida, SAIFUL I. KHONDAKER, Nanoscience Technology Center, Department of Physics, School of Electrical Engineering and Computer Science, University of Central Florida — Reduced graphene oxide (RGO) sheets consist of highly ordered graphene domain and structural defects including oxidized carbon atoms and topological defects. Charge transport properties of RGO sheets are strongly influenced by the degree of disorderliness which can be tuned by varying the amount of the reduction. We studied the hopping conduction of the RGO sheets with different reduction efficiency. We show that the low temperature charge transport properties of the RGO with various reduction efficiency can be well described by Efros-Shklovskii variable range hopping (ES VRH), $\rho \sim \exp[-(T/T)^{1/2}]$. We will discuss how the localization length varies with the degree of reduction. The result indicates that the coulomb interactions between graphene domains play an important role in the charge transport of the RGO sheets.

Monday, February 27, 2012 2:30PM - 5:30PM –
Session D13 DMP GMAG: Focus Session: Magnetic Nanostructures-Characterization (Scanning Probe, X-ray and Neutron) 211

2:30PM D13.00001 STM Studies of Mn₁₂-Ph on Highly Oriented Pyrolytic Graphite, K. REAVES, Department of Physics and Astronomy, Texas A&M University; WPI-AIMR, Tohoku University, Japan, K. KIM, K. IWAYA, T. HITOSUGI, Y.G. KIM, K. ITAYA, WPI-AIMR, Tohoku University, Japan, H. ZHAO, K.R. DUNBAR, Department of Chemistry, Texas A&M University, H.G. KATZGRABER, Department of Physics and Astronomy, Texas A&M University; ETH Zurich, W. TEIZER, Department of Physics and Astronomy, Texas A&M University; WPI-AIMR, Tohoku University, Japan — Mn₁₂-Ph displays tunneling of quantized magnetization below 3K. In other Mn₁₂ ligand variants this magnetic behavior can alter the electronic behavior of the molecule making it a good candidate for a molecular logic gate. Mn₁₂O₁₂(C₆H₅COO)₁₆ (Mn₁₂-Ph) has a Mn₁₂ core and 16 Phenyl ligands and is deposited onto the surface of highly oriented pyrolytic graphite (HOPG). The samples are then studied via scanning tunneling microscopy in air at 300K and in ultra high vacuum at 300K and 4.2K. At 300K, film formation is studied to optimize samples for subsequent low-temperature studies. Isolated objects are observed via STM on the surface, clearly distinct from the underlying graphite lattice. Topographic data are analyzed in an attempt to correlate apparent features to the internal molecular structure of Mn₁₂-Ph. Voltage spectra of locations thought to be associated with the molecular core are compared to other locations thought to be the HOPG and Phenyl. Spectroscopic data indicate a bias voltage dependence at locations associated with the internal molecular structure thought to be related to the metallic-core of the molecules.

2:42PM D13.00002 Room-temperature spin-polarized scanning tunneling microscopy of antiferromagnetic $\text{Mn}_3\text{N}_2(001)$ nanopylramids¹, KANGKANG WANG, ARTHUR SMITH, Ohio University Nanoscale and Quantum Phenomena Institute — Antiferromagnets play a key role in spintronic applications owing to the exchange bias effect. As devices miniaturize in size and dimension, novel magnetic structures dramatically different from the bulk often emerge. Here we apply spin-polarized scanning tunneling microscopy (SP-STM) at room temperature to study the local magnetization of antiferromagnetic nitride nanostructures. $\text{Mn}_3\text{N}_2(001)$ thin films have been grown on $\text{MgO}(001)$ substrates using molecular beam epitaxy and transferred *in situ* to a home-built SP-STM for magnetic imaging. Results show that the surface consists of alternating chemically in-equivalent atomic terraces. Using SP-STM with dI/dV mapping, different layers can be clearly discriminated due to their different conductances. These differences in conductance are a result of not only the different chemical environments, but also the spin ordering and broken symmetry at the surface. Contrary to expectations, a layer-wise alternating surface anisotropy in these nanopylramids is observed. The presented study enables further investigations of the interplay between growth defects and the formation of intriguing antiferromagnetic domains.

¹Authors gratefully acknowledge support from the U.S. DOE and the NSF.

2:54PM D13.00003 Atomic Force Microscopy Incorporated with Magnetic Sample Modulation: a new approach to detect the magnetic nanomaterials, JING-JIANG YU, Nanotechnology Measurements Division, Agilent Technologies, Inc., JAYNE GARNO, Department of Chemistry, Louisiana State University — A new imaging strategy using atomic force microscopy (AFM) for detecting magnetic nanomaterials with much higher spatial resolution and sensitivity than the traditional magnetic force microscopy (MFM) technique is developed [1,2]. This AFM-based imaging mode is referred to as magnetic sample modulation (MSM), since the flux of an AC-generated electromagnetic field is used to induce physical movement of magnetic nanomaterials on surfaces during imaging. The AFM is operated in contact mode using a soft, nonmagnetic tip to detect the physical motion of the sample. By slowly scanning an AFM probe across a vibrating area of the sample, the frequency and amplitude of vibration induced by the magnetic field is tracked by changes in tip deflection. Thus, the AFM tip serves as a force and motion sensor for mapping the vibrational response of magnetic nanomaterials. The investigations are facilitated by nanofabrication methods combining particle lithography with organic vapor deposition and electroless deposition of iron oxide to prepare designed test platforms of magnetic materials at nanometer length scales. Examples of detecting magnetic nanoparticles and magnetic biospecies at single molecular level will be presented [3,4].

[1] Li et al. Analytical Chemistry, 2009, 81, 4792-4802

3:06PM D13.00004 Uncompensated Magnetization in Antiferromagnets, and New Classification of Exchange Bias Systems, IGOR V. ROSHCHIN, Department of Physics and Astronomy and Materials Science and Engineering Program, Texas A&M University — Exchange bias (EB) is typically observed in a bilayer consisting of a ferromagnet (FM) and an antiferromagnet (AF) as a horizontal shift of the FM hysteresis loop. It is attributed to exchange coupling across the interface. Several experimental findings demonstrate, and most models agree that uncompensated magnetization (UM) in the AF plays an important role in EB. However, the origin of UM remains unknown for most EB systems. Using magnetometry and polarized neutron reflectivity (PNR) we observe UM in antiferromagnet-only, (110)- FeF_2 epitaxially grown on MgF_2 , thin-film samples. The PNR reveals the spatial distribution of the UM. This UM exhibits the so-called “intrinsic exchange bias”: a shift of the hysteresis loop of UM. This effect is similar to the “classical” EB observed in bilayers, except that here, it is observed in a single layer material. The surface is responsible for the macroscopically broken time-reversal symmetry, uncompensated magnetization (UM) in a nominally compensated antiferromagnet [1], and, ultimately, for a new magnetic state. In this magnetic state, zero remanent magnetization cannot be obtained isothermally, because the origin ($M(H=0)=0$) is outside of the major hysteresis loop. Using symmetry group arguments [1] and results of *ab-initio* calculations [2], we argue that it is an equilibrium state. Below T_N , the UM in FeF_2 is coupled to the bulk antiferromagnetic order parameter as supported by several experimental results, including high value of EB field, its temperature dependence, and the absence of the training effect. Based on the proposed origin of the UM and experimental observations for different EB systems, we discuss a new classification of exchange bias systems into two categories, explaining differences in the observed properties.

This work is done in collaboration with K. E. Badgley (TAMU), M. Zhernenkov (LANL and ANL), M. R. Fitzsimmons (LANL), M. Erekhinsky, I. K. Schuller (UCSD), K. D. Belashchenko (UNL), and A. H. Romero (CONACyT), and supported by Texas A&M University, TAMU-CONACyT Collaborative Research Grant Program, DOE, AFOSR, and NSF-9976899. PPPROALMEX-DAAD-CONACyT bi-national program. TACC at UT-Austin is acknowledged for providing HPC resources.

[1] K. D. Belashchenko, Phys. Rev. Lett. **105**, 147204 (2010).

[2] S. López-Moreno *et al.*, Phys. Rev. B (submitted).

3:42PM D13.00005 Modeling Scanning SQUID Magnetometry Images of Magnetic Dipoles, LISA QIAN, BEENA KALISKY, BRANNON KLOPFER, BO DWYER, KATHRYN MÖLER, Stanford University — Scanning superconducting quantum interference devices (SQUIDs) with sub-micron sized pick-up loops are the most sensitive detectors of local magnetic flux and can have spin sensitivities down to 100 $\mu\text{B}/\sqrt{\text{Hz}}$. This makes them the ideal candidate for detecting magnetic dipole signals from individual nanomagnets. However, because the image kernel of the SQUID is not usually well known, quantitative analysis of magnetometry images can often be difficult. By using similarly measured SQUID magnetometry of superconducting vortices, we show that it is possible to fit images of magnetic dipoles by combining images of two monopoles. This fitting technique allows us to extract the magnetic moment as well as the information on the spatial extent of the imaged dipole. To quantify the statistical errors of the fit and the systematic errors of the measurement, we fabricated and measured nanomagnet bars of different lengths. This analysis technique, in conjunction with scanning SQUID microscopy, can be used to study individual nanomagnets in a wide variety of fields, ranging from biology to condensed matter physics.

3:54PM D13.00006 ABSTRACT WITHDRAWN —

4:06PM D13.00007 Chemical Segregation in GdFeCo : An X-ray view on Magnetic Coercivity, ALEXANDER REID, SLAC National Accelerator Laboratory, CATHERINE GRAVES, BENNY WU, Dept. of Applied Physics, Stanford University, TIANHAN WANG, Stanford Institute for Materials and Energy Science, Stanford University, ALEXEY KIMEL, ANDREI KIRILYUK, Radboud University Nijmegen, The Netherlands, ARATA TSUKAMOTO, A. ITOH, Nihon University, Japan, JOACHIM STÖHR, SLAC National Accelerator Laboratory, THEO RASING, Radboud University Nijmegen, The Netherlands, HERMANN DÜRR, ANDREAS SCHERZ, SLAC National Accelerator Laboratory — The magnetic coercivity in intermetallic alloys is known to be dominated by microscopic inhomogeneities. These control the characteristics of magnetic switching as they provide nuclei for magnetic domain formation, and the pinning sites governing domain wall propagation. However, such regions exist on nanometer length scales with weak magnetic contrast to their surroundings; their characterization has therefore remained illusive. Here we demonstrate how resonant x-ray scattering is intrinsically sensitive to magnetic changes in a segregated phase. We utilize the fact that magnetic scattering asymmetry directly probes regions where this phase segregation occurs. Our measurements on GdFeCo show strongly temperature dependant magnetic canting in the segregated regions due to local changes in magnetic anisotropy. Understanding the origin and importance of these chemically segregated regions will allow a better understanding of the magnetic switching process in GdFeCo .

4:18PM D13.00008 Using X-Ray Diffraction Microscopy for Imaging Magnetic Domain Structures of Magnetic Thin Films, OLEG KRUPIN, European XFEL GmbH, Germany & SLAC National Laboratory, USA, J.J. TURNER, SLAC National Laboratory, USA, X. HUANG, London Centre for Nanotechnology, University College London, United Kingdom, K.A. SEU, Lawrence Berkeley National Lab, USA, D. PARKS, S. KEVAN, University of Oregon, USA, E. LIMA, K. KISLINGER, Brookhaven National Lab, USA, I. MCNULTY, Argonne National Lab, USA, R. GAMBINO, Material Science and Engineering, Stony Brook University, USA, S. MANGIN, Institut Jean Lamour, CNRS/Nancy-Universite, Nancy, France, S. ROY, P. FISCHER, Lawrence Berkeley National Lab, USA — We report the application of iterative phase retrieval from magnetic x-ray diffraction for imaging magnetic domain structures of magnetic thin films. Using coherent x-ray scattering at the x-ray photon energy corresponding to the $L_{3,2}$ absorption edges of the 3d material Co, we demonstrate that linearly polarized soft x rays can be used to obtain the element specific information about both the amplitude and the phase of magnetic domain structures existing in thin films. We successfully recovered an image of the magnetic structure of an amorphous terbium-cobalt thin film with a spatial resolution of about 75 nm and could differentiate between the magnetization directions, finding qualitative agreement with soft x-ray microscopy images recorded with Fresnel zone plate optics having better than 25 nm spatial resolution.

4:30PM D13.00009 Magnetic order and fluctuations in Fe_3O_4 nanoparticles via coherent X-ray magnetic scattering, KARINE CHESNEL, MATEA TREVINO, YANPING CAI, ANDREW MATTHEW, Physics department, BYU, ROGER HARRISON, Chemistry department, BYU, UT, ANDREAS SCHERZ, SLAC, Stanford, CA — Magnetite (Fe_3O_4) particles exhibit a superparamagnetic behavior when their sizes are in nanometer scale. Such nanoparticles could potentially be used for applications in the medical field. We are interested in investigating the magnetic order and fluctuation dynamics in self-assemblies of such nanoparticles. Our Fe_3O_4 nanoparticles are prepared by an organic route and range from 5 nm to 50 nm in size. They are deposited on membrane where they self-assemble. We have been studying the magnetic order using X-ray resonant magnetic scattering (XRMS) at the SSRL synchrotron facility in Stanford. This unique technique, combined with X-ray Magnetic Circular Dichroism (XMCD), provide information about the spatial distribution of the particles and their magnetic order (1). In addition, the use of coherent light at the SSRL beamline, combined with the application of magnetic field in-situ at different temperatures, allows for studying local magnetic disorder (2) and dynamics of fluctuations near the blocking temperature.

1. J.B.Kortright et al., PRB **71**, 012402 (2005)

2. K. Chesnel et al., PRB **83**, 054436 (2011)

4:42PM D13.00010 Magnetic x-ray scattering, transport and MFM study of strongly correlated $La_{1-x}Sr_xMnO_3$ nanowires¹, XIAOQIAN M. CHEN, TYLER R. NAIBERT, NICK BRONN, JAMES C.T. LEE, SHU WANG, JAMES N. ECKSTEIN, NADYA MASON, RAFFI BUDAKIAN, PETER ABBAMONTE, Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, XIAOFANG ZHAI, None, ANAND BHATTACHARYA, Argonne National Laboratory — Artificial patterning is a promising new approach to studying strongly correlated materials, since a boundary acts as a perturbation that can tip the balance among various competing ground states. We have fabricated large, periodic arrays of 80 nm wide nanowires from epitaxially grown $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) thin films. Their electronic and magnetic properties were studied with resonant soft x-ray scattering (RSXS), transport measurements and magnetic force microscopy (MFM). RSXS measurements revealed a series of structural diffraction peaks that arise from the periodic wire structure. Below the Curie temperature we also observed a series of magnetic superlattice reflections, indicating collective ordering of the magnetic moments into a pattern with a spatial period of five wires. Transport measurements also showed anomalous “telegraph” switching noise at temperatures below 15K, and MFM revealed unusual domain formation. We interpret these results as arising from unusual, boundary-induced magnetic domains interacting via long-ranged, classical magnetic dipole coupling.

¹This work was supported by the U.S. Department of Energy under grants DE-FG02-07ER46453 and DE-FG02-06ER46285.

4:54PM D13.00011 Local structure and magnetic properties of ultrathin Mn films grown on Si(001), SAMER KAHWAJI, THEODORE MONCHESKY, Dalhousie University, Halifax, Canada, DARYL CROZIER, ROBERT GORDON, Simon Fraser University, Burnaby, Canada — We report on the structural and magnetic properties of ultrathin Mn layers deposited onto Si(001) by molecular beam epitaxy (MBE) at low temperature. X-ray absorption fine structure (XAFS) studies reveal that the structure of the silicide layer that forms depends on the growth temperature of the capping layer. A capping layer grown at 200 °C on 0.35 monolayer (ML) Mn results in a metastable MnSi phase with a B2-like (CsCl) structure, whereas a cap grown at room temperature on 0.5 ML followed by annealing at 200 °C produces a lower coordinated MnSi phase with a B20-like structure. Increasing the Mn thickness from 0.5 to 4 monolayers does not trigger a structural transformation but drives the structure closer to MnSi-B20. Using SQUID magnetometry, we show that the sample with B2-like structure has the largest Mn magnetic moment of $0.33\mu_B/\text{Mn}$ at $T=2$ K, and a Curie temperature T_C above 250 K. MnSi-B20 layers showed lower moments and much lower T_C 's, in-line with those reported for MnSi-B20 thin films.

5:06PM D13.00012 Probing the surface magnetic properties via Auger-photoelectron coincidence spectroscopy, GIAN PAOLO BRIVIO, GUIDO FRATESI, Department of Materials Science, University of Milano Bicocca, Italy, MARIO ITALO TRIONI, CNR- National Research Council of Italy, ISTMI, Milano, Italy, ROBERTO GOTTER, IOM-CNR, Basovizza, Trieste, Italy, GIANNI STEFANI, Department of Physics, University of Roma Tre, Italy — Auger-photoelectron coincidence spectroscopy (APECS) via a dichroic effect is a suitable tool to study complex systems such as magnetic thin films and multilayers. We present clear evidence for such a dichroic effect in the M_{3VV} Auger line shape of Fe films on Cu(001) measured by angle resolved APECS showing final state spin selectivity (triplet vs. singlet components). Using the Fermi Golden rule and the density functional theory formalism, the Auger spectrum and its angular distributions are computed. For magnetic systems, the spin dependence of the Auger matrix elements allows one to work out the individual multiplet contributions to the Auger spectrum. For an accurate interpretation of experiments we also take into account the valence hole-hole interaction affecting the Auger line shape by the Cini-Sawatzky theory but considering a spin dependent on-site interaction U. The calculated angular distribution, in case of a non-spherical ionized core level (e.g. $l=1$, $m=0$), follows a non-trivial behavior in agreement with experiment.

5:18PM D13.00013 Polarized small angle neutron scattering of MnO/Mn_3O_4 nanocrystals, L. DEDON, Y. IJIRI, Department of Physics and Astronomy, Oberlin College, R. BOOTH, Department of Physics, Carnegie Mellon University, K. KRYCKA, J.A. BORCHERS, W.C. CHEN, S. WATSON, NIST Center for Neutron Research, NIST, J.J. RHYNE, Lujan Neutron Scattering Center, Los Alamos National Laboratory, S.A. MAJETICH, Department of Physics, Carnegie Mellon University — Monodisperse magnetic nanoparticles are of great interest for biomedical and data storage applications, particularly in cases where the core and shell can be carefully controlled to alter properties like magnetic anisotropy. However, it is often difficult to determine the underlying moment arrangements and correlations in these systems. Here, we focus on manganese (II) oxide/manganese (II,III) oxide core/shell nanoparticles, using polarized small angle neutron scattering (SANS) to probe the magnetic intra and interparticle interactions. The 30nm diameter particles with 4-5nm shell were prepared by solution chemistry methods and self-assembled into 3D nanocrystals. SANS measurements were conducted in magnetic fields from remanence-1T and temperatures from 10-300K. Magnetic and structural scattering components were separated using an algorithm previously described in [1]. The magnetic signature depended on the field and temperature history of the sample. Modeling work has been done to further quantify the interparticle length scales and the effects of crystal packing. This work was supported in part by NSF grants DMR-0454672, -0704178, -0804779, -1104489, and DOE grant DE-FG02-08ER40481. [1] K.L. Krycka, et al. Phys. Rev. Lett. 104, 207203 (2010).

Monday, February 27, 2012 2:30PM - 5:30PM –

Session D14 DMP GMAG: Focus Session: Spins in Carbon - Spins in Graphene 212

2:30PM D14.00001 Spin transport in graphene, BARBAROS ÖZYILMAZ, Department of Physics, National University of Singapore — Conventional electronic transistors involve the control of electronic charge at the nanoscale to realize memory, logic and communication functions. All these electronic charges, however, also carry a spin that remains unutilized in present commercial devices. This has motivated the search for new materials that propagate spin-polarized currents over large distances. Among the most promising materials for spintronics has been graphene. Micron-scale spin relaxation lengths have been previously demonstrated in single-layer graphene. Recently, we showed that bilayer graphene is a far more interesting candidate for spintronics. By fabricating spin valves on bilayer graphene we have achieved at room temperature spin relaxation times up to 2 nanoseconds, which are an order of magnitude higher than for single layer graphene [1]. Furthermore, the spin-relaxation time scales inversely with the mobility of BLG sample. This indicates the importance of D'yakonov-Perel' spin scattering in BLG. Last not but least, the presence of an electric field tunable band gap in bilayer graphene makes it particularly appealing. Our work provides fundamental insight into the unique properties of bilayer graphene for spintronic applications. Remarkably, a similar difference between single layer and bilayer graphene is also observed in large area graphene grown by the CVD method on copper. These results demonstrate the potential of CVD graphene in realistic spintronics devices [2].

[1] T - Y. Yang et al., Observation of Long Spin-Relaxation Times in Bilayer Graphene at Room Temperature, PRL (2011).

[2] A. Avsar et al., Towards Wafer Scale Fabrication of Graphene Based Spin Valve Devices, Nano Lett. (2011).

3:06PM D14.00002 Spin Transport in Epitaxial Graphene on SiC (0001), J. ABEL, A. MATSUBAYASHI, University at Albany, C. DIMITRAKOPOULOS, D.B. FARMER, ALI AFZALI, A. GRILL, C.Y. SUNG, IBM T.J. Watson Research Center, V.P. LABELLA, University at Albany — Long spin lifetimes in graphene make it an ideal candidate for the channel material in future spintronic devices. The long spin lifetimes arise due to the small intrinsic spin orbit coupling and low hyper-fine interaction of the electron spins with the carbon nuclei. Spin lifetimes are measured in epitaxially grown graphene on SiC from IBM. The spin lifetime is measured with non-local Hanle measurements to observe spin precession in the graphene. Spin lifetimes are then extracted by fitting to the solution of the Bloch equation with a diffusion term. A comparison will be presented between an injection and detection contact structure with a bare Co/graphene interface and a Co/HfO₂/graphene interface, where it was found that the HfO₂ interface results in an increased spin lifetime. Temperature dependent spin lifetimes and Hall mobilities were measured, and a comparison of the two measurements will also be presented to provide insight into the spin scattering mechanism in epitaxial graphene on SiC.

3:18PM D14.00003 ABSTRACT WITHDRAWN —

3:30PM D14.00004 Spin Dependent Scattering from Gated Obstacles in Graphene Systems¹, MAHMOUD ASMAR, SERGIO ULLÓA, Ohio University — We study scattering of Dirac fermions in the presence of both intrinsic and Rashba spin orbit interactions (SOIs). We use the analytical form of eigenstates in a system with cylindrical symmetry to calculate useful quantities for the scattering of Dirac particles such as phase shifts, and both transport and total cross sections, as well as the corresponding scattering times. At low energies the scattering from a gated obstacle in the absence of SOIs is anisotropic and predominantly forward [1]. In contrast, for energies close to the intrinsic SOI amplitude, the scattering becomes *isotropic*, which can be seen as arising from the effective Dirac mass generated by the SOI interaction. In the presence of Rashba fields we find that the spin-flip scattering is isotropic while it remains anisotropic and predominantly forward for spin-preserving scattering, leading to persistent spin polarization in the forward direction. At high energies, we find a series of resonances in the elastic scattering times, associated with particle trajectories orbiting the obstacle and characterized by long lifetimes. The Rashba SOI is found to double the number of long lived states in both spin-preserving and spin-flip scattering channels. [1]M.Monte Verde et al., PRL **104**,126801 (2010)

¹Supported by NSF-PIRE and NSF-MWN/CIAM.

3:42PM D14.00005 Tunnel spin injection into graphene through ALD-grown tunnel barrier, TAKEHIRO YAMAGUCHI, IIS, Univ. of Tokyo, SATORU MASUBUCHI, IIS and INQIE, Univ. of Tokyo, KAZUYUKI IGUCHI, RAI MORIYA, IIS, Univ. of Tokyo, TOMOKI MACHIDA, IIS and INQIE, Univ. of Tokyo, and PRESTO-JST — Graphene is a promising material for spintronics devices because of its long spin relaxation time due to weak spin-orbit interaction and hyperfine interaction. For the spintronics, it is very essential to develop a reliable method to inject spin polarized electrons into graphene from ferromagnetic electrodes. In this study, between ferromagnetic electrodes and graphene we fabricated a new type of Al₂O₃ tunnel barrier grown by atomic layer deposition (ALD). Before ALD of Al₂O₃, we functionalized the surface of graphene with a self-assembled monolayer of 3, 4, 9, 10 perylene tetracarboxylic acid (PTCA) to improve adhesion and growth of Al₂O₃. Using ALD-Al₂O₃/PTCA composite barrier, large nonlocal magnetoresistance of 30 Ω was observed at 45 K. Nonlocal magnetoresistance reached maximum around charge neutrality point, and *I* – *V* characteristics of the contacts are nonlinear. These results indicate the achievement of tunnel spin injection into graphene, revealing potentially high performance of ALD-Al₂O₃/PTCA tunnel barrier [1]. [1] T. Yamaguchi et al., J. Magn. Magn. Mater. (2011), doi: 10. 1016/j.jmmm. 2011. 09. 031

3:54PM D14.00006 ABSTRACT WITHDRAWN —

4:06PM D14.00007 Spin waves in finite graphene ribbons, ANDREA LATGE, FRANCISCO CULCHAC, ANTONIO COSTA, Instituto de Física, Universidade Federal Fluminense — In a previous work we have shown that the spin excitations of a graphene zigzag ribbon have a dispersion relation predominantly linear for large wave lengths, due to the antiferromagnetic coupling between the magnetizations of the opposite edges. Although the excitations are weakly damped in electrically neutral nanoribbons, the damping can be enhanced by the application of gate voltages. This allows control of the spin relaxation times by purely electrostatic means. Here we investigate spin excitations and also electronic transport in finite zigzag ribbons, connected to graphene-like metallic leads. The ground state is described self-consistently within a mean-field scheme. The spin excitations are extracted from transverse dynamic susceptibility. As a general result we found conductance gaps populated with localized states that are swept out as the length of the conductor increases. The magnetic moment is site dependent, differently from the infinite case, and diverse spin wave excitation modes are exhibited. We study the spin wave behavior and the dynamic susceptibility dependence on the coupling intensity between ribbon and leads. We analyze the role played by the coupling on the spin wave life times and the effects of external doping.

4:18PM D14.00008 GMAG Dissertation Award Talk: Spin Injection and Relaxation in Graphene, WEI HAN, University of California, Riverside — Graphene is a unique and promising candidate for spintronics due to its high mobility, low intrinsic spin-orbit and hyperfine couplings, which should lead to long spin lifetimes and relaxation lengths. Experimentally, the gate-tunable spin transport has been achieved at room temperature. However, the spin injection efficiency has been low and the spin lifetime is still much shorter (50- 200 ps) than expected theoretically (~micro seconds). To fulfill the potential of graphene for spintronics, two major advances are needed to be accomplished; enhance the spin injection efficiency and extend the spin lifetime. In this talk, I will focus on the contributing results for these advancements in graphene spintronics during my Ph. D. study. First, I develop a method to grow atomically smooth MgO tunnel barrier using Ti seeding layer prior the MgO growth on graphene. Then tunneling spin injection into graphene is achieved. The nonlocal spin signal is observed to be as high as 130 ohms at 300 K, with a spin injection efficiency of 30%. Second, using tunneling contacts to suppress the contact-induced spin relaxation, we observed the spin lifetimes as long as 771 ps at 300 K, 1.0 ns at 4 K in SLG, and 6.2 ns at 20 K in bilayer graphene (BLG). Furthermore, contrasting spin relaxation mechanisms are found in SLG and BLG. Third, the spin lifetimes on the same SLG spin valve with tunable mobilities are investigated. These results are important advances for graphene to be used for spin computing or spin logic applications.

4:54PM D14.00009 Magnetism in neutron irradiated graphene samples, YANCEN LI, JOEL THERRIEN, ECE U. Mass Lowell — Recent work in our lab has shown that graphene can become ferromagnetic by way of the addition of hydrogen. The graphene shows a weak but distinct magnetization loop at room temperature. Magnetic force microscopy shows that the magnetic effect can be added and subsequently removed by exposure to a cold hydrogen plasma followed by annealing at 400 Deg C. An outstanding question has been whether the effect observed is due to the interaction of the hydrogen with the graphene, or the addition of defects from the hydrogen. The role of the hydrogen vs. defects was studied using raman microscopy and magnetic force microscopy on graphene samples exposed to neutron irradiation for comparison of a sample containing defects without adatoms.

5:06PM D14.00010 Magnetic Moment Formation in Hydrogenated and Defected Graphene, KATHLEEN MCCREARY, ADRIAN SWARTZ, WEI HAN, ROLAND KAWAKAMI, University of California, Riverside — Recent experimental observations of magnetic moment formation and magnetic ordering in graphene and graphite have excited both theorists and experimentalists. Magnetic ordering in carbon based materials would provide an alternate material to the conventional d and f metals employed in current technologies and could contribute to new applications in nanotechnology, spintronics, medicine, and telecommunications. While still a young and controversial field, previous experimental and theoretical works suggest the presence of magnetic moments in carbon materials is attributed to impurities, boundaries, reduced dimensionality, or defects. In this study, we perform spin transport measurements on graphene devices in order to investigate magnetic moment formation in doped graphene. The graphene surface is modified inside an ultrahigh vacuum chamber through a variety of methods including hydrogen adsorption, Ar sputtering, and molecular beam deposition of transition metals. We observe signatures of paramagnetic moment formation associated with dopants and defects in graphene.

5:18PM D14.00011 Quantum Monte Carlo study of magnetic impurity in bilayer graphene, J.H. SUN, Department of Physics, The Chinese University of Hong Kong, F.M. HU, COMP/Department of Applied Physics, Aalto University, School of Science and Technology, H.K. TANG, HAI-QING LIN, Department of Physics, The Chinese University of Hong Kong — It is expected to observe many different properties in bilayer graphene when compared with single layer graphene due to the differences in crystal structure. Additionally, bilayer system offers a freedom of inducing a gap in the energy band by applying a shift in the electrochemical potential to two graphene layers. In this work, we study the magnetic properties of an Anderson magnetic adatom in Bernal stacking bilayer graphene and compare the results with those of single layer counterpart. Several different cases such as different adatom position and different potential bias of two layers are studied using the quantum Monte Carlo method. In all the cases, we find that the impurity local magnetic moment can be switched between relatively large and small values by tuning the chemical potential. We apply MaxEnT method to compute impurity spectral density and find its behavior to differ from that of an impurity in a single layer graphene. We also calculate various correlation functions and make comparisons.

Monday, February 27, 2012 2:30PM - 5:30PM – Session D15 DMP FIAP GMAG: Focus Session: Spins in Metals - Ultra Fast Dynamics 213

2:30PM D15.00001 Ultrafast Magnetism of Multi-component Ferromagnets and Ferrimagnets on the Time Scale of the Exchange Interaction, ILIE RADU, Radboud University Nijmegen, the Netherlands and Helmholtz-Zentrum Berlin, BESSY II, Germany — Revealing the ultimate speed limit at which magnetic order can be controlled, is a fundamental challenge of modern magnetism having far reaching implications for the magnetic recording industry [1]. Exchange interaction is the strongest force in magnetism, being ultimately responsible for ferromagnetic or antiferromagnetic spin order. How do spins react after being optically excited on a timescale of or even faster than the exchange interaction? Here, we demonstrate that femtosecond (fs) measurements of ferrimagnetic and ferromagnetic alloys using X-ray magnetic circular dichroism provide revolutionary new insights into the problem of ultrafast magnetism on timescales pertinent to the exchange interaction. In particular, we show that upon fs optical excitation the ultrafast spin reversal of GdFeCo - a material with antiferromagnetic coupling of spins - occurs via a transient ferromagnetic state [2]. The latter emerges due to different dynamics of the Gd and Fe magnetic moments: Gd switches within 1.5 ps while it takes only 300 fs for Fe. Thus, by using a single fs laser pulse one can force the spin system to evolve via an energetically unfavorable way and temporarily switch from an antiferromagnetic to a ferromagnetic type of ordering. In order to understand whether the observation of this temporarily decoupled and element-specific dynamics is a general phenomenon or just something strictly related to the case of ferrimagnetic GdFeCo, we have investigated the demagnetization of the archetypal ferromagnetic NiFe alloys. Essentially, we observe the same distinct magnetization dynamics of the constituent magnetic moments: Ni demagnetizes within ~300 fs being much faster than the demagnetization of Fe of ~800 fs. This distinct demagnetization behavior leads to an apparent decoupling of the Fe and Ni magnetic moments on a few hundreds of fs time scale, despite the strong exchange interaction of 260meV (~16 fs) that couples them. These observations supported by atomistic simulations, present a novel concept of manipulating magnetic order on different classes of magnetic materials on timescales of the exchange interaction [3].

[1] A. Kirilyuk, A.V. Kimel and Th. Rasing, *Rev. Mod. Phys.* **82**, 2731 (2010).

[2] I. Radu *et al.*, *Nature* **472**, 205 (2011).

[3] I. Radu *et al.*, *submitted* (2011).

3:06PM D15.00002 Uncovering the Ultrafast Angular Momentum Transfer Channels on the Nanoscale in GdFeCo, CATHERINE GRAVES, Stanford University, ALEX REID, Stanford Institute for Materials and Energy Science, BENNY WU, TIANHAN WANG, Stanford University, SANNE DE JONG, Stanford Institute for Materials and Energy Science, ILIE RADU, Radboud University Nijmegen, SASHA EPP, ROBERT HARTMANN, MPG-ASG Hamburg, ARATA TSUKAMOTO, Nihon University, Japan, RYAN COFFEE, MINA BIONTA, JOSHUA TURNER, WILLIAM SCHLOTTER, Linac Coherent Light Source, YVES ACREMANN, ETH Zürich, ALEXEY KIMEL, ANDREI KIRILYUK, Radboud University Nijmegen, JOACHIM STÖHR, Linac Coherent Light Source, THEO RASING, Radboud University Nijmegen, HERMANN DÜRR, ANDREAS SCHERZ, Stanford Institute for Materials and Energy Science — The ultrafast control of electron spins is of both fundamental scientific and technological interest. Recent experiments have shown that femtosecond laser excitation can act as a stimulus to switch the magnetization direction in ferrimagnetic GdFeCo, called all-optical switching. However, how angular momentum is transferred to result in a switched state remains unknown. To further understand this mechanism, we use 80fs x-ray pulses from LCLS to study how angular momentum transfer is triggered in GdFeCo by fs laser excitation using time-, element- and spatially-resolved x-ray resonant magnetic scattering. We present here the first-ever measurement of the fs magnetic response in GdFeCo with spatial resolution down to 10nm. Our results reveal drastically different behaviors on the nanoscale as compared to the bulk and provide insight into the angular momentum transfer channels.

3:18PM D15.00003 Ultrafast Demagnetization Measurements using Extreme Ultraviolet Light: Comparison of Electronic and Magnetic Contributions, CHAN LA-O-VORAKIAT, EMRAH TURGUT, CARSON A. TEALE, HENRY C. KAPTEYN, MARGARET M. MURNANE, JILA/University of Colorado, DENIS LVOVSKY, ROMAN ADAM, PATRIK GRYCHTOL, CLAUS M. SCHNEIDER, Peter Grünberg Institute, Jülich, Germany, STEFAN MATHIAS, MARTIN AESCHLIMANN, University of Kaiserslautern and Research Center OPTIMAS, JUSTIN M. SHAW, HANS NEMBACH, THOMAS J. SILVA, National Institute of Standards and Technology — Ultrashort pulses from high-harmonic generation provide new capabilities for uncovering coupled charge, spin, and phonon dynamics in magnetic materials by combining elemental selectivity with ultrafast time resolution in a tabletop source. In this talk, we address an important question in magneto-optics that has implications for understanding femtosecond magnetism: is the signal from the transverse magneto-optical Kerr effect at the M-shell absorption edges of a magnetic material purely magnetic or perturbed by non-magnetic optical artifacts? We conclusively show that high harmonics sensitively probe the magnetic state, with negligible contributions from electronic effects because of hot-electron dynamics. Finally, our measurements are in excellent agreement with conventional visible-wavelength magneto-optics probes and illustrate the power of high harmonics for probing the dynamics in magnetic materials.

3:30PM D15.00004 Theory of spin hot pockets in laser-induced demagnetization in ferromagnetic nickel¹, GUOPING ZHANG, Department of Physics, Indiana State University, MINGSU SI, Lanzhou University, YIHUA BAI, Center for Instruction, Research and Technology, Indiana State University, THOMAS F. GEORGE, University of Missouri-St. Louis — We will first review the current theory of the demagnetization process, with a particular focus on two distinctive contributions: (a) the optical dipole interaction (ODI) between a laser field and a magnetic system and (b) the spin expectation value change (SEC) between two transition states. We then introduce a new optical spin operator, a product of SEC and ODI between transition states. In ferromagnetic nickel, our first-principles calculation demonstrates that the larger the value of optical spin operator is, the greater the dynamic spin moment change is. This simple operator is very useful, as it directly links the time-dependent spin moment change $\Delta M_z^k(t)$ at every crystal-momentum k point to its intrinsic electronic structure and magnetic properties. Those hot spin pockets should be the focus of future research.

¹Supported by the U. S. Department of Energy under Contract No. DE-FG02-06ER46304, the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, and DE-AC02-06CH11357, and National Science Foundation of China (NSFC)

3:42PM D15.00005 Ultrafast Transport of Laser-Excited Spin-Polarized Carriers in Metallic Multilayers¹, ALEXEY MELNIKOV, Physical Chemistry Department, Fritz-Haber-Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — The ultrafast spin dynamics induced by a transport of spin polarized carriers is a hot topic motivated by the fundamental interest in magnetic excitations and applications like spintronics and data storage. To understand underlying elementary processes typically occurring on femtosecond time scales, we have developed a time-of-flight-like approach that probes the spin dynamics induced by hot carriers (HC) and demonstrated a *spin polarized* HC transport through an epitaxial Au/Fe/MgO(001) structure. Using a back pump-front probe configuration, we establish that HC induced in Fe by the pump laser pulse can form a nearly *ballistic* spin current (SC) in Au. Optical second harmonic (SH) generated at the Au surface by the probe pulse monitors the transient surface HC density and spin polarization (SP). Since HC with different SP are excited in Fe to different final energies and consequently have different lifetimes in Au, the HC pulse has steep leading part formed by ballistic HC with the negative SP and shallow trail part formed by diffusive HC with the positive SP. This leads to the SC sign change within the 1 ps overall SC pulse duration. We also make a step towards understanding the origin of laser-induced ultrafast demagnetization overcoming the limited ability of conventional pump-probe schemes to distinguish photon-, electron-, and phonon-mediated effects. Comparing the SH response of Fe to the direct optical excitation with that to the excitation by hot carriers generated in Au, we rule out coherent effects of the pump pulse electromagnetic field and show that the HC-induced spin dynamics is responsible for the ultrafast demagnetization.

¹Financial support by the DFG through ME 3570/1-1 is acknowledged.

4:18PM D15.00006 First-principles dynamical calculation of a pump-probe scenario for the spin flip on NiO, GEORGIOS LEFKIDIS, WOLFGANG HÜBNER, University of Kaiserslautern — Using a fully ab-initio approach we calculate in a dynamic way the time-dependent probe signal of a spin flip scenario on the antiferromagnetic NiO surface. We start from a first-principles calculation of the highly correlated, relativistic, electronic states of a doubly embedded NiO_5^{--8} cluster followed by the time-propagation of the system under the influence of the spin-flipping pump pulse *and* the detecting probe pulse. This way we treat both pulses on equal footing and, for the first time, consider the effects of the electronic non-equilibrium due to the concurrent presence of the pulses. Our time-resolved calculations reveal the subtle influence of the probe pulse itself on the detection signal, which cannot be completely treated solely by the time propagation of the pump pulse and the subsequent calculation of the static susceptibility tensor [1,2]. We also analyze the angular-momentum conservation and its distribution among the system and both laser pulses [3].

[1] G. P. Zhang, W. Hübner, G. Lefkidis, Y. Bai, and T. F. George, *Nature Physics* **5**, 499 (2009)

[2] G. P. Zhang, G. Lefkidis, W. Hübner and Y. Bai, *J. Appl. Phys.* **109**, 07D303 (2011)

[3] G. Lefkidis, G. P. Zhang and W. Hübner, *Phys. Rev. Lett.* **103**, 217401 (2009)

4:30PM D15.00007 Non-equilibrium coupling and femto-second oscillatory spin torque in non-collinear F/N/F magnetic multilayers¹, JIANWEI ZHANG, QIANG WANG, Dept. of Physics, Tongji University — By employing time-dependent diffusion theory, we study time-evolution behaviors of spin torque and spin current in non-collinear Ferromagnetic/Normal/Ferromagnetic tri-layers structure. We find in ferromagnetic layer spin torque has femto-second oscillatory in its initio building-up process, which indicates that excited itinerant electron's spin process alone background magnetization in femto-second period near the interfacial region. We also find even mismatch of background magnetization at each F/N interfaces is not enough to compensate discontinuity of spin current near interface, however, by introducing non-equilibrium coupling between two F/N interfaces, one can produce a continuous spin current state across both two interfaces without mandating any boundary conditions. In our study, we find a new universal time-dependent propagator to generate all directions continuous spin current across two F/N interfaces. This new spin propagator is also closely related to spin flip scatter at interface. In addition, we also find the coupling of two N/F interfaces enlarges transverse spin diffusion channels into magnetic layer. Finally, our time-dependent spin current and spin torque states also match our pervious self-consistent steady state results.

¹This work was supported by Science & Technology Commission of Shanghai Municipality (Grant No.10PJ1410300).

4:42PM D15.00008 Probing the timescale of the exchange interaction in a ferromagnetic alloy, EMRAH TURGUT, CHAN LA-O-VORAKIAT, MARK E. SIEMENS, MARGARET M. MURNANE, HENRY C. KAPTEYN, JILA, University of Colorado, Boulder, STEFAN MATHIAS, PATRICK GRANITZKA, STEFFEN EICH, MARTIN AESCHLIMANN, University of Kaiserslautern and Research Center OPTIMAS, Germany, PATRIK GRYCHTOL, ROMAN ADAM, CLAUS M. SCHNEIDER, Peter Grünberg Institute, Research Center Jülich, Germany, JUSTIN M. SHAW, HANS T. NEMBACH, THOMAS J. SILVA, National Institute of Standards and Technology, Boulder — The underlying physics of all ferromagnetic behavior is the cooperative interaction between individual atomic magnetic moments that results in a macroscopic magnetization. In this work, we use extreme ultraviolet pulses from high-harmonic generation as an element-specific probe of ultrafast, optically driven, demagnetization in a ferromagnetic Fe-Ni alloy (Permalloy). We show that for times shorter than the characteristic timescale for exchange coupling, the magnetization of Fe quenches more strongly than that of Ni. Then, as the Fe moments start to randomize, the strong ferromagnetic exchange interaction induces further demagnetization in Ni, with a characteristic delay determined by the strength of the exchange interaction. We can further enhance this delay by lowering the exchange energy by diluting the Permalloy with Cu. This measurement probes how the fundamental quantum mechanical exchange coupling between Fe and Ni in magnetic materials influences magnetic switching dynamics in ferromagnetic materials relevant to next-generation data storage technologies.

4:54PM D15.00009 Driving coherent spin reorientation transition with femtosecond laser pulses, VLADIMIR STOICA, ROY CLARKE, Physics Department, University of Michigan — Ultrafast studies of spin reorientation transition provide insight in magnetization switching processes and are important for the magnetic recording technology. Using femtosecond optical techniques, we demonstrate coherent control of the magnetization vector in epitaxial Fe films. These films feature uniaxial anisotropy that is thermally modulated by an optical pulse. We observe an optically-induced spin reorientation transition of first-order that provides an efficient route to ultrafast coherent magnetization switching. The switching is found to be a three-step temporal process: a coherent reorientation (~ 100 ps) is followed by a spin precession in a newly created metastable state (~ 300 ps), which evolves into a dual domain state that undergoes relaxation within $\sim 2 - 4$ ns. We provide a model to explain the experimental data and predict further applications of this technique. The details of the experiments compare favorably with the simulated magnetization trajectories, opening new pathways for coherent control of magnetic dynamics with pulsed lasers.

5:06PM D15.00010 Theory of the inverse Faraday effect driven by non-coplanar spin structures, KATSUHISA TAGUCHI, GEN TATARA, Tokyo Metropolitan University — We show theoretically that a new mechanism of the inverse Faraday effect exists in the presence of non-coplanar spin structures in metals even without the spin-orbit interaction. The spin density generated by the effect is proportional to the circular polarization of the light, $(\mathcal{E} \times \mathcal{E}^*)$ ($\mathcal{E}$ is the complex amplitude vector of the electric field of the circular light), and $\nabla \times \mathbf{j}_s^\alpha$, where $\mathbf{j}_s^\alpha \equiv (\mathbf{n} \times \nabla \mathbf{n})^\alpha$ is the spin current carried by the spin structure ($\mathbf{n}$ is the unit vector of the localized spin). The effect turns out to be larger than the conventional inverse Faraday effect, and the present mechanism is expected to be useful for the magnetization flip of the Skyrmion.

5:18PM D15.00011 Examination of spin waves in a two-dimensional magnetic superlattice¹, GLADE SIETSEMA, MICHAEL FLATTÉ, University of Iowa — We have studied the properties of spin waves in two-dimensional periodic superlattices of magnetic materials.[1] Frequencies and linewidths are calculated for square and hexagonal symmetry superlattices from the Landau-Lifshitz-Gilbert equations. Large differences in the saturation magnetizations and exchange stiffness constants of the materials are shown to be capable of producing gaps in the magnonic spectrum across the entire superlattice Brillouin zone. For example, with a hexagonal superlattice of Fe and YIG we find gaps of 0.5THz and 1THz within the lowest four bands. Additionally, calculations of the system's Green's functions are used to examine the superlattice's response to pulse excitations, such as from a spin torque oscillator.

[1]arXiv:1111.2506v1

¹This work supported by an ARO MURI.

Monday, February 27, 2012 2:30PM - 5:18PM – Session D16 DCMP: Strongly Correlated Numerics and Theory 251

2:30PM D16.00001 Local and non-local correlations in nanoscopic systems, GIORGIO SANGIOVANNI, A. VALLI, G. ROHRINGER, A. TOSCHI, K. HELD, Vienna University of Technology, H. DAS, Cornell University, T. SAHA-DASGUPTA, Bose National Centre for Basic Sciences — Tools for reliably treating nanoscopic systems, like coupled quantum-dots, ad-atoms on surfaces, macromolecules, etc., in the presence of electronic correlations are either missing or prohibitively expensive. We have implemented a new computational scheme based on a self-consistently defined set of local problems [1]. Our method scales linearly with the number of sites and allows us to perform large-scale sign-problem free Quantum Monte-Carlo simulations. We have studied the behavior of a single-atom junction formed upon stretching a metallic wire and found that a metal-insulator crossover is induced when the wire is about to break up. The combination with ab-initio techniques allowed us to study size-dependent properties of Manganite nano-clusters [2]. The simplest implementation of our method includes only local self-energy effects. We recently went beyond this and applied the resulting more sophisticated version of our method to an exactly solvable model finding results in remarkable agreement with the exact solution.

[1] A. Valli, G. Sangiovanni, O. Gunnarsson, A. Toschi and K. Held, PRL **104**, 246402 (2010)

[2] H. Das, G. Sangiovanni, A. Valli, K. Held and T. Saha-Dasgupta, PRL **107**, 197202 (2011)

2:42PM D16.00002 Quantum impurity solver based on truncated ED (RASCI) wave function expansion¹, DOMINIKA ZGID, EMANUEL GULL, CHRIS MARIANETTI, ANDREW MILLIS, DAVID REICHMAN, Columbia University, GARNET CHAN, Cornell University — Quantum impurity models appear in many applications, including nanoscience and the dynamical mean field approximation (DMFT). Many physically relevant impurity models are too large to be solved by exact diagonalization (ED), lack the interaction and hybridization structure required for quantum Monte Carlo (QMC) simulations, or suffer from a severe sign problem. We present an alternative impurity solver inspired by configuration interaction (RASCI) techniques of quantum chemistry and based on a controlled truncation of a wave function expansion. The method can access larger impurity models (impurities with 5 *d*-orbitals and 20 bath orbitals can be easily calculated on a single processor) than can ED and avoids the sign problems of QMC methods. The performance is demonstrated for a cluster DMFT approximation to the two dimensional Hubbard model and for the problem of a Co adatom on a Cu(111) surface.

¹This work was supported by the CMCSN program of the US Department of energy

2:54PM D16.00003 Modified Iterated perturbation theory in the strong coupling regime and its application to the 3d FCC lattice¹, LOUIS-FRANÇOIS ARSENAULT, (1) Departement de Physique and RQMP, Université de Sherbrooke, Sherbrooke, QC, Canada, PATRICK SÉMON, (1), B. SRIRAM SHASTRY, (2) Physics Department, University of California, Santa Cruz, CA 95064, USA, A.-M.S. TREMBLAY, (1,3) Canadian Institute for Advanced Research, Toronto, Ontario, Canada — The Dynamical Mean-Field theory(DMFT) approach to the Hubbard model requires a method to solve the problem of a quantum impurity in a bath of non-interacting electrons. Iterated Perturbation Theory(IPT)[1] has proven its effectiveness as a solver in many cases of interest. Based on general principles and on comparisons with an essentially exact Continuous-Time Quantum Monte Carlo (CTQMC)[2], here we show that the standard implementation of IPT fails when the interaction is much larger than the bandwidth. We propose a slight modification to the IPT algorithm by requiring that double occupancy calculated with IPT gives the correct value. We call this method IPT- D . We show how this approximate impurity solver compares with respect to CTQMC. We consider a face centered cubic lattice(FCC) in 3d for different physical properties. We also use IPT- D to study the thermopower using two recently proposed approximations[3] S^* and S_{Kelvin} that do not require analytical continuation and show how thermopower is essentially the entropy per particle in the incoherent regime but not in the coherent one.[1]H.Kajueter et al. Phys. Rev. Lett. 77, 131(1996)[2]P. Werner, et al. Phys. Rev. Lett. 97, 076405(2006)[3]B.S. Sriram Shastry Rep. Prog. Phys. 72 016501(2009)

¹NSERC, CRC, CIFAR, CFI, MDEIE (Québec), MIT-Harvard CUA

3:06PM D16.00004 Magnetic properties of the Hubbard model on the fcc lattice¹, HAO SHI, SHIWEI ZHANG, department of physics, college of william and mary — As a possible model for ferromagnetism, we study the magnetic properties of the Hubbard model on an fcc lattice. Near-neighbor and next-near-neighbor hopping parameters are included to examine the effect of band structure. We use exact diagonalization and the Constraint Path Monte Carlo (CPMC) ² methods. Several methodological improvements in CPMC, for example the release of the constraint, will be discussed. We present benchmark quality results on the paramagnetic ground state and partially polarized states, as a function of interaction strength. A magnetic phase diagram is obtained from our many-body calculations, and comparison will be made with results from Dynamical Mean Field theory ³.

¹Supported by ARO and NSF.

²S. Zhang, J. Carlson, and J. Gubernatis, Phys. Rev. B **55**, 7464 (1997); C.-C. Chang and S. Zhang, Phys. Rev. B **78**, 165101 (2008).

³ M. Ulmke, The Eur. Phys. J. B. **1**, 301 (1998)

3:18PM D16.00005 Dual fermion dynamical cluster approach for strongly correlated systems, SHUXIANG YANG, Department of Physics & Astronomy, Louisiana State University, HERBERT FOTSO, Department of Physics, Georgetown University, HARTMUT HAFERMANN, Centre de Physique Théorique, Ecole Polytechnique, CNRS, France, KA MING TAM, JUANA MORENO, Department of Physics & Astronomy, Louisiana State University, THOMAS PRUSCHKE, Department of Physics, University of Goettingen, Germany, MARK JARRELL, Department of Physics & Astronomy, Louisiana State University — A multi-scale many-body approach is developed for strongly-correlated electron systems by combining the dynamical cluster approximation (DCA) and the recently introduced dual fermion formalism. This approach systematically incorporates non-local corrections to the DCA by employing an exact mapping from a real lattice to a DCA cluster of linear size L_c embedded in a dual fermion lattice. The Green function in the dual space serves as a small parameter enabling the use of a diagrammatic perturbation calculation on the dual fermion lattice. For example, the dual fermion self-energy calculated with simple second-order perturbation theory scales as $\mathcal{O}(1/L_c^3)$. We demonstrate the effectiveness of the approach by applying it to the 2D Hubbard model.

3:30PM D16.00006 Extended Correlation in Strongly Correlated Systems, Beyond Dynamical Cluster Approximation, HERBERT FOTSO, Department of Physics, Georgetown University, SHUXIANG YANG, Department of Physics and Astronomy, Louisiana State University, HARTMUT HAFERMANN, Centre de Physique Théorique, Ecole Polytechnique, KA-MING TAM, JUANA MORENO, Department of Physics and Astronomy, Louisiana State University, THOMAS PRUSCHKE, Department of Physics, University of Goettingen, MARK JARRELL, Department of Physics and Astronomy, Louisiana State University, LOUISIANA STATE UNIVERSITY COLLABORATION, ECOLE POLYTECHNIQUE COLLABORATION, UNIVERSITY OF GOETTINGEN COLLABORATION — We present a new multi-scale approach for strongly correlated systems that combines the Dynamical Cluster Approximation and the recently introduced dual-fermion formalism. This approach employs an exact mapping from a real lattice to a DCA cluster of linear size L_c embedded in a dual fermion lattice. The short-length-scale physics is addressed by DCA cluster calculations, while the longer-length-scale physics is addressed diagrammatically using dual fermions. The bare and dressed dual fermionic Green functions scale as $\mathcal{O}(1/L_c)$, so perturbation theory on the dual lattice converges very quickly. E.g., the dual Fermion self-energy calculated with simple second order perturbation theory is of order $\mathcal{O}(1/L_c^3)$, with third order and three-body corrections down by an additional factor of $\mathcal{O}(1/L_c)$.

3:42PM D16.00007 Extension of dual-fermion formalism towards disordered systems, HANNA TERLETSKA, Louisiana State University, Brookhaven National Lab, SHUXIANG YANG, ZI YANG MENG, SANDEEP PATHAK, KA MING TAM, JUANA MORENO, MARK JARRELL, Louisiana State University — To study the correlation effects in disordered materials, we extend the recently developed dual fermion approach [1] to include systems with disorder. In particular, we consider the effect of nonlocal disorder-induced correlations in the non-interacting Anderson model. Within this method, such nonlocal effects are included in a systematic way as an expansion to the coherent potential approximation (CPA). The ability to properly treat the nonlocal correlations and provide non-local corrections to the CPA, is crucial for the description of the electron localization. In our analysis, we consider the density of states and localization effects and compare them with the existing results. [1] A.N. Rubtsov, et. al., Phys. Rev. B **79**, 045133 (2009).

3:54PM D16.00008 Application of the Dual Fermion-Dynamical Cluster Approach to the 1D Falicov Kimball Model, SANDEEP PATHAK, ZI YANG MENG, S.-X. YANG, MARK JARRELL, JUANA MORENO, Louisiana State University — The Falicov Kimball model is the simplest model for correlated electrons. It was introduced to study metal-insulator transitions. In one dimension, it is known to possess a charge density wave (CDW) instability at zero transition temperature (T_c). However, finite cluster methods like Dynamical Mean Field Theory (DMFT), Dynamical Cluster Approximation (DCA), Cellular Dynamical Mean Field Theory (CDMFT), etc. show finite temperature CDW transition. In this paper, we study the model using the recently developed Dual Fermion-Dynamical Cluster approach that takes into account large length scale correlations through the auxiliary particles known as dual Fermions. We find that T_c obtained from this method is lower than that obtained from the cluster methods. In particular, we study the scaling behavior of T_c with the linear cluster size and also the scaling of other one-particle and two-particle quantities near the criticality.

4:06PM D16.00009 Phase Separation and Charge-Ordered Phases of the $d = 3$ Falicov-Kimball Model at $T > 0$: Temperature-Density-Chemical Potential Global Phase Diagram from RG Theory¹, A. NIHAT BERKER, Sabanci University and MIT, OZAN S. SARIYER, Koc University and U of North Carolina, MICHAEL HINCZEWSKI, U of Maryland and F Gursay Res Inst — The global phase diagram of the spinless FK model in $d=3$ is obtained by renormalization-group theory, exhibiting 5 distinct phases. Four of these phases are charge-ordered (CO) phases, in which the system forms two sublattices with different electron densities. The CO phases occur near half filling of the conduction electrons, for the entire range of localized electron densities. Phase boundaries are second order, except for the intermediate and large interaction regimes, where a first-order phase boundary occurs in the central region of the phase diagram, resulting in phase coexistence near half filling of both localized and conduction electrons. These two-phase or three-phase coexistence regions are between different charge ordered phases, between charge-ordered and disordered phases, and between dense and dilute disordered phases. The second-order phase boundaries terminate on the first-order transitions via critical endpoints and double critical endpoints. The first-order phase boundary is delimited by critical points. The phase diagram cross-sections with respect to the chemical potentials and densities of the localized and conduction electrons, at all representative interaction strengths, hopping strengths, temperatures, are calculated and exhibit 10 distinct topologies.

¹Support by Humboldt Foundation, TUBITAK, TUBA

4:18PM D16.00010 Collective Excitations and Stability of the Excitonic Phase in the Extended Falicov–Kimball Model, DENIS I. GOLOSOV, Dept. of Physics, Bar-Ilan University, Israel — We consider the excitonic insulator state (often associated with electronic ferroelectricity), which arises on the phase diagram of an extended spinless Falicov–Kimball model (FKM) at half-filling. Within the Hartree–Fock approach, we calculate the spectrum of low-energy collective excitations in this state up to second order in the narrow-band hopping and/or hybridisation. This allows to probe the mean-field stability of the excitonic insulator. The latter is found to be unstable when the case of the pure FKM (no hybridisation with a fully localised band) is approached. The instability is due to the presence of another, lower-lying ground state and *not* to the degeneracy of the excitonic phase in the pure FKM. The excitonic phase, however, may be stabilised further away from the pure FKM limit. In this case, the low-energy excitation spectrum contains new information about the properties of the excitonic condensate (likely including the critical temperature).

4:30PM D16.00011 Propagation of entanglement in one-dimensional models of many-body localization, JENS H. BARDARSON, UC Berkeley & Lawrence Berkeley National Laboratory, FRANK POLLMANN, Max-Planck-Institute for the Physics of Complex Systems, JOEL E. MOORE, UC Berkeley & Lawrence Berkeley National Laboratory — An important and still unanswered fundamental question is whether a closed quantum system of many interacting particles can be localized by disorder. The time evolution of an initially unentangled state is studied for a 1D random-field XXZ Hamiltonian. Even for weak interactions, when the system is thought to be in a many-body localized phase, entanglement shows neither localized nor diffusive behavior: interactions act as a singular perturbation on the truly localized state with no interactions. The logarithmic time dependence of entanglement observed rather suggests a broad range of time scales typical of glassy behavior.

4:42PM D16.00012 Fidelity Spectrum in Quantum Phase Transitions, WING CHI YU, SHI-JIAN GU, HAI-QING LIN, The Chinese University of Hong Kong — A quantum phase transition (QPT) is incarnated by an abrupt change in the qualitative structure in the ground state wavefunction of a many-body system as the external driving parameter varies. The ground state fidelity, which is a measure of similarity between two states, is expected to show a sudden drop across the transition point and its possibility as a witness to QPTs has raised much interest in recent years. However, the ground state fidelity does not capture much information about the contribution of the low-lying excitations. In this presentation, we introduce the concept of fidelity spectrum, i.e. the matrix elements of $M = |\Psi(\lambda)\rangle\langle\Psi(\lambda + \delta\lambda)|$, where λ is the external driving parameter and $\Psi(\lambda)$ is the wavefunction of the system at λ . By studying the fidelity spectrum, we hope to shed light on the role of excited states played in QPTs. We investigate the fidelity spectrum in two many-body systems, namely the one-dimensional transverse-field Ising model and the two-dimensional Kitaev model defined on a honeycomb lattice. We found that in different phases, as well as at the critical points, the fidelity spectrum shows significant different behaviors.

4:54PM D16.00013 ABSTRACT WITHDRAWN —

5:06PM D16.00014 Quantum Monte Carlo calculation of reduced density matrices, LUCAS WAGNER, University of Illinois at Urbana-Champaign — Quantum Monte Carlo (QMC) methods offer an efficient way to approximate the interacting ground state and some excited states of realistic model Hamiltonians based on the fundamental Coulomb interaction between electrons and nuclei. Many highly accurate results have been obtained using this method; however, it is often a challenge to extract the important correlations that the QMC wave function contains. I will describe some new results using the reduced density matrices (RDM's) to understand the electron correlation in the many-body wave function. The RDM's have both informative usage for describing correlation and pragmatic uses in further improving the variational wave function.

Monday, February 27, 2012 2:30PM - 5:30PM —

Session D17 DMP: Focus Session: Surfaces and Interfaces in Nonoxide Nanostructures: Growth, Structure, and Characterization - Growth Dynamics 252A

2:30PM D17.00001 Factors that control the morphology of ice films on metal surfaces¹, NORMAN BARTELT, Sandia National Laboratories — Examination of the equilibrium nanoscale morphology of ice films provides important clues about the energetics of water-metal interactions [1]. In this talk I compare STM and DFT results for the structure of ice films on Pt(111) and Ni(111). Because the lattice constants of Ni and Pt differ by 10%, this comparison allows us to probe the effect of lattice misfit on ice nucleation and growth. On both substrates, STM suggests a first molecular water layer very different from bulk ice: besides the usual hexagonal rings they also both contain a motif of pentagons and heptagons [2]. Furthermore, at 140K, thicker films on both substrates dewet the substrate to lower interfacial energy by forming 3-dimensional ice crystallites several nanometers thick [3]. However, despite these similarities, there are striking differences in the submonolayer structure and in the kinetics of the dewetting process. Using DFT calculations as a guide, I will discuss how these differences can be related to substrate lattice constant and draw conclusions about the processes that control ice film morphology.

[1] A. Hodgson and S. Haq, Surf. Sci. Rep. 64, 381 (2009).

[2] S. Nie, P. J. Feibelman, N. C. Bartelt and K. Thürmer, Phys. Rev. Lett. 105, 026102 (2010).

[3] K. Thürmer and N. C. Bartelt, Phys. Rev. B 77, 195425 (2008); Phys. Rev. Lett. 100, 186101 (2008).

¹Joint work with K. Thuermer, S. Nie and P.J. Feibelman. Supported by the Office of Basic Energy Sciences, Division of Materials and Engineering Sciences, U.S. DOE under Contract No. DEAC04-94AL85000.

3:06PM D17.00002 Structure and dynamics of water nano-droplets on graphene, MING MA, ANGELOS MICHAELIDES, GABRIEL AEPPLI, London Centre for Nanotechnology, University College London — The wettability of graphene and the diffusion of water droplets across it is of central importance to many emerging applications in nanofluidics. Here we report an extensive set of molecular dynamics simulations for water clusters of varying sizes on graphene (20 to 2,000 water molecules), using force field parameters fitted to recent ab initio quantum Monte Carlo data [J. Ma, A. Michaelides, D. Alfe, L. Schimka, G. Kresse, and E. G. Wang, Phys. Rev. B 84, 033402 (2011)]. The contact angle for the water droplets obtained here, with our ab initio water - carbon interaction, is in very good agreement with experiments. A strong size dependence in the diffusion of the water droplets across the surface is also observed. This work is a step towards understanding surface transportation in carbon based nanofluidics.

3:18PM D17.00003 Large-scale simulations of glancing-angle deposition¹, JACQUES AMAR, XUEJING LIU, University of Toledo — While thin-films grown via glancing-angle deposition have interesting structural, mechanical, and optical properties, the large range of time- and length-scales makes realistic simulations difficult. Accordingly, while activated relaxation processes may be important at long time-scales, here we focus on the deposition process since we expect the effects of shadowing and deposition-induced relaxation to dominate for large deposition angles. In particular, by taking advantage of the speed of recently developed graphical-processing-units (GPUs) we have carried out “large-scale” GPU-enhanced MD simulations of Cu/Cu(100) growth up to 20 monolayers (ML) for deposition angles θ (corresponding to the angle with respect to the substrate normal) ranging from 50° to 85° and for both random and fixed azimuthal angles. In general, we find good agreement with experimental results for the dependence of thin-film porosity on deposition angle and film-thickness. Results for the dependence of the surface roughness, lateral correlation length and microstructure (e.g. defect density, vacancy density, and strain) on the deposition angle and film thickness will also be presented.

¹Supported by the U. of Toledo Center for Photovoltaics Innovation and Commercialization

3:30PM D17.00004 Shape transitions in strained Cu islands on Ni(100): kinetics versus energetics¹, YUNSHI SHIM, JACQUES AMAR, University of Toledo — We examine the shape transition from compact to ramified islands observed in submonolayer Cu/Ni(100) growth. Recently, it has been argued that this transition is not due to a growth instability but can be understood in terms of energetic arguments. In order to determine the responsible mechanisms we have carried out energetics calculations as well as temperature-accelerated dynamics (TAD) and kinetic Monte Carlo (KMC) simulations. Our results indicate that the shape transition cannot be explained by equilibrium arguments, but is instead due to kinetic effects which are mediated by strain. In particular, by calculating the relevant line-tension and strain energies, we find that the equilibrium critical island-width is at least four orders of magnitude larger than the experimentally observed arm-width. In contrast, our TAD simulations indicate that unexpected concerted motions occurring at step edges are responsible. The energy barriers for these concerted motions decrease with increasing island size and appear to saturate for islands larger than 300 - 400 atoms. By including these strain-induced kinetic processes in our KMC simulations of island-growth, we have been able to explain both the temperature- and coverage-dependence of the island morphology.

¹Supported by NSF-DMR 0907399

3:42PM D17.00005 Dewetting Processes in Ultra-thin Epitaxial Ag Films on Si(111), CHARLOTTE E. SANDERS, JISUN KIM, C.K. SHIH, UT Austin — The authors have recently reported the development of a technique to grow large-area, single-crystal, atomically smooth Ag films on Si(111), and have demonstrated the utility of such films for plasmonics applications: the films support surface plasmon polaritons with extremely low damping. Although the authors have observed that films with thickness on the order of several tens of nanometers can be relatively stable against dewetting—at least on a time scale long enough for fabrication and EOT probing under ambient conditions—they have also seen that very thin Ag films (e.g., 5 nm) start dewetting under ambient conditions within about 24 hours. This raises an important question: how and why does dewetting occur? The authors have now undertaken a detailed and systematic study of the mechanism of dewetting in epitaxial Ag films on Si(111) as a function of film thickness. The current presentation will focus on this work, and will attempt to shed light on the apparent robustness of films grown using their method.

3:54PM D17.00006 Diffusion of a Ga adatom on the GaAs(001)- $c(4 \times 4)$ -heterodimer surface: A first-principles study¹, SANJAY KHARE, JASON ROEHL, SANDEEP ARAVELLI, University of Toledo, RAY PHANEUF, University of Maryland — The adsorption and diffusion behavior of a Ga adatom on the GaAs(001)- $c(4 \times 4)$ -heterodimer surface were studied by employing ab initio density functional theory computations in the local density approximation. Structural and bonding features of the $c(4 \times 4)$ -heterodimer reconstruction surface were examined. A comparison with the $c(4 \times 4)$ -ss reconstruction² was performed. Minimum energy sites (MES) on $c(4 \times 4)$ -heterodimer surface were located by mapping the potential energy surface for a Ga adatom. Barriers for diffusion of a Ga adatom between the neighboring MES were calculated by using top and exchange diffusion mechanisms. We proposed two unique diffusion pathways for a Ga adatom diffusing between the global minimums of two neighboring unit cells. Signature differences between electronic structures of top- and exchange- diffusion mechanisms were studied for relevant atoms. We observed a higher diffusion barrier for exchange mechanism compared to top hopping.³

¹Submitted for publication.

²J. L. Roehl et al, Phys. Rev. B 82, 165335 (2010).

³Supported by NSF DMR 0705464, CNS 0855134.

4:06PM D17.00007 Voronoi Cell Patterns: theoretical model and application to submonolayer growth¹, DIEGO LUIS GONZÁLEZ², T.L. EINSTEIN, U. of Maryland — We use a simple fragmentation model to describe the statistical behavior of the Voronoi cell patterns generated by a homogeneous and isotropic set of points in 1D and in 2D. In particular, we are interested in the distribution of sizes of these Voronoi cells. Our model is completely defined by two probability distributions in 1D and again in 2D, the probability to add a new point inside an existing cell and the probability that this new point is at a particular position relative to the preexisting point inside this cell. In 1D the first distribution depends on a single parameter while the second distribution is defined through a fragmentation kernel; in 2D both distributions depend on a single parameter. The fragmentation kernel and the control parameters are closely related to the physical properties of the specific system under study. We apply our model to describe the Voronoi cell patterns of island nucleation for critical island sizes $i=0,1,2,3$. Experimental results for the Voronoi cells of InAs/GaAs quantum dots are also described by our model.

¹Supported primarily by NSF-MRSEC-DMR 05-20471, with partial support from DOE-BES-CMCSN and by CNAM at UMD

²Affiliation as of 1/12: Univ. del Valle, Cali, Colombia

4:18PM D17.00008 Aberration corrected Low Energy Electron Microscopy for Surface and Interface Studies, RUDOLF TROMP, IBM T.J. Watson Research Center — Correction of spherical and chromatic aberrations of the electron microscope objective lens constitutes one of the most significant and far-reaching breakthroughs in electron optics in the last 20 years. For instance, with the TEAM microscope it is now possible to image atoms with a spatial resolution of 50 picometers, providing a detailed real-space view of the carbon atoms in a single sheet of graphene. Similarly, the resolution on Low Energy Electron Microscopy (LEEM) has improved from a typical value of 5 nm, to less than 2 nm, at an electron energy of just a few eV. Photo Electron Emission Microscopy (PEEM) has recently achieved a resolution of 5 nm. In this talk I will discuss the successful implementation of electron-mirror based aberration correction in LEEM. Some of the details of the electron optical implementation will be discussed, in particular the unique optical properties of the electron mirror, and its mode of operation. Quantitative methods to verify proper control of the optical parameters and successful aberration correction have been developed and implemented in this new instrument. Spatial resolution has improved by more than a factor 2 as compared to the uncorrected instrument, and an ultimate spatial resolution below twice the wavelength of the electron at the sample appears to be achievable. In comparison, the highest resolution Transmission Electron Microscopes have a spatial resolution of about 20 electron wavelengths.

4:54PM D17.00009 LEEM and STM studies of Ag on Ge (110)¹, BRET STENGER, CORY MULLETT, MARSHALL VAN ZIJLL, EMILIE HUFFMAN, DYLAN LOVINGER, SHIRLEY CHIANG, University of California Davis — The growth of Ag deposited on Ge(110) was studied with low energy electron microscopy (LEEM) and scanning tunneling microscopy (STM). The LEEM studies showed the formation of long one dimensional islands as Ag was deposited above 430 °C. Island nucleation proceeded from defects in the Ge substrate. During deposition, the length of the islands increased while the width remained constant. The size and distribution of the islands was dependent on the substrate temperatures during deposition. At 480 °C, islands were 100 nm wide and 1-20 μm long at 9 ML of coverage. At 530 °C, islands were 200nm wide and 1-3 μm long at 9 ML of coverage. STM images showed that the islands were composed of Ag and that the surface regions between the islands exhibited a reconstruction which is characteristic of pure Ge.

¹Funded by NSF CHE-0719504 and NSF PHY-1004848.

5:06PM D17.00010 LEEM Observations of Ag/Ge(111) Structural Phases and Phase Transformations¹, SHIRLEY CHIANG, CORY MULLETT, University of California Davis — We use low energy electron microscopy (LEEM) to study the growth of, and transformations between structural phases of Ag deposited on Ge(111) above and below the Ag desorption temperature. Ag deposited on Ge(111) forms three main surface phases above 100 °C: (4x4), ($\sqrt{3}\times\sqrt{3}$)R30°, and (3x1). For deposition between 540-575 °C, a (3x1) phase grows. Upon the completion of the growth of the (3x1) phase, a ($\sqrt{3}\times\sqrt{3}$)R30° phase grows. For sufficiently high Ag deposition rates, we observed the same growth sequence above the Ag desorption temperature of 575 °C, up to 640 °C. Desorption above 575 °C proceeds with the reverse sequence: the ($\sqrt{3}\times\sqrt{3}$)R30° phase desorbs followed by desorption of the 3x1 phase. Above 640 °C, we observed the growth of the (3x1) phase but not the ($\sqrt{3}\times\sqrt{3}$)R30°. For 4x4 and ($\sqrt{3}\times\sqrt{3}$)R30° surfaces prepared by deposition between 200-500 °C we observe the transformation of these phases to a 1x1 disordered phase at the desorption temperature (575 °C), with desorption proceeding from the edges of disordered 1x1 domains.

¹Funded by NSF CHE-0719504 and NSF PHY-1004848.

5:18PM D17.00011 Crystalline Structure of the Pb/Si(111)7x7 Stable Wetting Layer, M. GRAMLICH, S.T. HAYDEN, YIYAO CHEN, U. Missouri, C. KIM, Kyun Hess U., Korea, M.C. TRINGIDES, Ames Lab-USDOE, P.F. MICELI, U. Missouri — The wetting layer formation in the Pb/Si(111)7x7 system has attracted extensive interest because of anomalously fast kinetics, which enables the formation of quantum size effect (QSE) nanoislands [Jeffrey et al. PRL **96**, 106105 (2006)]. However, previous studies of the wetting layer by x-ray diffraction and scanning-probes have led to *inconsistent* structural models; thus, the structure of this wetting layer has been unsolved. Furthermore, a recent investigation has revealed that the wetting layer is out-of-equilibrium over a surprisingly broad temperature range [Gramlich et al., PRB **84**, 075433 (2011)]. Using *in situ* x-ray scattering methods, we have solved the *stable*, low temperature annealed structure of the wetting layer. It exhibits a strained atomic layer where Pb atoms are in transition, from Si-7x7 sites towards 8x8-sites, with some Pb-atoms vertically closer to the Si-7x7. Interestingly, the Si adatoms shift to the edges of the unit cell. Funding is acknowledged from NSF DMR-0706278 (PFM, MWG, STH, YC, and the Ministry of Knowledge Economy of Korea 2009-F014-01 (CK). The experiments were performed on the 6IDC beam line, supported by the US-DOE (through Ames Lab, W-7405-Eng-82), at the Advanced Photon Source (US-DOE, W-31-109-Eng-38) located at Argonne National Laboratory.

Monday, February 27, 2012 2:30PM - 5:30PM —

Session D18 DMP: Focus Session: Nanostructures and Metamaterials, Growth, Structure, and Characterization – What is a good conductor for Metamaterials and Plasmonics 252B

2:30PM D18.00001 Manipulating Plasmons Using Graphene for One-Atom-Thick Optical Signal Processing, NADER ENGHETA, University of Pennsylvania — In this talk, we provide an overview of our recent theoretical work on merging the field of graphene with metamaterials and transformation optics. In particular, we show that the control and variation of graphene's conductivity, spatially and temporally, may offer a one-atom-thick platform for manipulation of optical signals propagating along the single sheet of graphene as the surface Plasmon polariton (SPP) surface waves. Since the phase velocity of the SPP surface wave directly depends on the graphene conductivity, tailoring the conductivity can be regarded as a “knob” to control and shape the propagation of such SPP across the graphene. We have shown that such inhomogeneous distribution of conductivity across the graphene gives rise to the notion of one-atom-thick transformation optics and metamaterials—essentially thinnest possible metamaterials [A. Vakil, N. Engheta, *Science*, **332**, 1291 (2011)]. Additionally we have demonstrated, theoretically and using computer simulations, that one can achieve optical signal processing functions such as Fourier transforming across a single layer of graphene [A. Vakil, N. Engheta, “Fourier Optics on Graphene” *ArXiv* 1108.5218 (2011)]. The graphene-based Fourier optics suggests prospects for multilayer signal processing, allowing for design of ultra-compact nanoscale signal processing systems. We are also investigating other optical manipulation, such as waveguiding, field confinement in cavities, graphene antennas, optical spectrometry, and optical mirror reflection, all on one-atom-thick structures. In this talk, we will present some of our results on these topics.

3:06PM D18.00002 Graphene, superconductors, and metals: What is a good conductor for metamaterials and plasmonics?¹, PHILIPPE TASSIN, Vrije Univ. Brussel and Ames Lab/Iowa State Univ. — Recent developments in the field of metamaterials and plasmonics have promised a number of exciting applications, in particular at terahertz and optical frequencies. Most metamaterials consist of carefully designed metallic structures that replace atoms in their role as the basic unit of interaction with electromagnetic radiation. Unfortunately, the noble metals are not particularly good conductors at optical frequencies, resulting in significant dissipative loss in metamaterials. In this communication, we address the question of what is a good conductor for use in metamaterials and in plasmonics. We develop a model based on the quasistatic response of the metamaterial constituents to an incident electromagnetic field in order to derive a figure of merit for conductors. We find (1) it is the resistivity of the material—rather than the conductivity or permittivity—that provides direct information on the dissipative loss in the metamaterial, and (2) the dissipative loss depends on certain geometric aspects of the system, such as the layer thickness. Subsequently, we apply the model to graphene, to superconductors (Nb and YBCO), to several noble and transition metals, and to some conducting oxides (like ITO).

¹Co-authors of this work are Thomas Koschny, Maria Kafesaki, and Costas M. Soukoulis. This work was supported by Ames Laboratory (U.S. DOE), the U.S. ONR (Award No. N000141010925), and the E.U. project NIMNIL (Grant. No. 228637).

3:42PM D18.00003 Quantum Plasmonics, REINIER HEERES, LEO KOUWENHOVEN, VALERY ZWILLER, TU Delft — Surface plasmon polaritons allow confinement of light to sub-wavelength length-scales. Due to the confinement the electro-magnetic fields involved are stronger, which can be used to enhance optical interactions. We use this fact to realize a plasmonic beam-splitter based on a directional-coupler geometry, i.e. two waveguides close to each other coupled by their evanescent fields. This beam-splitter can be much smaller than conventional dielectric structures. Integrated Niobium-Nitride superconducting single-photon detectors (SSPDs) allow to probe the plasmons directly in the near-field. This makes it possible to study the structure on the quantum level using photon pairs created in a spontaneous parametric down-conversion process. Our aim is to observe Hong-Ou-Mandel interference, a true quantum effect which causes indistinguishable photons arriving at the same time at both inputs to exit through the same port, i.e. bunch. This will prove the quantum nature of surface plasmons and could be used to build sub-wavelength quantum logic gates. We also show that resonant plasmonic antennas can greatly enhance the absorption and therefore detection efficiency of SSPDs.

3:54PM D18.00004 Application of metasurface description for multilayered metamaterials and an alternative theory for metamaterial perfect absorber¹, JIANGFENG ZHOU, University of South Florida, HOU-TONG CHEN, Los Alamos National Laboratory, THOMAS KOSCHNY, Ames Laboratory, Iowa State University, ABUL AZAD, ANTOINETTE TAYLOR, Los Alamos National Laboratory, COSTAS SOUKOULIS, Ames Laboratory, Iowa State University, JOHN O'HARA, Oklahoma State University — Recently, the metamaterial perfect absorber has attracted intense interest in metamaterial community. The impedance matching mechanism based on effective bulk permittivity and permeability is widely used to explain such structures. However, this model has difficulties, in particular, because such systems are usually asymmetric, assigning homogenous effective material parameters to these systems may lead to unphysical results. In our work, we use an effective medium model that treats each layer of the metamaterial as a metasurface with unique effective surface electric and magnetic susceptibility, χ_{se} and χ_{sm} . We then use a transfer matrix method to analyze the overall EM properties of multilayered metamaterials using the effective material parameters (surface susceptibilities) of each layer. We find that the functional mechanism is the Fabry-Perot interference resulting from the multiple reflections in the cavity bounded by two metamaterial layers. This contrasts with previous explanations based on bulk effective medium theory.

¹Los Alamos National Laboratory LDRD Program, Ames Laboratory was supported by the Department of Energy (Basic Energy Sciences) under contract No. DE-AC02-07CH11358. This was partially supported by the U.S. Office of Naval Research, Award No. N000141010925

4:06PM D18.00005 Active Core-Shell Nanowire Optical Antenna Absorbers¹, CARLOS ASPETTI, CHANG-HEE CHO, RITESH AGARWAL, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA — Core-shell dielectric-metal nanoparticles have demonstrated tunability of their absorption properties due to the size- and shape-dependence of the surface plasmon resonance. Recently, the core-shell semiconductor-insulator-metal nanowire was examined as a platform for manipulating the core emitter lifetimes due to the highly confined and intense electromagnetic fields mediated by whispering gallery surface plasmon polariton modes. Combining these two concepts we realize an active semiconductor-insulator-metal optical antenna, which demonstrates a highly tunable absorption spectrum. By directly contacting the semiconductor core, photocurrent data is coupled with simulations to show highly tunable, significant broad-band absorption enhancement; a general result for a range of material systems.

¹Research for this publication was conducted with Government support under and awarded by DoD, Air Force Office of Scientific Research, National Defense Science and Engineering Graduate (NDSEG) Fellowship, 32 CFR 168a.

4:18PM D18.00006 Genetic Optimization of Optical Nanoantennas, CARLO FORESTIERE, ALYSSA PASQUALE, Department of Electrical and Computer Engineering & Photonic Center, Boston University, ANTONIO CAPRETTI, Department of Electrical Engineering, Università degli Studi di Napoli Federico II, SYLVANUS LEE, Department of Electrical and Computer Engineering & Photonic Center, Boston University, GIOVANNI MIANO, Department of Electrical Engineering, Università degli Studi di Napoli Federico II, ANTONELLO TAMBURRINO, DAEIMI, Università degli Studi di Cassino, LUCA DAL NEGRO, Department of Electrical and Computer Engineering & Photonic Center, Boston University — Metal nanostructures can act as plasmonic nanoantennas (PNAs) due to their unique ability to concentrate the light over sub-wavelength spatial regions. However engineering the optimum PNA in terms of a given quality factor or objective function. We propose a novel design strategy of PNAs by coupling a genetic optimization (GA) tool to the analytical multi-particle Mie theory. The positions and radii of metallic nanosphere clusters are found by requiring maximum electric field enhancement at a given focus point. Within the optimization process we introduced several constraints in order to guarantee the physical realizability of the tailored nanostructure with electron-beam lithography (EBL). Our GA optimization results unveil the central role of the radiative coupling in the design of PNA and open up new exciting pathways in the engineering of metal nanostructures. Samples were fabricated using techniques and surface-enhancement Raman scattering measures were performed confirming the theoretical predictions.

4:30PM D18.00007 Plasmonic Anti-Hermitian Coupling for Nano-Manipulation of Light, ZILIANG YE, SHAUNG ZHANG, YUANG WANG, YONGSHIK PARK, GUY BARTAL, XIAOBO YIN, XIANG ZHANG, UC Berkeley — Open quantum systems consisting of coupled bound and continuum states have been studied in a variety of physical systems. In these systems, the effects of the continuum decay channels are accounted for by indirect anti-Hermitian couplings among the bound states. Here we propose a general scheme to control light in a nano-plasmonic system by utilizing the anti-Hermitian coupling between the individually designed resonances of each plasmonic element in the system. As a specific example, we experimentally show a realistic coupled plasmonic dipole antenna array with $\lambda/15$ separations, in which selective excitation of an individual antenna can be achieved by tuning the frequency of the incident light. Without the anti-Hermitian coupling, these antennas are indistinguishable from each other.

4:42PM D18.00008 Broadband scattering reduction using a hybrid inertial metamaterial design¹, THEODORE MARTIN, GREGORY ORRIS, Naval Research Laboratory — The ability to hide an object from an external wave through scattering reduction is one of the most sought-after goals of the metamaterials community. Using transformational optics, Pendry [1] demonstrated that a wave can be bent around an object using a conformal map that reduces the object's scattering cross section to zero. The transformational method has now been extended to transformational acoustics [2], but the traditional inertial method requires infinite mass at the boundary of the hidden object, which cannot be easily approximated in practice. Scattering reduction can also be obtained over a more limited bandwidth using wrapping layers that cancel some of the modal coupling between the object and the exterior environment [3]. Using multiple scattering theory, we demonstrate that a combination of an “imperfect” conformal map with a scattering cancellation layer can achieve improved scattering reduction over a broad bandwidth in an aqueous acoustic environment. Our “hybrid” design is amenable to a parameter-space constrained to within an order of magnitude of the background fluid in order to obtain a solution with realistic material properties. The introduction of a cancellation layer enables us to optimize performance over targeted frequency bands with only a small impact on the overall size of the design.

[1] J. B. Pendry, D. Schurig, and D. R. Smith, *Science* **312**, 1780 (2006).

[2] S. A. Cummer and D. Schurig, *New J. Phys.* **9**, 45 (2007).

[3] A. Alù and N. Engheta, *Phys. Rev. Lett.* **100**, 113901 (2008).

¹Supported by the Office of Naval Research

4:54PM D18.00009 Surface plasmon excitations in multicoaxial metamaterial cables: Zero magnetic field, BAHRAM DJAFARI-ROUHANI, University of Science & Technology of Lille, MANVIR KUSHWAHA, Rice University — By using an elegant response function theory, which does not require matching of the messy boundary conditions, we investigate the surface plasmon excitations in the multicoaxial cylindrical cables made up of negative-index metamaterials in the absence of an applied magnetic field. The multicoaxial cables with *dispersive* metamaterial components exhibit rather richer (and complex) plasmon spectrum with each interface supporting two modes: one TM and the other TE for (the integer order of the Bessel function) $m \neq 0$. The cables with *nondispersive* metamaterial components bear a different tale: they do not support simultaneously both TM and TE modes over the whole range of propagation vector. The computed local and total density of states enable us to substantiate spatial positions of the modes in the spectrum.¹ Such quasi-one dimensional systems as studied here should prove to be the milestones of the emerging optoelectronics and telecommunications systems.

¹M.S. Kushwaha and B. Djafari-Rouhani, *J. Opt. Soc. Am B* **27**, 605 (2010).

5:06PM D18.00010 Surface Plasmon Based Engineering of Semiconductor Nanowire Optics¹, CHANG-HEE CHO, CARLOS O. ASPETTI, Department of Materials Science and Engineering, University of Pennsylvania, MICHAEL E. TURK, JAMES M. KIKKAWA, Department of Physics and Astronomy, University of Pennsylvania, SUNG-WOOK NAM, RITESH AGARWAL, Department of Materials Science and Engineering, University of Pennsylvania — Emission from unthermalized (hot) excitons can be observed from high-quality crystals and quantum-well structures due to decreases in the exciton lifetimes but typically with low yields. By employing a plasmonic nanocavity, we observe efficient hot-exciton emission in core-shell CdS-SiO₂-Ag nanowires with intensities surpassing those from thermalized excitons [1]. These new spectral characteristics are mediated by whispering gallery plasmonic modes that yield highly intense electromagnetic fields. As a result, the exciton radiative lifetime is decreased by several orders of magnitude. The introduction of a high-quality hybrid plasmonic nanocavity structure significantly changes the photophysics of the host material, demonstrating an approach applicable to other material systems.

[1] Chang-Hee Cho, *et al*, *Nature Materials*, **10**, 669 (2011).

¹Transient optical work supported by the Department of Energy BES Award No. DESC0002158. Remaining work supported by ARO W911NF-09-1-0477, NIH Director's New Innovator Award Program, 1-DP2-7251-01, NSF-NSEC-DMR08-32802, and NSF IGERT DGE02-21664.

5:18PM D18.00011 Plasmonic nanostructures for multiscale light amplification, AIQING CHEN, ULRICH WELP, VITALII VLASKO-VLASOV, Argonne National Laboratory, MSD, RYAN MILLER, ELENA SHEVCHENKO, LEONIDAS OCOLA, STEPHEN GRAY, Argonne National Laboratory, CNM, EUGENE DEPRINCEIII, Georgia Institute of Technology — We demonstrate experimentally a multiscale plasmonic design for giant light amplification using gold nanoparticles self-assembled in gratings on a metal mirror with thin dielectric spacer. The successive increase of the light enhancement factors upon addition of individual plasmonic elements in the design is tested by measurement of the Raman signal from R6G and benzenethiol molecules on clusters of nanoparticles, their ordered arrays on dielectric, semiconducting, and metal substrates, and on metal substrate with gratings. High fidelity of our structures as SERS substrates are confirmed by areal maps of the Raman response. FDTD numerical calculations are in a good agreement with our experimental measurements.

Monday, February 27, 2012 2:30PM - 4:54PM –

Session D19 DCMP DMP: Invited Session: Novel Phases in Strongly Correlated Iridates 253AB

2:30PM D19.00001 Spin orbit coupling, electron correlations and exotic magnetism in 5d complex Ir oxides, HIDENORI TAKAGI, Department of Physics, University of Tokyo and RIKEN ASI — In 5d Iridium oxides, a large spin-orbit coupling of ~ 0.5 eV, inherent to heavy 5d elements, is not small as compared with the width of d bands and often modifies the landscape of the electronic structure substantially. This is distinct from those of 3d transition metal oxides and gives rise to a variety of novel electronic phases. Layered Ir⁴⁺ perovskite Sr₂IrO₄ is recently revealed to be a novel $J_{eff}=1/2$ Mott insulator [1,2], where even a moderate Coulomb U can open up a correlation gap because of the large spin-orbit coupling. In the three dimensional analogue of Sr₂IrO₄, SrIrO₃, the large spin-orbit coupling manifests itself in a contrasted way, where the interplay of strong spin-orbit coupling and lattice distortions brings the system almost to a band insulator. SrIrO₃ is in fact a very low carrier density semimetal with unusual transport and magnetic properties. If $J_{eff}=1/2$ Ir⁴⁺ is placed on a honeycomb lattice or a geometrically frustrated lattice such as pyrochlore lattice, even more exotic states might be anticipated, including a correlated topological insulator [3] and a Kiteav magnet [4]. Our attempt to explore such spin-orbit coupling induced states will be reported.

Work done in collaboration with T. Takayama, B.J.Kim, S.Fujiyama, K.Ohashi, J.Matsuno, H.Osumi and T.Arima.

[1] B.J.Kim *et al.*, *Phys Rev Lett* **101**, 076402 (2008).

[2] B. J. Kim, H. Ohsumi, T. Komesu, S. Sakai, T. Morita, H. Takagi, and T. Arima, *Science* **323**, 1329 (2009).

[3] Shitade *et al.*, *Phys. Rev. Lett.* **102**, 256403 (2009).

[4] J. Chaloupka, G.Jackeli, and G.Khalullin, *Phys. Rev. Lett.* **105**, 027204 (2010)

3:06PM D19.00002 Topological and spin-liquid phases in strongly correlated iridates, YONG BAEK KIM, University of Toronto — Recently, the emergence of topological phases in interacting electron systems such as topological insulators and spin liquid phases, has been a subject of intensive research. In particular, much attention has been given to 5d transition metal oxides where the strong spin-orbit coupling and intermediate strength of the electron interaction provide an ideal playground for the emergence of a number of interesting topological phases. We summarize recent theoretical efforts in this direction in the context of Iridates, or iridium oxides. We make connections to the existing and future experiments on a variety of iridates materials including pyrochlore iridates, honeycomb-lattice iridates, and hyperkagome-lattice systems.

3:42PM D19.00003 Possible proximity of the Iridates $(\text{Na,Li})_2\text{IrO}_3$ to a topologically ordered Mott insulator: Phase diagram of the Heisenberg-Kitaev model, SIMON TREBST, University of Cologne — Motivated by the recent experimental observation of a Mott insulating state for the layered Iridates $(\text{Na,Li})_2\text{IrO}_3$, we discuss possible ordering states of the effective Iridium moments taking into account the extreme sensitivity of these 5d transition metal oxides to crystal field effects and strong spin-orbit coupling. The microscopic exchange has been argued [1,2] to be a combination of isotropic Heisenberg and highly anisotropic Kitaev exchange, which can be tracked back to the spin and orbital components of the effective momenta. Depending on the relative strength of these two couplings, the system exhibits either various types of conventional magnetic order or a more exotic gapless spin-liquid ground state. Carefully studying [3] the stability of these phases at finite-temperatures – and the role of frustration, i.e. a considerable suppression of the ordering temperature from the Curie-Weiss temperature – allows us to connect back to thermodynamic experiments [4] on the Iridates $(\text{Na,Li})_2\text{IrO}_3$ and possibly estimate microscopic coupling parameters. Finally, we discuss the effects of a magnetic field applied in the [111] direction – perpendicular to the hexagonal lattice formed by the Iridium moments – and show that a topologically ordered ground state is found over a small range of coupling parameters [5], also indicating the existence of an exotic critical point whose location might not be far from actual material parameters.

Work done in collaboration with H.C. Jiang, Z.C. Gu, X.L. Qi, J. Reuther, and R. Thomale.

- [1] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. 102, 017205 (2009).
- [2] J. Chaloupka, G. Jackeli, and G. Khaliullin, Phys. Rev. Lett. 105, 027204 (2010).
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4:18PM D19.00004 Honeycomb lattice spin-orbit Mott insulators¹, PHILIPP GEGENWART, I. Physikalisches Institut, Georg-August University Goettingen — Iridates displaying a Mott insulating state caused by the interplay of electronic correlations and strong spin-orbit coupling have recently attracted considerable attention. We focus on the honeycomb material A_2IrO_3 ($\text{A}=\text{Na, Li}$), in which the topology of the underlying lattice leads to interesting magnetic properties [1]. The strong spin-orbit coupling in this 5d transition metal system is expected to result in orbital-dependent highly anisotropic magnetic in-plane exchange [2]. The combination of $J_{\text{eff}} = 1/2$ and the underlying honeycomb lattice makes A_2IrO_3 a promising candidate for the Kitaev model, which is exactly solvable and has a spin-liquid ground state. Our experimental data on Na_2IrO_3 prove a Mott insulating state of effective $J=1/2$ moments with predominant antiferromagnetic coupling, indicated by a Weiss temperature of $\theta = -120$ K. A bulk antiferromagnetic transition occurs at a much reduced temperature of $T_N = 15$ K and the reduced magnetic entropy suggests strong magnetic frustration and/or low-dimensional magnetic interactions. The nature of the ordered phase has also been studied by resonant x-ray spectroscopy near the Ir-L3 edge, providing evidence for an unconventional, most-likely zig-zag-type spin ordering [3]. The latter may be related to next-nearest neighbour exchange and/or a substantial Kitaev contribution in the Heisenberg-Kitaev model [2]. Upon replacing Na with the smaller Li, one may enhance the relative importance of the Kitaev contribution. For Mott insulating Li_2IrO_3 we observe a similar ordering temperature of 15 K, while the negative Weiss temperature is drastically reduced. These observations are compatible with an enhancement of the Kitaev contribution compared to the Na-system, suggesting that Li_2IrO_3 could be located close to the Kitaev limit [5].

- [1] Yogesh Singh and P. Gegenwart, Phys. Rev. B. 82, 064412 (2010).
- [2] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. 102, 017205, (2009).
- [3] X. Liu et al., Phys. Rev. B 83, 220403(R) (2011).
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¹Work in collaboration with Yogesh Singh and Soham Manni.

Monday, February 27, 2012 2:30PM - 5:30PM –
Session D20 FIAP: Invited Session: Advanced Electromagnetic Imaging and Remote Sensing:
From DC to Daylight 253C

2:30PM D20.00001 Advanced EM Modeling in Support of Buried Target Detection and Identification¹, EUGENE LAVELY, BAE Systems — The detection and discrimination of buried unexploded ordnance is essential for restoration of millions of acres of munitions testing grounds to public use. Public safety is paramount so high detection probability is essential, and accurate discrimination is key for economically feasible remediation. Time domain electromagnetic (TDEM) induction methods in principle have the capability to address these criteria. The transmitter loop current pulse generates a magnetic field in the target region. This changing applied field, especially as the pulse terminates, induces currents in the target, generating a scattered magnetic field. The decaying scattered field, following pulse termination, induces the measured voltage in the receiver loop. There are three different regimes that one may identify in the voltage time traces: early, intermediate, and late time. At very early time, immediately following pulse termination, the currents are confined to the immediate surface of the target. The initial diffusion of these currents into the target interior leads to a $1/2$ power law decay for nonferrous targets, ($3/2$ for ferrous targets). At intermediate time, as the currents penetrate the deeper target interior, the power law crosses over to a multi-exponential decay, representing the simultaneous presence of a finite set of exponentially decaying modes. Finally, at late time only the single, slowest decaying mode survives. At intermediate- to late-time our mean field algorithm models the dynamics by computing as large a number as possible of the modes, and determining the excitation level of each. At early time, the power law arises from a superposition of an essentially infinite number of exponentials, and a complementary theory, based on the detailed dynamics of the initial very thin surface current sheet, has been developed instead. We pre-compute intrinsic properties of modes containing all discrimination information of targets, and use this for nearly real-time inversion of TDEM measurement for target properties and subsequent discrimination.

¹Research supported by Strategic Environmental Research and Development Program (SERDP).

3:06PM D20.00002 Through-wall microwave imaging: some applications of physics to urban reconnaissance¹, PETER WEICHMAN², BAE Systems — I will review some recent physics-based modeling approaches in support of microwave through-wall building tomography. Building layout estimation is a nonlinear inverse problem with a large number of degrees of freedom (geometry, location, and scattering properties of major building elements, such as walls, floors, and ceilings, plus many other smaller elements such as windows, doorways, and stairways). The physics of microwave propagation in such environments is very complex, involving multiple reflection, transmission, and diffraction events. Careful control of measurement protocol, using well-focused and directed transmitter and receiver arrays, can mitigate this to some degree. However, even under the most optimistic scenarios, the number of interactions increases exponentially as the signal penetrates more deeply into the building. Multiple overlapping returns from different building elements quickly overwhelm one's ability to disambiguate their sources. To explore the fundamental limitations on solutions to the inverse problem, efforts to create physics-based models that capture the signal complexity as accurately as possible will be described. These models remain an approximate description of reality, but nevertheless enable one to understand the effects of the explosion of multiple scattering events on the inversion, and quantify the limits of the inversion quality under even the most optimistic scenarios for data diversity and precision.

¹Research supported by DARPA Contract No. HR0011-06-C-0110

²6 New England Executive Park, Burlington, MA 01803

3:42PM D20.00003 Advanced methods in synthetic aperture radar imaging, THOMAS KRAGH, BAE Systems — For over 50 years our world has been mapped and measured with synthetic aperture radar (SAR). A SAR system operates by transmitting a series of wideband radio-frequency pulses towards the ground and recording the resulting backscattered electromagnetic waves as the system travels along some one-dimensional trajectory. By coherently processing the recorded backscatter over this extended aperture, one can form a high-resolution 2D intensity map of the ground reflectivity, which we call a SAR image. The trajectory, or synthetic aperture, is achieved by mounting the radar on an aircraft, spacecraft, or even on the roof of a car traveling down the road, and allows for a diverse set of applications and measurement techniques for remote sensing applications. It is quite remarkable that the sub-centimeter positioning precision and sub-nanosecond timing precision required to make this work properly can in fact be achieved under such real-world, often turbulent, vibrationally intensive conditions. Although the basic principles behind SAR imaging and interferometry have been known for decades, in recent years an explosion of data exploitation techniques enabled by ever-faster computational horsepower have enabled some remarkable advances. Although SAR images are often viewed as simple intensity maps of ground reflectivity, SAR is also an exquisitely sensitive coherent imaging modality with a wealth of information buried within the phase information in the image. Some of the examples featured in this presentation will include: (1) Interferometric SAR, where by comparing the difference in phase between two SAR images one can measure subtle changes in ground topography at the wavelength scale. (2) Change detection, in which carefully geolocated images formed from two different passes are compared. (3) Multi-pass 3D SAR tomography, where multiple trajectories can be used to form 3D images. (4) Moving Target Indication (MTI), in which Doppler effects allow one to detect and geolocate moving targets within SAR images. (5) Real time video SAR, where one forms a continuously updated SAR image by “staring” at an area of interest.

4:18PM D20.00004 Multiple-input Multiple-output Ground Moving Target Indicator Radar: Theory and Practice, DAN BLISS, Lincoln Laboratory, Massachusetts Institute of Technology — Multiple-input multiple-output (MIMO) extensions to radar systems enable a number of advantages compared to traditional approaches. These advantages include improved angle estimation and target detection. In this paper, an overview of MIMO radar is provided, and the concept of coherent MIMO radar is defined. The principle focus of the paper is the discussion of MIMO ground moving target indication (GMTI). For GMTI radar modes, the advantages of a coherent MIMO architecture include improved angle estimation and enhanced slow speed target detection. To illustrate this, the concept of coherent MIMO radar is introduced and performance comparisons made between MIMO GMTI and traditional radar GMTI. These comparisons are supported by theoretical bounds, simulations, and experimental results for GMTI angle estimation accuracy and minimum detectable target velocity. For some applications, these results indicate significant potential improvements in clutter-mitigation, signal-to-noise ratio (SNR) loss, and reduction in angle-estimation error for slow-moving targets. The important effects of waveform characteristics is addressed.

4:54PM D20.00005 Image Formation in Bio-optical Sensing¹, ERIC MILLER, Tufts University — Over the past two decades a number of optical sensing methods have emerged with potential to provide complementary information to traditional medical imaging modalities in application areas ranging from basic science to disease diagnosis and treatment monitoring. Though still largely in the research and development stage, modalities including diffuse optical tomography (DOT), fluorescence molecular tomography (FMT), photo-acoustic tomography (PAT), and bio-luminescence tomography (BLT) have excited much interest due to their natural functional imaging capability, their relatively low cost, and the fact that none required the use of ionizing radiation. These advantages however are tempered by a number of challenges associated with the processing of these data. Specifically, these data types all rely in one way or another on the interaction of light with tissue. The diffusive nature of this interaction inherently limits the spatial resolution of these modalities. As a result the process of forming an image is a far more delicate task than is the case with more standard imaging modalities such as X-ray computed tomography (CT). Two basic methods have been explored to address the ill-posedness of these problems in order to improve the information content in the resulting images. The optical data may be augmented either through the use of spectral diversity or by attempting to integrate optical data types with information from other modalities such as CT or MRI. Alternatively, a mathematical technique known as regularization can be used to impose physically-based constraints on the reconstruction. In this talk, I shall provide an overview of the work in my group in optical image formation within the contexts of DOT for breast cancer imaging and FMT for small animal imaging. The focus of the talk will be on methods that integrate data augmentation and mathematical regularization. In the case of FMT, we shall discuss our work in combining the optical data with information provided by CT concerning the structural distribution of tissue classes within the region of interest. Here, we have developed a number of spatially-varying regularization methods which use the CT data to help constrain the FMT reconstruction and obtain imaging results that are substantially improved over classical regularization techniques. For DOT, we have recently been considering the use of hyperspectral data sets in which information from over 100 near infrared wavelengths is made available to the processing. When combined with a regularization scheme based on parameterizing the images in a geometric manner, we believe that it will be possible to produce a standalone DOT system with spatial resolution that is today only achieved by combining DOT with e.g., CT.

¹This work was supported in part by NIH Grant R01-CA154774.

Monday, February 27, 2012 2:30PM - 5:30PM — Session D21 DCMP: Multiband Superconductivity, mostly MgB₂ 254A

2:30PM D21.00001 STS studies of the pi-band superconductivity in MgB₂ in a transverse field¹, C. GRIGGS, M.R. ESKILDSEN, University of Notre Dame, N.D. ZHIGADLO, J. KARPINSKI, ETH — Since being discovered MgB₂ has become the paradigm for two-band/two-gap superconductivity. Early scanning tunneling spectroscopy (STS) measurements, showed a rapid suppression of the superconductivity in the isotropic π -band for modest applied fields $H \parallel c$. These measurements were performed with the tunnel current (I_t) parallel to the crystalline c -axis which couple, almost exclusively, to the π -band, and with the suppression attributed to vortex core overlap. Here we report STS measurements performed in a transverse field, such that $I_t \parallel c \perp H$. In this configuration no vortices are cutting through the image plane, and instead the superconducting phase is affected by the Meissner currents running within one penetration depth of the sample surface. Within this field orientation we observe far less suppression of the superconducting state in the π -band compared to the earlier measurements with $H \parallel c$. A clear gap is seen up to $H = 0.9$ T.

¹Supported by NSF award no. DMR-0804887.

2:42PM D21.00002 Measurement of penetration depth of MgB_2 using DC SQUID, DANIEL CUNNANE, KE CHEN, X.X. XI, Temple University — Penetration depth is an important parameter for the design of Rapid Single Flux Quantum (RSFQ) circuits. For MgB_2 , different values from 40 nm to 150 nm have been reported by different groups. We have measured the penetration depth of MgB_2 using MgB_2 DC SQUIDS. The SQUID was made using $\text{MgB}_2/\text{MgO}/\text{MgB}_2$ Josephson junctions with epitaxial MgB_2 electrodes deposited via Hybrid Physical-Chemical Vapor Deposition. The MgO was deposited by RF Magnetron Sputtering of an MgO target. The device shows good voltage modulation above 150 μV . The working temperature for these SQUIDS ranges from below 10K to 37K, with the optimum voltage modulation near 35K. The results will be discussed in comparison to the penetration depth reported by other measurement techniques.

2:54PM D21.00003 Effect of scattering on the gap distribution in tunneling spectra of $\text{MgB}_2/\text{I}/\text{Pb}$ junctions, WENQING DAI, QI LI, Department of Physics, Pennsylvania State University, University Park, PA 16802, KE CHEN, XIAOXING XI, Department of Physics, Temple University, Philadelphia, PA 19122 — We fabricated $\text{MgB}_2/\text{Native oxide}/\text{Pb}$ planar tunneling junctions using the MgB_2 films grown by the hybrid physical-chemical vapor deposition technique (HPCVD). Both π (~ 1.8 meV) and σ gaps (~ 7.9 meV) were observed in spectra due to tunneling from side of c -oriented MgB_2 grains on film surface on SiC (0001) substrates. We have previously observed a distribution of energy gap values within both bands in clean HPCVD films with long electron mean free path. Here we report an investigation of the tunneling spectra by systematically varying the MgB_2 film thickness and the thickness of native oxide barrier. We found the MgB_2 π gap distribution range narrows from ~ 1.7 meV to ~ 1.4 meV together with a loss of fine peak structures, as the MgB_2 film thickness decreases from 100 nm to 33 nm, in which the electron mean free path is limited by the thickness. In addition, fine peak structures also smear out when the junction resistance is large. The results show electron scattering from both inside the film and on the surface can smear out the gap distribution structures in tunneling spectra.

3:06PM D21.00004 Vortex Lattice Transition Dynamics in MgB_2 , C. RASTOVSKI, P. DAS, K. SCHLESINGER, M.R. ESKILDSEN, W.J. GANNON, University of Notre Dame, IN, USA, C.D. DEWHURST, Institut Laue-Langevin, France, N.D. ZHIGADLO, J. KARPINSKI, ETH Zurich, Switzerland — We present small-angle neutron scattering (SANS) studies of the vortex lattice (VL) in MgB_2 with $H \parallel c$. This material has three different VL phases, all with triangular symmetry but oriented differently with respect to the crystalline axes. Furthermore, a high degree of metastability between the VL phases of MgB_2 has been observed as the sample is cooled or heated across the equilibrium phase transitions. Here we present detailed studies of how the metastable (MS) VL phases transition to the ground state (GS), either driven by small changes of the DC magnetic field or by a transverse AC field. Our results show that the MS VL is not due to vortex pinning, and results are inconsistent with predictions based on the Bean model. Instead, we speculate that a “jamming” of counter rotated VL domains is responsible for the VL metastability. This is further supported by a power law dependence of the GS VL domain population upon the number of applied AC cycles. This work was supported by the Department of Energy, Basic Energy Sciences under Award No. DE-FG02-10ER46783.

3:18PM D21.00005 Non-linear Time Effects in Superconducting Polycrystalline MgB_2 , MURAT OLUTAS, ATILGAN ALTINKOK, ATILLA KILIC, KIVILCIM KILIC, Abant Izzet Baysal University — The time evolution of the voltage response (V-t curves) to a symmetric bi-directional square wave (BSW) current with long periods (P) applied to the MgB_2 sample was investigated at low dissipation levels. It was observed that regular sinusoidal-like voltage oscillations evolve at certain ranges of the amplitude (I_{BSW}) and period (P_I) of the BSW current, external magnetic field (H), and temperature (T). The regular sinusoidal-like oscillations were interpreted in terms of the dynamic competition between pinning and depinning processes. In this process, the interaction between flux lines and pinning centers could be elastic coupling because of rigidity of flux line lattice in MgB_2 . We suggest that the oscillating mode can be related to the drifting of flux lines which are in motion. In this case, due to the strong pinning and complex relaxation effects, the majority of flux lines traversing the sample does not leave it entirely and remains in an oscillating mode by moving forth and back as a function of time. We suggest that the flux dynamics associated with the oscillating mode is the ordered motion of defective flux line system. Fast Fourier Transform analysis of V-t oscillations showed that the period of oscillations is comparable to that of the BSW current. The oscillating mode was also discussed in terms of sliding charge density waves (CDWs).

3:30PM D21.00006 Study of MgB_2 Films for RF Cavity Applications¹, TENG TAN, CHENGGANG ZHUANG², ALEX KRICK, KE CHEN, XIAOXING XI, Department of Physics, Temple University — Magnesium diboride (MgB_2) is a promising superconducting material for RF cavity applications due to its high critical temperature T_c and large thermodynamic critical field H_c . Using Hybrid Physical-Chemical Vapor Deposition (HPCVD), we have grown 2"-diameter MgB_2 films on sapphire and metal substrates, including molybdenum, niobium, tantalum, and stainless steel. Measured by DC magnetization, the T_c 's of these films were between 38.2 to 39.2 K; the upper critical field H_{c2} 's were about 7 T, in consistent with previously reported value of clean MgB_2 films; the zero-field critical current density J_c 's were above 10^7 A/cm² and were suppressed rapidly by increasing applied magnetic field, indicating a lack of pinning in clean MgB_2 films. Multilayered MgB_2/MgO films were also investigated to prevent vortex penetrating the MgB_2 layer and increase the vortex penetration field (H_{c1}) following Gurevich's theoretical work [1]. The RF properties of these films were studied.

[1] A. Gurevich, *Appl. Phys. Lett.* 88, 012511 (2006).

¹This work is supported by DOE under grant No. DE-SC0004410

²Now at Corning Research Center, China

3:42PM D21.00007 Mesoscopic Nonlinear Electrodynamical Response of the Two Band Superconductor MgB_2 ¹, TAMIN TAI, University of Maryland-College Park, TENG TAN, XIAOXING XI, Temple University, BEHNOOD GHAMSARI, STEVEN ANLAGE, University of Maryland-College Park — Multi-gap superconductors are expected to have exotic physics associated with internal coupling between the multiple order parameters. 10 years after its discovery, MgB_2 is a two gap superconductor that still attracts much attention for both fundamental and practical reasons. A microwave measurement of the temperature dependent third harmonic response P_{3f} (T) is performed by applying a strong and localized (mesoscopic) RF magnetic field on high quality MgB_2 films. Comparing to the P_{3f} (T) result on Nb thin films, the low temperature nonlinearity of MgB_2 shows a complete harmonic cancelation at a temperature near the transition temperature of the proximity-induced π band. One possibility is that this phenomenon is due to an additional intrinsic nonlinearity arising from Josephson coupling between the σ and π bands. This nonlinear response then interferes with other nonlinear mechanisms coming from moving vortices and the intrinsic nonlinear Meissner effect of the two-gap system. To investigate further, we measure the magnitude and phase of the nonlinear response and compare to models of the three nonlinearity mechanisms.

¹This work is supported by the US DoE/High Energy Physics through grant # DESC0004950, and also by the ONR AppEl, Task D10, (Award No. N000140911190), and CNAM. The work at Temple University is supported by DOE under grant No. DESC0004410.

3:54PM D21.00008 Superconducting-to-Normal Switching and I-V Experiments showing Multiple Tunneling Channels in a Multi-Gap Superconductor¹, STEVE CARABELLO, JOSEPH LAMBERT, JEROME MLACK, Drexel University, WENQING DAI, YI. SHEN, QI LI, The Pennsylvania State University, DANIEL CUNNANE, C.G. ZHUANG, KE CHEN, X.X. XI, Temple University, ROBERTO RAMOS, Indiana Wesleyan University — Magnesium diboride is a BCS superconductor with many interesting properties, notably its two superconducting energy gaps associated with the disconnected sheets of its Fermi surface. A heterojunction, using the dual-gap MgB₂ and a single-gap superconductor as its superconducting electrodes, provides a system well-suited for exploring the unique properties of MgB₂, by exhibiting multiple tunneling channels. We present data from superconducting-to-normal state switching experiments and tunneling spectroscopy experiments to temperatures as low as 20mK that indicate multiple tunneling channels in this multiple-gap superconductor. We describe features of escape rates and I-V curves that may be consistent with recent published theoretical work on macroscopic quantum tunneling in multi-gap superconductors.

¹This research has been supported by a grant-in-aid from Sigma Xi.

4:06PM D21.00009 ABSTRACT WITHDRAWN —

4:18PM D21.00010 Multilayer Structures in MgB₂ superconducting thin films: influence on doping, pinning, and connectivity¹, MIKE SUMPTION, MIKE SUSNER, SCOT BOHNENSTIEHL, TED COLLINGS, Materials Science Dept, The Ohio State University — Pinning force density, connectivity, and doping were investigated for MgB₂ superconducting thin films. Pulsed Laser Deposition (PLD) was used to produce MgB₂ thin films on Al₂O₃ (0001), MgO (111), YSZ (111), and SiC (0001) substrates. The MgB₂ target was manufactured through high pressure and high temperature induction heating that produced a highly dense material. ZrB₂, SiC, or C targets were alternated with the MgB₂ target to produce films with various levels of doping and/or pinning centers. X-ray diffraction (XRD) was used to determine the substitution, strain, and epitaxy. Surface microstructures and grain sizes were compared via scanning electron microscopy (SEM). Transmission electron microscopy (TEM) was employed on ion-milled samples representing cross-sections of the film to determine the oxide content of the films as well as to confirm if the added dopants modified the superconducting properties of the MgB₂ via atomic substitution or increases in strain. Normal-state resistivity measurements were taken on the films to determine the connectivity as compared to literature single crystal values. Magnetic J_c s were taken of the films to determine the influence of the microstructure on the pinning properties.

¹Supported by the U.S. Department of Energy (DOE), Office of High Energy Physics, under Grant No. DE-FG02-95ER40900

4:30PM D21.00011 Effect of Carbon Nanotubes on Transport Properties of MgB₂¹, DEREK CAPLINGER, DANHAO MA, Department of Physics, The Pennsylvania State University, Altoona College, Altoona, PA 16601, USA, RUWANTHA JAYASINGHA, Department of Physics & Astronomy, University of Louisville, Louisville, KY 40292, USA, KOFI ADU, Department of Physics, The Pennsylvania State University, Altoona College, Altoona, PA 16601, USA, GAMINI SUMANASEKERA, Department of Physics & Astronomy, University of Louisville, Louisville, KY 40292, USA — Carbon nanotubes (CNT) and magnesium diboride (MgB₂) are two fascinating materials; with CNT exhibiting unique quantum electrical properties due to its 1-D structure and MgB₂ being a superconducting with transition temperature (T_c) at ~ 40 K. We report preliminary results on the effect of carbon nanotubes on the temperature dependent (300K to 4K) thermoelectric power (TEP) and resistivity of MgB₂. The normalized resistance ($(R-R_{300})/R_{300}$) shows very little dependence on the sample composition; however, the absolute resistance increases with increasing CNT concentration. At high CNT composition, the TEP mimic the characteristic TEP of CNT. However at low CNT composition, we see an upturn at about 30K.

¹This Work is Funded by The Pennsylvania State University, Altoona College and The Materials Research Institute

4:42PM D21.00012 Applicability of two-component Ginzburg-Landau model in two-band systems¹, MIHAIL SILAEV, Royal Institute of Technology and Institute for physics of microstructures RAS, EGOR BABAEV, Royal Institute of Technology and University of Massachusetts Amherst — We report a microscopic derivation of the conditions under which the two-band superconductors can be described by a two-component Ginzburg-Landau (GL) field theory. We also investigate the conditions when multicomponent GL-like expansions fail and one should resort to a microscopic description. We show that besides being directly applicable at elevated temperatures, a version of a minimal two-component GL theory in certain cases also gives an unexpectedly accurate description of certain aspects of a two-band system even substantially far from T_c . This shows that two-component GL model can be used for addressing a wide range of questions in multiband systems.

¹This work is supported by Knut and Alice Wallenberg Foundation through the Royal Swedish Academy of Sciences, Swedish Research Council, US NSF CAREER Award No. DMR-0955902, “Dynasty” foundation, Presidential Council (Grant No. MK-4211.2011.2) and RFBR

4:54PM D21.00013 Inter-band scattering effects in the Chevrel phase superconductors, ANSON CHEUNG, University of Cambridge — Recent scanning tunneling spectroscopy on the Chevrel phases SnMo₆S₈ and PbMo₆S₈ by Petrović et al. (PRL **106**, 017003 (2011)) demonstrates clear signatures of multi-band superconductivity. In contrast with MgB₂, where there is extremely weak scattering between the σ and π bands, the inter-band scattering rate is relatively high compared to the intra-band scattering rate in the Chevrel phases. We calculate the quasi-classical Green's function in the presence of strong inter-band scattering and derive comparable results to the measured density of states. We make predictions for proposed measurements on the vortex cores.

5:06PM D21.00014 Collective modes in three-band superconductors with repulsive interband interactions¹, VALENTIN STANEV, Materials Science Division, Argonne National Laboratory — I consider a simple model of a three-band superconductor with repulsive interband interactions. In such a system frustration associated with the odd number of gaps leads to the possible existence of intrinsically complex time-reversal symmetry breaking (TRSB) order parameter. I show that in this state the fluctuations of the *different* gaps are strongly coupled and this leads to the development of novel excitations, which mix the phase and amplitude oscillations. This is due to the non-trivial relative phase angle between the gaps. The energy of these excitations is less than 2Δ and thus they are true collective modes of the system.

¹This work is supported by the Center for Emergent Superconductivity, a DOE Energy Frontier Research Center, Grant No. DE-AC0298CH1088.

5:18PM D21.00015 Cryomagnetic STM imaging of the subsurface vortex lattice in the multi-band superconductor $2H\text{-NbSe}_2$ ¹, IGOR FRIDMAN, University of Toronto, V. LUKIC, Stevens Institute of Technology, C. KLOC, Nanyang Technological University, Singapore, C. PETROVIC, Brookhaven National Laboratory, J.Y.T. WEI, University of Toronto and Canadian Institute for Advanced Research — Using cryomagnetic scanning tunneling microscopy (STM) in a novel field geometry, we studied single crystals of the multiband superconductor $2H\text{-NbSe}_2$ under diamagnetically-induced superfluid momentum. Spectroscopy and conductance imaging were performed at 300 mK and in a field of up to 9 T, applied in the ab -plane.[1] Spatial maps of the Doppler effect on the quasiparticle tunneling spectrum revealed distinct stripe patterns that originate from in-plane vortices whose cores are buried in the bulk.[2] The stripe separation varies systematically as a function of the applied field. Our results are interpreted in terms of the interaction between vortical and screening currents, and demonstrate a general method for probing subsurface vortices, especially in emerging multiband superconductors such as the ferro-pnictides/chalcogenides.

[1] I. Fridman *et al.*, arXiv:1110.6490 (2011)

[2] I. Fridman *et al.*, Appl. Phys. Lett. **99**, 192505 (2011)

¹Work supported by NSERC, CFI/OIT, CIFAR, U.S. DOE and Brookhaven Science Associates (No. DE-Ac02-98CH10886)

Monday, February 27, 2012 2:30PM - 5:30PM –
Session D22 DMP DCOMP: Focus Session: Fe-based Superconductors - Crystal Growth, Structure, and Properties of $K_x\text{Fe}_{1-y}\text{Se}$ Phases 254B

2:30PM D22.00001 Superconductivity in $K_x\text{Fe}_{2-y}\text{Se}_{2-z}\text{S}_z$ ¹, CEDOMIR PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory — Single crystal alloys $K_x\text{Fe}_{2-y}\text{Se}_{2-z}\text{S}_z$ offer valuable insight into the strength of electronic correlations in the normal state and structural characteristics associated with superconductivity. I will discuss the evolution of the superconducting and magnetic ground states as a function of sulfur concentration z and some noticeable changes in the average and local crystal structure associated with this [1-4]. Conductivity and magnetic properties coincide with stoichiometry changes and with particular local environment of Fe atoms on the two Fe sites in the crystal structure. The ratio of superconducting T_c and Fermi temperature T_F is also suppressed by sulfur doping, indicating the suppression of electronic correlations. The superconductivity persists with relatively high T_c even when electronic correlations in the normal state are greatly reduced. The results for $z = 0$ will be compared with other experimental techniques that probe nanoscale phase separation and degree of vacancy order [5-6]. It will be shown that local structure and population of particular Fe sites is rather important for obtaining the bulk superconducting phase. Superconducting volume fraction and homogeneity of superconducting phase is in direct competition with Fe vacancy order [7].

[1] Hechang Lei *et al.*, Phys. Rev. Lett. **107**, 137002 (2011)

[2] Hechang Lei *et al.*, Phys. Rev. B **83**, 180503 (2011)

[3] Kefeng Wang *et al.*, Phys. Rev. B **74**, 0503 (2011)

[4] Kefeng Wang *et al.*, Phys. Rev. B **84**, 054526 (2011)

[5] Z. Wang *et al.*, Phys. Rev. B **83**, 140505 (2011)

[6] Y. J. Yan *et al.*, arXiv:1104.4941 (2011)

[7] Hyejin Ryu *et al.*, arXiv:1111.2597.

¹Work at Brookhaven is supported by the U.S. DOE under Contract No. DE-AC02-98CH10886 and in part by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. DOE, Office for Basic Energy Science (H.Lei).

3:06PM D22.00002 Crystal growth and detailed structural characterization of superconducting and non-superconducting phases in the $K_{1-x}\text{Fe}_{2-y}\text{Se}_2$ system, DANIEL SHOEMAKER, DUCK YOUNG CHUNG, MELANIE FRANCISCO, HELMUT CLAUS, SEVDA AVCI, Argonne National Laboratory, ANNA LLOBET, Lujan Neutron Scattering Center, Los Alamos National Laboratory, HEFEI HU, JIAN-MIN ZUO, University of Illinois at Urbana-Champaign, MERCOURI KANATZIDIS, Argonne National Laboratory and Northwestern University — Amid the flurry of activity on $K_{1-x}\text{Fe}_{2-y}\text{Se}_2$ superconductors, it remains established that the stoichiometric compound $K_2\text{Fe}_4\text{Se}_5$ is an antiferromagnetic semiconductor. This raises the question of whether subtle $\text{Fe}^{1+/3+}$ doping causes $K_{1-x}\text{Fe}_{2-y}\text{Se}_2$ to become a bulk superconductor, and if so, is there a structural distinction between superconducting and non-superconducting phases? We have grown $K_{1-x}\text{Fe}_{2-y}\text{Se}_2$ samples that show superconductivity with $T_C = 31$ K, even when growth conditions are starkly different from those reported in the literature. Here we present high-resolution synchrotron X-ray diffraction measurements, alongside single-crystal x-ray and electron diffraction, to elucidate the phase space in this system. Combined with magnetometry, heat capacity, and transport measurements, our structure-property relations help prescribe how chemical composition and heat treatment induce superconductivity and vacancy ordering in the $K_{1-x}\text{Fe}_{2-y}\text{Se}_2$ system.

3:18PM D22.00003 Suppression of superconductivity and spin-glass behavior in Cu-doped $\text{K}_0.8\text{Fe}_2\text{Se}_2$ ¹, RONGWEI HU, JOHNPIERRE PALIONE, SHANTA SAHA, RICHARD GREENE, Center for Nanophysics & Advanced Materials and Department of Physics, University of Maryland — Single crystals with nominal compositions of $\text{K}_0.8\text{Fe}_{2-x}\text{Cu}_x\text{Se}_2$ were grown and studied with low temperature electrical transport and magnetic susceptibility measurements. We show that the superconductivity present in undoped $\text{K}_0.8\text{Fe}_2\text{Se}_2$ crystals with transition temperature of 31 K is very quickly suppressed with Cu doping into the Fe site, and the system very quickly becomes insulating. We discuss anomalous behavior at higher doping, including spin-glass like behavior with further Cu doping.

¹This work was supported by AFOSR-MURI Grant FA9550-09-1-0603

3:30PM D22.00004 What is the true parent state in alkali-doped Iron Selenides, WEI LI, Fudan University, Shanghai, China, SHUAI DONG, Department of Physics, Southeast University, Nanjing, China, CHEN FANG, JIANGPING HU, Purdue University — By performing first-principles electronic structure calculations and analyzing effective magnetic model of alkali-doped iron selenides, we show that the materials without iron vacancies should approach a novel checkerboard phase in which each four Fe sites group together in tetragonal structure. The checkerboard phase is the ground state with a block antiferromagnetic (AFM) order and a small charge density wave order in the absence of superconductivity. Both of them can also coexist with superconductivity. The results explain mysterious 2 by 2 ordered patterns and hidden orders observed in various different experiments, clarify the missing link between AFM and superconducting phases, suggest that the block-AFM state is the parent state, and unify the understanding of various observed phases in alkali-doped iron selenides. (Reference: Wei Li, *et al.*, arxiv:1110.0372 (2011))

3:42PM D22.00005 Structural and Superconducting Properties of $K_{0.8}Fe_{1.6+x}Se_2$ single crystals, SU JUNG HAN, GENDA GU, QIANG LI, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973-5000, USA — We report structural and superconducting properties of $K_{0.8}Fe_{1.6+x}Se_2$ single crystals. Superconducting properties were studied by using transport, specific heat and magnetization measurements, and compared with that of $FeSe_{1-x}Te_x$. We found the *c*-axis resistive transition and specific heat behavior are distinctively different in these two classes of materials. Structural properties were studied via transmission electron microscopy and energy-dispersive X-ray spectroscopy. We found large scale structural and chemical disorder in the $K_{0.8}Fe_{1.6+x}Se_2$ samples. The relationship between structural and superconducting properties in $K_{0.8}Fe_{1.6+x}Se_2$ will be discussed.

3:54PM D22.00006 Imaging the coexistence of superconductivity and a charge density modulation in $K_{0.73}Fe_{1.67}Se_2$ superconductor, PENG CAI, CUN YE, WEI RUAN, XIAODONG ZHOU, State Key Laboratory of Low Dimensional Quantum Physics, Department of Physics, Tsinghua University, AIFENG WANG, MENG ZHANG, XIANHUI CHEN, Hefei National Laboratory for Physical Science at Microscale and Department of Physics, University of Science and Technology of China, YAYU WANG, State Key Laboratory of Low Dimensional Quantum Physics, Department of Physics, Tsinghua University — We report scanning tunneling microscopy studies of the local structural and electronic properties of the iron selenide superconductor $K_{0.73}Fe_{1.67}Se_2$ with $T_C = 32K$. On the atomically resolved FeSe surface, we observe well-defined superconducting gap and the microscopic coexistence of a charge density modulation with $\sqrt{2} \times \sqrt{2}$ periodicity with respect to the original Se lattice. We propose that a possible origin of the pattern is the electronic superstructure caused by the block antiferromagnetic ordering of the iron moments. The widely expected iron vacancy ordering is not observed, indicating that it is not a necessary ingredient for superconductivity in the intercalated iron selenides.

4:06PM D22.00007 Local Atomic and Electronic Structure of $K_{0.8}Fe_{1.6+x}Se_2$: Structural Order and Disorder, TREVOR TYSON, TIAN YU, New Jersey Institute of Technology, SU JUNG HAN, Brookhaven National Laboratory, MARK CROFT, Rutgers University, GENDA D. GU, IVO DIMITROV, QIANG LI, Brookhaven National Laboratory — The local structure of superconducting single crystals of $K_{0.8}Fe_{1.6+x}Se_2$ was studied by x-ray absorption spectroscopy. Near-edge spectra reveal that the average valence of Fe is 2+. The structure about the Se and Fe sites shows a high degree of order in the nearest neighbor Fe-Se bonds. On the other hand, the combined Se and K local structure measurements reveal a very high level of structural disorder in the K layers. The temperature dependence of the Fe-Se atomic correlation follows that of the Fe-As correlation in $LaFeAsO_{0.89}F_{0.11}$. In $K_{0.8}Fe_{1.6+x}Se_2$, the nearest neighbor Fe-Fe bonds has a lower Einstein temperature and higher structural disorder than in $LaFeAsO_{0.89}F_{0.11}$. For higher shells, an enhancement of the second nearest neighbor Fe-Fe interaction is found just below T_C and suggests that correlations between Fe magnetic ion pairs beyond the first neighbor are important in models of magnetic order and superconductivity in these materials. This research is supported by DOE BES Grant DE-FG02-07ER46402 (NJIT) for T.A.T and T.Y. and DOE BES Contract No. DE-AC0298CH10886. (BNL), for S.J.H, G.G, I.K.D, and Q. L.

4:18PM D22.00008 Interplay between structure and properties in $TlFe_{1.6}Se_2$ ¹, ANDREW MAY, HUIBO CAO, MICHAEL MCGUIRE, CLAUDIA CANTONI, BRYAN CHAKOUMAKOS, RADU CUSTELCEAN, BRIAN SALES, Oak Ridge National Laboratory — The degree to which Fe vacancies order greatly influences the properties of intercalated FeSe compounds. In this talk, we will consider the relationship between vacancy ordering and the properties of $TlFe_{1.6}Se_2$. Unlike the alkali-metal based compounds, such as $K_{0.8}Fe_{1.6}Se_2$, $TlFe_{1.6}Se_2$ does not become superconducting and always forms with the Tl-sites fully occupied. This results in reduced complexity and disorder, allowing the role of Fe vacancies to be probed directly. Common to all of these materials is $\sqrt{5}a \times \sqrt{5}a$ superstructure associated with ordering of the Fe vacancies, which appears coupled to a block-checkerboard antiferromagnetic order. Through subtle changes in composition and processing, the vacancies can order more or less completely, and this results in substantial variations in the magnetic properties of $TlFe_{1.6}Se_2$. The electronic behavior is relatively insensitive to these changes, though, as semiconducting behavior is observed in all cases. Finally, high resolution TEM reveals complex local structures, which are markedly different from those observed in $K_{0.8}Fe_{1.6}Se_2$.

¹This work was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

4:30PM D22.00009 Defect Structures and nonstoichiometry in the $K_xFe_{2-y}Se_2$ by X-ray diffraction., JOHN CLARIDGE, ALEXEY GANIN, ALEC MCLENNAN, JOHN BACSA, MATTHEW ROSSEINSKY, University of Liverpool, YASUHIRO TAKABAYASHI, KOSMAS PRASSIDES, Durham University — The mechanisms of charge carrier density control in the iron pnictide and chalcogenide superconductors are important as small changes in composition produce metal-insulator transitions and generate superconductivity at temperatures of up to 37K in chalcogenides and 55K in pnictides. All of the reported materials are based on a square FeX ($X = Se, As$) layer built from edge-sharing of FeX_4 tetrahedra. Insertion of alkali metal cations between FeSe layers affords superconductivity in $A_xFe_{2-y}Se_2$ ($A = K, Rb, Cs, Tl$; $0.7 < x < 1$, $0 < y < 0.5$) materials highlights the defect chemistry as the iron charge states close to +2 found in the other Fe-based superconductors require the creation of considerable defect concentrations on either or both iron and alkali metal sites. Ordering of the tetrahedral site vacancies in two crystals of refined compositions $K_{0.93(1)}Fe_{1.52(1)}Se_2$ and $K_{0.862(3)}Fe_{1.563(4)}Se_2$ produces a fivefold expansion of the parent $ThCr_2Si_2$ unit cell in the ab plane which can accommodate 20% vacancies on a single site within the square FeSe layer. The iron charge state is maintained close to +2 by coupling of the level of alkali metal and iron vacancies, doping mechanisms, which can operate at both average and local structure levels will be discussed. These structures will also be considered in terms of their local ordering and with relation to other defect chalcogenide layer structures and possible phase segregation.

4:42PM D22.00010 Local structural disorder and superconductivity in $K_xFe_{2-y}Se_2$, HYEJIN RYU, HECHANG LEI, Brookhaven National Lab, A.I. FRENKEL, Yeshiva University, C. PETROVIC, Brookhaven National Lab — We report significantly enhanced magnetic moment on $K_xFe_{2-y}Se_2$ single crystals after post-annealing and quenching process. In $K_xFe_{2-y}Se_2$ unit cell, there are two Fe sites, Fe1 which has higher symmetry with longer average Fe-Se bond length, and Fe2 which has lower symmetry with shorter average Fe-Se bond length. Temperature dependent X-ray absorption fine structure (XAFS) analysis results on quenched and as grown $K_xFe_{2-y}Se_2$ materials show that quenched $K_xFe_{2-y}Se_2$ materials have increased average Fe-Se bond length and decreased static disorder. This result indicates that occupancy of Fe1 sites increased after post-annealing and quenching process. This result provides clear evidence that Fe1 sites carry higher magnetic moment than Fe2 sites.

4:54PM D22.00011 Novel synthesis method of $K_xFe_{2-y}Se_2$ single crystal, TOSHINORI OZAKI, HIROYUKI TAKEYA, SATOSHI DEMURA, KEITA DEGUCHI, YASUNA KAWASAKI, HIROYUKI OKAZAKI, HIROSHI HARA, TAKAHIDE YAMAGUCHI, HIROAKI KUMAKURA, YOSHIHIKO TAKANO, National Institute for Materials Science — The discovery of superconductivity in $K_xFe_{2-y}Se_2$ with $\sim T_C$ 31 K has triggered a great interest in the field of iron-based superconductors [1]. $K_xFe_{2-y}Se_2$ superconductor has several practical advantages of relatively high T_C , high upper critical field (H_{c2}) and less toxicity compared to FeAs-based superconductors. However, the procedure for producing $K_xFe_{2-y}Se_2$ single crystal is complicated and time-consuming: At first, the FeSe precursor was prepared, and then the single crystals of $K_xFe_{2-y}Se_2$ were grown by the self-flux method. The simplification of the synthesis is really important for applications. We present a novel synthesis method of $K_xFe_{2-y}Se_2$ single crystal, which is very simple and quick. A superconducting transition of this sample appeared at $T \sim 31.6$ K. After quenching the sample, the calculated volume fraction from dc magnetic susceptibility was dramatically increased, consistent with the previous report [2]. We will also report the details of the synthesis, transport properties and microstructures of the samples. 1)J.Guo, *et al*, Phys. Rev. B **82**, 180520 (2010). 2)H. Lei, *et al*, arXiv: 1109.0534.

5:06PM D22.00012 Ordering driven superconductivity in an alkaline iron selenide¹, XIAO-JIA CHEN, Geophysical Laboratory, Carnegie Institution of Washington, Washington, D.C. 20015, QING-ZHEN HUANG, NIST Center for Neutron Research, National Institute of Standards and Technology Gaithersburg, MD 20899, JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, MINGHU FANG, Department of Physics, Zhejiang University, Hangzhou 310027, China, WEI BAO, Department of Physics, Renmin University of China, Beijing 100872, China, JIAN-BO ZHANG, LING-YUN TANG, Department of Physics, South China University of Technology, Guangzhou 510641, China, JINFU SHU, VIKTOR STRUZHNIKIN, RUSSELL HEMLEY, HO-KWANG MAO, Geophysical Laboratory, Carnegie Institution of Washington, Washington, D.C. 20015 — Combining the resistivity, synchrotron x-ray diffraction, and neutron diffraction measurements, we investigated the evolution of the structural, magnetic, and superconducting properties with pressure up to 37 GPa of superconducting $\text{Rb}_{0.347}\text{Ti}_{0.347}\text{Fe}_{1.752}\text{Se}_2$. Extended phase diagram of temperatures and pressure were established for this material. The results show the superconductivity is in reality driven by ordering.

¹This work is supported by the U.S. DOE under Grants No. DE-SC0001057.

5:18PM D22.00013 Pressure-tuned superconductivity of iron chalcogenides, LILING SUN, Institute of Physics, CAS, XIAO-JIA CHEN, Geophysical Laboratory, Carnegie Institution of Washington, Washington, D.C., JING GUO, PEIWEN GAO, Institute of Physics, CAS, HANGDONG WANG, MINGHU FANG, Department of Physics, Zhejiang University, China, XIAOLONG CHEN, GENFU CHEN, QI WU, DACHUN GU, CHAO ZHANG, XIAOLI DONG, XI DAI, Institute of Physics, CAS, HO-KWANG MAO, Geophysical Laboratory, Carnegie Institution of Washington, Washington, D.C., ZHONGXIAN ZHAO, Institute of Physics, CAS — In this talk, we present our recent progress in effect of pressure on superconductivity of newly discovered iron chalcogenide superconductors. We show that the either positive or negative pressure can tune superconductivity of this new kind of superconductors. Superconductivity with higher superconducting transition temperature T_c can reemerge after elimination of the initial superconducting phase upon compression. We find that the maximum T_c of the reemerging superconducting phase is as high as 48.7 K for $\text{K}_{0.8}\text{Fe}_{1.70}\text{Se}_2$ and 48 K for $\text{Ti}_{0.6}\text{Rb}_{0.4}\text{Fe}_{1.67}\text{Se}_2$, setting a new T_c record for chalcogenide superconductors. The presence of the second superconducting phase is proposed to be related to pressure-induced quantum criticality. Our findings open up the potential route for the exploration of high- T_c superconductivity in iron-based and other superconductors.

Monday, February 27, 2012 2:30PM - 5:18PM — Session D23 DCMP: Metals Theory Oxides Interfaces 255

2:30PM D23.00001 Transferable tight-binding description of the Fe-C interaction, NICHOLAS HATCHER, GEORG K.H. MADSEN, RALF DRAUTZ, ICAMS, Ruhr-Universität Bochum — A coherent transferable tight-binding (TB) parameterization including magnetism has yet to be developed for the Fe-C interaction. Although interatomic potentials have been obtained for this system, recent findings show that the results from these potentials are inconsistent with DFT calculations and do not give an accurate portrayal of chemical bonding in the system. Using dual DFT grid and LCAO calculations within GPAW, we obtain one electron wave functions expanded in a multiple- ζ LCAO basis. This is then down-folded onto an optimal minimal basis, giving a continuous and transferable description of Fe-C bonding. By constructing a TB energy functional using these bond integrals and a parameterized interatomic repulsion, we show how an accurate description of the energy hierarchy of interstitial carbon in Fe-structures can be achieved. Furthermore, we use the model to calculate elastic properties and energies of a variety of Fe-carbides, defects, and carbon diffusion paths. This simple model based on physical insights may be used to study systems containing thousands of atoms.

2:42PM D23.00002 Empirical potentials from a combined density functional theory / genetic algorithm approach: Illustration for Xe in UO₂, ALEXANDER THOMPSON, BRYCE MEREDIG, CHRIS WOLVERTON, Northwestern University — We have developed a new empirical potential for xenon in uranium dioxide with existing UO₂ potentials that achieves accurate xenon defect energetics. This potential was fit to several snapshots of DFT+U molecular dynamics of a single defect configuration using the genetic algorithm code Iterative Potential Refinement (IPR). In IPR, the forces, stresses, and energies from DFT calculations are used to parameterize empirical potentials. Several random sets of parameters are used to compare against DFT and the genetic algorithm minimizes the error of the parameters with respect to the DFT results. We compare this potential and other xenon potentials to DFT+U using a large set of defect calculations of xenon incorporated into sites with high, intermediate, low strain. Despite only being fit to a single configuration, our new empirical potential gives the very good agreement with DFT+U across a range of xenon incorporation sites and vastly outperforms existing xenon potentials.

2:54PM D23.00003 ABSTRACT WITHDRAWN —

3:06PM D23.00004 The dielectric response of single-crystal UO₂ probed by terahertz time-domain spectroscopy, YONG AN, MST-8, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, TREVOR TYSON, Department of Physics, New Jersey Institute of Technology, Newark, NJ 07102, USA, STEVEN CONRADSON, MST-8, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — We measured the complex dielectric function, $\varepsilon = \varepsilon_r + i\varepsilon_i$, of single-crystal UO₂ in the temperature (T) range of 5-500 K by terahertz (THz) time-domain spectroscopy to study its dielectric response. A critical temperature point of 60 K is found for the measured temperature dependence of $\varepsilon_r(T)$. The dispersion of $\varepsilon(\omega)$ in the THz range follows the trend of the damped resonant mode of the transverse optical phonon at $\omega_{TO}=8.4$ THz. Examining the Lyddane-Sachs-Teller relationship reveals mode-softening of ω_{TO} in the temperature range of 60-120 K. We then performed optical-pump THz-probe measurements to study the dynamic dielectric response of UO₂ following photoexcitation. We observe a small pump-induced change in ε that lasts for more than one millisecond, indicating heavy electron behavior of photoexcited 5f electrons resulting from strong electron-lattice interaction. The slow relaxation is attributed to the diffusion of optical phonons generated by photoexcited 5f electrons in the UO₂ crystal.

3:18PM D23.00005 Magnetocaloric Effect of NiFeCoCrPdx High Entropy Alloys¹, DUSTIN BELYEA, University of South Florida, C. BAUER, USF, M. LUCAS, Air Force Research Laboratory, J. HORWATH, AFRL; Wright State University, E. MICHEL, AFRL; UTC inc., CASEY W. MILLER, USF — FeCoCrNi is one of many “high entropy alloys” (HEAs), which are multicomponent alloys with high entropy of mixing. These materials often have high hardness, and resistance to wear and corrosion, making them attractive for applications. Here, we report on the magnetic entropy change and magnetocaloric effect of the FeCoCrNiPdx system. The addition of Pd to FeCoCrNi has been shown to enable the critical temperature to be tuned from 130 K for x=0 to 500 K for x=2. Isothermal magnetization measurements were made on samples with x ranging from 0 to 0.50 as functions of temperature. The magnetic entropy change (ΔS) was calculated using the thermodynamic Maxwell Relation. We find that Pd additions tune the peak ΔS temperature from 130 to 300K, while modestly increasing the peak ΔS magnitude. Interestingly, the addition of Pd leads to an almost doubling of the relative cooling power (RCP), as well as a notable change in the critical behavior of the material. The RCP of ~ 35 J/kg for a 1T field change puts the Pd-containing HEAs in competition with other magnetocaloric materials in the 100-200 K operating range. This alloy system's combination of durability and a tunable Curie temperature without appreciable change in cooling power may make this system interesting for magnetocaloric applications.

¹Supported by AFOSR and NSF

3:30PM D23.00006 Magnetic and crystallographic properties of Cr_{1-x}Fe_xGe, YUEN YIU, NIRMAL GHIMIRE, DAVID MANDRUS, University of Tennessee, STEPHEN NAGLER, MICHAEL MCGUIRE, Oak Ridge National Laboratory, DAVID MANDRUS COLLABORATION — According to previously published bulk measurements, Cr_{1-x}Fe_xGe exhibits a quantum critical point at $x=0.75$, where it turns from a paramagnet (for $x > 0.75$) into a ferromagnet (for $x < 0.75$). Cr_{1-x}Fe_xGe is a simple cubic B20 (FeSi) crystal. The endpoints of the alloy are binary compounds that have been studied to some degree. FeGe, the better known of the two, is a spiral ferromagnet similar to MnSi. However, less is known for CrGe, which is thought to be a weakly ferromagnetic paramagnet with bulk properties that may be explained by the paramagnon theory. We report new neutron scattering results on Cr_{1-x}Fe_xGe for $x=0.6, 0.7, 0.75, 0.8$.

3:42PM D23.00007 An *ab-initio* multiscale method to investigate chemical embrittlement of metals, GEORG SCHUSTERITSCH, Harvard University, THOMAS KÜHNE, Johannes Gutenberg University of Mainz, EFTHIMIOS KAXIRAS, Harvard University — We present a multiscale method, coupling a small region treated by first-principles quantum mechanics, to a large classical atomistics region. Our method is based on total energy arguments that are applicable to metals. We employ Kohn-Sham (KS) Density Functional Theory (DFT) in the region of interest and couple this to the classical Embedded Atom Method (EAM). Results for the chemical embrittlement of metals due to segregated impurities at grain boundaries (GB) are presented. We study the average interplanar strain surrounding the GB and use this as a measure of the atomic relaxation. We apply our method to study the chemical embrittlement of Cu by Bi and Pb impurities and compare this to the effect of Ag impurities, which are known to segregate to the GB but not embrittle Cu. We find that Bi and Pb weaken and hence embrittle the Cu GB. In contrast Ag impurities at the GB plane increase cohesion.

3:54PM D23.00008 Molecular dynamics study of the thermopower of Ag, Au, and Pt nanocontacts, F. PAULY, Molecular Foundry, Lawrence Berkeley National Laboratory, USA, J.K. VILJAS, Department of Physics, University of Oulu, Finland, M. BÜRKLE, Institute for Theoretical Solid State Physics, Karlsruhe Institute of Technology, Germany, M. DREHER, P. NIELABA, Department of Physics, University of Konstanz, Germany, J.C. CUEVAS, Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain — Using molecular dynamics simulations of many junction stretching processes combined with tight-binding-based electronic structure and transport calculations, we analyze the thermopower of silver (Ag), gold (Au), and platinum (Pt) atomic contacts. In all cases we observe that the thermopower vanishes on average within the standard deviation and that its fluctuations increase for a decreasing minimum cross section of the junctions. However, we find a suppression of the fluctuations of the thermopower for the s-valent metals Ag and Au, when the conductance originates from a single, perfectly transmitting channel. Essential features of the experimental results for Au, Ag, and copper (Cu) of Ludoph and van Ruitenbeek [Phys. Rev. B 59, 12290 (1999)], as yet unaddressed by atomistic studies, can hence be explained by considering the atomic and electronic structure at the disordered narrowest constriction of the contacts. For the multivalent metal Pt our calculations predict the fluctuations of the thermopower to be larger by one order of magnitude as compared to Ag and Au, and suppressions of the fluctuations as a function of the conductance are absent. Main features of our results are explained in terms of an extended single-level model.

4:06PM D23.00009 First-Principles Study of Hydrogen Permeation in Palladium-Gold Alloys, ANGELO BONGIORNO, SHUCHENG XU, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332 — Density functional theory and lattice model calculations are combined to study the permeability of hydrogen in Pd lightly alloyed with Au. This study shows that small amounts of Au substitutions in Pd lead to, respectively, an increase and decrease of the diffusivity and solubility of hydrogen in the alloy. The competition between these two phenomena depends on temperature and can yield dilute PdAu membranes with a hydrogen permeability higher than pure Pd.

4:18PM D23.00010 Hydrogen Embrittlement in Zirconium: a Quasi-Continuum Density Functional Theory Study¹, Q. PENG, Rensselaer Polytechnic Institute — The hydrogen embrittlement in Zirconium becomes a very important and emergent issue for academia, industry and policy makers as a result of the Japan nuclear accident. The hydride formation, diffusion and embrittlement in zircaloy will impact dramatically on the development of advanced nuclear energy systems, the life time extension of the current nuclear fleet and dry storage of spent nuclear fuel. Quasi-Continuum Density Functional Theory (QCDFE) is a powerful concurrent multiscale method based entirely on density functional theory (DFT) and allows quantum simulations of materials properties of a large system with billions of atoms. Using QCDFE modeling, we found that the presents of hydrogen at the cracktip of zirconium, both on crack surface and in-bulk, will form zirconium hydrides and embrittle the system. The concentration of hydrogen and orientation of crack plays important roles in such embrittlement. The mechanism of hydrogen embrittlement under various loading conditions will be discussed.

¹The authors would like to acknowledge the generous financial support from the Defense Threat Reduction Agency (DTRA) Grant # BRBA08-C-2-0130, and the U.S. Nuclear Regulatory Commission Faculty Development Program under contract # NRC-38-08-950.

4:30PM D23.00011 Effects of disorder on the T-dependent bandstructure of purple bronze Li₂Mo₁₂O₃₄, THOMAS JARLBORG, PIOTR CHUDZINSKI, THIERRY GIAMARCHI, DPMC, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Geneva 4, Switzerland — The band structures of ordered and disordered Li₂Mo₁₂O₃₄ are calculated by use of *ab-initio* DFT-LMTO method. The unusual band dispersion in the z-direction obtained in previous band calculations is confirmed for the ordered structure, and the overall band structure agree reasonably with existing photoemission data. The T-dependent band broadening is calculated from configurations with thermal disorder of the atomic positions within the unit cell. The band structure shows important band broadening of the two bands at the Fermi energy. The bands are particularly sensitive to in-plane movements of Mo sites. Already disorder due to zero-point motion makes a band broadening of the order of 20 meV and creates a sizable band overlap. The effect of Li vacancies on the two bands is relatively small.

4:42PM D23.00012 Metamagnetic transition self-propelled by the spin injection, ALEXANDER ZYUZIN, University of Waterloo, A.YU. ZYUZIN, A.F. Ioffe Physico-Technical Institute — We study metamagnetic phase transition of itinerant electrons controlled by the spin injection mechanism. The current flow between a ferromagnetic metal and a metamagnetic metal produces the non-equilibrium shift of chemical potential for spin-up and spin-down electrons. This shift acts as an effective magnetic field driving the metamagnetic transition between low and high magnetization states of the metamagnet in the vicinity to the contact with the ferromagnet. We show that high magnetization state of the metamagnet self propels into the bulk of the metamagnet and the length of this state has threshold dependence on the electrical current.

4:54PM D23.00013 Generalized Statistical Thermodynamics Applied to Small Material Systems, ROBERT CAMMARATA, Johns Hopkins University — When characterizing the behavior of small material systems, surface effects can strongly influence the thermodynamic behavior and need to be taken into account in a complete thermal physics analysis. Although there have been a variety of approaches proposed to incorporate surface effects, they are often restricted to certain types of systems (e.g., those involving incompressible phases) and often invoke thermodynamics parameters that are often not well-defined for the surface. It is proposed that a generalized statistical mechanics based on the concept of thermodynamic availability (exergy) can be formulated from which the surface properties and their influence on system behavior can be naturally and rigorously obtained. This availability-based statistical thermodynamics will be presented and its use illustrated in a treatment of nucleation during crystallization.

5:06PM D23.00014 $d + id$ superconductivity on the honeycomb bilayer, MILICA MILOVANOVIC, JAKSA VUCICEVIC, DARKO TANASKOVIC, Institute of Physics Belgrade — We demonstrate that for interlayer attractive interactions on bilayer honeycomb lattice with large interlayer hopping, a time reversal symmetry breaking d -wave topological superconductor is a dominant phase. We find that small momentum order parameter expansion has $d_{x^2-y^2} + id_{xy}$ symmetry around both Dirac points and discuss a possible relevance of this state for experiments on graphene bilayer.

Monday, February 27, 2012 2:30PM - 5:30PM —
Session D24 FIAP: Bionanotechnology and Nanostructured Sensors 256

2:30PM D24.00001 Zirconium tungstate/epoxy resin nanocomposites with negative coefficient of thermal expansion for all-dielectric cryogenic temperature sensors, ERICH SEE, Virginia Tech, VLADIMIR KOCHERGIN, LAUREN NEELY, MADRAKHIM ZAYETNIKOV, MicroXact Inc., GIANLUIGI CIOVATI, Jefferson Lab, HANS ROBINSON, Virginia Tech — The α -phase of zirconium tungstate (ZrW_2O_8) has the remarkable property that its coefficient of thermal expansion (CTE) is negative over its entire range of thermal stability (0-1050K), and through this range it has a nearly constant negative CTE. When ZrW_2O_8 nanoparticles are mixed into a polymer resin, the resulting composite has a reduced CTE when compared with that of the pure polymer. However, previous research on such composites has occurred only near room temperature. We show that at cryogenic temperatures, it is possible to make ZrW_2O_8 /resin nanocomposites with negative CTE. By coating a fiber-optic Bragg grating with such a composite, we were able to create an all-optical temperature sensor without the use of metals, which would be of particular use in superconducting RF cavities. The sensor has sensitivity down to at least 2 K, six times lower than previous fiber-optic temperature sensors.

2:42PM D24.00002 ABSTRACT WITHDRAWN —

2:54PM D24.00003 Strong two-photon-fluorescence from semiconducting polymer nanoparticles for high contrast imaging of cancerous cells, SOUMITRA SATAPATHI, Department of Physics and Applied Physics, University of Massachusetts Lowell, Lowell, MA, 01854, ANOOP PAL, Biomedical Engineering and Biotechnology Program, University of Massachusetts Lowell, Lowell, MA, 01854, LIAN LI, US Army Natick Soldier Research, Development & Engineering Center, Natick, MA, 01760, SURESH GADDE, Nanodelivery Laboratory, Brigham and Women's Hospital, Harvard Medical School, Boston, MA 02115, DHIMITER BELLO, Biomedical Engineering and Biotechnology Program, University of Massachusetts Lowell, Lowell, MA, 01854, LYNNE SAMUELSON, University of Massachusetts Lowell, Lowell, MA, 01854, JAYANT KUMAR, Department of Physics and Applied Physics, University of Massachusetts Lowell, Lowell, MA, 01854 — Strong two-photon-induced fluorescence was observed from a series of novel fluorescent semiconducting polymer nanoparticles using femtosecond laser pulses at 800 nm. The conjugated polymer nanoparticles were fabricated by a simple technique known as the "mini emulsion" technique. The quadratic dependence of the two-photon-fluorescence was confirmed by varying the laser intensity. The two-photon-absorption cross-sections of the nanoparticles were determined in aqueous dispersions by comparing with that of Rhodamine 6G. The deep penetration of the near-infrared laser together with large absorption cross-section demonstrated here, renders these fluorescent polymer nanoparticles as ideal candidates for high contrast in vivo fluorescent imaging of certain tumor cells.

3:06PM D24.00004 Surface Modified Gadolinium Phosphate Nanoparticles as MRI Contrast Agents¹, MATTHIEU F. DUMONT, Dept. Physics. and NHMFL, Univ. Florida, CELINE BALIGAND, Dept. Physiol. Func. Genomics, Univ. Florida, ELISABETH S. KNOWLES, MARK W. MEISEL, Dept. Physics. and NHMFL, Univ. Florida, GLENN A. WALTER, Dept. Physiol. Func. Genomics, Univ. Florida, DANIEL R. TALHAM, Dept. Chem., Univ. Florida — Nanoparticles of $\text{GdPO}_4\cdot\text{H}_2\text{O}$ were synthesized in a water/oil microemulsion using IGEAL CO-520 as surfactant resulting in 50 nm to 100 nm particles that are dispersible and stable in water. Using surface modification chemistry previously established for zirconium phosphonate surfaces,² the particles are directly modified with 5'-phosphate terminated oligonucleotides, and the specific interaction of the divalent phosphate with Gd^{3+} sites at the surface is demonstrated. The ability of the modified nanoparticles to act as MRI contrast agents was determined by performing MR relaxivity measurements at 14 T. Solutions of nanopure water, Feridex® and Omniscan® (FDA cleared contrast agents) in 0.25% agarose were used for comparison and control purposes. MRI data confirm that $\text{GdPO}_4\cdot\text{H}_2\text{O}$ nanoparticles have relaxivities (r_1, r_2) comparable to commercially available contrast agents.³ In addition, biofunctionalization of the surface of the nanoparticles does not prevent their function as MRI contrast agents.

¹Supported by NSF CHE-0957155 (DRT), DMR-0701400 (MWM), and DMR-0654118 (NHMFL).

²J. Monot et al., *J. Am. Chem. Soc.* 130 (2008) 6243.

³H. Hifumi et al., *J. Am. Chem. Soc.* 128 (2006) 15090.

3:18PM D24.00005 ABSTRACT WITHDRAWN —

3:30PM D24.00006 Surface Plasmon Resonance Imaging of the Enzymatic Degradation of Cellulose Microfibrils, KYLE REITER, ADAM RAEGER, Department of Physics, University of Guelph, ANTHONY CLARKE, Department of Molecular and Cellular Biology, University of Guelph, JACEK LIPKOWSKI, Department of Chemistry, University of Guelph, JOHN DUTCHER, Department of Physics, University of Guelph — As the largest component of biomass on Earth, cellulose represents a significant potential energy reservoir. Enzymatic hydrolysis of cellulose into fermentable sugars, an integral step in the production of biofuel, is a challenging problem on an industrial scale. More efficient conversion processes may be developed by an increased understanding of the action of the cellulolytic enzymes involved in cellulose degradation. We have used our recently developed quantitative, angle-scanning surface plasmon resonance imaging (SPRI) device to study the degradation of cellulose microfibrils upon exposure to cellulolytic enzymes. In particular, we have studied the action of individual enzymes, and combinations of enzymes, from the *Hypocrea Jecorina* cellulase system on heterogeneous, industrially-relevant cellulose substrates. This has allowed us to define a characteristic time of action for the enzymes for different degrees of surface coverage of the cellulose microfibrils.

3:42PM D24.00007 Non-destructive method for measuring the Ca/P ratio in human bone, ALEXANDER SLEPKO, ALEXANDER DEMKOV, The University of Texas at Austin — Hydroxyapatite (HA) $[\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2]$ is the main mineral constituent in human bone. It crystallizes in hexagonal and monoclinic phase, which are very similar in structure and properties. A critical measure for healthy bones is the Ca/P ratio which in turn affects the dielectric constant of the mineral constituent. The dielectric constant of HA varies between 5 and 20 depending on the Ca/P ratio in the sample [*J. Mater. Sci.: Mater. Med.* **21**, 399]. We suggest exploiting this large span in the dielectric constant in a non-destructive method to measure the Ca/P ratio in bone by optical spectroscopy. Using density functional theory we calculate the long-range corrected phonon dispersion. We find that only modes around 330 cm^{-1} are strongly affected by the dielectric constant. The shifts in frequency can be up to 20 cm^{-1} as you span the range of the dielectric constant. Thus, by measuring the optical shift and comparing with calibrated samples it is possible to draw conclusions on the Ca/P ratio in the mineral. Importantly, we find the same modes in both the monoclinic and hexagonal phases to be sensitive to changes in the dielectric constant.

3:54PM D24.00008 Surface Functionalized Nanocoax Biosensors¹, BINOD RIZAL, MICHELLE ARCHIBALD, GREGORY MCMAHON, Boston College, NATASHA ERDMAN, Joel USA, Inc., STEPHEN SHEPARD, MICHAEL J. BURNS, THOMAS C. CHILES, MICHAEL J. NAUGHTON, Boston College — We have adapted the nanocoax array architecture for high sensitivity, all-electronic chemical and biological sensing. We previously demonstrated ppb concentration level detection sensitivity to volatile organic compounds in dry air using the nanocoax array with nanoporous coax annuli [1]. Here, we report progress toward modifying/functionalizing the coax metal surfaces to enable specific binding of target molecules (e.g. proteins, toxins, pathogenic organisms), followed by electronic interrogation via capacitance/impedance spectroscopy. As a proxy for target molecules, and in order to confirm the ability to selectively functionalize desired surfaces in our nanopillar / nanocoax geometry, we have selectively attached streptavidin-functionalized core-shell CdSe/ZnS quantum dots to gold nanopillars. Next steps will include substituting antibodies for the quantum dots, and measuring the capacitance and impedance response to the introduction of protein (PSA , CA-125, etc.) in serum. Ref. [1]: H.Z. Zhao, B. Rizal, G. McMahon, H. Wang, P. Dhakal, T. Kirkpatrick, Z.F. Ren, T.C. Chiles, D. Cai and M.J. Naughton (submitted).

¹Supported by the National Cancer Institute CA137681.

4:06PM D24.00009 Magnetic wire trap arrays for biomarker-based molecular detection, GREGORY VIEIRA, The Ohio State University Department of Physics, KALPESH MAHAJAN, GANG RUAN, JESSICA WINTER, The Ohio State University William G. Lowrie Department of Chemical and Biomolecular Engineering, R. SOORYAKUMAR, The Ohio State University Department of Physics — Submicrometer-scale magnetic devices built on chip-based platforms have recently been shown to present opportunities for new particle trapping and manipulation technologies. Meanwhile, advances in nanoparticle fabrication allow for the building of custom-made particles with precise control of their size, composition, and other properties such as magnetism, fluorescence, and surface biomarker characteristics. In particular, carefully tailored surface biomarkers facilitate precise binding to targeted molecules, self-actuated construction of hybrid structures, and fluorescence-based detection schemes. Based on these progresses, we present an on-chip detection mechanism for molecules with known surface markers. Hybrid nanostructures consisting of micelle nanoparticles, fluorescent quantum dots, and superparamagnetic iron oxide nanoparticles are used to detect proteins or DNA molecules. The target is detected by the magnetic and fluorescent functionalities of the composite nanostructure, whereas in the absence of the target these signals are not present. Underlying this approach is the simultaneous manipulation via ferromagnetic zigzag nanowire arrays and imaging via quantum dot excitation. This chip-based detection technique could provide a powerful, low cost tool for ultrasensitive molecule detection with ramifications in healthcare diagnostics and small-scale chemical synthesis.

4:18PM D24.00010 Strategies to enhance the bioavailability of curcumin: a potential antitumor drug, ABHISHEK KUMAR, JOSHNA CHITTIGORI, University of Massachusetts Lowell, LIAN LI, LYNNE SAMUELSON, U.S. Army Natick Soldier Research, Development & Engineering Center, DANIEL SANDMAN, JAYANT KUMAR, University of Massachusetts Lowell — Curcumin is a polyphenol which has elicited considerable interest for its antioxidant and anti tumor properties. Although curcumin may be used as potential therapeutic drug, it is very sparingly soluble in water which makes it less bioavailable under physiological conditions. We report two approaches to make curcumin more bioavailable. The first approach involves fabricating colloidal dispersions of curcumin in the range of tens of nanometers. The second approach involves functionalization of curcumin with polyethylene glycol (PEG) to render it water dispersible or soluble. Since curcumin is a fluorescent molecule as well as a potential drug, its interactions with cells have been investigated using one and two photon confocal fluorescence imaging. We have also observed strong interaction between curcumin and metal ions, which may have physiological implications.

4:30PM D24.00011 Comparison anti-bacterial effect of silver/polystyrene nanocomposites on gram negative and positive bacteria, AKHTAROLMOLOOK KAZEMI, Biochemical and Bioenvironmental Engineering Research Center, Sharif University of Technology, MARYAM RAFTARI, Department of physics and Astronomy, University of Sheffield, Sheffield, UK, SAJJAD TOLLABI-MAZRAEHNO, Johannes Kepler University, Altenberger Str. 69, 4040 Linz, Austria, MOHAMMAD MAHDAVI, Department of Physics, Sharif University of Technology, AZAM IRAJIZAD, Institute for Nanoscience and nanotechnology, Sharif University of Technology — Silver nanoparticles/polystyrene nanocomposites were prepared via casting the solution of polystyrene in a mixture of carbon tetrachloride and acetone containing silver nanoparticles. Colloidal silver nanoparticles in acetone were synthesized by pulsed laser ablation (PLA) of pure bulk silver. Casting the colloidal silver nanoparticles in a solution of polystyrene results in a yellowish transparent polymeric sheet. TEM images show rather spherical nanoparticles with mean diameter of 5 nm. Ag/PS nanocomposites were characterized by UV-VIS spectroscopy. In this study, we also investigated the antimicrobial activity of silver nanocomposites against Escherichia coli (E.coli) and Staphylococcus aureus (S.aureus) as a model for Gram negative and Gram positive bacteria. Antibacterial tests were performed against E. coli and S.aureus, on LB agar plates containing different amount of nanoparticles. Our results showed at all these concentrations, the nanoparticles caused a growth delay of E. coli, increasing the concentration of nanoparticles increased this growth delay.

4:42PM D24.00012 Luminescence of Rare-Earth-Doped Nanoparticles with Aromatic Linker Molecules, TESS SENTRY, MOHITA YALAMANCI, YANWEI ZHANG, ANYA LEACH, MOHINDAR SEEHRA, XIAODONG SHI, ALAN BRISTOW, West Virginia University — Rare-earth-doped vanadate glasses retain their luminescence when formed as shells around magnetic cores [1]. This property has prompted speculation that composite magneto-photoluminescent (CMPL) structures can be used in biological applications. For example, CMPL nanoparticles can be magnetically tuned to separate cells, proteins and nucleic acids [2]. A crucial step in realizing this goal is to attach organic linkers (between the rare-earth-doped shell and bio-probes), which do not affect the luminescence. We demonstrate with IR spectroscopy that Eu:YVO₄ nanoparticles treated with benzoic acid, 3-nitro 4-chloro-benzoic acid and 3,4-dimethoxy benzoic acid all result in the modification of the surface states, replacing the native metal-hydroxyl bond with a longer chain aromatic linker, which can be later functionalized. Photoluminescence spectra under UV-excitation show that the dominant ⁵D₀ → ⁷F₂ transition at ~620 nm is unaffected by the chemical treatment. The result provides a platform to facilitate the attachment of bio-probes to Eu:YVO₄ nanoparticles and related CMPL nanostructures with Fe₂O₄ cores.

[1] N. B. McDowell et al, J. Appl. Phys. 107, 09B327 (2010).

[2] T. R. Sathe et al, Anal. Chem. 78, 5627 (2006).

4:54PM D24.00013 Light-powered nanoparticle – MEMS hybrid, EVGENIYA MOISEEVA, TOMAS LUCAS, GUANDONG ZHANG, ANDRE GOBIN, CINDY HARNETT, University of Louisville, ELECTRICAL AND COMPUTER ENGINEERING DEPARTMENT TEAM, BIOENGINEERING DEPARTMENT TEAM — This work presents a light-actuated microelectromechanical (MEMS) structure with bistable elements and its applications in cellular-scale actuation. These devices are built using a metal/oxide bilayer with a stress mismatch. In the hybrid design that uses gold nanoparticles for localized heating, a nanoparticle coating is patterned onto the selected part of the device by Parylene micro-stenciling before releasing the structures from the planar substrate. These gold nanoparticles are attractive for use in μ TAS and biotechnology due to their biocompatibility and inertness, the ability to conjugate to the surface via thiol chemistry or electrostatic interaction, and especially their strong tunable absorption in the near infrared region. Integration of the near infrared (IR)-resonant gold nanoparticles with bistable MEMS structures creates light-driven hybrid actuators that quickly respond to narrow-band IR light. The movement of the MEMS device is achieved through controlled thermal expansion, with actuation speed in the millisecond range.

5:06PM D24.00014 Motion observation and SPR measurements of kinesin motility on microtubules, A. SIKORA, D. OLIVEIRA, K. KIM, WPI-AIMR, Tohoku University, Japan, A.L. LIAO, WPI-AIMR, Tohoku University, Japan and Materials Science and Engineering, Texas A&M University, M. UMETSU, T. ADSCHIRI, WPI-AIMR, Tohoku University, Japan, W. HWANG, Materials Science and Engineering, Department of Biomedical Engineering, Texas A&M University, W. TEIZER, WPI-AIMR, Tohoku University, Japan; Materials Science and Engineering and Department of Physics and Astronomy, Texas A&M University — Motor proteins convert chemical energy directly into mechanical work with high efficiency (~50%). One of these proteins, kinesin, is used in the cell to transport organelles. It “walks” along biopolymer tracks called microtubules and, depending on the type, can reach speeds of a few micrometers per second. Kinesin can carry intracellular cargo over long distances against several piconewtons of loads and is barely limited by the cargo size. Motion of streptavidin-coated quantum dots carried by kinesin on microtubules will be presented. We have expressed biotinylated Kinesin-1 using *Escherichia coli*. Attachment to quantum dots was performed using the strong binding affinity between streptavidin and biotin. Microtubules, labeled with rhodamine, allow visualization by fluorescence microscopy. The measured speed of our kinesin fits well with results found in the literature. Surface Plasmon Resonance (SPR) measurements allow the identification and strength evaluation of bonding. Using this technique, we will present results on the binding between our expressed kinesin and microtubule.

5:18PM D24.00015 Construction of Quantum Dot Micro/Nano-track as a Seedbed for Kinesin Motor Proteins, K. KIM, WPI-AIMR, Tohoku University, Japan, A. L. LIAO, WPI-AIMR, Tohoku University, Japan; Materials Science and Engineering, Texas A&M University, A. SIKORA, D. OLIVEIRA, M. UMETSU, T. ADSCHIRI, WPI-AIMR, Tohoku University, Japan, W. HWANG, Materials Science and Engineering, Department of Biomedical Engineering, Texas A&M University, W. TEIZER, WPI-AIMR, Tohoku University, Japan; Materials Science and Engineering and Department of Physics and Astronomy, Texas A&M University — Kinesin is a motor protein engaged in motion on microtubules. It is involved in various subcellular processes such as cell division and transportation of intracellular cargo. The system of (1) kinesin, (2) *in-vitro* polymerized microtubules and (3) specifically functionalized quantum dots has been employed to realize kinesin motility *in-vitro*. Selective attachment of the kinesin motor protein to a surface is an important prerequisite for the development of artificial bio-engineered devices utilizing these dynamic processes in *in-vitro* systems. We will elucidate the feasibility of using a micro/nano-track paved with streptavidin coated quantum dots as fluorescently traceable linkers for biotinylated kinesins. This will be based on results from fluorescence microscopy observations of recent motility assays and quantum dot distributions observed on structured PMMA (polymethyl-methacrylate) surfaces patterned by electron beam lithography.

Monday, February 27, 2012 2:30PM - 5:06PM –
Session D25 DCOMP GSCCM DMP: Focus Session: Matter at Extreme Conditions - New Experimental Capabilities 257A

2:30PM D25.00001 Ultrafast, high resolution, phase contrast imaging of shock response with synchrotron radiation: opportunities and challenges, S.N. LUO, B.J. JENSEN, D.E. HOOKS, K.J. RAMOS, J.D. YEAGER, K. KWIATKOWSKI, T. SHIMADA, D.A. FREDENBURG, Los Alamos National Lab, K. FEZZAA, Argonne National Lab — Designing materials that function at dynamic extremes and predicting dynamic materials response require experimental investigations of their time, rate and microstructure dependences. Key to such experiments are *in situ*, in-volume, temporally and spatially resolved measurements (e.g., x-ray imaging and diffraction). Here we report ultrafast (<100 ps), high resolution (~3 μm), dynamic phase contrast imaging (PCI) measurements during high strain-rate loading (100 ns scale). A gas gun was installed at 32ID beamline of the Advanced Photon Source for dynamic loading, and dynamic PCI measurements were performed with a single x-ray pulse on representative materials/processes, including cylinder impact and penetration, large-cell foam compaction, cerium jet formation and granular material compression. We present overall experimental scheme and opportunities for dynamic materials research as seen from the preliminary results, as well as challenges both for photon sources and detectors.

2:42PM D25.00002 Probing Matter at an Atomic Unit of Pressure using convergent compression, JAMES HAWRELIAK, DAMIAN SWIFT, JON EGGERT, DAVE BRAUN, LLNL, STEVE ROTHMAN, AWE, GILBERT COLLINS, LLNL — Geometric confinement significantly increases the shock pressure as a spherically-converging shock approaches the central focus. Inertial confinement fusion is one area where this technique enables the 100 MBar ablation pressure to multiply to the several-GBar pressure required for fusion. We are using x-ray radiography of a spherically convergent shock wave in a solid sphere to explore material equations of state at pressures which exceed the atomic unit of pressure ($E_h/a_0 = 300\text{MBar}$); the energy density of a hydrogen atom. Measuring materials properties above this pressure will breach yet another significant barrier in our quest to understand extreme states, and will open a completely new realm where the atomic nature of matter is very strongly perturbed. We will discuss initial experiments performed on the Omega laser facility and plans for future experiments on the NIF.

2:54PM D25.00003 High-resolution phase contrast imaging of brittle failure during impact loading, KYLE RAMOS, BRIAN JENSEN, LUO SHENGNIAN, DANIEL HOOKS, JOHN YEAGER, KRIS KWIATKOWSKI, TSUTOMU SHIMADA, Los Alamos National Laboratory, KAMEL FEZZAA, Advanced Photon Source — Heterogeneous processes involved in brittle failure necessitate *in situ*, spatially resolved observation. An impact capability has recently been developed in which synchrotron phase contrast imaging (PCI), at the 32-ID beamline of the Advanced Photon Source, can be used to resolve crack interfaces during dynamic deformation. The imaging is both fast and high-resolution as images with approximately 3 micrometer resolution are obtained from single x-ray pulses (<100 ps duration). Experiments have been performed to investigate questions regarding velocimetry interpretation, the effect of stress states, and whether cracking can occur under uniaxial compression. Uniaxial compression and tension in planar impact configurations and cylindrical impact penetration has been used to vary stress states and observe failure. PCI and velocimetry results from these experiments will be presented for a range of brittle materials spanning glasses and ceramics.

3:06PM D25.00004 Deformation and material dynamics under ultrafast compression, MICHAEL ARMSTRONG, Lawrence Livermore National Laboratory — For decades, dynamic compression experiments have been used to determine the equation of state of materials, and examine material deformation at high strain rates. Within the last 15 years, ultrafast optical methods have been used to characterize deformation at strain rates in excess of $10^{10}/\text{s}$. Recently such experiments have found broad consistency with empirical laws formulated at orders of magnitude lower strain rates, but have also discovered intriguing phenomena on short time scales, such as elastic stress orders of magnitude beyond the yield strength. These experiments explore the ultimate limits of material relaxation via deformation, and the results suggest exciting possibilities for practical and scientific application of ultrafast compression, including nonequilibrium material synthesis, determination of the equation of state with a small scale experiment, and the investigation of ultrahigh density with a table top laser. Here we will talk about our experiments on the ultrafast deformation of metals, including aluminum and iron, and the ultrafast compression of deuterium.

3:42PM D25.00005 High-resolution phase contrast imaging of jet formation in shocked cerium to examine material strength, BRIAN JENSEN, SHENG LUO, FRANK CHERNE, GUY DIMONTE, GUILLERMO TERRONES, DANIEL HOOKS, KYLE RAMOS, JOHN YEAGER, KRIS KWIATKOWSKI, TSUTOMU SHIMADA, Los Alamos National Laboratory, KAMEL FEZZAA, Argonne National Laboratory — Understanding the dynamic properties of metals has been a long-standing scientific challenge. Experiments are needed to locate phase boundaries, to obtain equation-of-state data within those boundaries, and to examine properties such as material strength in the relevant phases. Efforts have been underway in recent years to examine the multiphase equation-of-state for cerium largely because of its complex phase diagram that exists at relatively moderate pressures and temperatures. To date, experiments have been performed to determine the Hugoniot, the shock-melt transition, and to examine the low-pressure phases through the critical point. In the current work, we present novel data that uses ultrafast, high-resolution phase contrast imaging (PCI) to examine jet-formation in cerium for impact stresses that span the alpha-phase up to the melt boundary. These experiments were performed using a recently developed capability at the 32-ID beamline of the Advanced Photon Source that couples the PCI method with an impact system to obtain real-time, spatially resolved images during dynamic compression. Experimental results will be presented and compared with recent efforts that use more traditional shock-release and double-shock loading to examine strength.

3:54PM D25.00006 High Resolution Diagnostics for Simultaneous Measurements of Velocity and Density in Shock-Driven Instabilities, RICARDO MEJIA-ALVAREZ, SRIDHAR BALASUBRAMANIAN, GREG ORLICZ, KATHY PRESTRIDGE, Los Alamos National Laboratory — The interaction between a shock wave and the interface between two fluids of different density might induce macroscopic mixing of the fluids. It is generally accepted that baroclinic vorticity, resulting from misalignments between the density gradient across the interface and the pressure gradient of the shock wave, impels this macroscopic mixing. So far, the Extreme Fluids Team at Los Alamos National Laboratory has conducted the only detailed studies of the structure of the developing instability. These studies encompass simultaneous measurements of velocity and density via combined Particle Image Velocimetry (PIV) and Planar Laser Induced Fluorescence (PLIF). Using this approach, the above mentioned Team has conducted extensive studies over a varicose curtain of heavy gas (SF_6). Since a curtain implies two succeeding interfaces, a new Vertical Shock Tube (VST) was developed for simultaneous characterization of velocity and density fields of single-interface shock-driven flows. This talk is intended to present some of the results obtained for double-interface shock driven flows, as well as describing the characteristics, challenges, and range of possibilities of the laser diagnostics incorporated in the VST.

4:06PM D25.00007 LCLS: A new frontier for time-resolved in situ lattice measurements in materials at extreme conditions, DESPINA MILATHIANAKI, SLAC National Accelerator Laboratory, DAMIAN SWIFT, JAMES HAWRELIAK, Lawrence Livermore National Laboratory, RICHARD LEE, SLAC National Accelerator Laboratory — While laser-based pump-probe experiments have provided significant insights into the processes induced by dynamic loading (e.g. shock-induced phase transitions, elastic-plastic response), the material behavior at the lattice level has been extremely difficult to unveil due to the temporal and signal-to-noise limitations of laser-based x-ray techniques. Here we present recent dynamic x-ray diffraction measurements on the shock-induced behavior of polycrystalline Mg in the 10-40 GPa regime, followed by future experiments in the field of dynamic high pressure science using the free electron laser at LCLS as an ultrafast x-ray probe.

4:18PM D25.00008 Progress towards Single Shot Spectroscopic Techniques for Time-Resolved Measurements in the Diamond Anvil Cell, DOUGLAS ALLEN DALTON, Geophysical Laboratory, Carnegie Institution of Washington, R. STEWART MCWILLIAMS, M.F. MAHMOOD, Howard University and Geophysical Laboratory, ALEXANDER F. GONCHAROV, Geophysical Laboratory — We will discuss how we are bridging the gap between static diamond anvil cell and dynamic shock experiments using various spectroscopic techniques which utilize nonlinear optics. Using pulsed laser techniques, we can achieve extreme temperatures while probing optical and chemical changes on fast time scales. Recent developments incorporating broadband spectroscopy into the laser heated diamond anvil cell have indicated that probing phase transitions while measuring temperature is possible [1]. Various methods for incorporating nonlinear vibrational spectroscopy (such as CARS) into the diamond anvil cell will be discussed. The application of these optical diagnostics to pulsed laser heating and table-top shock experiments [2] will be presented.

[1] R.S. McWilliams et al., in preparation.

[2] M.R. Armstrong et al., J. Appl. Phys., **108**, 023511, (2010).

4:30PM D25.00009 Phase diagram of shock and ramp-compressed tin, AMY LAZICKI, JONATHON EGGERT, RYAN RYGG, DAMIAN SWIFT, JAMES MCNANEY, GILBERT COLLINS, Lawrence Livermore National Laboratory — We will present powder x-ray diffraction results on laser-ramp-compressed solid tin up to 600 GPa, and discuss new methods for detecting the melting transition. Tin has a complex phase diagram with multiple observed and predicted high pressure phases and a moderate melting temperature, making it an ideal subject for a fundamental study of material properties using new techniques. Ramp compression in the solid allows access to extremely dense condensed phases and in the liquid the possibility for dynamically freezing molten tin. With newly developed x-ray diffraction methods we examine crystal structure, strength and texture in the dynamically compressed phases, and explore the possibility of a new method for mapping out melting curves.

4:42PM D25.00010 Ultrafast Shock Interrogation of Hydrogen Peroxide/Water Mixtures: Thermochemical Predictions of Shock Condition Chemistry¹, JOSEPH ZAUG, MICHAEL ARMSTRONG, SORIN BASTEA, JEFFREY CARTER, I-F. WILLIAM KUO, JONATHAN CROWHURST, CHRISTIAN GRANT, Lawrence Livermore National Laboratory, X-CHEM TEAM — Hydrogen peroxide is a powerful oxidizer and its concentrated aqueous solutions exhibit very high reactivity, even sustaining detonation under strong enough confinement. Due to its simple composition and basic expected decomposition kinetics hydrogen peroxide is very suitable for studying the interplay of high pressures, temperatures and reactivity and their effect on the equation of state, particularly at the boundary between detonating and non-detonating behavior. To this end we performed speed of sound and picosecond time resolved shock measurements on solutions of hydrogen peroxide of concentrations from 30 to 90 percent, and analyzed the results in terms of common assumptions of chemical equilibrium in reactive fluid mixtures. Experimental shock states were achieved up to a maximum pressure of 20 GPa with corresponding shock velocities of 6-7 km/sec.

¹This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344. We acknowledge the LLNL Laboratory Directed Research and Development office for support.

4:54PM D25.00011 Simulation of Forward and Inverse X-ray Scattering From Shocked Materials, JOHN BARBER, QUINN MARKSTEINER, CRIS BARNES, Los Alamos National Laboratory — The next generation of high-intensity, coherent light sources should generate sufficient brilliance to perform in-situ coherent x-ray diffraction imaging (CXDI) of shocked materials. In this work, we present beginning-to-end simulations of this process. This includes the calculation of the partially-coherent intensity profiles of self-amplified stimulated emission (SASE) x-ray free electron lasers (XFELs), as well as the use of simulated, shocked molecular-dynamics-based samples to predict the evolution of the resulting diffraction patterns. In addition, we will explore the corresponding inverse problem by performing iterative phase retrieval to generate reconstructed images of the simulated sample. The development of these methods in the context of materials under extreme conditions should provide crucial insights into the design and capabilities of shocked in-situ imaging experiments.

Monday, February 27, 2012 2:30PM - 5:30PM –

Session D26 DCOMP DMP: Focus Session: Physics of Energy Storage Materials - Catalysis and H₂ Storage 257B

2:30PM D26.00001 Design Principles for Oxygen Reduction and Evolution on Oxide Catalysts

, YANG SHAO-HORN, Massachusetts Institute of Technology — Driven by growing concerns about global warming and the depletion of petroleum resources, developing renewable energy production and storage technologies represent one of the major scientific challenges of the 21st century. A critical element in pursuit of this quest is the discovery of efficient and cost-effective catalysts used in solar fuel production via electrochemical energy conversion processes such as oxygen evolution reaction (OER) and oxygen reduction reaction (ORR), both of which are central to the efficiencies of direct solar and electrolytic water-splitting devices, fuel cells, and metal-air batteries. Although the Sabatier's principle provides a qualitative argument in tuning catalytic activity by varying the bond strength between catalyst surface and reactant/product (neither too strong nor too weak leading to the maximum activity at moderate bond strength), it has no predictive power to find catalysts with enhanced activity. Identifying a "design principle" that links catalyst properties to the catalytic activity is critical to accelerate the search for highly active catalysts based on abundant elements, and minimize the use of precious metals. Here we establish a molecular principle that governs the activities of oxygen evolution reaction (OER) and oxygen reduction reaction (ORR) for oxide catalysts, where the activities primarily correlate to the σ^* orbital ("e_g") occupation of surface transition metal cations established by systematic examination of more than ten to fifteen transition metal oxides. The intrinsic ORR and OER activities exhibit a volcano-shaped dependence on the e_g occupancy and the activities peak at an e_g occupancy close to unity. Our findings reflect the critical influence of the σ^* orbital on the energetics of surface reaction intermediates on surface transition metal ions such as the O₂²⁻/OH⁻ displacement and the OH⁻ regeneration, and thus highlight the importance of surface oxide electronic structure in controlling catalytic activities. Using the established molecular principle, we further demonstrate that an alkaline earth cobalt oxide with a chemical formula of Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3δ} (BSCF), catalyzes the OER with intrinsic activity that is at least an order of magnitude higher than the state-of-the-art iridium oxide catalyst in basic solutions.

[1] J. Suntivich, H.A. Gasteiger, N. Yabuuchi, H. Nakanishi, J. B. Goodenough and Y. Shao-Horn, Design Principles for Oxygen Reduction Activity on Perovskite Oxide Catalysts for Fuel Cells and Metal-Air Batteries, *Nature Chemistry*, **3**, 546–550 (2011).

[2] Jin Suntivich, Kevin J. May, Hubert A. Gasteiger, John B. Goodenough and Yang Shao-Horn, A Perovskite Oxide Optimized for Oxygen Evolution Catalysis from Molecular Orbital Principles, *ScienceExpress*, Science DOI: 10.1126/science.1212858, (2011).

3:06PM D26.00002 Modeling of hydrogen evolution reaction on the surface of GaInP₂¹, WOON

IH CHOI, BRANDON WOOD, ERIC SCHWEGLER, TADASHI OGITSU, LLNL, QUANTUM SIMULATION GROUP TEAM — GaInP₂ is promising candidate material for hydrogen production using sunlight. It reduces solvated proton into hydrogen molecule using light-induced excited electrons in the photoelectrochemical cell. However, it is challenging to model hydrogen evolution reaction (HER) using first-principles molecular dynamics. Instead, we use Anderson-Newns model and generalized solvent coordinate in Marcus-Hush theory to describe adiabatic free energy surface of HER. Model parameters are fitted from the DFT calculations. We model Volmer-Heyrovsky reaction path on the surfaces of CuPt phase of GaInP₂. We also discuss effects of surface oxide and catalyst atoms that exist on top of bare surfaces in experimental circumstances.

¹LLNL-LDRD

3:18PM D26.00003 ABSTRACT WITHDRAWN —

3:30PM D26.00004 In situ Raman Evidence for Reversible Room-Temperature Hydrogenation

in Pt-doped Carbons¹, XIAOMING LIU, PSU Materials Research Laboratory, YOUJIAN TANG, ENSHI XU, PSU Department of Physics, THOMAS FITZGIBBONS, PSU Department of Chemistry, HUAN-HSIUNG TSENG, MING-SHENG YU, CHENG-SI TSAO, Taiwan Institute of Nuclear Energy Research, JOHN BADDING, PSU Department of Chemistry, VINCENT CRESPI, PSU Department of Physics, ANGELA LUEKING, PSU Department of Chemical Engineering and EMS Energy Institute, ANGELA D. LUEKING TEAM, JOHN V. BADDING TEAM, VINCENT H. CRESPI TEAM, CHENG-SI TSAO COLLABORATION — Atomic hydrogen spillover was investigated by in situ Raman spectroscopy and density functional theory. In the presence of Pt nanoparticles, modes related to Basal plain hydrogenation were observed for activated carbon and graphene, respectively, during Raman measurements in 100 bar H₂. The modes were absent when Pt, carbon, or H₂ were omitted from the experiment. Substituting H₂ with D₂ led to the expected isotopic shift for a hydrogen-dominated vibrational mode. The mode disappeared and reappeared over several cycles of exposure to H₂ or He at room temperature, consistent with room-temperature reversibility of H chemisorbed to the activated carbon in the presence of Pt nanoparticles. Reversibility apparently arises from a facilitated transition of H from a chemisorbed state to a more mobile physisorbed state, followed by recombination and release. Reversibility for Pt/graphene was much less pronounced, suggesting that structural heterogeneities in the sample carbon support and/or catalyst-carbon contact are important factors.

¹This work was supported by DOE-BES Awards DE-FG02-09ER466556 and DE-SC0002157 and EERE Award DE-FG36-08GO18139

3:42PM D26.00005 Hydrogen storage on calcium coated boron (hetero-)fullerenes: A DFT study

, SULEYMAN ER, Harvard University, GEERT BROCKS, University of Twente, GILLES A. DE WIJS, Radboud University Nijmegen — Using density functional theory (DFT), we investigate hydrogen storage properties of calcium-coated molecular systems of B₈₀ boron fullerene, C₄₈B₁₂ boron-doped heterofullerenes, and well-known C₆₀ fullerene. Here, we consider the most common and low-lying isomers of B₈₀ and C₄₈B₁₂. We find that the Ca-coated molecules have the following properties: (1) The binding of metal atoms to B₈₀ or to C₄₈B₁₂ molecules is much stronger than their binding to a C₆₀ molecule. (2) B₈₀ and C₄₈B₁₂ have larger electron affinities than their carbon only counterpart, and accordingly discharge the surface Ca atoms more efficiently. (3) B₈₀ molecule, however, shows structural deformations upon reacting with Ca atoms. (4) C₄₈B₁₂Ca₆, however, is stable at elevated temperatures. C₄₈B₁₂ has well-exposed, positively charged Ca atoms on its surface, and binds up to six hydrogen molecules per metal center with hydrogen binding energies of 0.17-0.14 eV/H₂, that are suitable for ambient temperature hydrogen storage.

3:54PM D26.00006 Role of nano in catalysis: Pd catalyzed H desorption from MgH₂, WEIYU XIE,

DAMIEN WEST, YIYANG SUN, SHENGBAI ZHANG, Rensselaer Polytech Inst — Magnesium hydride (MgH₂) is promising for on-board hydrogen (H) storage with the major hurdle being the slow desorption kinetics. H desorption from ball-milled MgH₂ peaks at two slightly different temperatures, which further split in the presence of palladium catalyst. It has been experimentally demonstrated that nanostructuring can eliminate the high temperature peak. However, the effect of nanostructuring cannot be explained by thermodynamic destabilization due to quantum size effect. Our first-principles calculation reveals that there exist two reaction pathways for H desorption from MgH₂. One involves H vacancy (SV) diffusion at surface, while the other one involves H atom diffusion in bulk. The SV pathway self-terminates as dehydrogenation eventually eliminates the exposed MgH₂ region. Therefore, it is size-sensitive and fully functions only when the surface-to-bulk ratio is large, which is available only in nanostructures. Our calculation further shows that the SV pathway significantly lowers the desorption barrier, because it decouples the H transport process with the surface liftoff process and benefits from a fact that diffusion of vacancies at surface can have significantly lower barrier than that in bulk.

4:06PM D26.00007 Particle-size dependence of the activation energy for decomposition of lithium amide¹, CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara, KHANG HOANG, Naval Research Laboratory, ANDERSON JANOTTI, Materials Department, University of California, Santa Barbara — Lithium amide (LiNH_2) is a promising material for reversible hydrogen storage, yet atomistic mechanisms behind the dehydrogenation process are unknown. The activation energy for LiNH_2 decomposition has been observed to strongly vary with ball milling, suggesting a dependence of the thermodynamics and kinetics of the decomposition on the particle size. We have examined these mechanisms based on first-principles calculations for native point defects and defect complexes in LiNH_2 . We propose that the decomposition of LiNH_2 into lithium imide (Li_2NH) and ammonia (NH_3) occurs through two competing mechanisms, one involving the formation of native defects in the interior of the material and the other at the surface. As a result, the prevailing mechanism and hence the activation energy depend on the surface-to-volume ratio, or the specific surface area, which changes with the particle size. We explain the observed variations of activation energy, and address the role played by LiH in the dehydrogenation of ($\text{LiNH}_2 + \text{LiH}$) mixtures. The relationship between the structure of hydrogen-related defects and the end products in the decomposition reaction can be extended to other complex hydrides.

¹Work supported by DOE.

4:18PM D26.00008 Deliquescence of NaBH_4 computed from density functional theory, PING LI, WISSAM AL-SAIDI, KARL JOHNSON, University of Pittsburgh — Complex hydrides are promising hydrogen storage materials and have received significant attention due to their high hydrogen-capacity. The hydrolysis reaction of NaBH_4 releases hydrogen with both fast kinetics and high extent of reaction under technical conditions by using steam deliquescence of NaBH_4 . This catalyst-free reaction has many advantages over traditional catalytic aqueous phase hydrolysis. The first step in the reaction is deliquescence, i.e. adsorption of water onto NaBH_4 surface and then formation of a liquid layer of a concentrated NaBH_4 solution, which is quickly followed by hydrogen generation. We have used periodic plane wave density functional theory to compute the energetics and dynamics of the initial stages of deliquescence on the (001) surface of NaBH_4 . Comparison of results from standard generalized gradient approximation functionals with a dispersion-corrected density functional show that dispersion forces are important for adsorption. We used DFT molecular dynamics to assess the elementary steps in the deliquescence process.

4:30PM D26.00009 Electronic Structure and Molecular Dynamics Calculations for KBH_4 ¹, DIMITRIOS PAPACONSTANTOPOULOS, ANDREW SHABAEV, KHANG HOANG, George Mason University, MICHAEL MEHL, Naval Research Laboratory, NICHOLAS KIOUSSIS, UC at Northridge — In the search for hydrogen storage materials, alkali borohydrides MBH_4 ($\text{M}=\text{Li}, \text{Na}, \text{K}$) are especially interesting because of their light weight and the high number of hydrogen atoms per metal atom. Electronic structure calculations can give insights into the properties of these complex hydrides and provide understanding of the structural properties and of the bonding of hydrogen. We have performed first-principles density-functional theory (DFT) and tight-binding (TB) calculations for KBH_4 in both the high temperature (HT) and low temperature (LT) phases to understand its electronic and structural properties. Our DFT calculations were carried out using the VASP code. The results were then used as a database to develop a tight-binding Hamiltonian using the NRL-TB method. This approach allowed for computationally efficient calculations of phonon frequencies and elastic constants using the static module of the NRL-TB, and also using the molecular dynamics module to calculate mean-square displacements and formation energies of hydrogen vacancies.

¹The work at GMU is supported by DoE.

4:42PM D26.00010 Dehydrogenation of LiBH_4 nanoclusters: A first-principles study, EBRAHIM HAZRATI, FILIPE VASCONCELOS, ESM, IMM, Radboud University, GEERT BROCKS, CMS, University of Twente, ROBERT DE GROOT, GILLES DE WIJS, ESM, IMM, Radboud University — Recent experimental studies^{1,2} show faster desorption kinetics, improved reversibility and more favorable thermodynamics for confined LiBH_4 nanoparticles than the bulk. Using density functional theory calculations, we first discuss the geometries and energetics of LiBH_4 , LiH , LiB , Li and B clusters. Secondly, we study the effects of particle size on the decomposition pathway of LiBH_4 clusters. Our calculations show that only very small clusters of LiBH_4 (up to 12 formula units) are significantly destabilized relative to the bulk. High stability of small clusters of LiBH_4 originates from the fact that surface energies are very low for bulk LiBH_4 . (100), (010), (101) and (011) surfaces are almost degenerate with surface energies of 0.113, 0.102, 0.115 and 0.097 J/m², respectively. Clusters of LiH , LiB , Li and B are more strongly destabilized than the LiBH_4 clusters upon decreasing the cluster size. We show that, in contrast to the bulk, destabilized clusters of LiBH_4 decompose to $(\text{LiB})_n$ clusters. Finally, we present some of our preliminary NMR chemical shift results for different LiBH_4 surface terminations.

¹A.F. Gross et al. J. Phys. Chem. C 112, 5651, 2008

²X. Liu et al. Chem. Mater. 23, 1331, 2011

4:54PM D26.00011 First-principles Modeling of Diffusion during Hydrogenation of LiBH_4 , CHAO YU, VIDVUDS OZOLINS, Department of Materials Science and Engineering, University of California, Los Angeles — LiBH_4 has been studied extensively because of its high volumetric and gravimetric hydrogen content. However, experiments show that hydrogen release is very slow at temperatures up to 300 C, which severely limits applications in mobile storage. Using density-functional theory calculations, we systematically study bulk diffusion of defects during solid-state hydrogenation reactions. The defect concentration and concentration gradients are calculated for a variety of defects, including charged vacancies and interstitials. We find that low concentration gradients limit the rate of hydrogen desorption.

5:06PM D26.00012 Bulk diffusion of defects in $\text{LiAlH}_4/\text{Li}_3\text{AlH}_6$, BILJANA ROLIH, VIDVUDS OZOLINS, UCLA — From various experimental studies on decomposition of hydrogen storage materials it has been proposed that bulk diffusion of metal species may be the rate limiting step in hydrogen storage reactions. A recently developed theoretical model uses density functional theory to study the underlying processes involved in bulk diffusion. To date this model has been applied to study dehydrogenation of NaAlH_4 . However further study of alkaline and alkali earth metals merits attention, particularly LiAlH_4 with a high gravimetric hydrogen density, accessible at moderate temperatures. This study uses density functional theory to obtain concentration gradients and diffusivities of native charged and neutral defects in Li_3AlH_6 and LiAlH_4 . The flux of each defect is obtained and thus the activation energy for each defect. Our results show that diffusion of metal species is a possible rate limiting process in the system.

5:18PM D26.00013 First-Principles Study of the Li-Na-Ca-N-H System: Compound Structures and Hydrogen-Storage Properties, PATTANASAK TEERATCHANAN, FEI ZHOU, University of California, Los Angeles, KYLE MICHEL, Northwestern University, VIDVUDS OZOLINS, University of California, Los Angeles — Mixed-metal amides and imides are being widely investigated as potential hydrogen storage materials. Using a combination of first-principle DFT calculations, grand-canonical linear programming, and prototype electrostatic ground state (PEGS) approaches, we predict hydrogen storage reactions in the Li-Na-Ca-N-H system. The enthalpies, entropies, static, zero-point, and $T > 0\text{K}$ vibrational energies of known compounds together with our predictions of some incomplete experimental crystal structures are presented.

Monday, February 27, 2012 2:30PM - 5:30PM – Session D27 DMP GERA: Invited Session: Materials for Energy Applications 258AB

2:30PM D27.00001 The DOE SunShot Initiative: Science and Technology to enable Solar Electricity at Grid Parity, RAMAMOORTHY RAMESH, US DOE / UC Berkeley — The SunShot Initiative's mission is to develop solar energy technologies through a collaborative national push to make solar Photovoltaic (PV) and Concentrated Solar Power (CSP) energy technologies cost-competitive with fossil fuel based energy by reducing the cost of solar energy systems by ~ 75 percent before 2020. Reducing the total installed cost for utility-scale solar electricity to roughly 6 cents per kilowatt hour ($1\$/\text{Watt}$) without subsidies will result in rapid, large-scale adoption of solar electricity across the United States and the world. Achieving this goal will require significant reductions and technological innovations in all PV system components, namely modules, power electronics, and balance of systems (BOS), which includes all other components and costs required for a fully installed system including permitting and inspection costs. This investment will re-establish American technological and market leadership, improve the nation's energy security, strengthen U.S. economic competitiveness and catalyze domestic economic growth in the global clean energy race. SunShot is a cooperative program across DOE, involving the Office of Science, the Office of Energy Efficiency and Renewable Energy and ARPA-E.

3:06PM D27.00002 Integrating the multifunction necessary for electrochemical energy storage into energy- and size-scalable ultraporous nanoarchitectures¹, DEBRA ROLISON², U.S. Naval Research Laboratory — Designing high performance energy-storage devices that combine nanometric feature size with well-wired transport paths requires an architectural perspective. We chose carbon aerogel-like nanofoam papers as attractive plug-and-play electrode substrates because of such desirable properties as high specific surface area, electronic conductivity, and through-connected pore structure. Achieving this blend of desirable properties requires an optimal balance of critical architectural features: (1) open, 3D interconnected macropores sized at 100 to 300 nm (a difficult-to-obtain size range in porous carbons) and (2) pore walls of a size that reduce dead weight and volume (preferably ca. 20-nm wall thickness for 100- to 300-nm voids), yet retain mechanical strength and flexibility without compromising electronic conductivity (preferably ca. 20 S/cm). Carbon nanofoam papers provide a low cost and scalable nanocomposite that exists within this "Goldilocks zone" of desirable properties and which has catalyzed breakthroughs in our work with asymmetric electrochemical capacitors, air cathodes for metal/air batteries, lithium-ion batteries, 3D batteries, and semifuel cells. New charge-storage or catalytic functionality is imparted to internal carbon walls simply by transporting reactants within the 3D macroporous. Self-limiting modification strategies allow us to incorporate conformal, nanoscopic "paints" of metal (Mn, Ti, Ru, Fe) or polymer (redox-active or electron insulating) or to specifically adsorb metal nanoparticles (Pt, Au, Pd, Ag) throughout the macroscopic thickness (0.07 to 0.3 mm) of carbon nanofoam papers as dictated by the requirements of a specific end application. For instance, modification with 10-nm MnO_x increases the mass-, geometric-, and volume-normalized capacitance (2- to 10-fold) relative to the native carbon nanofoam without significantly altering its high-rate character and provides a structure that can be used in an asymmetric electrochemical capacitor or used to an air cathode in a Zn/air cell to electrocatalyze oxygen reduction and provide pulse power. Our redesigned carbon nanofoam offers a versatile design platform for much-needed advances in a broad range of multifunctional energy storage and conversion.

¹This work was supported by the U.S. Office of Naval Research.

²In collaboration with Jeffrey W. Long, Megan B. Sassin, Christopher N. Chervin, Joseph F. Parker, Jean Marie Wallace, Natalie L. Brandell, Bradley T. Willis, and Nathan W. Kucko.

3:42PM D27.00003 Bio-inspired Approaches to Solar Energy Conversion, MICHAEL WASIELEWSKI, Department of Chemistry and ANSER Center, Northwestern University, Evanston, IL 60208-3113 — Natural photosynthesis is carried out by organized assemblies of photofunctional tetrapyrrole chromophores and catalysts within proteins that provide specifically tailored environments to optimize solar energy conversion. Artificial photosynthetic systems for practical solar fuels production must collect light energy, separate charge, and transport charge to catalytic sites where multi-electron redox processes will occur. The primary goal of our research in this field is to understand the fundamental principles needed to develop integrated artificial photosynthetic systems. These principles include how to promote and control: 1) energy capture, charge separation, and long-range directional energy and charge transport, 2) coupling of separated charges to multi-electron catalysts for fuel formation, and 3) supramolecular self-assembly for scalable, low-cost processing from the nanoscale to the macroscale. The central scientific challenge is to develop small, functional building blocks, having a minimum number of covalent linkages, which also have the appropriate molecular recognition properties to facilitate self-assembly of complete, *functional* artificial photosynthetic systems. This lecture will describe our use of ultrafast optical spectroscopy and time-resolved EPR spectroscopy to understand charge transport in self-assembled structures for artificial photosynthesis.

4:18PM D27.00004 Quantum-well and quantum-dot structures for high-efficiency photovoltaics, EDWARD YU, The University of Texas at Austin — Quantum-well and quantum-dot semiconductor heterostructures offer a variety of opportunities for achieving photovoltaic power conversion efficiencies in excess of the Shockley-Queisser limit for single-homojunction solar cells. However, realization of such efficiencies is likely to require a combination of very high quality epitaxial growth or nanostructure synthesis to minimize carrier trapping and recombination, detailed understanding and analysis of optical absorption and nonequilibrium carrier transport processes, and light trapping to enable efficient optical absorption in very thin device layers. We discuss work in which GaAs/InGaAs/InAs semiconductor quantum-well and quantum-dot solar cells are realized in designs that enable efficient collection of photogenerated carriers from quantum-wells and dots, and combined with subwavelength-scale metal and dielectric structures that enable incident photons to be scattered into guided optical modes within a thin-film device, thereby enabling increased absorption efficiency in very thin device layers. Several aspects of this work will be addressed. Measurement of electric-field-dependent photocurrent response enables design of structures in which photogenerated carriers are collected efficiently from quantum-well or quantum-dot structures in the intrinsic region of a p-i-n junction solar cell. Processing to remove epitaxially grown device layers from their original growth substrate enables metal and dielectric nanostructures to be designed and integrated with the semiconductor epitaxial layer structures to scatter incident photons into strongly guided optical modes within the semiconductor. Finally, detailed analysis of quantum-well and quantum-dot optical absorption as well as optical mode structure within the device enables optimization of the absorption and mode profiles to achieve maximum power conversion efficiency. Both computational and experimental results derived from these approaches will be described.

4:54PM D27.00005 Combined conversion of heat and light with Photon Enhanced Thermionic Emission for solar energy harvesting, NICHOLAS MELOSH, Materials Science and Engineering, Stanford University — Recently a new mechanism for solar energy harvesting based on photon-enhanced thermionic emission (PETE) was proposed. This two-step process uses photons to excite carriers into the conduction band, followed by thermionic emission from the conduction band, and electron collection at a low-workfunction anode. This process effectively combines both heat and light, and its efficiency was calculated to exceed ideal single junction photovoltaics since it harvests some of the heat that is normally lost within PV devices. Experimental measurements demonstrated this mechanism in GaN materials, yet the quantum efficiency was very low. Here we discuss the loss mechanisms in the PETE process, and several approaches to overcome them. In particular we focus on surface recombination effects and absorption losses, and demonstrate a heterostructured device that increases the quantum efficiency by two orders of magnitude. Prospects for combined-cycle devices incorporating a PETE converter as a topping cycle on conventional thermal cycles are also analyzed.

Monday, February 27, 2012 2:30PM - 5:30PM –

Session D28 DMP: Focus Session: Dopants and Defects in Semiconductors - Oxides and Interfaces 258C

2:30PM D28.00001 Interdiffusion, Unintentional Doping and Electronic Reconstruction at Polar/nonpolar Oxide Interfaces¹

, SCOTT CHAMBERS, Pacific Northwest National Laboratory — The observation of conductivity at the interface of insulating polar and non-polar perovskites (general form ABO_3) has sparked considerable interest worldwide, with much of the work to date being focused on the $LaAlO_3/SrTiO_3(001)$ heterojunction. Many attribute the interface conductivity to an electronic reconstruction alleviating the polar discontinuity via a film-to-interface charge transfer. However, the possibility of dopant- and/or defect-mediated conductivity cannot be ruled out, especially when the interfaces are not atomically abrupt. Electronic reconstruction requires an electric field within the film to facilitate the charge transfer process. However, x-ray photoemission spectroscopy studies reveal little or no electric field in the LAO film either above or below the critical thickness for conductivity, calling into question the validity of the electronic reconstruction model. In order to gain deeper insight into the electronic properties, it is worthwhile to manipulate the interface by changing the B-site cation in the polar perovskite. There are no low-lying d -derived bands in $LaAlO_3$. Therefore, if conductivity occurs, it ought to be driven by either the wholesale transfer of charge from the $LaAlO_3$ O2p-derived band into the STO (i.e. electronic reconstruction), or unintentional doping and/or defect creation. By replacing Al with a transition metal cation, we inject a new degree of freedom into the band structure – partially occupied d orbitals – and, thus, enable other mechanisms of charge redistribution. We have explored this concept by placing Cr(III) at the B-site and describe the electronic properties of epitaxial $LaCrO_3/STO(001)$ heterojunctions. To minimize defect creation, the films were deposited using molecular beam epitaxy (MBE), in which the incoming atom energies are very low (<0.1 eV). Core-level and valence-band x-ray photoemission spectra measured for MBE-grown $LaCrO_3/SrTiO_3(001)$ yield band offsets and potential gradients within the $LaCrO_3$ sufficient to trigger an electronic reconstruction to alleviate the polarity mismatch. Yet, the interface is insulating. Based on first principles calculations, we attribute this unexpected result to interfacial cation mixing combined with charge redistribution within CrO_2 layers, enabled by low-lying d states within $LaCrO_3$, which suppresses an electronic reconstruction.

¹This work was supported by the U.S. Department of Energy, Office of Science, Division of Materials Sciences and Engineering under Award #10122 (film growth) and Division of Chemical Sciences under Award #48526 (photoemission measurements and modeling).

3:06PM D28.00002 Calculation of charge transition levels of oxygen vacancies in rutile TiO_2 using the GW method¹

, ANDREI MALASHEVICH, MANISH JAIN, STEVEN G. LOUIE, UC Berkeley and Lawrence Berkeley National Laboratory — Titanium dioxide (TiO_2) is a semiconductor displaying photovoltaic and photocatalytic properties and is widely used in numerous technological applications, such as solar cells, hydrolysis of water, photocatalysis, etc. Defects are important for optical properties of TiO_2 , e.g. they play a crucial role in photocatalytic reactions. Gaining a deep understanding of the influence of intrinsic defects, such as vacancies and interstitials, on the properties of this material is highly desirable. In spite of many theoretical and experimental investigations of defects in TiO_2 , controversies still remain. In this work, the charge transition levels of oxygen vacancies are studied in the rutile form of TiO_2 . For this purpose the GW method is employed for the calculation of the band gap and the position of the defect levels in the gap. The effects of lattice relaxations for systems with various charge states are taken into account. This is done with the help of hybrid functionals, since LDA or PBE mean fields do not describe defect levels properly, which may result in incorrect lattice relaxations. To account for spurious effects due to periodic images of the charged defects, appropriate electrostatic correction techniques are used.

¹This work was supported by NSF Grant No. DMR10-1006184 and by DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC and NICS.

3:18PM D28.00003 Strain effect on diffusion properties of oxygen vacancies in bulk and sub-surface of rutile TiO_2 ¹

, DAJUN SHU, ZHAOWU WANG, MU WANG, School of Physics, Nanjing University — The influences of external strain on diffusion properties of the bulk and subsurface oxygen vacancy (OV) in rutile TiO_2 are systematically studied using first-principle calculations. For OVs in bulk, we find that tensile (compressive) strain applied in the [001] direction or isotropically applied in the equivalent [110] and $[\bar{1}\bar{1}0]$ directions reduces (increases) the energy barriers of diffusion. Anisotropic strain applied in [110] and $[\bar{1}\bar{1}0]$ increases the energy barriers of diffusion in the two directions. Meanwhile it results in anisotropic diffusion behaviors. Between [110] and $[\bar{1}\bar{1}0]$, the bulk OV prefers to diffuse along the one in which more compressive or less tensile strain is applied. From subsurface to surface, the most energetically favorable OV pathway is along the [110] rows terminated with the surface bridging oxygen atoms. The diffusion barrier of the OV in the first trilayer is much lower than that of a bulk OV. External in-plane tensile strain can further reduce the energy barrier of the subsurface OV diffusion, and thus help to improve the diffusion of OVs from bulk to surface.

¹This work was supported by NSF of China (under Grant Nos. 10974079, 11174123, and 11034005) and Jiangsu

3:30PM D28.00004 Vibrational spectroscopy of O-H and O-D centers in TiO_2 ¹

, FIGEN BEKISLI, MICHAEL STAVOLA, W. BEALL FOWLER, Lehigh University — While the vibrational properties of O-H centers in TiO_2 have been studied for many years, recent experiments suggest a new picture of their behavior. In the 1970s, Bates and Perkins found a single, sharp, strongly polarized O-H line in TiO_2 , and similarly for O-D and O-T [1]. On the contrary, recent studies by Herklotz *et al.* [2] find three closely spaced O-H (O-D) lines that were assigned to two different charge states of an O-H (O-D) shallow donor. We have in our possession the very TiO_2 samples studied many years ago by Bates and Perkins. We have introduced H and D into these samples and also into TiO_2 samples obtained recently. High-resolution vibrational spectroscopy performed as a function of temperature at Lehigh provides new insight into the different vibrational properties seen for O-H in TiO_2 in the 1970's and in recent studies by Herklotz *et al.* [1] J.B. Bates and R.A. Perkins, Phys. Rev. B **16**, 3713 (1977). [2] F. Herklotz *et al.*, Phys. Rev. B **83**, 235202 (2011)..

¹Supported by NSF Grant DMR 0802278

3:42PM D28.00005 Intrinsic Spin-Orbit Effects in Strontium Titanate

, CUNEYT SAHIN, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa, Iowa City, Iowa 52242, USA, GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA, MICHAEL E. FLATTÉ, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa, Iowa City, Iowa 52242, USA — We have calculated spin relaxation times via the Elliott-Yafet mechanism for strontium titanate as a function of temperature. The approach uses a low-energy effective spin-orbit Hamiltonian constructed from a tight-binding model with atomic spin-orbit interactions. The intrinsic spin Hall conductivity for strontium titanate has also been calculated from the same low-energy Hamiltonian using a Berry's phase technique. Modifications to the spin relaxation and spin Hall conductivity from elastic strain at an interface will also be described. This work was supported by an ARO MURI.

3:54PM D28.00006 Prediction of a “half semiconductor” for spintronics in non-compensated n-p codoped TiO_2 ¹, WENGUANG ZHU, University of Tennessee & Oak Ridge National Laboratory, XING-QIU CHEN, Institute of Metal Research, CAS, China, HANNO WEITERING, University of Tennessee & Oak Ridge National Laboratory, ZHENYU ZHANG, University of Science and Technology of China & Harvard University, G. M. STOCKS, Oak Ridge National Laboratory — Based on hybrid density functional calculations, we predict that by doping non-compensated Cr-N pairs a normal wide-band-gap semiconductor TiO_2 can be altered to a “half semiconductor”, in which both the top and the valence band and the bottom of the conduction band are fully spin-polarized and exclusively contributed by the same spin component. The underlying formation mechanism of such an unusual band structure is revealed via detailed electronic structure analysis. The magnetic property of the material will also be discussed in this talk. Such a “half semiconductor” material may provide a new twist to generate and manipulate spin currents for spintronics.

¹Research supported by the DOE, Office of BES, Materials Sciences and Engineering Division.

4:06PM D28.00007 Charged and neutral oxygen vacancies at MgO surfaces under realistic temperature and pressure conditions, NORINA A. RICHTER, SERGEY V. LEVCHENKO, MATTHIAS SCHEFFLER, Fritz Haber Institute of the Max Planck Society — Surface O vacancies (F-centers) can strongly influence catalytic properties of MgO and metal clusters supported on MgO, but the experimental determination of their concentration at catalytic conditions is difficult. We employ density-functional theory and the *ab initio* atomistic thermodynamics approach to determine concentration and charge states of F-centers at (111) and flat and stepped (100) surfaces of MgO at realistic (T , p) conditions. Slab models and the virtual-crystal approximation [1] are used to model charged defects at surfaces. We find a strong dependence of F^+ and F^{2+} formation energy on the exchange-correlation (XC) functional. Varying the amount of screening and fraction of exact exchange within the HSE functional, we find a linear correlation between defect formation energies and calculated valence-band width of the host material, in line with recent results for bulk systems [2]. Using this correlation and extrapolating to experimental band width, we conclude that only F^{2+} centers can be present in significant concentrations at the (100) terraces at realistic conditions. — [1] L. Vegard, Z. Phys. **5**, 17 (1921); M. Scheffler, Physica **146B**, 176 (1987); [2] R. Ramprasad *et al.*, subm. to Phys. Rev. Lett.

4:18PM D28.00008 Pressure dependence of the large polaron transport in anatase TiO_2 single crystals, JAČIM JAČIMOVIĆ, CRISTIAN VAJU, HELMUTH BERGER, ARNAUD MAGREZ, Laboratory of Physics of Complex Matter Physics, Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland, VIKTOR CEROVSKI, RADOMIR ŽIKIĆ, Institute of Physics, Belgrade, Serbia, RICHARD GAÁL, LÁSZLÓ FORRÓ, Laboratory of Physics of Complex Matter Physics, Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland — Anatase is a TiO_2 polymorph which is a 3.2 eV gap semiconductor interesting for several applications, including catalysis, photocatalysis, and, especially, dye-sensitized solar cells. Surprisingly, transparent single crystals of anatase grown in our laboratory show a metallic resistivity above 60 K which origin is a shallow donor level created by oxygen vacancies. The high value of the resistivity and its T^3 temperature dependence are the result of the polaronic nature of the charge carriers which is supported by the Seebeck coefficient (S). The application of hydrostatic pressure fails to close the donor level and to extend the conducting state to the entire temperature range. Instead, we have found a non-monotonic variation of the low temperature activation energy with applied pressure which is ascribed to the change of polaron's mobility. Thermo-electric power exhibits an unconventional temperature and pressure dependence shedding an additional light on the conductivity mechanism in this compound. The pressure dependence of S is governed by the transport of the large entropy associated with the polaron formation.

4:30PM D28.00009 Revisiting the mechanism of photocatalytic activities in N-doped TiO_2 ¹, NAOITO UMEZAWA, National Institute for Materials Science, JST PRESTO, JINHUA YE, National Institute for Materials Science, MANA — Photocatalysis possesses a great potential for environmental remediation and fuel production [1]. Nitrogen doped TiO_2 is a well-known visible-light sensitive photocatalyst where deep impurity states associated with substitutional nitrogen at oxygen sites (N_O) are believed to be the source of the red shift in photo-absorption edge. However, such a deep level should trap hole carriers, degrading oxidation process. The contradiction between the deep N_O level and rather a high oxidation power of N-doped TiO_2 has been an unsolved puzzle. Here, we propose a convincing mechanism which successfully solves the riddle. N_O strongly binds with a titanium atom at an interstitial site, forming a defect-impurity band, which consists of bonding and anti-bonding states of nitrogen p and titanium d and narrows the band gap. Such a newly formed band, which is connected to the valence band maximum of the host TiO_2 , becomes the migration path of photo-induced hole carriers, assisting carrier transfer to the surface. This clearly explains the photocatalytic activity of N-doped TiO_2 both for the visible-light absorption and the oxidation reaction. [1] Hua Tong, Shuxin Ouyang, Yingpu Bi, Naoto Umezawa, Mitsutake Oshikiri, and Jinhua Ye, Advanced Materials DOI: 10.1002/adma.20110275

¹This work was supported by the JSPS KAKENHI (21760030) and the JST PRESTO program.

4:42PM D28.00010 Femtosecond laser doped and nanostructured TiO_2 for photocatalysis, KATHERINE PHILLIPS, ELIZABETH LANDIS, CYNTHIA FRIEND, ERIC MAZUR, Harvard University — We present a novel method for femtosecond-laser doping of titanium dioxide (TiO_2) for above bandgap absorbance by irradiating titanium metal in the presence of oxygen and dopants. With a bandgap of 3.2 eV for the anatase crystalline phase, TiO_2 most strongly absorbs in the UV range ($\lambda < 387$ nm). However, doping with metals and nitrogen has been shown to create intermediate states in the bandgap. Using femtosecond laser doping techniques on titanium in a gaseous environment, we produce laser-induced periodic surface structures. Altering the gas composition and pressure does not change the surface morphology, but it does impact the chemical composition of the surface. We present compositional data from x-ray photoelectron and Raman spectroscopy and structural data from scanning electron microscopy. Our research presents an innovative approach using laser scanning techniques to alter the structure of TiO_2 and generate a new material for visible-light photocatalysis that has the potential for watersplitting.

4:54PM D28.00011 First-principles study of interstitial hydrogen in yttria-stabilized zirconia.¹, APOSTOLOS MARINOPOULOS, CEMDRX, Physics Department, University of Coimbra, CEMDRX, PHYSICS DEPARTMENT, UNIVERSITY OF COIMBRA TEAM — Hydrogen is a common impurity in oxides and has been known to exhibit a dual behavior: either by being a dopant or alternatively an amphoteric impurity with the transition (pinning) level, $E(+/-)$, lying inside the gap [1]. By means of calculations based on density-functional theory (DFT) and a hybrid-functional scheme (Heyd-Scuseria-Ernzerhof) we have studied the incorporation of hydrogen in yttria-stabilized zirconia. Equilibrium sites and formation energies were determined and the role of intrinsic oxygen vacancies needed to stabilize the cubic phase of the oxide was particularly examined. Whereas, in its positively-charged state, H^+ , hydrogen was found exclusively to form a dative-type bond with O ions, the neutral paramagnetic H^0 displayed a coexistence with deep interstitial configurations with minimal lattice relaxation of the host lattice. A number of atomic-level mechanisms and migration paths were explored in order to understand this site interplay and the dynamics of neutral H^0 in a way that is consistent with the existing experimental data. [1] C.G. Van de Walle and J. Neugebauer, Nature **423**, 626 (2003).

¹This work was supported by the program COMPETE: FCOMP-01-0124-FEDER-010450 and by the Portuguese Fundação para a Ciência e a Tecnologia (FCT) under the Ciência 2007 and PTDC/FIS/102722/2008 programs.

5:06PM D28.00012 Fundamental limits on optical transparency of transparent conducting oxides: free-carrier absorption in SnO_2 ¹, HARTWIN PEELAERS, Materials Department, University of California, Santa Barbara, California, EMMANOUIL KIOUPAKIS, Materials Department, UC Santa Barbara, California; Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, California — Transparent conducting oxides (TCOs) are a technologically important class of materials used as transparent contacts in optoelectronic devices, such as flat-panel displays, touch screens, solar cells, and light-emitting diodes. These applications are possible because the TCOs combine high electrical conductivity with transparency to visible light. However, the large concentration of free electrons introduces a source of absorption that forms a fundamental limit to the transparency. We evaluated the importance of phonon-assisted free-carrier absorption in SnO_2 completely from first principles. We also provide insight into the mechanisms that govern absorption in different wavelength regimes. Our results show that the absorption is weak in the visible, but it increases by as much as a factor of 5 in the UV. For the infrared region, we show that the absorption increases with the wavelength, and that this increase is proportional to the third power of the wavelength. We also explain this third power dependency.

¹This work was supported by the BAEF, NSF MRSEC, and DOE.

5:18PM D28.00013 Self-trapping of holes in p-type oxides: Theory for small polarons in MnO ¹, HAOWEI PENG, STEPHAN LANY, National Renewable Energy Laboratory — Employing the *p-d* repulsion to increase the valence band dispersion and the energy of the VBM is an important design principle for p-type oxides, as manifested in prototypical p-type oxides like Cu_2O or CuAlO_2 which show a strong Cu-*d*/O-*p* interaction. An alternative opportunity to realize this design principle occurs for Mn(II) compounds, where the *p-d* orbital interaction occurs dominantly in the fully occupied d^5 majority spin direction of Mn. However, the ability of Mn to change the oxidation state from +II to +III can lead to a small polaron mechanism for hole transport which hinders p-type conductivity. This work addresses the trends of hole self-trapping for MnO between octahedral (rock-salt structure) and tetrahedral coordination (zinc-blende structure). We employ an on-site hole-state potential so to satisfy the generalized Koopmans condition. This approach avoids the well-known difficulty of density-functional calculations to describe correctly the localization of polaronic states, and allows to quantitatively predict the self-trapping energies. We find that the tetrahedrally coordinated Mn is less susceptible to hole self-trapping than the octahedrally coordinated Mn.

¹Supported by the US Department of Energy, Office of Basic Energy Sciences as part of an Energy Frontier Research Center.

Monday, February 27, 2012 2:30PM - 5:30PM — Session D29 GQI: Focus Session: Qubits in Diamond II 259A

2:30PM D29.00001 Quantum information and quantum sensing with NV diamond, PHILIP HEMMER, Texas A&M University — No abstract available.

3:06PM D29.00002 Control of hybrid quantum registers in diamond, TIM HUGO TAMINIAU, TOENO VAN DER SAR, MACHIEL S. BLOK, GIJS DE LANGE, HANNES BERNIEN, WOLFGANG PFAFF, LUCIO ROBLEDO, RONALD HANSON, Kavli Institute of Nanoscience Delft, Delft University of Technology, PO Box 5046, 2600 GA Delft, The Netherlands — Nitrogen Vacancy (NV) centers in diamond provide a robust quantum register consisting of the NV electron spin, the nuclear spin of the associated nitrogen atom and nearby nuclear spins of carbon impurities (^{13}C). The constituents of this hybrid system each have different properties that make them ideal for different roles. For example, the electron spin is readily polarized and read-out optically using spin-dependent fluorescence, whereas long coherence times make the nuclear spins ideal quantum memories. However, because all these systems evolve and decohere on very different time scales, it is challenging to control the register and to protect it from decoherence due to the surrounding environment at the same time. Here we discuss our recent progress in initializing, controlling and reading out all the spins in such few-qubit NV quantum registers. To this end, we combine dynamical decoupling of the electron spin with control of all the nuclear spins, and explore different initialization schemes. These few qubit registers might then be used to implement quantum search algorithms and error correction protocols.

3:18PM D29.00003 Quantum interference of single photons from two remote Nitrogen-Vacancy centers in diamond, ALEXANDER KUBANEK, ALP SIPAHIGIL, EMRE TOGAN, MICHAEL GOLDMAN, YIWEN CHU, NATHALIE DE LEON, ALEXANDER ZIBROV, MIKHAIL LUKIN, Harvard University — The interference of two identical photons impinging on a beam splitter leads to perfect photon coalescence where both photons leave through the same output port. This fundamental effect, known as Hong-Ou-Mandel (HOM) interference [1], can be used to characterize the properties of quantum emitters with high accuracy. This is a particularly useful tool for quantum emitters embedded in a solid state matrix because their internal properties, unlike those of atoms in free space, can vary substantially from emitter to emitter due to interactions with the environment. Here, we demonstrate HOM interference of photons emitted from two single Nitrogen-Vacancy (NV) centers in diamond that are spatially separated by 2 meters. The frequencies of the photons are controlled by tuning individual optical transitions of associated NVs via a DC electric field. The indistinguishability of the photons paves the way for entanglement generation between remote solid state qubits. [1] C. K. Hong, Z.Y. Ou, and L. Mandel, Phys. Rev. Lett. 59, 2044 (1987).

3:30PM D29.00004 Coherent excitation dynamics of single spins in diamond¹, A.L. FALK, G.D. FUCHS², D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106, V.V. DOBROVITSKI, Ames Laboratory and Iowa State University, Ames, IA, 50011 — The spin dynamics of nitrogen vacancy (NV) centers in diamond during non-resonant optical excitation are fundamentally important for both optical initialization and fluorescence-based spin read-out. While such processes rely on the preservation of the longitudinal spin projection, an NV center's lack of orbital coherence at room temperature might suggest that its quantum phase would be destroyed during excitation. We address this question using Ramsey experiments, quantum process tomography and theoretical modeling and establish limits on the coherence loss of an NV center during optical excitation [1]. By treating the excitation and spin precession as a quantum process, we measure a process fidelity of $F = 0.87 \pm 0.03$, which includes excited state dephasing during measurement. Extrapolation to the moment of optical excitation yields $F \approx 0.95$. These results provide a new understanding of NV centers' spin coherence during optical excitation and are crucial for efforts to use coherent evolution in the excited state for spin control.

[1] G. D. Fuchs, A. L. Falk, V. V. Dobrovitski, and D. D. Awschalom, *submitted* (2011)

¹This work is funded by AFOSR, ARO, and DARPA.

²School of Applied and Engineering Physics, Cornell University, NY 14853

3:42PM D29.00005 Optimizing the resolution and the sensitivity of a scanning NV magnetometer, SUNGKUN HONG, PATRICK MALETINSKY, MICHAEL GRINOLDS, LAN LUAN, BIRGIT HAUSMANN, MIKHAIL LUKIN, RONALD WALSWORTH, MARKO LONCAR, AMIR YACOBY, Harvard University — A nitrogen-vacancy (NV) center in diamond has been recently considered as an outstanding atomic-scale magnetic field sensor. At the heart of NV based magnetometry is the ability to control the position of an NV within few nanometers to a sample, while preserving its spin coherence and readout fidelity. To this end, we previously developed a fabrication procedure for creating a monolithic scanning diamond nanopillar containing a single NV center. Here we present further optimization of our devices by locating NV centers with nanoscale accuracy as well as improving their magnetic field sensitivity. For locating the NV center, we developed a nanoscale imaging of a NV center in the device via near-field fluorescence quenching, which facilitates post selection of devices with NV centers being closer to the surface. In addition to enhancing photon collection via wave guiding through the nanopillar, we also significantly improved the spin coherence times of our devices via dynamic decoupling. This results in a magnetic field sensitivity of 30 nT/sqrt(Hz), unprecedented for scanning NV centers.

3:54PM D29.00006 High Dynamic Range Magnetometry with a Single Spin in Diamond¹, N.M. NUSRAN, M. UMMAL MOMEEN, M.V. GURUDEV DUTT, University of Pittsburgh — Detection of the weak magnetic fields associated with nanometer sized volumes of spins could allow for non-invasive, element-specific probing of a variety of important physical and biological systems. Averaging out random noise which is the commonly used standard measurement strategy (SM) in most nano-sensors, will at best lead to a field variance that is inversely proportional to the total averaging time. Further, there exists a trade-off between the field sensitivity and the dynamic range in the SM. In this work, we demonstrate an alternative approach for accurate magnetic sensing, using novel phase estimation algorithms (PEA), implemented on a single electronic spin associated with the nitrogen-vacancy (NV) defect center in diamond. The field variance in our approach scales down faster than the SM. The trade-off between the field sensitivity and the dynamic range no longer exists in this approach. Our results show an improvement of $\sim 6.25dB$ in the field sensitivity compared to the SM, over a large field sensing range ($\sim \pm 0.3mT$). Besides their direct impact on applications in demonstrated nanoscale magnetic sensing and imaging, this may also open the way for application of other quantum feedback and control techniques to magnetometry.

¹This work was supported by NSF, DOE and the Alfred P. Sloan Research Fellowship.

4:06PM D29.00007 Room temperature solid-state quantum bit with second-long memory, GEORG KUCSKO, PETER MAURER, CHRISTIAN LATTA, Harvard University, DAVID HUNGER, LMU Munich, LIANG JIANG, Caltech, FERNANDO PASTAWSKI, Max-Planck-Institut für Quantenoptik, NORMAN YAO, STEVEN BENNET, Harvard University, DANIEL TWITCHEN, Element Six, IGNACIO CIRAC, Max-Planck-Institut für Quantenoptik, MIKHAIL LUKIN, Harvard University, LUKIN GROUP TEAM, CIRAC GROUP COLLABORATION — Realization of stable quantum bits (qubits) that can be prepared and measured with high fidelity and that are capable of storing quantum information for long times exceeding seconds is an outstanding challenge in quantum science and engineering. Here we report on the realization of such a stable quantum bit using an individual ¹³C nuclear spin within an isotopically purified diamond crystal at room temperature. Using an electronic spin associated with a nearby Nitrogen Vacancy color center, we demonstrate high fidelity initialization and readout of a single ¹³C qubit. Quantum memory lifetime exceeding one second is obtained by using dissipative optical decoupling from the electronic degree of freedom and applying a sequence of radio-frequency pulses to suppress effects from the dipole-dipole interactions of the ¹³C spin-bath. Techniques to further extend the quantum memory lifetime as well as the potential applications are also discussed.

4:18PM D29.00008 Mechanism for optical initialization of spin in NV⁻ center in diamond¹, SANGKOOK CHOI, MANISH JAIN, STEVEN G. LOUIE, University of California, Berkeley and Lawrence Berkeley National Laboratory — Optical initialization of the negatively charged nitrogen-vacancy (NV⁻) center in diamond, the experimental manipulation of its degenerate mixed ground state into an un-entangled spin state through optical means, makes it one of the best candidates for realization of individually addressable spins in the solid state for quantum computing and other studies under ambient conditions. However, its exact mechanism is still not clear. Based on exact diagonalization of a many-electron Hamiltonian with parameters derived from ab initio GW calculations, the present study elucidates the electronic structure of the NV⁻ center and puts forward a concrete optical initialization mechanism. We calculated the ordering and energy surfaces of the low-energy many-body states and the relaxation processes of photo-excitation responsible for the optical initialization. Intersystem crossings are shown to be essential.

¹Supported by NSF DMR10-1006184, US DOE No. DE-AC02-05CH11231, Samsung Foundation, and computer resources from Teragrid and NERSC.

4:30PM D29.00009 Long-range quantum gates using dipolar crystals, HENDRIK WEIMER, Harvard University, ITAMP, NORMAN YAO, Harvard University, CHRIS LAUMANN, Harvard University, ITAMP, MIKHAIL LUKIN, Harvard University — We propose to use the magnetic dipole interaction in high density arrays of nitrogen-vacancy centers to enable long-range quantum logic between distant spin qubits. In our approach, an effective interaction between remote qubits is achieved by adiabatically following the ground state of the dipolar chain across a quantum phase transition [1]. We demonstrate that the proposed quantum gate is particularly robust against disorder and enables coherent coupling between qubits on distances that are compatible with sub-wavelength addressing techniques.

[1] H. Weimer et al., arXiv:1009.1003 (2011).

4:42PM D29.00010 Magnetic imaging of a single electron spin using a scanning NV magnetometer under ambient conditions, MICHAEL GRINOLDS, SUNGKUN HONG, PATRICK MALETINSKY, LAN LUAN, RONALD WALSWORTH, MIKHAIL LUKIN, AMIR YACOBY, Harvard University — It has long been an outstanding challenge to develop a magnetometer capable of detecting individual spins under ambient conditions. Nitrogen-vacancy (NV) centers are an attractive candidate for such a sensor, as even at room temperature their spins can be initialized and read out optically, have long coherence times, and are localized on atomic length scales. Here we present measurements using a scannable NV center to magnetically image the dipole field of a single electron spin. For a target spin, we chose to use an additional NV spin as it can be initialized and driven independently from other proximal spins, allowing us to perform dynamical decoupling schemes on both sensing and target NV spins. Magnetic images are taken under ambient conditions and are achieved through optimizing NV magnetic sensitivity (<60 nT/sqrt(Hz)) as well as minimizing the distance between the NV center and our target spin (<50 nm).

4:54PM D29.00011 Fabrication of thin diamond membranes for quantum information processing, IGOR AHARONOVICH, JONATHAN LEE, ANDREW MAGYAR, EVELYN HU, Harvard University — Coupling of nano-photonic devices to color centers in diamond offers exceptional opportunities to enhance our understanding of light-matter interactions. The formation of thin single crystal diamond membranes containing such centers, is an important prerequisite for the fabrication of diamond based devices. However, there are challenges in forming such membranes in ways that do not compromise the quality of the cavities or the optical properties of the emitters. Here we report the formation of optically active diamond membranes and the subsequent fabrication of optical cavities. In our approach, 1.7 μ m thick diamond membranes were generated by forming a sacrificial layer using ion implantation, followed by thermal annealing. These membranes then served as templates for the epitaxial overgrowth of ~ 300 nm of diamond using CVD. Remarkably, the regrown films reveal the presence of optically active defects which were *not* present in the template, such as silicon-vacancy (SiV) or nitrogen vacancy centers. Microdisk cavities were then formed from the regrown single crystal diamond membranes. Whispering gallery modes (WGMs) with quality factors of ~ 3000 were measured from the diamond cavities. Spectral overlap of WGMs with the zero phonon line of SiV centers was observed and lifetime reduction of the coupled emitter – cavity system was measured. The demonstration of coupling between diamond emitters and a single crystal diamond cavity is a crucial step towards diamond integrated nano-photonic networks.

5:06PM D29.00012 Noises of spin baths for qubits in diamond, ZHIHUI WANG, ANIRBAN DAS, DANIEL LIDAR, SUSUMU TAKAHASHI, University of Southern California — Nitrogen-vacancy (NV) center in diamond is a promising qubit candidate for quantum information processing and high precision magnetometry and is an excellent platform for studying quantum spin dynamics [1,2]. Overcoming spin decoherence of NV centers is critical to the applications. Coupling to spin baths of paramagnetic impurities and nuclei is a major decoherence source for NV centers. Therefore, recent theoretical and experimental efforts have aimed at suppressing the bath noises. In this presentation, we will discuss effects of the spin baths on the qubits at different regimes including high magnetic fields where the degree of the electron spin polarization is almost complete [3]. We will also discuss dynamical decoupling sequences to investigate spin bath noises.

- [1] R. Hanson et al., *Science*. **320**, 352 (2008).
- [2] G. de Lange et al., *Science*. **330**, 60 (2010)
- [3] S. Takahashi et al., *Phys. Rev. Lett.* **101**, 047601 (2008)

5:18PM D29.00013 Spectroscopy of composite solid-state spin environments for improved metrology with spin ensembles, NIR BAR-GILL, LINH PHAM, CHINMAY BELTHANGADY, DAVID LESAGE, Harvard University, PAOLA CAPPELLARO, MIT, JERONIMO MAZE, Pontificia Universidad Catolica de Chile, MIKHAIL LUKIN, AMIR YACOBY, RONALD WALSWORTH, Harvard University — For precision coherent measurements with ensembles of quantum spins the relevant Figure-of-Merit (FOM) is the product of spin density and coherence lifetime, which is generally limited by the dynamics of spin coupling to the environment. Significant effort has been invested in understanding the causes of decoherence in a diverse range of spin systems in order to increase the FOM and improve measurement sensitivity. Here, we apply a coherent spectroscopic technique to characterize the dynamics of a composite solid-state spin environment consisting of Nitrogen-Vacancy (NV) color centers in room temperature diamond coupled to baths of electronic spin (N) and nuclear spin (¹³C) impurities. For diamond samples with a wide range of NV densities and impurity spin concentrations we employ a dynamical decoupling technique to minimize coupling to the environment, and find similar values for the FOM, which is three orders of magnitude larger than previously achieved in any room-temperature solid-state spin system, and thus should enable greatly improved precision spin metrology. We also identify a suppression of electronic spin bath dynamics in the presence of a nuclear spin bath of sufficient nuclear spin concentration. This suppression could inform efforts to engineer samples with even larger FOM for solid-state spin ensemble metrology and collective quantum information processing.

Monday, February 27, 2012 2:30PM - 5:30PM –
Session D30 GQI: Focus Session: Quantum Information for Quantum Foundations - Entanglement and Causal Structure 259B

2:30PM D30.00001 Quantum measurement bounds beyond uncertainty relations, SETH LLOYD, MIT, VITTORIO GIOVANNETTI, Scuola Normale Pisa, LORENZO MACCONE, University of Pavia — Quantum measurements are limited by bounds such as the Heisenberg uncertainty relations which limit the accuracy of measuring a quantity via the standard deviation of the conjugate one. This talk shows that the accuracy of measuring a quantity such as phase or time is limited by the expectation value of the conjugate quantity. This result proves the long-standing conjecture – recently challenged – that the ultimate phase-precision limit in interferometry is lower bounded by the inverse of the total number of photons employed in the estimation process.

2:42PM D30.00002 Quantum sharability: Entanglement is less monogamous than you think, PETER JOHNSON, Dartmouth College, BENJAMIN SCHUMACHER, Kenyon College, LORENZA VIOLA, Dartmouth College — One of the essential features of entanglement is monogamy. However, it is well known that there are entangled states which are not monogamous. A generalization of the monogamy property is provided by the concept of sharability. For bipartite states, we say a state (or relationship) is $1-n$ sharable if a subsystem can simultaneously share this relationship with n other subsystems. Any state with a limited sharing capacity is entangled, and the strictness of the limit corresponds to how entangled the state is. We present the most interesting findings of sharability of bipartite qubit and qudit states and describe an application to quantum teleportation.

2:54PM D30.00003 New entanglement properties in systems of higher-spin particles, JAY LAWRENCE, University of Chicago and Dartmouth College, MARIO GAETA, ANDREI KLIMOV, University of Guadalajara, Jal., Mexico — We describe a new entanglement property of four-qutrit states that is inaccessible to any number of qubits. In such states, every particle is equally entangled with all others, as in GHZ states, but the entanglement is more robust than that of any four-qubit state. We describe the entanglement properties of related generalized graph states of three-state and five-state particles, and show how these suggest that new entanglement properties will emerge more generally for systems of $p+1$ particles, each having p states, where p is a prime number.

3:06PM D30.00004 Optimal Probabilistic Simulation of Quantum Channels from the Future to the Past, DINA GENKINA, University of Maryland, GIULIO CHIRIBELLA, LUCIEN HARDY, Perimeter Institute — We introduce the study of probabilistic protocols that simulate quantum channels transforming input states in the future into output states in the past. The maximum probability for such a simulation is set by causality and, we claim, depends on the amount and type (classical or quantum) of information the given channel can transmit. In particular, we focus on probabilistic teleportation with multiple copies of input and output. We show that as the number of input copies increases, the maximum probability of successful teleportation increases, a feature that is impossible in classical physics. As the number of input copies tends to infinity, the teleportation probability converges to the maximum probability for the simulation of an ideal classical channel from the future to the past.

3:18PM D30.00005 The asymmetry properties of pure quantum states, IMAN MARVIAN, Institute for Quantum computing & Perimeter Institute for theoretical Physics, Waterloo, Canada, ROBERT SPEKKENS, Perimeter Institute for theoretical Physics, Waterloo, Canada — The *asymmetry properties* of a state relative to some symmetry group specify how and to what extent the given symmetry is broken by the state. Characterizing these is found to be surprisingly useful for addressing a very common problem: to determine what follows from a system's dynamics (possibly open) having that symmetry. We demonstrate and exploit the fact that the asymmetry properties of a state can be understood in terms of information-theoretic concepts. We show that for a pure state ψ and a symmetry group G , they are completely specified by the characteristic function of the state, defined as $\chi_\psi(g) \equiv \langle \psi | U(g) | \psi \rangle$ where $g \in G$ and U is the unitary representation of interest. Based on this observation, we study several important problems about the interconversion of pure states under symmetric dynamics such as determining the conditions for reversible transformations, deterministic irreversible transformations and asymptotic transformations.

3:30PM D30.00006 Equilibration of Global Observables to Microcanonical Measure for Complex Systems, JOSEPH EMERSON, Dept of Applied Math and IQC, University of Waterloo, COZMIN UDUDEC, Dept of Physics, University of Waterloo — In the last few years we have seen significant progress in understanding how the canonical features of quantum statistical mechanics can be derived rigorously from an exact treatment of the underlying quantum mechanical system. Here we consider a related problem: we determine sufficient conditions under which one can derive an effective equilibration to the microcanonical ensemble for the measurement statistics of the global observables of a closed system. Our central assumption is that the unitary time-evolution operator of the system is sufficiently complex when expressed in the eigenbasis of the observable of interest that its eigenstates can be modeled by a typical unitary chosen from the Haar measure (or Circular Unitary Ensemble). This assumption is well-motivated from numerical studies in the field of quantum chaos where this property has been observed for simple model systems whose classical counterparts are globally chaotic. Further, we discuss the time scale on which equilibration occurs in the context of two models for the eigenvalues of the dynamical system. We argue that our results are a natural consequence of an epistemic view of pure quantum states, but may be surprising or even controversial for adherents of other interpretational perspectives.

3:42PM D30.00007 Coarse-graining makes it hard to see micro-macro entanglement¹, SADEGH RAEISI, Institute for Quantum Computing, University of Waterloo, PAVEL SEKATSKI, Université de Genève, CHRISTOPH SIMON, IQIS, University of Calgary — Observing quantum effects such as superpositions and entanglement in macroscopic systems requires not only a system that is well protected against environmental decoherence, but also sufficient measurement precision. Motivated by recent experiments, we study the effects of coarse-graining in photon number measurements on the observability of micro-macro entanglement that is created by greatly amplifying one photon from an entangled pair. We compare the results obtained for a unitary quantum cloner, which generates micro-macro entanglement, and for a measure-and-prepare cloner, which produces a separable micro-macro state. We show that the distance between the probability distributions of results for the two cloners approaches zero for a fixed moderate amount of coarse-graining. Proving the presence of micro-macro entanglement therefore becomes progressively harder as the system size increases.

¹We acknowledge AITF, NSERC, iCORE, and the Swiss NFS for financial support.

3:54PM D30.00008 On the quantification of resourcefulness in quantum information¹, YUVAL SANDERS, University of Waterloo, BEN FORTESCUE, Southern Illinois University, GILAD GOUR, University of Calgary — Quantum information processing tasks cannot be performed for free; several types of informational resource must be consumed. Such resources are often expensive: entanglement, for example, is quite difficult to distribute between distant parties. Efficient consumption of informational resources is therefore desirable for practical quantum information processing. Determination of the efficiency of a given protocol requires some method of quantifying the resources present before and after the implementation of a protocol. In the prototypical case of entanglement, one or several entanglement monotones are often used to determine the entanglement cost of a protocol. The mathematical definition of an entanglement monotone has undergone multiple revisions since its formal introduction by Vidal. Currently, a real-valued function of quantum states is considered an entanglement monotone if the function is monotonically decreasing under application of channels that can be enacted using only local operations with classical communication. In this lecture, I argue that even this simple definition is unnecessarily restrictive for fully characterising the entanglement of a state and propose a more general scheme of relative quantifiers of entanglement.

¹Partially supported by NSERC

4:06PM D30.00009 Scalar Fields via Causal Tapestries, WILLIAM SULIS, McMaster University/University of Waterloo — Causal tapestries provide a framework for implementing an explicit Process Theory approach to quantum foundations which models information flow within a physical system. We consider event-transition tapestry pairs. An event tapestry O is a 4-tuple (L, K, M, l_p) where K is an index set of cardinality κ , $M = M \times F(M) \times D \times P(M')$ a mathematical structure with M a causal space, $F(M)$ a function space, D a descriptor space, $P(M')$ either a Lie algebra or tangent space on a manifold M' , l_p an event tapestry. L consists of elements of the form $[n] \langle \alpha \rangle \{G\}$, n in K , α in M and G an acyclic directed graph whose vertex set is a subset of L_p . Likewise, a transition tapestry Π is a 4-tuple (L', K', M', l'_p) where $M' = M' \times F(M') \times D' \times P'(M')$. The dynamic generates a consistent succession of $O - \Pi$ pairs by means of a game based on the technique of forcing used in logic to generate models. This dynamic has previously been shown to be compatible with Lorentz invariance. An application of this approach to model scalar fields is presented in which each informon is associated with a function of the form $f(\pi k_1/\sigma_1, \dots, \pi k_N/\sigma_N) \sin(\sigma_1 t_1 - \pi k_1) / (\sigma_1 t_1 - \pi k_1) \dots \sin(\sigma_N t_N - \pi k_N) / (\sigma_N t_N - \pi k_N)$ and the WSK interpolation theorem is used to generate the resulting scalar field on the causal manifold.

4:18PM D30.00010 Topology of Quantum Discord¹, NGA NGUYEN, ROBERT JOYNT, Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA — Quantum discord is arguably a more sensitive measure of quantum correlations than quantum entanglement, and may be able to serve as a resource for quantum computation. All quantum correlations are subject to destruction by external noise. The route by which this destruction takes place depends on the shape of the hypersurface of zero discord in the space of generalized Bloch vectors. In the case of 2 qubits, we show that, except at the origin, this hypersurface is a 9-dimensional manifold with boundary embedded in a 15-dimensional background space. This is done by computing the tangent vectors explicitly and verifying that there are no self-intersections. We discuss the implications for the time evolution of discord in physical models, which contrasts sharply with the evolution of entanglement.

¹This project is funded by the Darpa Quest program, Contract No. FA9550-09-0033.

4:30PM D30.00011 ABSTRACT WITHDRAWN —

4:42PM D30.00012 Quantumness versus entanglement in quantum measurements¹, GERARDO ADESSO, School of Mathematical Sciences, The University of Nottingham, MARCO PIANI, Institute for Quantum Computing and Department of Physics and Astronomy, University of Waterloo — We analyze a hierarchy of quantumness measures for composite systems, defined in terms of the entanglement necessarily created between systems and apparatus during local measurements. We prove that the quantumness so defined is always greater than intra-systems entanglement, establishing a firm ordering relation between different non-classical features of correlations. We analyze qualitatively and quantitatively the flow of correlations in iterated measurements, showing that quantumness and entanglement can never decrease along von Neumann chains. Our results provide a comprehensive framework to understand and quantify general signatures of quantumness in multipartite states, and prove how useful the broader study of the quantumness of correlations can be to shed light on issues in quantum information processing, in the quantum theory of measurement and in quantum foundations.

¹MP acknowledges support by NSERC, CIFAR, Ontario Centres of Excellence. GA was supported by a Nottingham Early Career Research and Knowledge Transfer Award.

4:54PM D30.00013 Operational interpretation of the G-asymmetry for Abelian groups¹ , MICHAEL SKOTINIOTIS, GILAD GOUR, University of Calgary — In a reference frame alignment protocol the sender, Alice, prepares a quantum system in a state $ket\psi$, that serves as a token of her reference frame, and sends this system to a receiver, Bob, who performs a measurement and learns about the reference frame. We derive the state and measurement that maximize the accessible information in a reference frame alignment protocol. We show that in the limit where a large number of systems are sent, the accessible information per copy equals the Holevo bound. The latter was shown to be equal to the relative entropy of frameness, or G -asymmetry, of the state $ket\psi$, a measure of resourcefulness analogous to the relative entropy of entanglement. We show that for a reference frame alignment protocol, associated with a finite abelian group, Z_N , or the continuous group $U(1)$, associated with the important case of photon number super-selection, the rate of accessible information is quantified by the linearized, regularized G -asymmetry. Our result provides an information theoretic operational interpretation for the G -asymmetry that has been thus far lacking.

¹Natural Sciences and Engineering Research Council, and United States Army Research Office.

5:06PM D30.00014 Considerations of Closed Systems that Measure Particles , MICHAEL STEINER, RONALD RENDELL, Inspire Institute, Inc. — The Measurement Problem has been of fundamental concern since the discovery of Schrodinger's equation. We have been developing a framework for which this problem can be considered under the assumption that the detector is a closed system. Considerations that such systems satisfy will be presented. Questions of whether or not such a framework is possible for which the various considerations can be met will be presented. Related existing work in the literature will be presented.

5:18PM D30.00015 Is entanglement signaling really impossible? , JACK SARFATTI, Retired — Quantum entanglement cannot be used as a communication channel without an auxiliary light speed limited classical key to unlock the message at the receiver? Hermitian observables guarantee orthogonal sender base states that erase any nonlocal influence of the sender settings on the detection probabilities at the receiver. However, this is no longer true when the entangled whole has different macro-quantum coherent Glauber sender states. Glauber states are non-orthogonal eigenstates of the non-Hermitian photon destruction operator. The Born probability interpretation breaks down because of "phase rigidity" (P.W. Anderson's "More is different"). This is a new regime that is to orthodox quantum theory what general relativity is to special relativity. Antony Valentini has argued that the breakdown of the Born probability rule entails "signal non locality" (aka entanglement signals). The space-time interval between the sending and the receiving irreversible measurements is irrelevant depending only on the free will of the local observers. That is, this is a pre-metrical topological information effect. There is asymmetry between the sending and the receiving. Therefore, there is no ambiguity between active (retro) cause and passive effect.

Monday, February 27, 2012 2:30PM - 5:30PM —
Session D31 DMP: Focus Session: Topological Insulators: Synthesis & Characterization - Thin Films 260

2:30PM D31.00001 Epitaxial growth of high quality Bi_2Se_3 thin films on CdS , XUFENG KOU, LIANG HE, University of California, Los Angeles, FAXIAN XIU, Iowa State University, MURONG LANG, University of California, Los Angeles, YONG WANG, The University of Queensland, ALEXEI FEDEROV, Lawrence Berkeley National Laboratory, XINXIN YU, University of California, Los Angeles, JIN ZOU, The University of Queensland, KANG WANG, University of California, Los Angeles, UNIVERSITY OF CALIFORNIA, LOS ANGELES TEAM, IOWA STATE UNIVERSITY COLLABORATION, THE UNIVERSITY OF QUEENSLAND COLLABORATION, LAWRENCE BERKELEY NATIONAL LABORATORY COLLABORATION — We report the experiment of high quality epitaxial growth of Bi_2Se_3 thin films on lattice-matched hexagonal CdS (0001) substrates using a solid source molecular-beam epitaxy system. Layer-by-layer growth of single crystal Bi_2Se_3 has been observed from the first quintuple layer with larger surface triangular terraces. The improved film quality facilitates the characterization of surface states during magneto-transport measurements, such as high Hall mobility of $\sim 6000\text{ cm}^2/\text{Vs}$, a distinct Shubnikov-de Haas (SdH) oscillations and weak anti-localization cusp in the magnetic field dependent longitudinal resistance. These characteristics of Bi_2Se_3 thin films promise a variety of potential applications in ultra-fast, low-power dissipation devices.

2:42PM D31.00002 Fabrication of High Quality Topological Insulator Thin Films and Heterostructures , LI ZHANG, ROBERT HAMMOND, MERAV DOLEV, MAC BEASLEY, AHARON KAPITULNIK, Stanford University, GLAM TEAM — In this talk, I will present a method of fabrication high quality topological insulator thin films and heterostructures with ferromagnet materials using MBE with a RF Selenium cracker cell and pulsed laser deposition. I will also show some preliminary results on the physical properties of those films, including topography, crystal structure and transport properties.

2:54PM D31.00003 MBE growth and transport of the topologically tunable $(Bi_{1-x}In_x)_2Se_3$ system , MATTHEW BRAHLEK, NAMRATA BANSAL, NIKESH KOIRALA, Rutgers University Physics and Astronomy, SUYANG XU, ZAHID HASAN, Princeton University Physics, SEONGSHIK OH, Rutgers University Physics and Astronomy — A current challenge in the field of topological insulators (TI) is identifying a clear transport signal of the surface conduction. The structural similarity between Bi_2Se_3 and In_2Se_3 allowed us to combine the two to obtain $(Bi_{1-x}In_x)_2Se_3$; Bi_2Se_3 has inverted bands, and thus is a non-trivial insulator. In_2Se_3 has no inverted bands and is therefore a trivial band insulator with energy gap 1.3-1.9eV. The mixing ratio x can be thought of as a knob to switch the system from a trivial to a non-trivial state. I will briefly discuss our scheme for producing atomically smooth molecular beam epitaxial grown thin films. I will also discuss our work on transport in the TI-to-non TI regime, and the metal to insulator regime, and compare these results with angle resolved photo emission spectroscopy data.

3:06PM D31.00004 Hybrid Physical-Chemical Vapor Deposition of Bi_2Se_3 Thin films on Sapphire , JOSEPH BROM, YUE KE, RENZHONG DU, JAROD GAGNON, QI LI, JOAN REDWING, The Pennsylvania State University — High quality thin films of topological insulators continue to garner much interest. We report on the growth of highly-oriented thin films of Bi_2Se_3 on c-plane sapphire using hybrid physical-chemical vapor deposition (HPCVD). The HPCVD process utilizes the thermal decomposition of trimethyl bismuth (TMBi) and evaporation of elemental selenium in a hydrogen ambient to deposit Bi_2Se_3 . Growth parameters including TMBi flow rate and decomposition temperature and selenium evaporation temperature were optimized, effectively changing the Bi:Se ratio, to produce high quality films. Glancing angle x-ray diffraction measurements revealed that the films were c-axis oriented on sapphire. Trigon crystal planes were observed in atomic force microscopy images with an RMS surface roughness of 1.24 nm over an area of $2\mu\text{m}\times 2\mu\text{m}$. Variable temperature Hall effect measurements were also carried out on films that were nominally 50-70 nm thick. Over the temperature range from 300K down to 4.2K, the carrier concentration remained constant at approximately $6\times 10^{18}\text{ cm}^{-3}$ while the mobility increased from $480\text{ cm}^2/\text{Vs}$ to $900\text{ cm}^2/\text{Vs}$. These results demonstrate that the HPCVD technique can be used to deposit Bi_2Se_3 films with structural and electrical properties comparable to films produced by molecular beam epitaxy.

3:18PM D31.00005 Pulsed Laser Deposition of Epitaxial Topological Insulator Thin Films: Bi_2Te_3 and $\text{Bi}_2\text{Te}_2\text{Se}$, SHIXIONG ZHANG, LI YAN, JINGBO QI, MUJIN ZHUO, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, YONGQIANG WANG, Materials Science and Technology Division, Los Alamos National Laboratory, ROHIT P. PRASANKUMAR, QUANXI JIA, S. TOM PICRAUX, Center for Integrated Nanotechnologies, Los Alamos National Laboratory — While high quality epitaxial thin films of topological insulators have been achieved by molecular beam epitaxy, there has been little progress using other thin film growth techniques. Here, we report the growth of high quality epitaxial Bi_2Te_3 and $\text{Bi}_2\text{Te}_2\text{Se}$ thin films on silicon (111) and YSZ (111) substrates by pulsed laser deposition (PLD). Systematic structural characterization of the films using x-ray diffraction and transmission electron microscopy has demonstrated that a low laser pulse rate is the key to achieving high quality epitaxial films. Rutherford backscattering spectrometry measurements suggest that the film composition is strongly influenced by the growth temperature and background gas pressure. The electrical transport properties of the films grown at the optimal conditions will also be discussed. Since PLD is an excellent tool to grow a variety of functional oxides, including multiferroics, magnetic semiconductors and high temperature superconductors, the growth of epitaxial topological insulator thin films by the same technique paves the way to synthesize multi-layered heterostructures of the above materials and search for novel physics arising from the resulting interfacial couplings.

3:30PM D31.00006 Growth and properties of half-Heusler DyPdBi ¹, BRIAN MULCAHY, MAO ZHENG, CAROLYN KAN, JAMES ECKSTEIN, University of Illinois Urbana-Champaign — Some half-Heusler phases have been predicted by Chadov, *et al.*, to exhibit topological electronic structure. In addition to providing an exciting new topological system, the breadth of the elemental parameter space for this system opens the door for investigation of the interplay between many novel physical states with the topological system. We have grown thin films of one of these phases, the cubic half-Heusler material DyPdBi , using carefully flux matched molecular beam epitaxy. Crystalline quality was monitored via *in situ* RHEED and verified by *ex situ* x-ray diffraction measurements. Transport measurements indicate the emergence of interesting correlated behavior at low temperature.

¹This work is supported by the NSF.

3:42PM D31.00007 Vacancy Reduction, Structural and Electronic Studies of Epitaxial Films of Topological Insulators¹, F. KATMIS, V. FATEMI, H. STEINBERG, L. ORONA, Department of Physics, MIT, Cambridge, USA, P. WEI, FBML, MIT, Cambridge, USA, P. JARILLO-HERRERO, J. MOODERA², Department of Physics, MIT, Cambridge, USA — We have developed methods for controlling the carrier concentration via a vacancy concentration reduction procedure in the MBE grown epitaxial topological insulator (TI) thin film on various substrates to reach the intrinsic features of TI. Our single crystalline TI thin films allowed us to systematically investigate the nature of coherent transport in this system. For structural characterization of TI thin films, various non-destructive methods, such as x-ray and electron based diffraction techniques, were used as a local probe to understand the long-, short-range atomic ordering and also lattice site occupation. Besides the improved electronic properties of the layers, as grown crystalline films density increased by 20% due to controlled vacancy reduction, determined by *in-situ* x-ray diffraction. Furthermore, correlation of vacancies and Se ion migration was observed to be the likely reason for lowering the carrier concentration. Our study also shows the dependence of carrier mobility and the vacancy concentration which has been optimized.

¹Work supported by MIT Lincoln Laboratory, ONR grant N00014-09-1-0177, and NSF grant DMR 0504158.

²FBML, MIT, Cambridge, USA

3:54PM D31.00008 Growth and in-situ ultra-high resolution ARPES studies of the Bi-Te family of topological insulators¹, JAMES LEE, FELIX SCHMITT, ROB MOORE, INNA VISHIK, MING YI, Z.X. SHEN, Stanford University — Topological insulators have received intense focus in the condensed matter community due to their academic and technical potential. The Quantum Anomalous Hall state is an example of the exotic physics that could have a major industry impact if it can be realized and controlled. While the topologically protected states live at interfaces between insulators of two topological classes, investigations of the underlying electronic structure via angle resolved photoemission spectroscopy requires pristine surfaces. Here we present results from *in situ* ultra-high resolution laser ARPES investigations at low temperatures of the doped Bi-Te family of topological insulator thin films grown via molecular beam epitaxy. Electronic structure evolution as a function of dopant, dopant level and thickness will be presented and compared to theoretical predictions.

¹Support given by the DOE and Stanford Graduate Fellowship.

4:06PM D31.00009 Fabrication of Bismuth Selenide Topological Insulating Samples, LUCAS ORONA, HADAR STEINBERG, VALLA FATEMI, FERHAT KATMIS, JAGADEESH MOODERA, PABLO JARILLO-HERRERO, MIT — In this talk, I will discuss fabrication of nanometric topological insulator Bi_2Se_3 devices. Our group uses two fabrication methodologies: Epitaxial thin films and single crystal exfoliation. I will discuss the benefits and drawbacks of each methodology. I will also address the effects on device performance by various steps of the fabrication process.

4:18PM D31.00010 Interfacing 2D and 3D Topological Insulators: $\text{Bi}(111)$ Bilayer on Bi_2Te_3 , TORU HIRAHARA, Department of Physics, University of Tokyo, GUSTAV BIHLMAYER, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, YUSUKE SAKAMOTO, MANABU YAMADA, Department of Physics, University of Tokyo, HIDETOSHI MIYAZAKI, SHIN-ICHI KIMURA, UVSOR Facility, Institute for Molecular Science, STEFAN BLÜGEL, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, SHUJI HASEGAWA, Department of Physics, University of Tokyo — Topological insulators (TI) are insulating materials but have metallic edge states that carry spin currents and are robust against nonmagnetic impurities [1]. While there have been a large number of reports on three-dimensional (3D) TI, only few works have been done in terms of two-dimensional (2D) TI. In the present paper, we report the successful formation of bilayer Bi, which was theoretically predicted to be a 2D TI [2]. We deposited bilayer Bi on a 3D TI Bi_2Te_3 , which the lattice mismatch is very small. From angle-resolved photoemission spectroscopy measurements and *ab initio* calculations, the electronic structure of the system can be understood as an overlap of the band dispersions of bilayer Bi and Bi_2Te_3 . Our results show that the Dirac cone is actually robust against nonmagnetic perturbations and imply a unique situation where the topologically protected one- and two-dimensional edge states are coexisting at the surface [3].

[1] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).

[2] S. Murakami, Phys. Rev. Lett. **97**, 236805 (2006).

[3] T. Hirahara *et al.*, Phys. Rev. Lett. **107**, 166801 (2011).

4:30PM D31.00011 Fabrication of Bi_2Te_3 Nanodots by Droplet Epitaxy on GaAs substrates

ZHAOQUAN ZENG, CHEN LI, Department of Physics, University of Arkansas, Fayetteville, AR 72701, DONGSHENG FAN, Department of Electrical Engineering, University of Arkansas, Fayetteville, AR 72701, YUSUKE HIRONO, TIMOTHY MORGAN, XIAN HU, Department of Physics, University of Arkansas, Fayetteville, AR 72701, JIAN WANG, MEENAKSHI SINGH, The Center for Nanoscale Science and Department of Physics, The Pennsylvania State University, University Park, PA 16802, ZHIMING WANG, State Key Laboratory of Electronic Thin Films and Integrated Devices, University of Electronic Science and Technology of China, SHUI-QING YU, Department of Electrical Engineering, University of Arkansas, Fayetteville, AR 72701, AQIANG GUO, GREGORY SALAMO, Department of Physics, University of Arkansas, Fayetteville, AR 72701, GREGORY J. SALAMO TEAM, SHUI-QING YU TEAM, ZHIMING WANG TEAM, JIAN WANG TEAM — Bi_2Te_3 , as a three-dimensional topological insulator, causes wide attention. Here, we report the fabrication of Bi_2Te_3 nanodots on GaAs substrate by droplet epitaxy using molecular beam epitaxy (MBE). Reflection high energy electron diffraction (RHEED), atomic force microscopy (AFM), x-ray photoelectron spectroscopy (XPS), and Raman measurement revealed the existence of Bi_2Te_3 nanodots. Several approaches were developed to control the size and density of as-grown Bi_2Te_3 nanodots. Temperature and density dependent magneto-transport measurements were investigated. This may provide a platform for the interaction investigation among topological insulators, semiconductors, ferromagnets and superconductors.

4:42PM D31.00012 AFM, Raman and electrical transport studies of topological insulating materials subjected to argon plasma etching

ISAAC CHILDRES, JIFA TIAN, IRENEUSZ MIOTKOWSKI, YONG CHEN, Purdue University — Plasma etching is an important tool in nano-device fabrication. We report a study on argon plasma etching of exfoliated flakes of topological insulator materials Bi_2Se_3 , Bi_2Te_3 , Sb_2Te_3 and $\text{Bi}_2\text{Te}_2\text{Se}$. We present data from atomic force microscopy (AFM), Raman spectroscopy and low-temperature magneto-transport measurements. The thickness of our samples measured by AFM is observed to decrease approximately linearly with plasma exposure time. We extract an etching rate for each type of material. For the initial increase in plasma exposure time, we observe increasing intensity and width of the characteristic E_g^2 Raman peak with little change in peak position. The width of this peak for etched flakes becomes larger than those of unetched samples of the same thickness. Additionally, we find that even moderate etching can significantly reduce the conductivity and hall mobility. These results indicate disorder is generated by plasma etching and impedes both phonon and carrier transport. Our findings are valuable for understanding the effects of argon plasma etching on topological insulator materials and using irradiation as a potential method to introduce controlled disorder in such materials.

4:54PM D31.00013 Tuning the spatial location of topological surface states via proximity effects¹

GUANGFEN WU, Univ. of Sci. & Tech. of China, Southeast Univ., China, YAN SUN, Shenyang National Lab for Materials Science, China, HUA CHEN, Univ. of Tennessee, Univ. of Texas at Austin, XIAO GUANG LI, Fudan Univ., Univ. of Sci. & Tech. of China, PING CUI, Univ. of Sci. & Tech. of China, JINLAN WANG, Southeast Univ., China, XINGQIU CHEN, Shenyang National Lab for Materials Science, China, ZHENYU ZHANG, Univ. of Sci. & Tech. of China, Harvard University — In order to exploit promising applications of topological insulators in quantum computing, spintronics, and catalysis, one prerequisite is to gain effective manipulation of the spatial distribution of the topological surface states (TSS). We use first-principles calculations to investigate the interfacial proximity effects on the TSS for hybrid systems consisting of semiconducting thin films with different bandgaps, spin-orbital coupling (SOC) strengths, and lattice mismatches grown on the TI substrate of Bi_2Se_3 . Our results show that the spatial location of the robust TSS can be tuned by the interplay of the effects associated with the SOC strength and the band gap size of the semiconductor. Potential experimental confirmations of these strong predictions are also discussed.

¹Supported by DMSE of USDOE, USNSF, and NNSF of China.

5:06PM D31.00014 Metal-Supported High Crystalline Bi_2Se_3 Quintuple Layers

JEONG HEUM JEON, WON JUN JANG, JONG KEON YOON, SANG-YOUN WEON, SE-JONG KAHNG, Dept. of Physics, Korea University — Atomically flat thin films of Bi_2Se_3 were grown on Au(111) metal substrate using molecular beam epitaxy. Hexagonal atomic structures and quintuple-layer steps were observed at the surfaces of grown films using scanning tunneling microscopy. Multiple sharp peaks from (003) family layers were characterized by X-ray diffraction measurements. The atomic stoichiometry of Bi and Se was considered using X-ray photoemission spectroscopy. Moiré patterns were obtained at the surfaces of one quintuple layer films due to lattice mismatch between Bi_2Se_3 and Au. Our experiments suggest that Au is a reasonable material for electrodes in Bi_2Se_3 devices.

5:18PM D31.00015 Ab initio study of epitaxial graphene on top of Sb_2Te_3 topological insulator

KYUNG-HWAN JIN, Department of Physics, POSTECH, SEUNG-HOON JHI, Department of Physics and Division of Advanced Materials Science, POSTECH — Understanding topological phase as observed in Dirac materials such as graphene and topological insulator (TI) has been a central issue in the field of condensed matter physics. Graphene and TI exhibit unique 2D electronic structures that attract great attention for potential application to spintronic devices. Heterostructures of graphene and TI provide interesting platforms to explore exotic electronic and transport properties of Dirac materials. Electronic structures of graphene in contact with TI were investigated using first-principles methods and tight-binding models. The Dirac cones of graphene on top of TI surface show several interesting features including band-gap opening and band splitting. By fitting first-principles calculations to tight-binding models, we analyzed the origin of the changes in the Dirac cones. We found that both intrinsic and extrinsic spin-orbit couplings are enhanced significantly due to proximity to topological insulator Sb_2Te_3 and that graphene turns into quantum spin-Hall phase. Our results suggest that graphene is also useful as a probe of TI surface states.

Monday, February 27, 2012 2:30PM - 5:30PM —

Session D32 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides
- Lattice Dynamics 261

2:30PM D32.00001 Dynamical couplings in ferroelectrics and multiferroics¹

DAWEI WANG, Xi'an Jiaotong University — First-principle-based molecular dynamics simulations are developed and used to investigate dynamical phenomena in the $\text{Pb}(\text{Zr,Ti})\text{O}_3$ (PZT) ferroelectric solid solutions and in the multiferroic BiFeO_3 system^{2,3}. Several interesting effects are reported, including: (1) the existence of two E modes in PZT in the 50–75 cm^{-1} range for temperatures smaller than $\simeq 200$ K when the system is in its $R3c$ phase. Such existence originates from a *linear* coupling between ferroelectric (FE) motions and tiltings of oxygen octahedra; (2) a Fermi resonance (FR) emerging from a *nonlinear* coupling between FE distortions and oxygen octahedra tilts. This FR manifests itself as the doubling of a nominally-single FE mode in a purely FE phase, when the resonant frequency of the FE mode is close to the first overtone of the oxygen octahedra tiltings; and (3) the prediction of an electromagnon peak, that results from specific interactions between magnetic dipoles, FE motions and oxygen octahedra tiltings, in BiFeO_3 . Some of these results have been confirmed by recent Raman scattering experiments, and analytical models are also developed to better understand such effects.⁴

¹This work is mostly supported by the DOE, Office of Basic Energy Sciences, under Contract No. ER-46612. D.W. also acknowledge support from the National Natural Science Foundation of China under Grant No. 10904122.

²D. Wang, J. Weerasinghe, and L. Bellaiche, Phys. Rev. B **83**, 020301(R) (2011).

³D. Wang, E. Buixaderas, J. Íñiguez, J. Weerasinghe, H. Wang, and L. Bellaiche, Phys. Rev. Lett. **107**, 175502 (2011).

⁴This work is done in collaboration with L. Bellaiche (University of Arkansas), J. Hlinka (Institute of Physics, Czech Republic), E. Buixaderas (Institute of Physics, Czech Republic), J. Íñiguez (Institut de Ciència de Materials de Barcelona, Spain) and J. Weerasinghe (University of Arkansas)

3:06PM D32.00002 A-site ion vibrational modes in ABO₃ polar perovskites, JIRI HLINKA, Institute of Physics ASCR, Na Slovance 2, 182 21 Prague 8 — It is well known that Pb(B'B'')O₃ family of complex perovskites contains materials with very useful dielectric, piezoelectric and ferroelectric properties. The overall electromechanical response of these system is believed to be related to their characteristic micro-to nanoscale structural correlations (chemical clusters, polar nanoregions or nanotwins). At the level of the ABO₃ unit cell, the remarkable polarizability of these materials originates from lead-ion displacements, and the anharmonic motion of these ions, loosely linked to the core oxygen octahedra network, largely dominates in the low-frequency phonon modes in the system. Therefore, the investigation of the low-frequency phonon modes in these systems is of a great importance. The aim of this contribution is to report recent experimental studies of such low-frequency vibrations by inelastic X-ray, neutron and light scattering techniques, in materials like lead zirconate titanate, lead magnesium niobium titanate or lead titanate. In particular, attention will be paid to our recent inelastic X-ray scattering studies of PZT lattice dynamics.

3:42PM D32.00003 Fully-atomistic first-principles approach to the temperature-dependent lattice-dynamical properties of perovskite oxides, MATHIAS LJUNGBERG, JACEK WOJDEL, JORGE INIGUEZ, ICMAB-CSIC — We present a methodology for the parametrization of effective Hamiltonians for ferroelectric perovskites that provides a fully atomistic description of the materials. The parameters in our effective models are obtained from first-principles calculations; no experimental input is used. The potential energy surface is represented by a truncated Taylor expansion around the ideal cubic perovskite structure, and is, up to second order, exactly equivalent to the first-principles computed one. Higher order terms are determined by fitting to the first-principles energetics and phonon dispersion relations of the relevant low-symmetry phases. By treating all structural degrees of freedom explicitly, our models allow us to investigate the competition between the soft modes that drive the ferroelectric phase transitions in these materials and other, secondary modes. We will show that such an interaction is of significant importance in the prototypical ferroelectric compound PbTiO₃; our method's ability to capture it constitutes a considerable improvement upon earlier approaches. We will also report on our current work to extend this methodology to treat inhomogeneous materials, as e.g. superlattices.

3:54PM D32.00004 Lattice dynamics of cubic PbTiO₃¹, IZUMI TOMENO, Akita University, JAIME A. FERNANDEZ-BACA, KAROL J. MARTY, ORNL, YORIIHIKO TSUNODA, Waseda University, KUNIIHIKO OKA, AIST — The lattice dynamics of cubic PbTiO₃ has been investigated using inelastic neutron scattering. We found four kinds of soft modes in cubic PbTiO₃: (1) the TO modes toward the Γ point, (2) the TA Λ_3 mode toward the R point, (3) the TA Λ_3 mode around the midpoint (1/4,1/4,1/4), and (4) the TA branches in the entire range. Moreover, the TO Σ_4 branch becomes flat away from the zone center. The steep dispersion of the TO modes toward Γ is isotropic and confined to the region $\xi < 0.2$. The temperature dependence of the Γ_{15} mode up to 1173 K is explained by a combination of the Lydanne-Sachs-Teller relation and the Curie-Weiss law. In contrast, the TA Λ_3 modes at the midpoint and R point are weakly temperature dependent. The coexistence of the soft Γ_{15} and R_{25} modes is in agreement with the predicted phonon instability. The midpoint softening suggests the tendency toward forming a fourfold periodicity along the [1,1,1] direction. The energy of the TO Δ_5 branch for cubic PbTiO₃ is considerably higher than that for Pb(Zn_{1/3}Nb_{2/3})O₃. This indicates that the TO modes are dominated by the B-site atom motion.

¹U.S.-Japan cooperative program on neutron scattering

4:06PM D32.00005 BaTiO₃ nanocrystals studied by Raman spectroscopy¹, A.K. FARRAR, T. ENGMAN, D.A. TENNE, Department of Physics, Boise State University, S. ADIREDDY, G. CARUNTU, Advanced Materials Research Institute, Department of Chemistry, University of New Orleans — Variable-temperature Raman spectroscopy study of BaTiO₃ nanocrystals of varied sizes (from 8 to 20 nm) will be presented. Highly uniform cube-shaped BaTiO₃ nanocrystals have been prepared by solvothermal synthesis at temperatures below 140 °C and characterized by x-ray diffraction and transmission electron microscopy. Raman spectra (measured with ultraviolet and visible excitation) show that all nanocrystals studied are ferroelectric; nanocrystal size effect on the Curie temperature has been investigated. Temperature evolution of Raman spectra (10–600K) demonstrates that the ferroelectric phase of the nanocrystals is different from the bulk BaTiO₃. The transitions from tetragonal to orthorhombic and from orthorhombic to rhombohedral phases, which are characteristic for bulk BaTiO₃, have not been observed in the nanocrystals; the ferroelectric phase in the nanocrystals is the same in the entire temperature range below T_c , and is different from any of the bulk phases. The observed behavior may be explained by complex polarization patterns theoretically predicted for zero-dimensional ferroelectrics.

¹Supported in part by NSF Grants DMR-0705127, DMR-1006136, EPS-1003897 and DMR-1004869, DARPA Grant HR 0011-09-0047, and Research Corporation for Science Advancement Grant 7134.

4:18PM D32.00006 Raman spectra and lattice dynamics of disordered complex perovskite BaMg_{1/3}Ta_{2/3}O₃, SEVERIAN GVASALIYA, DAN HÜVONEN, Laboratorium für Festkörperphysik, ETH Honggerberg, 8093 Zurich, Switzerland, SERGEY LUSHNIKOV, Ioffe Physico-Technical Institute, 194021, St Petersburg, Russia, ELENA POPOVA, St. Petersburg State University, Department of Crystallography, 199034, Russia & Ioffe Physico-Technical Institute, 194021, St Petersburg, Russia, TATIYANA SHAPLYGINA, Ioffe Physico-Technical Institute, 194021, St Petersburg, Russia, ANDREY ZHELUDEV, Laboratorium für Festkörperphysik, ETH Honggerberg, 8093 Zurich, Switzerland — In relaxor ferroelectrics the chemical and the displacive ionic disorders coexist and may cause a relaxation of the selection rules for Raman scattering. We performed a Raman scattering study of BaMg_{1/3}Ta_{2/3}O₃ (BMT), which is chemically disordered cubic perovskite showing no evidences for displacive disorder. Polarized Raman spectra from a single crystal of BMT were collected in the temperature range of 5 — 550 K. We are going to discuss the symmetry assignments of the observed modes and their temperature evolution. Simplified shell-model for the lattice dynamics of BMT will be presented. The results for BMT will be compared to the well-known observations for the Raman spectra from related relaxor ferroelectrics PbMg_{1/3}Ta_{2/3}O₃ and PbMg_{1/3}Nb_{2/3}O₃. In particular, the lowest Raman line observed in BMT is at ~ 110 cm⁻¹, whereas the doublet line in PbMg_{1/3}Ta_{2/3}O₃ is observed around 50 cm⁻¹. Also, we found out that the width of well-isolated A_{1g} line of BMT is approximately two times narrower than that observed in relaxors.

4:30PM D32.00007 Frequency shift of Raman modes due to an applied electric field and domain inversion in LiNbO₃, GREG STONE, BRIAN KNORR, Lehigh University, VENKATRAMAN GOPALAN, Pennsylvania State University, VOLKMAR DIEROLF, Lehigh University — We report changes in the frequency of several Raman modes in congruent and near-stoichiometric lithium niobate that are observed under the application of external applied electric fields parallel to the ferroelectric axis and after domain inversion. A comparison of the direction of the frequency shifts due to an applied electric field and domain inversion reveals that after forward poling there is a reduction of the internal field that is dependent on the intrinsic defect concentration present in the crystal. Upon back poling, the internal field returns to its original state. A further inspection of the Raman peaks reveals that the magnitude of the frequency shift is not consistent between an applied electric field and domain inversion. This indicates that the change in the local internal field introduced by domain inversion is not limited to the ferroelectric axis, but the fields orthogonal to the ferroelectric axis change. Work supported by the grants: NSF-DMR 0602986 and 1008075

4:42PM D32.00008 Infrared phonon anomaly and magnetic excitations in single-crystal $\text{Cu}_3\text{Bi}(\text{SeO}_3)_2\text{O}_2\text{Cl}^1$, KEVIN H. MILLER, C. MARTIN, X. XI, Department of Physics, University of Florida, H. BERGER, Ecole Polytechnique Federal de Lausanne, G.L. CARR, Photon Sciences, Brookhaven National Laboratory, D.B. TANNER, Department of Physics, University of Florida — Infrared reflection as a function of temperature has been measured on the anisotropic single-crystal $\text{Cu}_3\text{Bi}(\text{SeO}_3)_2\text{O}_2\text{Cl}$. The complex dielectric function and optical properties along all three crystal axes of the orthorhombic cell were obtained via Kramers-Kronig analysis and by fits to a Drude-Lorentz model. Below 110 K drastic anomalies in the phonon spectrum (e.g., new modes and splitting of existing modes) are observed along all three crystal axes. Transmission in the terahertz region as a function of temperature has revealed magnetic excitations originating below the ferromagnetic ordering temperature, $T_c=24$ K. The origin of the excitations in the magnetic state will be discussed in terms of their polarization and externally-applied magnetic field dependence.

¹Supported by the US DOE through contract DE-FG02-02ER45984 at UF and DE-AC02-98CH10886 at the NSLS

4:54PM D32.00009 Hydrogen diffusion and tunneling in KTaO_3 from first principles¹, HAZEM ABU FARSACKH, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — The high proton conductivity in many perovskites has attracted interest for potential applications, such as in fuel cells. A promising approach to increase their conductivity at lower temperatures involves enhancing quantum-mechanical tunneling. In order to determine the role of tunneling for H in KTaO_3 we employ first principles calculations for H interstitial atoms. We identify H binding sites and diffusion channels and calculate the associated activation energies. In addition, we analyze the effect of lattice relaxations on the diffusion barriers. Through calculating the 3D potential energy surface of H, we determine accurate H tunneling rates by numerically solving Schrödinger's equation for H in the 3D potential energy surface. Finally, we examine lattice vibrations and analyze their role in assisting proton tunneling.

¹This work was supported by IARPA

5:06PM D32.00010 Scaling of Flat Band Potential and Dielectric Constant as a Function of Ta Concentration in Ta-TiO₂ Epitaxial Films¹, Y.L. ZHAO, A. ROY BARMAN, S. DHAR, A. ANNADI, NUSNNI-NanoCore, NUS, M. MOTAPOTHULA, CIBA,NUS, J.H. WANG, H.B. SU, Material science, NTU, M. BREESE, CIBA,NUS, T. VENKATESAN, NUSNNI-NanoCore, NUS, Q. WANG, Material science, NUS — Electrochemical impedance spectroscopy measurements of pulsed laser deposited single crystal anatase TiO₂ thin films with various concentrations of Ta substituting for Ti were carried out. UV-visible measurements show a systematic increase of the bandgap with Ta incorporation. Corresponding Mott-Schottky plot was applied to obtain a continuous shift of the flat band potential with increasing free charge carrier concentration. This was verified theoretically by ab initio calculation which shows that extra Ta d-electrons occupy Ti t_{2g} orbital with increasing Ta concentration, thereby pushing up the Fermi level. The Mott-Schottky results were consistent when compared with Hall effect and temperature dependent resistivity measurements. From the measured deviation of carrier densities from Hall and Mott-Schottky measurements we have estimated the static dielectric constant of the TiO₂ as a function of Ta incorporation. We are able to estimate the shifts of both the conduction and valence bands from these measurements.

¹This work is supported by NUSNNI-Nanocore start-up fund and NRF-CRP grants “Tailoring Oxide Electronics by Atomic Control” (NRF2008NRF-CRP002-024). The theoretical work performed at NTU is supported in part by a MOE AcRf-Tier-1 grant (no. M52070060)

5:18PM D32.00011 Raman spectroscopic studies of $\text{Ti}_{1-x}\text{Ta}_x\text{O}_2$ alloy thin films¹, S. SAHA, A. ROY-BARMAN, NUSNNI-NanoCore, National University of Singapore, C.B. TAY, Department of Electrical and Computer Engineering, National University of Singapore, T. SARKAR, Y. ZHAO, NUSNNI-NanoCore, National University of Singapore, S. TRIPATHY, IMRE, A*STAR, Singapore, S. DHAR, - ARIANDO, NUSNNI-NanoCore, National University of Singapore, S.J. CHUA, Department of Electrical and Computer Engineering, National University of Singapore, T. VENKATESAN, NUSNNI-NanoCore, National University of Singapore — Anatase $\text{Ti}_{1-x}\text{Ta}_x\text{O}_2$ thin films have been of interest not only because of the recently found defect originated room temperature ferromagnetism, but also because of the wide possibilities of its application as transparent conducting oxide in flat panel displays, light emitting diodes and solar cells. The incorporation of a foreign element in a host oxide crystal has conventionally been referred to as doping. However, recently we have experimentally shown that even with as less as 1% Ta incorporation in TiO₂, a totally new alloy system is formed. Here we present a Raman and x-ray diffraction study of anatase $\text{Ti}_{1-x}\text{Ta}_x\text{O}_2$ thin films grown on (100) LaAlO_3 substrate by PLD to understand the crystal structure and defects in the Ta-incorporated TiO₂ thin films. We find that as Ta is incorporated in the TiO₂ lattice the out-of-plane phonons undergo red-shift while the in-plane phonon undergoes a blue-shift, suggesting an expansion of the TiO₂ lattice along the out-of-plane direction with a concomitant in-plane contraction.

¹We acknowledge NRF-CRP (Grant No. NRF2008NRFCRP002-024), NUS YIA, NUS cross-faculty grant, FRC, BMBF and NUSNNI.

Monday, February 27, 2012 2:30PM - 5:18PM – Session D33 GERA: Physics of Batteries and Fuel Cells 106

2:30PM D33.00001 Effect of Iron-based Impurities on the performance of nanostructured C-LiFePO₄ cathode materials for Li ion Batteries, P. VAISHNAVA, Kettering University, A. DIXIT, K. BAZZI, M.B. SAHANA, C. SUDAKAR, Wayne State University, M. NAZRI, Applied Sciences, Inc. Cedarville, Ohio, V. NAIK, University of Michigan - Dearborn, V.K. GARG, A.C. OLIVEIRA, Universidade de Brasilia, Brazil, G.A. NAZRI, R. NAIK, Wayne State University — We report synthesis of pure and C-LiFePO₄ nanoparticles in 20-30 nm size by sol-gel method. Three samples of C-LiFePO₄ were prepared by mixing 0.25M, 0.50M, and 1M lauric acid in the precursor solutions for carbon coating the particles. The samples were characterized by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), IR spectroscopy, SQUID magnetometry, Raman spectroscopy, and Fe⁵⁷ Mössbauer spectroscopy. All the samples were thoroughly investigated for their electrochemical properties. The XRD measurements showed all the samples are single phase materials with no impurity phase. However, we identified at least three residual non crystalline impurity phases simultaneously using Fe⁵⁷ Mössbauer spectroscopy, XPS, and the magnetic measurements. The elemental chemical states for Fe 2p, P 2p, and O 1s are analyzed using XPS for LiFePO₄ and compared with those of C-LiFePO₄ materials. SQUID magnetometry measurements suggest an antiferromagnetic transition ~50 K in both pure LiFePO₄ and C-LiFePO₄ samples. The role of various phases, such as FeP, Fe₂P, α-Fe and Fe₂O₃ identified and analyzed by Fe⁵⁷ Mössbauer spectroscopy and XPS, will be discussed in relationship to the electrochemical properties of the cathode materials.

2:42PM D33.00002 Role of Ce and In doping in the performance of LiFePO₄ cathode material for Li ion Batteries, BALAJI MANDAL, MARIAM NAZRI, Wayne State University, PREM P. VAISHNAVA, Kettering University, VAMAN M. NAIK, University of Michigan-Dearborn, GHOLAM A. NAZRI, RATNA NAIK, Wayne State University — Recently, the olivine LiFePO₄ has attracted attention as a promising cathode material for Li ion batteries. However, its poor electronic conductivity is a major challenge for its industrial applications. Different approaches have been taken to address this problem. Here, we report a method of improving its conductivity by doping In and Ce ions at the Fe site. We prepared the samples by sol-gel method followed by annealing at 650 °C in Ar (95%) +H₂(5%) atmosphere for 5 hrs. XRD and Raman spectroscopy confirm that the olivine structure remains unchanged upon doping with In and Ce up to 5 wt%. XRD analysis shows the values of the lattice parameters increase with doping as the ionic radii of Ce and In ions are larger than that of the Fe²⁺ ion. This observation also suggests that both Ce and In ions replace Fe ions and not the Li ions in the material. Upon doping, ionic conductivity was found to increase from 10⁻⁹ to 10⁻⁴ Ohm⁻¹cm⁻¹. Interestingly, Ce doped LiFePO₄ showed a higher conductivity than In doped LiFePO₄. SEM measurements show a bigger grain size of ~300-500 nm in doped LiFePO₄ which decreased to ~50 nm when the materials were synthesized using 0.25M lauric acid as a precursor. The electrochemical characteristics of the doped LiFePO₄ along with conductivity and Raman data will be presented.

2:54PM D33.00003 Formation of small polarons in Li₂O₂ and implications for Li-air batteries¹, JOONGGO KANG, National Renewable Energy Laboratory, Golden, Colorado 80401, USA, YOON-SEOK JUNG, Ulsan National Institute of Science and Technology, Ulsan, Korea, SU-HUAI WEI, ANNE DILLON, National Renewable Energy Laboratory, Golden, Colorado 80401, USA — Lithium-air batteries (LABs) have recently been revitalized as a promising electrical energy storage system due to their exceptionally high theoretical energy density. However, its usage is limited by poor rate capability and large polarization in the cell voltage due primarily to the formation of Li₂O₂ in the air cathode. Here, using hybrid density functional theory, we found that the formation of small polarons in Li₂O₂ is the origin that limits the electron transport in Li₂O₂. Consequently, the low electron mobility contributes to the hysteresis in cell voltage and limits the power density of the LABs. We suggest that similar behavior should exist in other peroxides, and p-type doping in Li₂O₂ could significantly improve the performance of LABs at high current densities.

¹This work was funded by the NREL LDRD program (DE-AC36-08GO28308).

3:06PM D33.00004 The Li-induced Conversion Reaction of Ultra-Thin FeF₂ Films¹, RYAN THORPE, SYLVIE RANGAN, ROBERT BARTYNSKI, OZGUR CELIK, LESZEK WIELUNSKI, Rutgers University — Iron (II) fluoride has recently gained interest as a possible cathode material in Li-ion conversion batteries. Conversion materials like this could potentially store 2-3 times more energy than conventional intercalation battery materials by utilizing the full range of charge states in their constituent transition metal ions, i.e., Fe⁽²⁺⁾F₂ + 2Li⁺ + 2e⁻ → Fe⁰ + 2LiF. Using surface science techniques, we are able to observe this reaction at the FeF₂-Li interface. We have grown 5nm films of high-purity polycrystalline FeF₂ in ultra-high vacuum and deposited atomic Li on the surface to simulate the conversion reaction in the absence of external contaminants. Using UV photoemission (UPS), x-ray photoemission (XPS), and inverse photoemission (IPE) spectroscopies, we have measured the composition and charge states of these materials. XPS of the FeF₂ sample after various Li exposures indicate a direct conversion from Fe²⁺ to Fe⁰, with no intermediary phases. The growth of a Fermi edge in UPS and IPE also indicates the formation of metallic Fe, while peaks characteristic of LiF can be seen in UPS after sufficient Li exposure. These results are consistent with those of recent TEM measurements on real electrochemical cells.

¹This material is based upon work supported as part of NECCES, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001294.

3:18PM D33.00005 Electrochemical Performance of Lithium Iron Phosphate Doped with Tungsten, HANU ARAVA, ANDREW TRENCHARD, GAN LIANG, HUI FANG, Sam Houston State University — Due to its high thermal stability, low cost and high theoretical charge capacity, LiFePO₄ has emerged as one of the most promising cathode materials for large-scale lithium ion batteries. In this work, we systematically investigated the effect on structure and electrochemical properties brought by W doping on Fe site of LiFePO₄. LiFe_{1-x}W_xPO₄ (x= 0, 0.01, 0.02, 0.03) samples with and without carbon coating were prepared by using solid-state reaction. The phase and structure of as prepared powders were characterized by X-ray diffraction and scanning electron microscope. Cycling charge and discharge measurement at various C-rates and cyclic voltammetry were employed to reveal the electrochemical properties. Results showed that carbon coating dramatically improved the capacity at fast C-rate. 2 at.% W doping was observed to have the highest charge capacity with 143 mAh/g at 0.1C and a 109 mAh/g for 1C.

3:30PM D33.00006 Model conversion reaction: Li reactivity on iron oxifluorides, SYLVIE RANGAN, RYAN THORPE, OZGUR CELIK, ROBERT BARTYNSKI, Rutgers University — Iron fluorides have gained interest as choice materials for conversion reaction-based batteries. Owing to their large band gaps and their ability to store up to three electrons per formula unit, batteries using these materials operate at high voltages and high energy densities. However the large band gap inhibits charge conduction and thus impedes efficient charging and discharging cycles. Two paths have been taken to overcome this limitation: 1) The use of nanoparticles embedded into a conducting carbon matrix improves both ionic and electronic conduction; and 2) The use of iron oxifluorides, which are characterized by a slightly reduced energy gap that facilitates electronic conduction. It is the latter point that is central to this study as, curiously, relatively little is known about the electronic structure of iron oxifluorides and their interaction with Li, a key aspect of a storage cell's electrochemistry. Model conversion reactions have been studied by evaporating Li on FeF₂ and FeF_xO_y samples. Using X-ray and UV photoemission as well as inverse photoemission spectroscopies, the occupied states and the unoccupied electronic states of the resulting samples have been probed. Transmission electron microscopy has been used in parallel to investigate phase analysis.

3:42PM D33.00007 Shape and volume changes in Lithiated Silicon anodes for batteries, EKIN CUBUK, WEI WANG, EFTHIMIOS KAXIRAS, Harvard University — Silicon is one of the most promising materials for use as an anode for Lithium-ion batteries due to its capacity to hold a large number of Li atoms (up to 4.4 Li per Si atom). One of the biggest challenges in using Silicon as anode material is mechanical failures due to large volume expansion during the lithiation process. Recently detailed experiments have been reported on the dependence of volume change on the crystal orientation, especially for nano-scale structures. We investigate the microscopic mechanisms for shape changes during lithiation of Si by comparing the reaction mechanisms of Li atoms on different surfaces of crystalline Si using first-principles calculations.

3:54PM D33.00008 Effect of carbon support on catalytic efficiency and durability in fuel cells, CECILE MALARDIER-JUGROOT, MICHAEL GROVES, DEBORAH DURBIN, MANISH JUGROOT, Royal Military College of Canada — New nanomaterials already play a key role in several emerging technologies. For instance, in fuel cell technology, catalytic efficiency can be greatly enhanced due to the high surface area of nanomaterials. Improving the durability and efficiency of a platinum catalyst is an important step in increasing its utility when incorporated as the anode or cathode of a proton exchange membrane fuel cell (PEMFC). The authors have shown using Density Functional Theory methods [1] that doping the carbon support of the Pt catalyst can increase the durability and efficiency of the catalyst. This paper will present the effect of doping of the carbon support on the complete reaction path of the Oxygen Reduction Reaction using *ab initio* structural methods as well as a complete *ab initio* molecular dynamics characterization of the reaction. In addition, the electronic structure of the carbon support was shown to improve the metal/CO interaction for the development of a membrane to prevent catalyst poisoning [2]. The paper will also emphasize the effect of the solvent, which is experimentally shown to be crucial. [1] M. Groves, A. Chan, C. Malardier-Jugroot and M. Jugroot, *Chem. Phys. Letters*, 481(4-6), 214-219, 2009 [2] D. Durbin and C. Malardier-Jugroot, *J. Phys. Chem. C*, 115 (3), 808-815, 2011

4:06PM D33.00009 Probing the Reversibility Limit of Lithium Ion Transport in Solid Film Batteries¹, HOWARD WANG, LIWEI HUANG, KAIKUN YANG, Institute for Material Research and Department of Mechanical Engineering, State University of New York, Binghamton, NY 13902, GREGORY DOWNING, Material Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, MD 20899, ALEC TALIN, PAUL NANEY, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD 20899, JASON ZHANG, Energy and Environment Directorate, Pacific Northwest National Laboratory, Richland, WA 99352, JON OWEJAN, JEFFREY GAGLIARDO, JEANETTE OWEJAN, Electrochemical Energy Research Laboratory, General Motors Company, Honeoye Falls, NY 14472 — Time-resolved neutron depth profiling (TR-NDP) has been used to measure the lithium distribution in electrode layers of thin film batteries during charge/discharge cycles. TR-NDP data demonstrate quantitatively that ionic transport in electrodes follows the electric current in the external circuits under normal charge/discharge conditions whereas deviates upon sudden structural changes. The reversibility limit of ionic transport has been quantified to indicate the onset of battery failure.

¹The NIST/ARRA funding through GM is greatly appreciated

4:18PM D33.00010 Energy Storage and Generation from Thermopower Waves, JOEL ABRAHAMSON, SAYALEE MAHAJAN, WONJOON CHOI, NICOLE SCHONENBACH, JUNGSIK PARK, MICHAEL WALSH, JARED FORMAN, JAE-HEE HAN, Massachusetts Institute of Technology, KOUROSH KALANTAR-ZADEH, RMIT University, MICHAEL STRANO, Massachusetts Institute of Technology — We have demonstrated through simulation and experiment that the nonlinear coupling between an exothermic chemical reaction in a fuel and a nanowire or nanotube with large axial heat conduction accelerates the thermal reaction wave along the nano-conduit. The thermal conduit rapidly transports energy to unreacted fuel regions, and the reaction wave induces a concomitant thermopower wave of high power density, producing electrical current in the same direction. At up to 14 W/g, this can be substantially larger than the power density offered by current micro-scale power sources (e.g. fuel cells, batteries) and even about seven times greater than that of commercial Li-ion batteries. MEMS devices and wireless sensor networks would benefit from such high power density sources to enable functions such as communications and acceleration hampered by present power sources.

4:30PM D33.00011 In-situ TEM observations of the nanoscale electrochemistry in a Li-ion cell, JIANYU HUANG, Sandia National Laboratories, UNIVERSITY OF PITTSBURGH COLLABORATION — The lithiation-delithiation processes of anode materials in lithium ion batteries were observed by in-situ electron microscopy. The lithiation-delithiation was strongly materials, size, and orientation dependent. Upon charging of SnO₂ nanowires, we observed high density of dislocations in the reaction front, while in charging of ZnO nanowires, we observed discrete cracks in the reaction front. In charging Si nanowires, we found the volume expansion was highly anisotropic, resulting in a dumbbell-shaped cross-section and cracking, eventually splitting the single nanowire into sub-wires. Carbon coating not only increases rate performance but also alters the lithiation-induced strain of SnO₂ nanowires. The radial expansion of the coated nanowires was completely suppressed. The lithiation process of individual Si nanoparticles was strongly size-dependent, i.e., there exists a critical particle size with a diameter of ~ 150 nm, below which the particles neither cracked nor fractured upon lithiation, above which the particles first formed cracks and then fractured.

4:42PM D33.00012 Gasoline-powered series hybrid cars cause lower life cycle carbon emissions than battery cars, CHRISTOPH MEINRENKEN, KLAUS S. LACKNER, Columbia University — Battery cars powered by grid electricity promise reduced life cycle green house gas (GHG) emissions from the automotive sector. Such scenarios usually point to the much higher emissions from conventional, internal combustion engine cars. However, today's commercially available series hybrid technology achieves the well known efficiency gains in electric drivetrains (regenerative braking, lack of gearbox) even if the electricity is generated onboard, from conventional fuels. Here, we analyze life cycle GHG emissions for commercially available, state-of-the-art plug-in battery cars (e.g. Nissan Leaf) and those of commercially available series hybrid cars (e.g., GM Volt, at same size and performance). Crucially, we find that series hybrid cars driven on (fossil) gasoline cause fewer emissions (126g CO₂eq per km) than battery cars driven on current US grid electricity (142g CO₂eq per km). We attribute this novel finding to the significant incremental emissions from plug-in battery cars due to losses during grid transmission and battery dis-/charging, and manufacturing larger batteries. We discuss crucial implications for strategic policy decisions towards a low carbon automotive sector as well as relative land intensity when powering cars by biofuel vs. bioelectricity.

4:54PM D33.00013 Design and Characterization of a Microcombustor for Thermophotovoltaic Devices, ABBEY LICHT, MICHAEL MOTOLA-BARNES, METH BANDARA, HAN CHEN, TOM VANDERVELDE, Tufts University — While batteries are currently used to provide power to devices in remote areas, their low energy density (.5MJ/kg) increases carrier weight, limiting the range of applications. Microcombustor systems, on the other hand, rely on hydrocarbon fuels which have a much greater energy density (40MJ/kg) and generate the same power at a fraction of the weight. The microcombustor when paired with a high-efficiency energy extracting device, such as a thermophotovoltaic cell, presents a complete micro-power system. This work describes the fabrication and characterization of a catalytic microcombustor designed specifically to optimize the power production of a thermophotovoltaic cell.

5:06PM D33.00014 Reverse electrowetting – a new approach to high-power harvesting of mechanical energy, TOM KRUPENKIN, J. ASHLEY TAYLOR, SUPONE MANAKASETTTHARN, University Wisconsin - Madison — Over the last decade electrical batteries have emerged as a critical bottleneck in portable electronics development. High-power mechanical energy harvesting can potentially provide a valuable alternative to the use of batteries, but until now, its adoption has been hampered by the lack of an efficient mechanical-to-electrical energy conversion technology. In this talk a novel mechanical-to-electrical energy conversion method is discussed. The method is based on reverse electrowetting (REWOD) – a novel microfluidic phenomenon. Electrical energy generation is achieved through the interaction of arrays of moving microscopic liquid droplets with novel nanometer-thick multilayer dielectric films. Advantages of this process include the production of high power densities, up to 1 KW sq. m; the ability to directly utilize a very broad range of mechanical forces and displacements; and the ability to directly output a broad range of currents and voltages, from several volts to tens of volts. We hope that the REWOD-based energy harvesting can provide a novel technology platform for a broad range of new electronic products and enable reduction of cost, pollution, and other problems associated with the wide-spread battery use.

Monday, February 27, 2012 2:30PM - 5:30PM –
Session D34 DCP: Focus Session: Nano I – Clusters 107A

2:30PM D34.00001 Cluster Structure and Reactions: Gaining Insights into Catalytic Processes, A. WELFORD CASTLEMAN, Penn State University — To many researchers outside the field of cluster science it comes as a surprise that much can be learned of its relevance to catalysis, even restricting the discussion to ionized systems. The objective of this talk is to present how fundamental insights into reaction mechanisms can be gained through employing alternative approaches that complement rather than supersede more conventional methods in the field of catalysis. In view of the well acknowledged role of defect centers in effecting reactivity, and the preponderance of recent papers presenting evidence of the importance of charged sites, the desire to conduct repetitive experiments is clear. Presented herein are approaches using clusters to accomplish this in order to unravel fundamental catalytic reaction mechanisms, and to use identified superatoms and the concepts of element mimics to tailor catalysts with desired functionality.

3:06PM D34.00002 Photoelectron Angular Distributions of Transition Metal Dioxide Anions - a joint experimental and theoretical study, IVAN IORDANOV, Department of Physics, Pennsylvania State University, DASITHA GUNARATNE, CHRISTOPHER HARMON, Department of Chemistry, Pennsylvania State University, JORGE SOFO, Department of Physics, Pennsylvania State University, A.W. CASTLEMAN, JR, Department of Chemistry, Pennsylvania State University — Angular-resolved photoelectron spectroscopy (PES) studies of the MO_2^- ($\text{M}=\text{Ti}, \text{Zr}, \text{Hf}, \text{Co}, \text{Rh}$) clusters are presented for the first time along with theoretical calculations of their properties. We confirm previously reported non-angular PES results for the vertical detachment energies (VDE), vibrational energies and geometric structures of these clusters and further explore the effect of the 'lanthanide contraction' on the MO_2^- clusters by comparing the electronic spectra of 4d and 5d transition metal dioxides. Angular-resolved PES provides the angular momentum contributions to the HOMO of these clusters and we use theoretical calculations to examine the HOMO and compare to our experimental results. First-principles calculations are done using both density functional theory (DFT) and the coupled-cluster, singles, doubles and triples (CCSD(T)) methods.

3:18PM D34.00003 Stability and Spectroscopic Properties of Singly and Doubly Charged Anions, SWAYAMPRAKASH BEHERA, PURU JENA, Virginia Commonwealth University — Considerable interest currently exists in expanding the pool of hetero-atomic negative ions which have electron affinities much higher than that of halogen atoms. These molecules, called superhalogens, usually consist of a metal atom (M) at the core surrounded by halogen atoms (X) and are represented by the formula MX_{n+1} where n is the maximal valence of the metal atom. We have studied the possibility if pseudohalogens such as CN, which mimic the chemistry of halogen atoms, can be used as building blocks of new superhalogens. Using density functional theory, Moller-Plesset perturbation theory and coupled clusters methods we have studied systematically the structure and spectroscopic properties of $\text{M}(\text{CN})_n$ systems ($\text{M}=\text{Na}, \text{Mg}, \text{Al}$; $n=1-3$ for Na, 1-4 for Mg, and 1-5 for Al) and compared the results to that of corresponding MCl_n clusters. We find that there is a significant difference between these two systems. This is because pseudohalogens have a tendency to dimerize and hence, we find that for these clusters the values of adiabatic detachment energy and the electron affinity may not be the same. Also, we have studied the dianions of $\text{M}(\text{CN})_n$ and MCl_n complexes to determine the critical size required for their stability. We show that CN moieties stabilize a dianion better than halogen atoms do due to the increase in the phase space over which added electrons are delocalized. This could play an important role in interpreting future experimental data on $\text{M}(\text{CN})_n$ complexes.

3:30PM D34.00004 Structure and stability of the $\text{M}_{8-n}\text{N}_n\text{C}_{12}$ ($\text{M}=\text{Ti}, \text{Zr}$; $\text{N}=\text{Sc}, \text{Y}$ and $n=1,2,3$) Met-Cars as building blocks of cluster-assembled materials, CUNEYT BERKDEMIR, SHI-BO CHENG, A. WELFORD CASTLEMAN JR., Department of Chemistry and Physics, The Pennsylvania State University, JORGE O. SOFO, Department of Physics and Materials Research Institute, The Pennsylvania State University — Clusters can be used as building blocks for new materials. However, in order to form a bulk material with clusters, they should be chemically stable. This stability can be characterized by a closed-shell electronic configuration having a large HOMO-LUMO gap. Met-Cars, metal-carbon species composed of early transition metals bonded to carbon, are stable but very reactive. We propose a method to lower their reactivity by metal atom substitution with lower atomic number atoms. We report DFT results on $\text{M}_{8-n}\text{N}_n\text{C}_{12}$ ($\text{M} = \text{Ti}, \text{Zr}$; $\text{N} = \text{Sc}, \text{Y}$, and $n=1,2,3$) Met-Cars in the neutral, cationic and anionic charge states. Our results show that the isoelectronic $\text{M}_6\text{N}_2\text{C}_{12}$, $\text{M}_5\text{N}_3\text{C}_{12}^-$ and $\text{M}_7\text{N}_1\text{C}_{12}^+$ Met-Cars have closed-shell electronic configurations and larger HOMO-LUMO gaps (1.0-1.7 eV) than that of the M_8C_{12} . The intercluster interaction between two isolated neutral $\text{M}_6\text{N}_2\text{C}_{12}$ Met-Cars is relatively weak compared to the M_8C_{12} dimers. Due to the weak interaction of the isolated neutral Met-Cars, their unique properties would be retained during assembly.

3:42PM D34.00005 Interplay of geometric and electronic structure in metalloid gallium clusters, DMITRI SCHEBARCHOV, NICOLA GASTON, Industrial Research Ltd. — Over the last two decades, the so-called "renaissance of main group chemistry" has led to significant advances in the synthesis, isolation and characterization of metalloid gallium clusters. What distinguishes these from other metalloid species (e.g. ligand-protected gold, silver, palladium, etc.) is their structural diversity, with the existence of four different Ga_{22} frameworks being a particularly striking example. To gain more insight into this polymorphism, we carried out electronic structure calculations using density functional theory. Our calculations verify that two of the ligand-protected Ga_{22} isomers can to some degree be viewed as superatom complexes - their respective metalloid cores are more or less close-packed, roughly spherical, and exhibit a well-defined electronic shell structure with a completely filled outer-most shell. The other two frameworks contain a slightly distorted icosahedral Ga_{12} core without a central atom - an unusual arrangement for metals - and the underlying electronic structure is more complex. This talk will serve as a summary of our calculations and illustrate the interplay of geometric and electronic structure in metalloid gallium clusters.

3:54PM D34.00006 Cluster Structure Selection Based on High Vertical Electron Affinity: The Case of TiO_2 Clusters, NOA MAROM, Institute for Computational Engineering and Sciences, The University of Texas at Austin, MINJUNG KIM, Institute for Computational Engineering and Sciences and Department of Chemical Engineering, The University of Texas at Austin, JAMES CHELIKOWSKY, Institute for Computational Engineering and Sciences and Departments of Chemical Engineering and Physics, The University of Texas at Austin — We study the structure and electronic properties of $(\text{TiO}_2)_{2-10}$ clusters using basin hopping based on density functional theory (DFT), combined with many-body perturbation theory in the GW approximation. We show that in photoemission experiments performed on anions the isomers with the high electron affinity are selectively observed rather than those with the lowest energy. These isomers possess a highly reactive Ti^{3+} site. The selectivity for highly reactive clusters may be exploited for applications in catalysis.

4:06PM D34.00007 Growing Ag Clusters in Superfluid He Droplets¹, LUIS F. GOMEZ, Department of Chemistry, University of Southern California, Los Angeles, CA, EVGENY LOGINOV, SICPA SA, Prilly, Switzerland, NAIHAO CHIANG, AVIK HALDER, NICHOLAS GUGGEMOS, VITALY KRESIN, Department of Physics, University of Southern California, Los Angeles, CA, ANDREY F. VILESOV, Department of Chemistry and Department of Physics, University of Southern California, Los Angeles, CA — Here we report on the growth and study of Ag clusters, ranging in size from 10 to 10^7 atoms, in a beam of superfluid He droplets. The droplets were used to capture Ag atoms from a hot oven, which then recombined in the interior of the droplet at sub-Kelvin temperature. The structure of the obtained Ag clusters was studied in situ via laser spectroscopy of their plasmon resonance. Furthermore, the clusters were surface-deposited and studied via transmission electron microscopy. The images have provided for a measure of the cluster flux and size distribution, which is in good agreement with an estimate based on the energy balance of Ag cluster growth in He droplets. The images also reveal an astounding change in shape of the deposited clusters to elongated and track-shaped with increased droplet size. This is ascribed to the formation of vortices within the He droplets whose cores are traced by the Ag atoms and clusters. The possible formation mechanism of the vortices and their stability will also be discussed.

¹This work was supported by NSF grant CHE-1112391.

4:18PM D34.00008 Atomic and Electronic Structure of Ag_n ($n \leq 13$) Clusters and their Reactivity with O_2^1 , GABRIEL U. GAMBOA, ARTHUR C. REBER, SHIV N. KHANNA, Department of Physics, Virginia Commonwealth University. — First principles theoretical studies on the atomic structure, stability, and electronic structure of neutral and anionic Ag_n clusters have been carried out within a gradient corrected density functional approach. It is shown that the clusters are marked by planar or layered structures. For most clusters, the ground state of anions has lowest spin multiplicity. To examine the reactivity of clusters, containing even number of electrons, with O_2 , we calculated the spin excitation energy representing the energy required to excite the cluster to the triplet configuration. It is shown that several of these even electron anionic species and in particular Ag_{13}^- have high spin excitation energy indicating that they should be inert towards reactivity with oxygen. The theoretical predictions are shown to be in agreement with preliminary experimental data on the reactivity of anionic species.

¹We gratefully acknowledge funding by the U.S. Department of the Army through a MURI grant W911NF-06-1-0280.

4:30PM D34.00009 On the Reactivity of $\text{Al}_{13}\text{I}_n^-$ and $\text{Al}_{14}\text{I}_n^-$ Clusters with Methanol¹, M.B. ABREU, A.C. REBER, S.N. KHANNA, Department of Physics, Virginia Commonwealth University — Al_{13} and Al_{14} cluster anions act as halogen or alkaline earth superatoms respectively when bound by I atoms. $\text{Al}_{13}\text{I}_2^-$ and $\text{Al}_{14}\text{I}_3^-$ have enhanced resistance to oxidation by oxygen because of the clusters' closed electronic shells, however the reactivity of aluminum clusters with methanol depends on the presence of complementary active sites. We have examined the reactivity of $\text{Al}_{13}\text{I}_n^-$ and $\text{Al}_{14}\text{I}_m^-$ with methanol to identify if the presence of electronegative iodine may induce active sites on the cluster. The presence of a single iodine atom on Al_{13}^- is insufficient to activate the cluster, however two adjacent ligands induce an active site and makes the cluster highly reactive. The $\text{Al}_{14}\text{I}_m^-$ clusters are found to be reactive with methanol highlighting the importance of geometric shell closures in ligand protected clusters.

¹We gratefully acknowledge financial support from Air Force Office of Scientific Research (AFOSR) through grant #FA9550-09-1-0371.

4:42PM D34.00010 Bonding and Electronic Structure of Cluster Assemblies with Metal Carbonyls¹, MEICHUN QIAN, ARTHUR REBER, SHIV KHANNA, Department of Physics, Virginia Commonwealth University, SUKHENDU MAN-DAL, HECTOR SAAVEDRA, Department of Chemistry, The Pennsylvania State University, PAUL WEISS, Department of Chemistry, The Pennsylvania State University and California Nanosystems Institute, University of California at Los Angeles, AYUSMAN SEN, Department of Chemistry, The Pennsylvania State University — Understanding the factors controlling the band gap energies of cluster-assembled materials is an important step towards creating nano-assemblies with tailored properties. To this end, we have investigated the band gap energies of cluster assemblies involving arsenic clusters bound to metal carbonyl charge-transfer complexes, $[\text{As}_7\text{M}(\text{CO})_3]^{3-}$ $\text{M} = \text{Cr}, \text{Mo}, \text{W}$. The binding of a single charge-transfer complex is shown to have a small effect on the band gap energy as the arsenic lone pair orbital and metal carbonyl orbitals are closely aligned in energy, resulting in a gap similar to the original cluster. The band gap energy is also found to be insensitive to the architecture of the assembled material. In the case where two charge-transfer complexes are bound to the cluster, the bottom of the conduction band is shown to be localized on a solvent molecule bound to the metal carbonyl.

¹We gratefully acknowledge funding by the U.S. Department of the Army through a MURI grant W911NF-06-1-0280.

4:54PM D34.00011 Stability and Shell Magnetism in Transition Metal Doped Calcium clusters¹, VICTOR M. MEDEL-JUAREZ, J. ULISES REVELES, S.N. KHANNA, Virginia Commonwealth University, V. CHAUHAN, P. SEN, Harish-Chandra Research Institute, Chhatnag Road Jhansi, Allahabad 211019, India — Clusters of many metallic elements are known to exhibit enhanced stability at valence electron counts 2, 8, 18, 20, 34, 40, ... that can be understood within a simple spherical confined nearly free electron gas model. In this work we show a magnetic species whose stability is rationalized on a modification of the above shell sequence through deformations of the spherical geometry and through enhanced exchange splitting of the electronic shells via impurity atoms with large atomic orbital exchange splitting. Through first principles theoretical studies of the electronic structure and stability of TMCa_8 ($\text{TM} = \text{Sc}, \text{Ti}, \text{V}, \text{Cr}, \text{Mn}, \text{Fe}, \text{Co}, \text{Ni}, \text{Cu}$ and Zn) clusters we identify a stable magnetic FeCa_8 cluster of 24 valence electrons distributed into a closed 1S2 1P6 1D10 2S2 shell sequence of 20 paired electrons and with 4 electrons occupying the majority $2D_{xy}2D_{x-y}^2$, $2D_{xz}$ and $2D_{yz}$ levels while the unfilled $2D_z^2$ level is separated by a large energy gap of 0.61 eV arising from atomic deformation.

¹We gratefully acknowledge support from U. S. Department of Energy (DOE) through grant DE-FG02-11ER16213.

5:06PM D34.00012 On the stability and oxidation of Pd_n ($n=1-7$) clusters on rutile $\text{TiO}_2(110)$ ¹, S. VINCENT ONG, SHIV KHANNA, Virginia Commonwealth University, DEPT OF PHYSICS, VIRGINIA COMMONWEALTH UNIVERSITY TEAM — First principles theoretical studies of the atomic and electronic structure of Pd_n ($n=1-7$) clusters supported on a $\text{TiO}_2(110)$ surface, and O_2 activation by such clusters, have been carried out within a gradient corrected density functional approach. It is shown that the supported Pd_n cluster geometries are driven by competing effects including intra-cluster interactions favoring compact geometries and cluster support interactions that favor geometries that flatten out in the $\text{TiO}_2(110)$ surface channel. When exposed to O_2 , a single Pd atom only activates the O-O bond while all other clusters energetically favor a broken O-O bond. The differing behavior of the Pd atom is proposed to originate from the minimal amount of charge transferred from Pd to O_2 and its spin excitation energy. For Pd_nO_2 ($n=2-7$), it is shown that while the first O is adsorbed on the Pd_n cluster, the second O occupies a site above a lattice Ti site at the Pd-Ti interface and is indicative of spill over O atoms. The theoretical findings are compared with recent experiments on the structure and oxidation of CO by supported clusters in the presence of O_2 .

¹This material is based upon work supported by the Air Force Office of Scientific Research (AFOSR) Award: FA9550-08-1-0400

5:18PM D34.00013 Strengthening of Au-Au bonds in small gold clusters by adsorbing noble gases, LUCA M. GHIRINGHELLI, SERGEY LEVCHENKO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut, D-14195, Berlin — In state-of-the-art experiments for the vibrational spectra of metal clusters in the gas phase, photodissociation spectroscopy is performed on clusters complexed with noble gas (RG) atoms, where a RG atom is usually expected to form a weak van der Waals bond. By employing DFT (PBE functional with selected comparisons to PBE0, and to MP2 and CCSD(T) calculations), we surprisingly find a partially covalent bond of *neutral* dimers with RG. For $\text{RG} = \text{Ar}, \text{Kr}, \text{Xe}$ one or two RG atoms can bind in a linear molecule with Au_2 . While both Hirschfeld and Mulliken analyses show a small electron transfer from the RG to Au_2 , the Au-Au bond *shortens* and the Au-Au stretch frequency increases. This is inconsistent with the expected effect of electron transfer to the antibonding orbital of the dimer. Electron-density (n) differences between the bonded systems and the isolated fragments show an accumulation of n between RG and the neighboring Au atom, and between the gold atoms. The analysis of the projected density of states reveals that, although only non-bonding orbital interactions and no charge transfer occurs between RG and Au_2 , the d -electrons of Au_2 are redistributed due to the interaction with RG in such a way that the Au-Au σ_s bond is strengthened.

Monday, February 27, 2012 2:30PM - 5:30PM –
Session D35 DCP: Focus Session: DFT II: Molecular Conductance; Charge Transfer 107B

2:30PM D35.00001 On the derivative discontinuity in molecular junctions¹, CHARLES STAFFORD, University of Arizona — Both the wave and particle aspects of the electron play essential roles in transport through single-molecule junctions. The wave character is implicit both in the Landauer formula used to understand nanoscale transport and in the very chemical bonds holding the junction together, while the particle aspect is manifested in phenomena such as Coulomb blockade and shot noise. The dominant computational paradigm for transport in single-molecule junctions involves local or semilocal approximations to density functional theory combined with nonequilibrium Green's functions. This approach does exceptionally well at describing the wave aspect of the electron, but fails to describe the particle aspect—due to the omission of the derivative discontinuity in the exchange-correlation potential that arises in the limit of vanishing lead-molecule coupling. To understand the role of the derivative discontinuity in molecular junctions, we investigated the transport and occupancy of a simple Anderson model of a molecular junction. We showed² that the exact single-particle Kohn-Sham potential of density functional theory reproduces the linear-response transport of the Anderson model exactly, despite the lack of a Kondo peak in its spectral function. Using Bethe ansatz techniques, we calculated this potential exactly for all coupling strengths, including the cross-over from mean-field behavior to charge quantization caused by the derivative discontinuity. The implications of our results for more complex molecular junctions will be discussed.

¹This work was supported in part by the Department of Energy under Award Number DE-SC0006699.

²Justin P. Bergfield, Zhenfei Liu, Kieron Burke, Charles A. Stafford, arXiv:1106.3104v2

3:06PM D35.00002 A density functional that works for transport through Anderson junction¹, ZHENFEI LIU, JUSTIN BERGFELD, KIERON BURKE, Departments of Chemistry and Physics, University of California, Irvine, CHARLES STAFFORD, Department of Physics, University of Arizona — Transport through an Anderson junction can be exactly described by density functional theory, at zero temperature and in the linear response regime. Using Bethe ansatz, we calculate the exact Kohn-Sham potential delivering the exact transmission. We propose a simple parametrization for the Kohn-Sham potential, using a known exact condition. Our parametrization faithfully reproduces numerical results, including the gradual development of the derivative discontinuity that is essential in describing Coulomb blockade correctly.

¹This work is funded by the U.S. Department of Energy (Grant No. DE-FG02-08ER46496).

3:18PM D35.00003 Non-steady state in quantum transport, ELHAM KHOSRAVI, Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany, STEFAN KURTH, Nano-Bio Spectroscopy Group, Departamento de Física de Materiales, Universidad del País Vasco, Avenida de Tolosa 72, E-20018 San Sebastian, Spain, GIANLUCA STEFANUCCI, Dipartimento di Fisica, Università di Roma Tor Vergata, Via della Ricerca Scientifica 1, 00133 Rome, Italy, E.K.U. GROSS, Max Planck Institute of Microstructure Physics, Weinberg 2, D - 06120 Halle, Germany — The standard approach to quantum transport combines the Landauer-Büttiker (LB) formalism with ground-state density functional theory (DFT). The basic assumption of this approach is that a steady state is achieved after turning on a DC bias. Here we show that this assumption is “not” valid in general and give examples for which no steady state develop within several adiabatic (time-local) approximations as well as in non-interacting systems. In these cases a time-dependent description of transport is essential. For the non-interacting case, the presence of bound states in a biased system is shown analytically and numerically to lead to persistent, localized current oscillations which can be much larger than the steady part of the current (PCCP. 11, 4535(2009)). For the interacting case, the discontinuity of the exchange-correlation potential of DFT in the context of electron transport for an interacting nanojunction attached to biased leads, gives rise to a dynamical state characterized by correlation-induced current oscillations in the Coulomb-blockade regime (PRL. 104, 236801(2010)). In addition, for multistable systems, the time-dependent approach describes if and how a solution can be reached through time evolution.

3:30PM D35.00004 DFT methods for conjugated materials: From benchmarks to functionals, JOHN SEARS, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia 30332-0400, JEAN-LUC BREDAS, School of Chemistry and Biochemistry, Georgia Institute of Technology — From a theoretical standpoint, many of the problems of interest in the study of pi-conjugated materials for organic electronics applications pose a particular challenge for many modern density functional theory methods. Systematic errors have been observed, for instance, in the description of charge-transfer excitations at donor/acceptor interfaces, in linear and non-linear polarizabilities, as well as in the geometric and electronic properties of conjugated polymers [1,2]. We will discuss recent results in our lab aimed at: (i) understanding the sources of error for some of these problems; (ii) addressing these errors using tuned long-range corrected functionals; and (iii) using these results to guide the development of state-of-the-art methodologies in a new open-source DFT code.

[1] J. S. Sears, T. Korzdorfer, C. R. Zhang, and J. L. Bredas, J. Chem. Phys. 135 151103 (2011)

[2] T. Korzdorfer, J. S. Sears, C. Sutton, and J. L. Bredas, J. Chem. Phys., accepted.

3:42PM D35.00005 Fundamental and excitation gaps in molecules of relevance for organic photovoltaics from an optimally tuned range-separated hybrid functional, SIVAN REFAELY-ABRAMSON, Weizmann Institute of Science, Israel, ROI BAER, Hebrew University, Jerusalem, Israel, LEEOR KRONIK, Weizmann Institute of Science, Israel — The fundamental and optical gaps of relevant molecular systems are of primary importance for organic-based photovoltaics. Unfortunately, whereas optical gaps are accessible with time-dependent density functional theory (DFT), the highest -occupied - lowest-unoccupied eigenvalue gaps resulting from DFT calculations with semi-local or hybrid functionals routinely and severely underestimate the fundamental gaps of gas-phase organic molecules. Here, we show that a range-separated hybrid functional, optimally tuned so as to obey Koopmans' theorem, provides fundamental gaps that are very close to benchmark results obtained from many-body perturbation theory in the GW approximation. We then show that using this functional does not compromise the possibility of obtaining reliable optical gaps from time-dependent DFT. We therefore suggest optimally-tuned range-separated hybrid functionals as a practical and accurate tool for DFT-based predictions of photovoltaically relevant and other molecular systems. For more details, see S. Refaely-Abramson, R. Baer, L. Kronik, Phys. Rev. B 84, 075144 (2011).

3:54PM D35.00006 (1) Modeling emissive charge-transfer states in solution phase functionalized silsesquioxanes. (2) On symmetry hidden charge transfer states: Lessons for the design of functionals¹, BARRY D. DUNIETZ, SHAOHUI ZHENG, HEIDI PHILLIPS, EITAN GEVA, University of Michigan — Range separate hybrid functionals are used to study the charge transfer processes in chromophores attached to silsesquioxanes molecular species. We investigate the experimentally observed red shifting of the emission spectra in comparison to the spectral shift for the individual ligand. Solvent effects are accounted for via a combination of constrained density functional theory and the polarizable continuum (PCM) model. We quantitatively reproduce the experimental red shift and identify the emissive state as a ligand-to-ligand, rather than a ligand-to-silsesquioxane, charge-transfer state. We also find that the enhanced red-shift cannot be explained without accounting for solvation effects and demonstrate the importance of using a range-separated hybrid functional, as opposed to more traditional functionals such as B3LYP, to obtain reliable predictions regarding the emissive state. If time allows we will also discuss the limitations and successes of RSH functionals in treating the case of charge transfer processes that are hidden by system symmetry. We use related models to draw insight for designing improved functionals.

¹This work is pursued as part of the Center for Solar and Thermal Energy Conversion, an Energy Frontier Research Center funded by the US Department of Energy Office of Science, Office of Basic Energy Sciences under 390 Award No. DE-SC0000957.

4:06PM D35.00007 Density Functional Methods and Electronic Processes in Organic Materials¹, QIN WU, Brookhaven National Lab — When modeling the fundamental processes in organic electronic materials, ab initio calculations play an important role because they provide an independent source of information. It is thus critical to use accurate and reliable ab initio methods. In this talk, we will share our experience in using density functional methods to study charge generation and transport in some organic systems. These include prototypical polythiophene and polyfluorene, as well as some newly synthesized conjugated molecules. They all have strong dispersion forces and strong electron-vibration coupling; both are well-known difficult effects for density functional methods to capture accurately. We will describe our effort in exploring ways to do meaningful calculations. Close collaborations with experimental work will also be emphasized.

¹Research is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

4:18PM D35.00008 Modelling Charge Transfer Reactions and Excitations with Subsystem DFT¹, MICHELE PAVANELLO, Leiden University, JOHANNES NEUGEBAUER, Technical University Braunschweig — The subsystem formulation of DFT known as Frozen Density Embedding (FDE) offers an excellent platform for studying charge transfer reactions in solvated systems, such as biosystems. We present the necessary theory developments for the calculation of the electronic couplings as well as the charge transfer excitations from FDE derived densities. We present preliminary calculations on DNA oligomers radical cations that include donor-bridge, donor-bridge-acceptor, and fully solvated systems.

¹M.P. acknowledges funding by a Marie Curie Fellowship of the European Commission (PIIF-GA-2009-254444). J.N. is supported by a VIDI grant (700.59.422) of the Netherlands Organization for Scientific Research (NWO).

4:30PM D35.00009 Ab initio molecular dynamics study of the electric double-layer capacitance at solution-electrode interfaces, YASUNOBU ANDO, YOSHIHIRO GOHDA, SHINJI TSUNEYUKI, Department of Physics, The University of Tokyo — Electric double-layer (EDL) is known as an important stage for electrochemical reactions at electrode-liquid interfaces. It has also attracted growing interest for its applications to electronic devices, called EDL capacitors (supercapacitors) and EDL transistors. In efficient development of each device, predicting the EDL capacitance in light of the material features is required. However, Helmholtz capacitance, the part of the EDL capacitance depending on the microscopic structure, has still not been estimated theoretically. Therefore, to evaluate that, we calculated the structure of solution-electrode interfaces by using ab initio molecular dynamics with effective screening medium method. As a result, we made it possible to estimate the Helmholtz capacitance taking the effect of the molecular orientation of the water and the electronic polarization in the water molecules due to the electric field into account. Apparent dielectric constant of the water near the interface can also be calculated. Interestingly, the results reveal that the existence of a first layer of the water molecules near the electrode determines the distance of closest approach of hydrated ions. Moreover, the estimated dielectric constant of the first layer differs from that predicted by the classical theory.

4:42PM D35.00010 Assessing the fitness of various exchange-correlation functionals for TD-DFT studies of charge-transfer excitations in organic dyes¹, PRATIBHA DEV, SAURABH AGRAWAL, NIAL ENGLISH, School of Chemical & Bioprocess Engineering, University College Dublin, SEC STRATEGIC CLUSTER TEAM — Dye Sensitized Solar Cells (DSSCs) are a possible alternative to the more expensive silicon-based cells. Theoretical research in this field has highlighted some of the issues with time-dependent density functional theory (TD-DFT) that is widely used to study electronic excitations of matter. The situation is complicated by the fact that several classes of approximations to the exchange correlation functional can be employed, however, not one of these strictly outperforms the others in its description of charge-transfer excitations. In this work, UV-Vis spectra are calculated using TD-DFT for several organic dyes – alizarin, squaraine, 4-(N, N-dimethylamino) benzonitrile, polyene-linker dyes and triphenylamine-donor dyes. We studied the dyes within three approximations (PBE, B3LYP and CAM-B3LYP) to the exchange-correlation functional. In the dyes considered here, a correlation exists between the functional performance and the spatial overlap of the states involved in the excitations. This overlap can be quantified to provide a good guideline for choosing the right functional when studying intramolecular charge transfer in dyes. It will be an invaluable tool when studying these molecules within more challenging systems, such as dye-titania complexes in DSSCs.

¹We acknowledge the computational support provided by ICHEC. PD acknowledges financial support for this work through EMPOWER fellowship granted by IRCSET. SA is supported by the Science Foundation Ireland under Grant No. [07/SRC/B1160].

4:54PM D35.00011 Electronic density functional theory in the grand canonical ensemble, electrochemistry, and the underpotential deposition of Cu/Pt(111)¹, RAVISHANKAR SUNDARARAMAN, KENDRA WEAVER, TOMAS ARIAS, Physics Department, Cornell University — The study of electrochemical systems within electronic density functional theory requires the handling of non-neutral electronic systems in the plane-wave basis in order to accurately describe charged metallic surfaces; this can be accomplished in joint density functional theory by adding an electrolyte with Debye screening². This capability opens up the opportunity to work in the grand canonical ensemble at fixed chemical potential μ for the electrons, which corresponds directly to the experimental setting in electrochemistry. We present efficient techniques for electronic density functional calculations at fixed μ , and demonstrate the improvement in predictive power over conventional neutral calculations using the underpotential deposition of Cu/Pt(111) as an example: for the first time, we calculate absolute voltages for electrochemical processes in excellent agreement with experiment, instead of voltage shifts alone.

¹This work was supported as a part of the Energy Materials Center at Cornell (EMC2), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001086.

²K. L. Weaver and T. A. Arias (under preparation)

5:06PM D35.00012 First-Principles Studies of Structure and Energy Level Alignment of Thiophene Assemblies on Methyl-Terminated Si(111), MIN YU, PETER DOAK, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory — Adsorption of organic molecules on semiconductor photocatalysts has attracted significant attention for energy conversion applications. In this work, we use density functional theory and many-body perturbation theory within the GW approximation to study the geometry, binding energetics, and energy level alignment of a model ligand, thiophene (C₄H₄S), chemisorbed via a C-Si bond on methyl-terminated silicon(111) substrates. We quantify the impact of coverage, interface dipoles, hybridization, and polarization effects on level alignment. For sufficiently weakly-coupled frontier orbitals, we explore the extent to which the self-energy change upon adsorption relative to the gas phase is dominated by nonlocal electrostatic polarization effects [1]. The implications of our results for other thiophene-related ligands, and future spectroscopic experiments, will be thoroughly discussed. We acknowledge DOE for support through JCAP, and NERSC for computational resources.

[1] J. B. Neaton, M. S. Hybertsen and S. G. Louie, Phys. Rev. Lett. 97, 216405 (2006).

5:18PM D35.00013 Electronic level alignment at a metal-molecule interface from a short-range hybrid functional, ARIEL BILLER, Weizmann Institute of Science, Israel, ISAAC TAMBLYN, JEFFERY B. NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, LEEOR KRONIK, Weizmann Institute of Science, Israel — Hybrid functionals often exhibit a marked improvement over semi-local functionals in the description of the electronic structure of organic materials. Because short-range hybrid functionals, notably the Heyd-Scuseria-Ernzerhof (HSE) functional, can also describe the electronic structure of metals reasonably well, it is interesting to examine to which extent they can correctly describe the electronic structure at metal-organic interfaces. Here, we address this question by comparing HSE calculations with many-body perturbation theory calculations in the GW approximation, or with experimental photoemission data, for two prototypical systems: benzene on graphite and benzene diamine on gold. For both cases, we find that while HSE yields results that are somewhat closer to experiment than those of semi-local functionals, the HSE prediction is still lacking quantitatively by ~ 1 eV. We show that this quantitative failure arises because HSE does not correctly capture the fundamental gap of the organic, or its renormalization by the metal. These discrepancies are traced back to missing long-range exchange and correlation components, an explanation which applies to any conventional or short-range hybrid functional.

Monday, February 27, 2012 2:30PM - 5:30PM –
Session D36 DCP: Focus Session: Environment I: Aerosols and Aqueous Solutions 107C

2:30PM D36.00001 Uncovering the formation mechanism of atmospheric nanoparticles¹, HANNA VEHKAMAKI, University of Helsinki — Atmospheric aerosol affect human health, visibility and radiation budget of the Earth. The current estimate is that 20-80% of aerosols particles are formed in the atmosphere by condensable gases. Experimental and theoretical data indicates that the formation of new particles in the atmosphere in most cases very likely involves sulphuric acid assisted with some base molecules. The role of ions in atmospheric particle formation is has been widely discussed during recent years. The diameter of the forming clusters is 1-2nm, falling between the smallest size where brute force quantum mechanical treatment is possible, and macroscopic size where bulk thermodynamics is applicable. Recent experiments at the CLOUD chamber in CERN have provided molecular-level information on the charged fraction of the nucleating clusters, but the theoretical framework needed to convert this into information on neutral clusters is still lacking. We have used a cost-effective multi-step computational chemistry method involving automated configurational sampling, density functional theory geometry optimizations and coupled-cluster energy calculations, to study the stability of charged and neutral sulfuric acid clusters containing ammonia and dimethylamine. Combined with a cluster dynamics model ACDC, we are able to replicate the formation rates observed in the CLOUD chamber, as well as match observed formation rates in Hyytiälä Smear II station in Finland.

¹ERC project 257360-MOCAPAF, Academy of Finland

3:06PM D36.00002 Molecular dynamics of binary and ternary nanodroplets with a miscibility gap¹, GERALD WILEMSKI, FAWAZ HRAHSHEH, Missouri University of Science and Technology — The structure of nanodroplets plays an important role in many natural processes including particle nucleation and aerosol formation in the atmosphere. Among other factors, chemical miscibility and surface tension strongly affect the structure of multicomponent nanodroplets at low temperature. Here, we investigate the structure of water/nonane and water/butanol/nonane nanodroplets using molecular dynamics (MD). Our MD results confirm our theoretical predictions of nonspherical nanodroplet (Russian-Doll) structures at low temperatures using density functional and lattice Monte Carlo techniques. We systematically study the variation of the droplet structure with temperature and with butanol concentration.

¹Supported by National Science Foundation Grant No. CBET-1033387.

3:18PM D36.00003 Organization at the Air-Aqueous Interface by Heterodyne-detected Phase-Sensitive Sum Frequency Spectroscopy¹, HEATHER ALLEN, The Ohio State University — Water and ions organize at the air – aqueous interface and the ion distributions within this region give rise to interfacial electric double layers. Geochemical solid-aqueous and atmospheric aerosol relevant air-aqueous interfaces were studied using vibrational sum frequency generation (VSFG), and in some cases, heterodyne-detected VSFG spectroscopy. Solid-aqueous and air-liquid interfaces were also investigated using total internal reflection Raman spectroscopy, infrared reflection absorption spectroscopy (IRRAS), and Brewster angle microscopy (BAM), respectively. Here, we show results from aqueous solutions containing salts such as sulfates and chlorides where surface adsorption and electric field direction reversal was observed. Of the salts studied at the air-aqueous interface with heterodyne-detected VSFG, the magnitude of the electric field in the surface extending to the subsurface regions decreases in the order: $(\text{NH}_4)_2\text{SO}_4 > \text{Na}_2\text{SO}_4 > \text{Na}_2\text{CO}_3 \geq \text{CaCl}_2 > \text{NaCl}$; the electric field is opposite in direction for the sulfates and carbonate relative to the chloride salts.

¹Support acknowledged from DOE-BES Geosciences and NSF-CHE ECS

3:54PM D36.00004 First-principles study of the infrared spectrum of the ice Ih (0001) surface¹, HUANG PATRICK, Lawrence Livermore National Laboratory, Livermore, California, 94550, T. ANH PHAM, University of California, Davis and Lawrence Livermore National Laboratory, Livermore, California, 94550, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, Livermore, California, 94550, GIULIA GALLI, University of California, Davis — Ice particles catalyze a number of processes relevant to atmospheric and environmental chemistry, and the elucidation of these reactions require knowledge of the ice surface structure. Although it is well known that the structure of bulk ice-Ih is proton disordered, the understanding of the microscopic structure of the ice surface is still limited. Recent theoretical studies ^{1,2} suggest that the basal (0001) surface of ice Ih is significantly more proton ordered than the bulk. In this work we compute infrared (IR) spectra of several ordered and disordered models of the (0001) surface of ice, and investigate the sensitivity of these spectra to the microscopic details of the surface structure. In particular we discuss possible signatures of disorder in the computed spectra. [1] D. Pan et al., Phys. Rev. Lett. 101, 155703 (2008); [2] V. Buch et al., Proc. Natl. Acad. Sci. U.S.A. 105, 5969 (2008)

¹Prepared by LLNL under Contract DE-AC52-07NA27344

4:06PM D36.00005 1st principle simulations of ions in water solutions: Bond structure and chemistry in the hydration shells of highly charged ions, JOHN WEARE, University of California, San Diego — Methods of direct simulation (Monte Carlo and molecular dynamics) have provided new insights into the structure and dynamics of electrolyte solutions. However, these methods are limited by the difficulty of developing reliable ion-solvent and solvent-solvent potential interactions in the highly perturbed hydration region. To model the interactions in this region methods of simulation that are based on the direct on the fly solution to the electronic Schrödinger equation (ab-initio molecular dynamics, AIMD) are being developed. However, 1st principle methods have their own problems because the solution to the electronic structure problem is intractable unless rather uncontrolled approximations are made (e.g. density functional theory, DFT) and there is high computational cost to the solution to the Schrödinger equation. To test the accuracy of AIMD methods we have directly simulated the XAFS spectra for a series of transition metal ions Ca^{2+} , Cr^{3+} , Mn^{2+} , Fe^{3+} , Co^{2+} , Ni^{2+} , Cu^{2+} , and Zn^{2+} . Despite DFT's well known deficiencies, the agreement between the calculated XAFS spectra and the data is almost quantitative for these test ions. This agreement supports the extension of the interpretation well beyond that of the usual XAFS analysis to include higher-order multiple scattering signals in the XAFS spectra, which provide a rigorous probe of the first shell distances and disorders. Less well resolved features of the spectra can still be analyzed and are related to 2nd shell structure. The combination of XAFS measurements and the parameter free AIMD method leads to new insights into the hydration structure of these ions. While strictly local DFT +gga provides excellent agreement with data, the addition of exact exchange seems to provide slightly better structural agreement. The computational complexity of these calculations requires the development of simulation tools that scale to high processor number on massively parallel supercomputers. Our present algorithm scales to nearly 100,000 processors. However, even with high scaling the time to solution is very long. We are also developing and testing new methods to improve the performance of simulation and new sampling methods that more efficiently explore phase space and can reach longer time frames. Results of calculation of the hydration structure and dynamics of highly charged ions and free energy calculations of ion association will be presented.

4:42PM D36.00006 Reactions of Solvated Electrons Initiated by Sodium Atom Ionization at the Vacuum-Liquid Interface¹, JUSTIN WIENS, University of Wisconsin-Madison, WILLIAM ALEXANDER, Montana State University-Bozeman, GILBERT NATHANSON, University of Wisconsin-Madison, TIMOTHY MINTON, Montana State University-Bozeman — Solvated electrons are powerful reagents in the liquid phase that break chemical bonds and create new reactive species, including hydrogen atoms. Electrons and hydrogen atoms born near the surface, however, behave differently than those created within the liquid. We explore this behavior by exposing liquid glycerol to a beam of sodium atoms. The Na atoms ionize in the surface region, generating electrons that react with deuterated glycerol, $\text{C}_3\text{D}_5(\text{OD})_3$, to produce D atoms, D_2 , D_2O , and glycerol fragments. Surprisingly, 40% of the D atoms desorb into vacuum before attacking C-D bonds to produce D_2 . These D atoms must traverse the interfacial region before desorbing, demonstrating that Na ionization prepares reactive species that reside momentarily at the surface and often escape before reacting with the solvent.

¹This work was supported by National Science Foundation as part of the Center for Energetic Non-Equilibrium Chemistry at Interfaces

4:54PM D36.00007 Heterogeneous Photochemistry and Optical Properties of Mineral Dust Aerosol, VICKI GRASSIAN, University of Iowa — It is now widely recognized that heterogeneous reactions of mineral dust aerosol with trace atmospheric gases impact the chemical balance of the atmosphere and the physicochemical properties of these particles. Field studies using single particle analysis, have now shown that the chemistry is mineralogy specific and follows the trends expected from laboratory studies. These laboratory studies, which were initiated over a decade ago, have focused on the nighttime chemistry of mineral dust aerosol which is really only "half" the story. This talk will focus on two aspects of solar light interaction with mineral dust aerosol. First, the heterogeneous photochemistry of adsorbed chromophores (e.g. nitrate ion) and light absorbing components of mineral dust (iron oxides and titanium dioxide) is discussed. These heterogeneous photochemical reactions are poorly understood and laboratory studies to better quantify these reactions in order to determine the impact on the chemical balance of the atmosphere are needed, as will be discussed. Second, the optical properties of mineral dust aerosol measured by extinction infrared spectroscopy and visible light scattering show that shape effects are extremely important for mineral dust aerosol.

Monday, February 27, 2012 2:30PM - 5:18PM – Session D37 SPS: SPS Undergraduate Research II 108

2:30PM D37.00001 Low Temperature Resistive Switching Behavior in a Manganite, CHRISTOPHER SALVO, MELINDA LOPEZ, STEPHEN TSUI, California State University San Marcos — The development of new nonvolatile memory devices remains an important field of consumer electronics. A possible candidate is bipolar resistive switching, a method by which the resistance of a material changes when a voltage is applied. Although there is a great deal of research on this topic, not much has been done at low temperatures. In this work, we compare the room temperature and low temperature behaviors of switching in a manganite thin film. The data indicates that the switching is suppressed upon cooling to cryogenic temperatures, and the presence of crystalline charge traps is tied to the physical mechanism.

2:42PM D37.00002 Atomic Steps on Thermally Annealed Oxide Substrates¹, ICON MAZZACCARI, RAFIYA JAVED, AMLAN BISWAS, Department of Physics, University of Florida — Atomically smooth perovskite oxide substrates are necessary for high quality thin-film growth. We have optimized the annealing conditions for the substrates, LaAlO_3 , SrTiO_3 and NdGaO_3 , which are commonly used substrates for growing thin-film perovskite oxides. The optimal annealing temperatures were between 950 °C and 1050 °C and the annealing time for each sample was varied by approximately 20%. Atomic force microscopy was used to compare the surfaces of the annealed substrates with the unannealed ones. These images capture the terrace steps that occur due to the annealing process, and we have confirmed that the heights of the steps are approximately one unit cell (0.4 nm). Currently, we are investigating methods for determining the site termination of the substrates and their effects on thin-film growth.

¹NSF DMR-0804452

2:54PM D37.00003 Field-Induced Phase Transitions in the $S=1/2$ Quasi-1D Antiferromagnet $\text{BaCo}_2\text{V}_2\text{O}_8$ ¹, GIOVANNI FRANCO-RIVERA, University of Puerto Rico at Mayaguez, N.A. FORTUNE, Smith College, S.T. HANNAHS, H.D. ZHOU, National High Magnetic Field Lab, H. TSUJII, Kanazawa University, Y. TAKANO, University of Florida — We have performed magnetocaloric effect and specific heat measurements in the $S=1/2$ quasi-one-dimensional Ising-like antiferromagnet $\text{BaCo}_2\text{V}_2\text{O}_8$ in magnetic fields up to 24 T at temperatures down to 0.3 K. The magnetocaloric effect measurements were made in order to investigate the field-direction dependence of a magnetic transition near 3.7 T. The specific heat and magnetocaloric effect measurements were employed to determine the H-T phase diagram when the field is applied parallel to the *c* axis of the sample. We have found a new antiferromagnetically ordered phase between 19.7 T and 23.1 T, most likely a spin-flop phase. At low fields, our results agree with the known Néel ordered phase boundary.

¹This work was supported in part by the University of Florida Physics REU program under NSF and DOD Grant No. DMR-0851707

3:06PM D37.00004 Magnetism in Transition Element Doped In_2O_3 Dilute Magnetic Semiconductors¹, M. LANGHOFF, E. NAHLIK, Department of Physics, Astronomy, and Materials Science, Missouri State University, Springfield, MO 65897, Y. KOLEKAR, Department of Physics, University of Pune, Pune, India, P. KAHOL, K. GHOSH, Department of Physics, Astronomy, and Materials Science, Missouri State University, Springfield, MO 65897 — There is currently a tremendous research effort in the area of dilute magnetic semiconductors (DMS). It is proposed that a DMS exhibiting ferromagnetic properties at room temperature could be used in a new class of devices termed spintronics. Whereas standard electronics work on the principle of manipulation of charge properties of an electron, spintronics work on controlling electron spin. Indium oxide is a wide band gap semiconductor with unique optical and electrical properties. Defect concentrations such as transition metal doping and oxygen vacancies in In_2O_3 can tune the electrical/magnetic behavior from ferromagnetic metal-like to ferromagnetic semiconducting to paramagnetic insulating. Bulk materials of magnetic element (Fe, Co and Cr) doped In_2O_3 have been made using a standard solid state reaction method. Structural and magnetic properties have been measured using standard techniques. XRD analysis confirmed single phase In_2O_3 with no impurity phases due to addition of magnetic elements. Magnetization as a function of applied magnetic field and temperature were collected on all the samples using a SQUID magnetometer. Detailed structural and magnetic properties will be presented in this talk.

¹This work is supported by National Science Foundation (Award Number DMR-0907037).

3:18PM D37.00005 Magnetic Properties of Ordered Nanoporous Nickel Films¹, JIABIN LIU, HAN-CHANG YANG, X.M. CHENG, Bryn Mawr College — Nanoporous materials have been of great interest for applications such as biosensors and energy storage. Magnetic properties and the magnetization reversal mechanism of nanoporous magnetic materials remain to be fully understood. In this work, we report the fabrication and magnetic properties of ordered nanoporous nickel (Ni) films. The fabrication involved the following steps: self-assembly of monodispersed polystyrene spheres, electrochemical deposition of desired materials, and sphere removal by a dissolution process. Scanning electron microscopy (SEM) images confirmed the highly ordered three-dimensional hexagonal closed pack structures of the Ni films. We characterized magnetic properties of the three-dimensional nanoporous Ni films using vibrating sample magnetometer (VSM). Magnetic hysteresis loops and first-order reversal curves (FORCs) were measured on the nanoporous Ni films of 200 nm pore size with different thicknesses. Analysis on hysteresis loops and FORC distributions shed light on the reversal mechanism of magnetization and magnetostatic interactions of ordered three-dimensional porous structures.

¹The work at Bryn Mawr College is supported by the National Science Foundation under Grant No. 1053854.

3:30PM D37.00006 Electrical characterization of CVD graphene, YARELY DÁVILA, NICHOLAS PINTO, University of Puerto Rico - Humacao, ZHENG TANG LUO, ALAN JOHNSON JR., University of Pennsylvania — Graphene is a one atom thick carbon sheet that can be obtained via exfoliation of graphite or via chemical vapor deposition (CVD). By using a very simple shadow masking technique, gold contact pads were evaporated over the graphene thereby eliminating chemical etching that is required when using photolithography and often leads to sample contamination. CVD graphene was electrically characterized in a FET configuration under different experimental conditions that include UV exposure, gas sensing and temperature. Our measurements yielded a carrier mobility of up to $3000 \text{ cm}^2/\text{V-s}$ for some devices. Exposure to UV dopes graphene in a controlled manner. The doping level could be maintained indefinitely in vacuum or could be completely reversed by slight heating in air without loss of device performance. The FET's were also tested at different temperatures with little change in the transconductance response. Exposure to ammonia gas *n*-doped graphene while exposure to NO_2 *p*-doped it.

3:42PM D37.00007 Electronic Structure Properties of Graphene/Boron Nitride Layered Systems¹, MAX PETULANTE, University of Maryland, NAM LE, LILIA WOODS, University of South Florida — We explore the properties of systems composed of two or three layers of graphene and hexagonal boron nitride (hBN) using the Vienna Ab-Initio Simulation Package (VASP), a software package for performing first principles simulations based on density functional theory (DFT). Particular attention is given to the contribution of inter-layer dispersion interactions, which are modeled within VASP by the “DFT-D2” method of Grimme. We obtain the binding and van der Waals energies, and inter-layer separations for the most stable stacking configurations of each of the following systems: hBN/graphene, graphene/hBN/graphene, hBN/graphene/hBN, hBN/hBN/graphene, and graphene/graphene/hBN. We observe that the addition of hBN layers to graphene structures induces a band gap, ranging from 0.024 eV, for the graphene/hBN/graphene arrangement, to 0.16 eV, for the hBN/graphene/hBN arrangement. These results, specifically band gaps on the same order as those of silicon and germanium, indicate that graphene/hBN layered structures may have applications in electronics.

¹This work was supported by NSF REU program (award No DMR-1004873).

3:54PM D37.00008 Magnetoresistance of Strained Rare Earth Manganese Oxide Thin Films: Effect of Post-Deposition Thermal Treatment¹, TYLER GOEHRINGER, PARUL SRIVASTAVA, E. KEVIN TANYI, DAVID SCHAEFER, RAJESWARI KOLAGANI, Towson University — We have studied the effects of thermal treatment (annealing) on the properties of thin films of manganese oxide materials $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$ and $\text{La}_{0.67}\text{Ba}_{0.33}\text{MnO}_3$, which are known to exhibit colossal magnetoresistance (CMR) and an insulator to metal transition. These materials show properties which are desirable for applications such as magnetic sensors, bolometric infrared sensors, or field effect devices. Two properties of interest, magnetoresistance (MR) and insulator metal transition are especially sensitive to strain because of the relationship between the properties and the symmetry of the crystal. The properties are also sensitive to the oxygen stoichiometry of the film due to changes in the valence state of the manganese which determines the charge carrier density. Recent results from our laboratory have shown a large magnetoresistance in strained films grown on lattice mismatched substrates. The MR continues to increase with decreasing temperature in these films. In order to understand the contribution of strain to the observed MR behavior, in we employ ‘thermal annealing’ to allow for relaxation of strain. Annealing also serves to achieve the optimum oxygen stoichiometry. We will present the results of our annealing studies and their implications for understanding the MR in strained films.

¹TG acknowledges support from Undergraduate Research grants from Fisher College of Science and Mathematics and Towson University Undergraduate research Committee.

4:06PM D37.00009 Grain Boundaries In Thin Film Organic Semiconductors¹, CORTNEY BOUGHER, SHAWN HUSTON, EITAN LEES, Appalachian State University, JEREMY WARD, ABDUL OBAID, Wake Forest University, MARSHA LOTH, JOHN ANTHONY, University of Kentucky, OANA JURCHESCU, Wake Forest University, BRAD CONRAD, Appalachian State University — We utilize conductive atomic force microscopy (C-AFM) and tunneling atomic force microscopy (TUNA) to characterize dynamics of electronic transport across fluorinated triethylsilyl ethynyl anthradithiophene (diF-TES ADT) grain boundaries. The crystallization of diF-TES ADT grown on SiO_2 will be discussed and related to comparable molecules. The resulting voltage drop between individual crystals as a function of dopants will be discussed in terms of charge transport models and compared to current device work.

¹This research is supported by the Ralph E. Powe Junior Faculty Enhancement Award, Appalachian State University, the Appalachian State University Office of Student Research, and the NC Space Grant Consortium

4:18PM D37.00010 Formation of Interfacial Carbide Layers in Multilayer Ti/DLC Thin Films

JASEN SCARAMAZZA, ZACHARY BUCK, TYLER DONATO, BRITTANY CURRAN, C.A. LUNK, S.E. LOFLAND, J.D. HETTINGER, Department of Physics and Astronomy, Rowan University — Titanium (Ti)/Diamond-like-carbon (DLC) and Chromium (Cr)/Carbon (C) multilayer films were prepared on c-axis oriented single crystal sapphire (Al_2O_3) substrates using magnetron sputtering. Interfacial properties of the films were analyzed using x-ray reflectivity and scanning electron microscopy. When DLC is sputtered on a layer of Ti, an interfacial layer of titanium carbide (TiC) forms which is reported for the first time. Energy provided by the substrate bias necessary to facilitate DLC sp^3 bond formation is suspected of allowing TiC to synthesize in a thin layer before DLC forms. It was also found that DLC has difficulty forming on Cr. These results are relevant to biomedical applications where DLC is applied as a low friction/wear film that can be formed on the surface of implants composed mainly of titanium. Further investigation into the medical and tribological effects of TiC interfacial layers is suggested.

4:30PM D37.00011 Properties of Cr_2AlC MAX phase thin films prepared by reactive magnetron sputtering

ZACHARY BUCK, TYLER DONATO, CHRISTOPHER ROTELLA, CARL LUNK, S.E. LOFLAND, J.D. HETTINGER, Department of Physics and Astronomy, Rowan University — $\text{M}_{n+1}\text{AX}_n$ (MAX) phases, where n is 1, 2, and 3, M is an early transition metal, A is an A-group element, and X is either C or N, are ternary carbides with unique properties such as low density, easy machinability, and good oxidation resistance. The MAX phase Cr_2AlC is of particular interest for industrial applications to its excellent high-temperature oxidation resistance and relatively low synthesis temperature. We prepared Cr_2AlC thin films on c-axis oriented single crystal Al_2O_3 , glassy carbon and Si thermal oxide substrates using reactive magnetron sputtering as precursor materials for carbide-derived carbon (CDC) films for “on-chip” supercapacitors. Film deposition was optimized using elemental composition data obtained by WDXRF. Optimized films were characterized using XRD and scanning electron microscopy. It was found that textured Cr_2AlC films only form when the composition was Al-rich allowing the formation of a Cr_5Al_8 interfacial layer. As film composition was optimized, the interfacial layer did not form but the XRD peaks associated with the Cr_2AlC also decreased in magnitude. Extremely high-textured films were grown when a thin buffer layer of CrAl_2 was deposited on the substrate before depositing the Cr_2AlC films. This result suggests that Cr_2AlC films may not be ideal for CDC applications since the films may “lift-off” during conversion due to the existence of the naturally occurring buffer-layer.

4:42PM D37.00012 Fluid-like conducting regions in solid manganite thin films¹

RAFIYA JAVED, HYOUNGJEEN JEEN, AMLAN BISWAS, Department of Physics, University of Florida — Hole-doped manganese oxides (manganites) exhibit a fluid-phase separated state in which the conducting and ferromagnetic phase (FMM) behaves like a fluid embedded in an insulating background phase [1]. While the manganite remains a solid, its local electrical properties behave as a fluid. The fluid behavior of the conducting regions can be tested by observing the effect of an electric field on the shape of the FMM regions. This change in shape is expected to result in anisotropic resistivity. This property was tested by designing microstructures of the manganite film, which simplify the experiment by localizing the electric field to a region the size of the FMM regions. We are testing for possible magnetic anisotropy since the conducting regions are also ferromagnetic. We will also discuss the size effect on the magnetic properties. [1] Dhakal et. al., Phys. Rev. B 75, 092404 (2007)

¹NSF DMR 0804452

4:54PM D37.00013 The intrinsic coupling of polarization with terahertz pulses in a ferroelectric nanowire¹

KIMBERLY SCHULTZ, Carthage College, RYAN HERCHIG, KEVIN MCCASH, INNA PONOMAREVA, University of South Florida — We use first-principles-based molecular dynamics simulations to study the interaction of a terahertz (THz) radiation with polarization in a ferroelectric ultrathin nanowire made of a lead zirconate titanate alloy. In our computational experiment, a 12 nm thick nanowire is first annealed down to temperature of 300 K and then subjected to a wide variety of THz pulses which differ in width, strength and frequency. Such nanowire develops an electrical polarization along the nanowire axial direction which couples strongly with incoming THz radiation. The atomistic resolution of our computational experiments allows us to trace the intrinsic polarization response and energy propagation/dissipation mechanisms that occur at the scale of femtoseconds. Our simulations were carried out under MVE and MVT conditions and the results did not vary significantly between the two ensembles. We further explore how the unique features of such response could be utilized in an ultrafast THz nanoswitches.

¹This work was supported by NSF REU program (award No DMR-1004873)

5:06PM D37.00014 Magnetic Element Doped Transparent Conducting In_2O_3 Thin Films for Spintronic Applications¹

E. NAHLIK, A. LAUDARI, M. LANGHOFF, K. GHOSH, Department of Physics, Astronomy and Materials Science, Missouri State University, Springfield, MO 65897 — Tremendous research efforts are underway to exploit the property of electron spin in spintronics. Spintronic devices critically depend on the availability of a specific materials system for spin injection, manipulation and detection. Transition metal (Cr, Fe, or Co) doped wide band gap oxide semiconductors possess these properties. Indium oxide (In_2O_3) is a wide band gap semiconductor with unique optical and electrical properties. Here, we investigate the effect of Cr, Fe, or Co doping on electrical and optical properties of In_2O_3 thin films. Thin films have been grown on sapphire and quartz substrates using pulse laser deposition method. Electrical and optical characteristics have been measured using UV-VIS spectroscopy and magneto-transport techniques. Optical transmittance and electrical parameters such as carrier concentration and carrier mobility vary with growth parameters such as growth temperature of the substrate and oxygen pressure of the chamber. These details will be discussed during this presentation.

¹This work is supported by National Science Foundation (Award Number DMR-0907037)

Monday, February 27, 2012 2:30PM - 5:18PM —

Session D39 GQI: Quantum Protocols: Tomography, Communication, and Coding 109B

2:30PM D39.00001 Practical characterization of quantum devices without tomography

OLIVIER LANDON-CARDINAL, U. de Sherbrooke, STEVEN FLAMMIA, IQI, Caltech, MARCUS SILVA, Raytheon BBN Technologies, YI-KAI LIU, NIST, DAVID POULIN, U. de Sherbrooke — Quantum tomography is the main method used to assess the quality of quantum information processing devices, but its complexity presents a major obstacle for the characterization of even moderately large systems. Part of the reason for this complexity is that tomography generates much more information than is usually sought. Taking a more targeted approach, we develop schemes that enable (i) estimating the fidelity of an experiment to a theoretical ideal description, (ii) learning which description within a reduced subset best matches the experimental data. Both these approaches yield a significant reduction in resources compared to tomography. In particular, we show how to estimate the fidelity between a predicted pure state and an arbitrary experimental state using only a constant number of Pauli expectation values selected at random according to an importance-weighting rule. In addition, we propose methods for certifying quantum circuits and learning continuous-time quantum dynamics that are described by local Hamiltonians or Lindbladians.

2:42PM D39.00002 Quantum tomography with small number of copies: a simple estimator for qubit states, HUI KHOON NG, Centre for Quantum Technologies, National University of Singapore, BERTHOLD-GEORG ENGLERT, Centre for Quantum Technologies and the Department of Physics, National University of Singapore — In quantum tomography, one performs repeated measurements on N copies of a given but unknown state and constructs an estimator for the state from the gathered data. A common way of converting the data into an estimator is the maximum-likelihood (ML) method, where the estimator is the state with the largest probability of giving rise to the observed data. ML methods work well for large N , since the likelihood function for large N is sharply peaked around its maximum. For small N , however, there is a significant neighborhood of states around the maximum with nearly equal probability of giving rise to the data. One can then imagine using the likelihood function as a weight to construct an estimator as an average over states. This motivates the introduction of the “mean estimator,” also previously discussed for quantum tomography in the spirit of Bayesian estimation by Blume-Kohout [NJP 12, 043034(2010)]. Here, we extend the mean estimator for a classical die problem to an estimator for qubit states, and demonstrate its advantage over ML estimators. We also discuss a way of overcoming the common complaint of rank-deficiency in ML estimators for our estimator. This simple estimator should be useful as a convenient first estimate for any qubit tomography experiment.

2:54PM D39.00003 Joint quantum tomography of state preparation and measurements using only known quantum operations¹, MARCUS DA SILVA, Raytheon BBN Technologies, JAY GAMBETTA, IBM T.J. Watson Research Center — An important problem in quantum information is the complete characterization of quantum devices, which is usually referred to as “quantum tomography”. Quantum tomography procedures exist for the characterization of quantum states (quantum state tomography), operations (quantum process tomography) and measurements (quantum measurement tomography) — and each of these procedures can be performed using only product states, local unitary operations and local projective measurements. Here we consider the problem of jointly characterizing both the initial state as well as the measurement observable of a system using only well characterized quantum operations. We find that neither local unitaries nor local completely-positive trace-preserving maps are sufficient for obtaining a complete description of the state preparation and measurement of the system, and describe a scheme that uses non-unital trace-reducing physical maps to obtain such a description.

¹We acknowledge support from IARPA under Contract No. W911NF-10-1-0324

3:06PM D39.00004 Single shot quantum state estimation via continuous measurement in a strong back-action regime, ROBERT COOK, IVAN DEUTSCH, University of New Mexico — Quantum state reconstruction is a fundamental task in quantum information science. The standard approach employs many projective measurements on a series of identically prepared systems in order to collect sufficient statistics of an informationally complete set of observables. An alternative procedure is to reconstruct quantum state by performing weak continuous measurement collectively on an ensemble, while simultaneously applying time varying controls [1]. For known dynamics, the measurement history determines the initial state. In current implementations the shot noise of the probe dominates over projection noise so that measurement-induced backaction is negligible. We generalize this to the regime where quantum backaction can play a significant role, even for small numbers of particles. Using the framework of quantum filtering theory, we model the reconstruction of the state of a qubit through collective spin measurement via the Faraday interaction and magnetic field controls, and develop a maximum-likelihood estimate based on the Fisher information contained in the measurement record.

[1] A. Silberfarb and I. H. Deutsch, “Quantum-state reconstruction via continuous measurement,” Phys. Rev. Lett. 95, 030402 (2005).

3:18PM D39.00005 Beyond maximum-likelihood estimation, BERGE ENGLERT, Natl Univ of Singapore — When the estimators in quantum state tomography or quantum process tomography are obtained by maximizing the likelihood, which has become the method of choice, a unique result is not obtained if the data are informationally incomplete. By combining maximum-likelihood (ML) estimation with Jaynes’s maximum-entropy (ME) principle, a unique estimator can be determined, and this is possible by an efficient iterative algorithm. The resulting estimators, however, can have the familiar deficiencies of maximum-likelihood estimators. Alternative estimation procedures that avoid these drawbacks are wanted. The talk reports on MLME estimation as well as alternative approaches with a Bayesian touch. [References: Phys. Rev. Lett. 107 (2011) 020404; arXiv:1110.1202]

3:30PM D39.00006 Experimental Realization of Adaptive Qubit Tomography, DYLAN H. MAHLER, CQIQ and IOS, Department of Physics, University of Toronto, JOSHUA COMBES, Department of Physics and Astronomy, University of New Mexico, LEE A. ROZEMA, ARDAVAN DARABI, CQIQ and IOS, Department of Physics, University of Toronto, CHRIS FERRIE, Institute for Quantum Computing and Department of Applied Mathematics, University of Waterloo, AEPHRAIM STEINBERG, CQIQ and IOS, Department of Physics, University of Toronto, ROBIN BLUME-KOHOUT, Theoretical Division, Los Alamos National Lab and CQIC, University of New Mexico — In quantum state tomography, an informationally complete set of measurements is made on N identically prepared quantum systems and from these measurements the quantum state can be determined. In the limit as $N \rightarrow \infty$, the estimation of the state converges on the true state. The rate at which this convergence occurs depends on both the state and the measurements used to probe the state. To characterize the quality of a set of measurements the fidelity of the estimation with the true state, averaged over a prior distribution of states, is used as a figure of merit. It is known [1] that for states very close to the surface of the Bloch sphere, the average infidelity $(1 - F)$ goes down with a rate proportional to $\frac{1}{\sqrt{N}}$. It has also been shown that there exists a gap between collective measurement protocols and local measurement protocols, but that local *adaptive* measurement protocols can come close to saturating the collective measurement bound of $\frac{1}{\sqrt{N}}$ [2]. Here we present an experimental demonstration of one qubit tomography that achieves a rate of convergence of $\frac{1}{\sqrt{N}}$ with only a single adaptive step and local measurements.

[1] Phys. Rev. A 78, 052122 (2008)

[2] Phys. Rev. Lett. 97, 130501 (2006)

3:42PM D39.00007 Scalable estimation of computational gate fidelities, EASWAR MAGESAN, University of Waterloo-Institute for Quantum Computing, JAY GAMBETTA, IBM T.J. Watson Research Center — Scalable methods for characterizing the noise affecting a quantum system are of significant interest in theoretical and experimental quantum information theory. Since completely characterizing the noise is exponentially hard in the number of qubits comprising the system, there has been significant effort in developing scalable methods for characterizing particular features of the noise. In particular, “randomized benchmarking” has been shown to be a robust and scalable method for estimating the average error rate over the set of quantum computational gates. We propose a new protocol that allows for benchmarking individual quantum gates rather than the average over the entire set. The protocol consists of a mixture of deterministic and random applications of computational gates and is shown to be scalable in the number of qubits comprising the system. The method is robust against state preparation and measurement errors and is valid provided the average variation of the noise over the gate set can be sufficiently bounded.

3:54PM D39.00008 Quantum controlled paths for perfect discrimination of no-signalling channels, GIULIO CHRIBELLA, Perimeter Institute — A no-signalling channel transforming systems in Alice’s and Bob’s local laboratories is compatible with two different causal structures: one where Alice’s output can be sent to Bob’s input and another where Bob’s output can be sent to Alice’s input. I show that a quantum superposition of circuits operating within these two causal structures enables the perfect discrimination between two no-signalling channels that could not be perfectly distinguished by any ordinary circuit [1]. Such a quantum superposition can be in principle achieved by introducing a qubit that controls the path followed by quantum systems, routing them to different ports of the given no-signalling channel.

[1] G. Chiribella, *Perfect discrimination of no-signalling channels via quantum superposition of causal structures*, arXiv:1109.5154.

4:06PM D39.00009 Experimental characterization of coherent dynamics in a spin chain, CHANDRASEKHAR RAMANATHAN, Dartmouth College, JAMES LEE, Oxford University, PAOLA CAPPELLARO, Massachusetts Institute of Technology, LORENZA VIOLA, Dartmouth College, DAVID CORY, Institute for Quantum Computing and University of Waterloo — We experimentally characterize the coherent room-temperature magnetization dynamics of a spin chain evolving under an effective double-quantum Hamiltonian. Our results indicate that a localized magnetic moment travels down the chain with a group velocity of $6.04 \pm 0.38 \mu\text{m/s}$, corresponding to coherent transport over $N \approx 26$ spins on the timescale of the experiment. We also characterize the influence of the ends of the chains on the magnetization dynamics. Our results are in excellent agreement with a nearest-neighbor-coupled analytical model that predicts that the dynamics are restricted to a Liouville space that only grows quadratically with the number of spins. This suggests that the long-range couplings present in the experimental system only cause a slow leakage out of the subspace. As the double-quantum Hamiltonian is related to the standard one-dimensional XX Hamiltonian by a similarity transform, our results can be directly extended to XX quantum spin chains, which have been extensively studied in the context of both quantum magnetism and quantum information processing

4:18PM D39.00010 Experimental Monte Carlo Quantum Process Certification, LARS STEFFEN, ARKADY FEDOROV, MATTHIAS BAUR, ETH Zurich, MARCUS PALMER DA SILVA, Raytheon BBN Technologies, ANDREAS WALLRAFF, ETH Zurich — Experimental implementations of quantum information processing have now reached a state, at which quantum process tomography starts to become impractical, since the number of experimental settings as well as the computational cost of the post processing required to extract the process matrix from the measurements scales exponentially with the number of qubits in the system. In order to determine the fidelity of an implemented process relative to the ideal one, a more practical approach called Monte Carlo quantum process certification was proposed in Ref. [1]. Here we present an experimental implementation of this scheme in a circuit quantum electrodynamics setup. Our system is realized with three superconducting transmon qubits coupled to a coplanar microwave resonator which is used for the joint-readout of the qubit states. We demonstrate an implementation of Monte Carlo quantum process certification and determine the fidelity of different two- and three-qubit gates such as CPHASE-, CNOT-, 2CPHASE- and Toffoli-gates. The obtained results are compared with the values obtained from conventional process tomography and the errors of the obtained fidelities are determined.

[1] M. P. da Silva, O. Landon-Cardinal and D. Poulin, arXiv:1104.3835(2011)

4:30PM D39.00011 Quantum filtering one bit at a time¹, JASON RALPH², NEIL OXTOBY, University of Liverpool, UK — We consider the purification of a quantum state using the information obtained from a continuous measurement record, where the classical measurement record is digitized to a single bit per measurement after the measurements have been made. Analysis indicates that efficient and reliable state purification is achievable for one- and two-qubit systems. We also consider quantum feedback control based on the discrete one-bit measurement sequences.

¹Financial support from UK EPSRC grant number EP/G007918

²Member of Institute of Physics (UK)

4:42PM D39.00012 New results in fault-tolerant quantum computing¹, GERALD GILBERT, YAAKOV WEINSTEIN, MITRE Quantum Information Science Group — We compare the accuracy of two methods used to construct a logical zero state appropriate for the $[[7,1,3]]$ CSS quantum error correction code in a non-equiprobable Pauli operator error environment. The first method is to apply error correction, via syndrome measurement, on seven physical qubits all in the state zero, using four-qubit Shor states to implement the syndrome measurements. The second method is to directly implement the $[[7,1,3]]$ encoding gate sequence. We find surprising results that show that even at the most basic level there is still much to be learned about achieving fault tolerance.

¹The authors are grateful for the support provided by the MITRE Innovation Program.

4:54PM D39.00013 On the Use of Shor States for the $[[7,1,3]]$ Quantum Error Correcting Code, YAAKOV WEINSTEIN, MITRE, SIDNEY BUCHBINDER, California Institute of Technology — We explore the effect of Shor state construction methods on logical state encoding and quantum error correction for the $[[7,1,3]]$ Calderbank-Shor-Steane quantum error correction code in a nonequiprobable error environment. We determine the optimum number of verification steps to be used in Shor state construction and whether Shor states without verification are usable for practical quantum computation. These results are compared to the same processes of encoding and error correction where Shor states are not used. We demonstrate that the construction of logical zero states with no first order error terms may not require the complete edifice of quantum fault tolerance. With respect to error correction, we show for a particular initial state that error correction using a single qubit for syndrome measurement yields a similar output state accuracy to error correction using Shor states as syndrome qubits. In addition, we demonstrate that error correction with Shor states has an inherent sensitivity to bit-flip errors.

5:06PM D39.00014 Quantum codes with low weight stabilizers¹, ALEXEY A. KOVALEV, Department of Physics & Astronomy, University of California, Riverside, California 92521, USA, ILYA DUMER, Department of Electrical Engineering, University of California, Riverside, California 92521, USA, LEONID P. PRYADKO, Department of Physics & Astronomy, University of California, Riverside, California 92521, USA — We study quantum cyclic stabilizer codes whose stabilizer can be always defined by one or two stabilizer generators. Our main goal is to construct low-weight stabilizer generators that can yield quantum codes with high code rate and simple error correction. To do so, we apply the classical quaternary representation of stabilizer codes and extend our recent study of one-generator cyclic codes [1]. For any stabilizer generator of weight four or five, we formulate a necessary and sufficient condition for its commutativity. We then proceed with a design of additive cyclic codes with such generators. In some cases, we also extend our commutativity condition and code design to generators of weight six. In particular, quantum cyclic codes with stabilizers of weight four are mapped to the generalized toric codes. Here we also extend the notion of toric codes using a translationally invariant generator and periodic boundary conditions on a two dimensional lattice. Some of our numerically constructed codes can be redefined by means of Code Word Stabilized (CWS) representation [1] as quantum versions of repetition codes. We particularly concentrate on codes with a fixed nonzero rate for which the minimum distance asymptotically grows as the blocklength grows.

[1] arXiv:1108.5490v1

¹ARO grant W911NF-11-1-0027 (LP and ID), NSF grant 1018935 (LP)

Monday, February 27, 2012 2:30PM - 5:18PM —

Session D40 DBIO GSNP: Focus Session: Systems Biology and Biochemical Networks I 156A

2:30PM D40.00001 Optimal Information Processing in Biochemical Networks, CHRIS WIGGINS, Columbia University — A variety of experimental results over the past decades provide examples of near-optimal information processing in biological networks, including in biochemical and transcriptional regulatory networks. Computing information-theoretic quantities requires first choosing or computing the joint probability distribution describing multiple nodes in such a network — for example, representing the probability distribution of finding an integer copy number of each of two interacting reactants or gene products while respecting the 'intrinsic' small copy number noise constraining information transmission at the scale of the cell. I'll give an overview of some recent analytic and numerical work facilitating calculation of such joint distributions and the associated information, which in turn makes possible numerical optimization of information flow in models of noisy regulatory and biochemical networks. Illustrating cases include quantification of form-function relations, ideal design of regulatory cascades, and response to oscillatory driving.

3:06PM D40.00002 Adaptation at the output of the chemotaxis signaling pathway¹, JUNHUA YUAN, RICHARD BRANCH, BASARAB HOSU, HOWARD BERG, Department of Molecular and Cellular Biology, Harvard University — The chemotaxis signaling pathway allows bacterial cells to sense and respond to changes in concentrations of chemical attractants or repellents. In *E. coli*, the machinery required for bacterial chemotaxis includes two large membrane-embedded multiprotein complexes, one that processes input (receptor clusters) and the other that generates output (flagellar motors). These complexes are coupled by diffusion of a small phosphorylated cytoplasmic protein, CheY-P, which binds to the flagellar motors, increasing the probability that they spin clockwise. Receptor output (the steady-state concentration of CheY-P) varies from cell to cell. However, the motor is ultrasensitive, with a narrow [CheY-P] operating range. How might the receptor output and motor input be matched? By combining various techniques such as FRET, single-motor TIRF, and single-motor bead assay, we showed that the motor shifts its operating range to match the receptor output by changing its composition. The number of FliM subunits in the C-ring increases in response to a decrement in the concentration of CheY-P, increasing motor sensitivity. Such adaptive remodeling is likely to be a common feature in the operation of many molecular machines.

¹This work was supported by National Institutes of Health Grant AI016478.

3:18PM D40.00003 The energy cost of accurate adaptation in networks with incoherent type-1 feed-forward loop, GANHUI LAN, YUHAI TU, IBM T. J. Watson Research Center — The incoherent type-1 feed forward loop (I1-FFL) is a common regulatory motif in many biochemical networks, some of which are responsible for accurate sensory adaptation. In this work, we analyze the sensitivity and adaptation function of the I1-FFL type enzymatic reaction networks. We show that detailed balance is broken in I1-FFL and continuous energy dissipation is needed to improve both the sensitivity and the adaptation accuracy of the network. Our study revealed a relation between the performance improvement and the energy dissipation rate. We find that this energy-assisted improvement is bounded (limited) by intrinsic properties of the molecular reaction system. The performance-energy relation in I1-FFL is similar to the recently obtained Energy-Speed-Accuracy relation in networks with negative-feedback-loop, another key motif for accurate sensory adaptation.

3:30PM D40.00004 Noise places constraints on eukaryotic gradient sensing and chemotaxis¹, BO HU, DANNY FULLER, WILLIAM LOOMIS, University of California - San Diego, WEN CHEN, University of Maryland - College Park, WOUTER-JAN RAPPEL, HERBERT LEVINE, University of California - San Diego — Chemotaxis is characterized by the directional cell movement following external chemical gradients. It plays a crucial role in a variety of biological processes including neuronal development, wound healing and cancer metastasis. Ultimately, the accuracy of gradient sensing is limited by the fluctuations of signaling components, e.g. the stochastic receptor occupancy on cell surface. We use concepts and techniques from statistical physics, estimation theory, and information theory to quantify the stochastic and nonlinear information processing in eukaryotic chemotaxis. We mainly address the following questions: (1) What are the physical limits of eukaryotic spatial gradient sensing? (2) How to characterize the movements of chemotactic cells? (3) How much gradient information can be reliably gained by a chemotactic cell? By answering those questions, we expect to derive new insights for general biological signal processing systems.

¹This work was supported by NIH Grant No. P01 GM078586 and NSF Grant No. PHY-0822283.

3:42PM D40.00005 Process-driven inference of biological network structure: feasibility, minimality, and multiplicity¹, CHEN ZENG, Department of Physics, The George Washington University, Washington, DC 20052 — For a given dynamic process, identifying the putative interaction networks to achieve it is the inference problem. In this talk, we address the computational complexity of inference problem in the context of Boolean networks under dominant inhibition condition. The first is a proof that the feasibility problem (is there a network that explains the dynamics?) can be solved in polynomial-time. Second, while the minimality problem (what is the smallest network that explains the dynamics?) is shown to be NP-hard, a simple polynomial-time heuristic is shown to produce near-minimal solutions, as demonstrated by simulation. Third, the theoretical framework also leads to a fast polynomial-time heuristic to estimate the number of network solutions with reasonable accuracy. We will apply these approaches to two simplified Boolean network models for the cell cycle process of budding yeast (Li 2004) and fission yeast (Davidich 2008). Our results demonstrate that each of these networks contains a giant backbone motif spanning all the network nodes that provides the desired main functionality, while the remaining edges in the network form smaller motifs whose role is to confer stability properties rather than provide function. Moreover, we show that the bioprocesses of these two cell cycle models differ considerably from a typically generated process and are intrinsically cascade-like.

¹The work is supported by National Science Foundation (NSF) Grant CMMI-0941228

4:18PM D40.00006 Communication channels between membrane bound proteins, JAMES SETHNA, BENJAMIN MACHTA, Department of Physics, Cornell University, SARAH VEATCH, Department of Biophysics, University of Michigan, Ann Arbor — Much of what might be called biological computation takes place on the plasma membrane, a 2D liquid composed of a diverse soup of lipids and embedded proteins. Motivated by the recent discovery that these membranes seem to be tuned close to a 2D liquid-liquid critical point, we set out to understand the different channels through which membrane bound proteins can communicate. Diffusing proteins can carry out reactions like phosphorylation when they come in contact with each other. Near criticality, proteins can also exert long-ranged critical Casimir forces on one another by coupling to the local composition order parameter. By modulating the growth and breakdown of the rigid cytoskeleton, they can direct forces on even more distant regions. In addition, proteins can control the release and production of second messengers that diffuse either through the bulk, or in the plane of the membrane itself. By making simple models for these processes we bound functional measures for them as communication channels. These include information theoretic measures of bandwidth, as well as physical measures of energetic efficiency and speed. Our results will likely shed light on the functional role of clustering and other collective behaviors often seen in experiments.

4:30PM D40.00007 Maximum entropy principle for predicting response to multiple-drug exposure in bacteria and human cancer cells, KEVIN WOOD, SATOSHI NISHIDA, Harvard University, EDUARDO SONTAG, Rutgers University, PHILIPPE CLUZEL, Harvard University — Drugs are commonly used in combinations larger than two for treating infectious disease. However, it is generally impossible to infer the net effect of a multi-drug combination on cell growth directly from the effects of individual drugs. We combined experiments with maximum entropy methods to develop a mechanism-independent framework for calculating the response of both bacteria and human cancer cells to a large variety of drug combinations comprised of anti-microbial or anti-cancer drugs. We experimentally show that the cellular responses to drug pairs are sufficient to infer the effects of larger drug combinations in gram negative bacteria, *Escherichia coli*, gram positive bacteria, *Staphylococcus aureus*, and also human breast cancer and melanoma cell lines. Remarkably, the accurate predictions of this framework suggest that the multi-drug response obeys statistical rather than chemical laws for combinations larger than two. Consequently, these findings offer a new strategy for the rational design of therapies using large drug combinations.

4:42PM D40.00008 Robust regulation of oscillatory Min-protein patterns¹, JACOB HALATEK, ERWIN FREY, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München — Robust spatial patterning was crucial just from the beginning of cellular evolution, and is key to the development of multicellular organisms. In *E. Coli*, the oscillatory pole-to-pole dynamics of MinCDE proteins functionality prevent improper cell divisions apart from midcell. Min-oscillations are characterized by the remarkable robustness with which spatial patterns dynamically adapt to variations of cell geometry. Moreover, adaption, and therefore proper cell division, is independent of temperature. These observations raise fundamental questions about the underlying core mechanisms, and about the role of spatial cues. With a conceptually novel and universal approach to cellular geometries, we introduce a robust model based on experimental data, consistently explaining the mechanisms underlying pole-to-pole, striped and circular patterns, as well as the observed temperature-dependence. Contrary to prior conjectures, the model predicts that MinD and cardiolipin domains are not colocalized. The key mechanisms are transient sequestration of MinE, and highly canalized transfer of MinD between polar zones. MinD channeling enhances midcell localization and facilitates stripe formation, revealing the potential optimization process from which robust Min-oscillations originally arose.

¹This project has been supported by the German Excellence Initiative via the program “Nanosystems Initiative Munich” (NIM).

4:54PM D40.00009 Mathematical Analysis of Biomolecular Network Reveals Connections Between Diseases¹, GUANYU WANG, The George Washington University — Connections between cancer and metabolic diseases may consist in the complex network of interactions among a common set of biomolecules. By applying singularity and bifurcation analysis, the phenotypes constrained by the AKT signaling pathway are identified and mapped onto the parameter space, which include cancer and certain metabolic diseases. By considering physiologic properties (sensitivity, robustness and adaptivity) the AKT pathway must possess in order to efficiently sense growth factors and nutrients, the region of normal responses is located. The analysis illuminates the parameter space and reveals system-level mechanisms in regulating biological functions (cell growth, survival, proliferation and metabolism) and how their deregulation may lead to the development of diseases. The analytical expressions summarize the synergistic interactions among many molecules, which provides valuable insights into therapeutic interventions.

¹This work was supported by an Institutional Research grant (IRG-08- 091-01) from the American Cancer Society to The George Washington University Cancer Institute.

5:06PM D40.00010 Modeling the mammalian circadian clock, CRAIG JOLLEY, HIROKI UEDA, RIKEN Center for Developmental Biology, Laboratory for Systems Biology — In biology, important processes often depend on a temporal schedule. The 24-hour periodicity of solar illumination caused by the earth's rotation has consequences for environmental factors such as temperature and humidity as well as ecological factors such as the presence of food, predators, or potential mates. As a result, many organisms have evolved to develop a circadian clock that allows them to anticipate these environmental changes in the absence of direct temporal cues. In recent years, extensive efforts have been made to deconstruct the biological clockwork from various organisms, develop mathematical models of circadian function, and construct synthetic analogues to test our understanding. My present work has two major foci. First, we have used regulatory principles revealed by recent experimental work to construct a model of the core genetic oscillator of the mammalian circadian system that captures key system-level behaviors. Second, we are exploring the possibility of a post-translational phosphorylation-based oscillator that is coupled to the core oscillator, conferring enhanced robustness and stability on the complete system. A simple model of this post-translational oscillator reveals key design constraints that must be satisfied by any such oscillator.

Monday, February 27, 2012 2:30PM - 4:54PM –

Session D42 DBIO: Focus Session: Physics of Cancer I – Evolution and Resistance 156C

2:30PM D42.00001 Drug Resistance and the Kinetics of Metastatic Cancer¹, KRASTAN B. BLAGOEV, National Science Foundation — Most metastatic cancers after initial response to current drug therapies develop resistance to the treatment. We present cancer data and a theory that explains the observed kinetics of tumor growth in cancer patients and using a stochastic model based on this theory we relate the kinetics of tumor growth to Kaplan-Meier survival curves. The theory points to the tumor growth rate as the most important parameter determining the outcome of a drug treatment. The overall tumor growth or decay rate is a reflection of the balance between cell division, senescence and apoptosis and we propose that the deviation of the decay rate from exponential is a measure of the emergence of drug resistance. In clinical trials the progression free survival, the overall survival, and the shape of the Kaplan-Meier plots are determined by the tumor growth rate probability distribution among the patients in the trial. How drug treatments modify this distribution will also be described. At the end of the talk we will discuss the connection between the theory described here and the age related cancer mortality rates in the United States.

¹This work was supported by the National Science Foundation. Any opinion, finding, and conclusions or recommendations expressed in this material; are those of the authors and do not necessarily reflect the views of the National Science Foundation.

3:06PM D42.00002 Lattice Boltzmann simulations of lymphatic pumping, CHRISTIAN KUNERT, TIM P. PADERA, LANCE L. MUNN, Massachusetts General Hospital/ Harvard medical school — Lymphatic flow plays an important role in the progress of many diseases, including lymphedema and metastasis. However lymphatic pumping and flow is poorly understood. Here, we present a computer model that is based on biological observations of lymphatic pumping. Fluid flow is simulated by a D2Q9 lattice Boltzmann model. The boundary of the vessels moves according to shear-induced nitric oxide production, and wall motion transfers momentum to the fluid to induce flow. Because the model only includes local properties, it can be highly parallelized. In our case we utilize graphic processors (GPU) to achieve high performance computation. We show that the model provides stable pumping over a wide range of parameter values, with optimum flow achieved in the biological ranges. Furthermore, we investigate the efficiency by analyzing the flow rate and pumping frequency in order to compare the behavior of the model with existing in vivo data.

3:18PM D42.00003 Mechanical and Structural Changes of the Pericellular Coat during Cell Proliferation, LOUIS T. MCLANE, School of Physics, Georgia Institute of Technology, ANNA GRANQVIST, The Renal Center, The Wallenberg Laboratory for Cardiovascular Research, Sahlgrenska University Hospital, PATRICK CHANG, ANTHONY KRAMER, JENNIFER E. CURTIS, School of Physics, Georgia Institute of Technology — The organization of a hyaluronan and proteoglycan-rich pericellular coat at the cell surface has been shown to facilitate cell migration and mitosis. These several microns thick, swollen grafted polymer matrices are directly correlated with efficient proliferation, migration, and in extreme cases have been associated with the metastatic spread of cancer. For example, hyaluronan synthesis is enormously increased when oncogenic viruses transform fibroblasts and elevated levels of hyaluronan are associated with the hyperproliferative and malignant phenotypes in melanoma and various carcinomas. Studies on cancer cell lines have shown that overproduction of hyaluronan and excess proteoglycan enhances their anchorage independent growth, tumorigenicity and metastatic potential. It has long been suspected that the mechanical and structural changes associated with enhanced pericellular matrix are in part responsible for these effects. Here we present measurements of pericellular coat mechanics and structure, investigating how it changes with cell cycle as well as increased or decreased proteoglycan content.

3:30PM D42.00004 Can low energy electrons lead to strand breaks in DNA under realistic conditions?, JORGE KOHANOFF, MAEVE SMYTH, Queens University Belfast — It is widely accepted that low energy electrons produced by ionizing radiation play an important role in causing DNA damage [B. Boudaïffa et al., *Science* **287**, 1658 (2000)]. Understanding the behaviour of DNA components in the condensed phase due to such electrons is a fundamental step towards modelling this damage within a realistic environment. Here we present a computational study of the effect of low energy electrons in condensed phase models of solvated DNA fragments. First we show that excess electrons, which are initially found delocalized, quickly localize around the nucleobases within a 15 fs time scale. Energies and time scales are comparable for each of the bases [M. Smyth and J. Kohanoff, *Phys. Rev. Lett.* **106**, 238108 (2011)]. The phosphodiester bond C_{3'}-O_{3'}, which under normal conditions is very stable, weakens significantly upon electron attachment both, in the gas and in the condensed phase. Computation of free energy profiles show that barriers for bond cleavage are in the region of 5-8 kcal/mol for all the solvated nucleotides, thus suggesting that this kind of event is quite likely at ambient temperature. This supports the notion that ionizing radiation can actually lead to DNA strand breaks in the physiological environment.

3:42PM D42.00005 Emergence of fractal behavior and other changes of cell surface during malignant transformation: AFM study of human cervical epithelial cells, MAXIM DOKUKIN, NATALIYA GUZ, CRAIG WOODWORTH, IGOR SOKOLOV, Clarkson University — Fractal behavior, self-similarity when zooming in or out, is frequently found in natural patterns emerged from chaos or any far from equilibrium systems. While expected and observed for tissues, the emergence of fractal behavior associated with malignant transformations was not observed at the level of single cell. Here report on the appearance of fractal behavior when normal human cervical epithelial cells become malignant. This was found by analyzing the adhesion maps imaged with AFM working in HarmoniX mode. Normal and malignant (a mix of cancerous and precancerous) cells were enzymatic only extracted from cervical tissue of healthy individuals and cancer patients, respectively. A surprising 100% discrimination of malignant and normal cells was observed. Although we previously reported differences in surface (brush) layer of cancer cells, the unambiguous quantitative divergence of the fractal behavior of the adhesion maps is a surprise (in particular, when compared to no difference found in the regular AFM images). The nature of the observed difference in the adhesion behavior will be discussed. These results may suggest that the fractal dimensionality can be treated as a new potential “physicomarker” for detection of individual cervical cancer cells.

3:54PM D42.00006 Improved survival in rats with glioma using MRI-guided focused ultrasound and microbubbles to disrupt the blood-brain barrier and deliver Doxil, MUNA ARYAL, BWH, Harvard Medical School/Department of Physics, Boston College, YONG ZHI ZHANG, NATALIA VYKHODTSEVA, JUYOUNG PARK, CHANIKARN POWER, NATHAN MCDANNOLD, Department of Radiology, BWH, Harvard Medical School — Blood-brain-barrier (BBB) limits the transportation of most neuropeptides, proteins (enzymes, antibodies), chemotherapeutic agents, and genes that have therapeutic potential for the treatment of brain diseases. Different methods have been used to overcome this limitation, but they are invasive, non-targeted, or require the development of new drugs. We have developed a method that uses MRI-guided focused ultrasound (FUS) combined with circulating microbubbles to temporarily open BBB in and around brain tumors to deliver chemotherapy agents. Here, we tested whether this noninvasive technique could enhance the effectiveness of a chemotherapy agent (Doxil). Using 690 kHz FUS transducer and microbubble (Definity), we induced BBB disruption in intracranially-implanted 9L glioma tumors in rat's brain in three weekly sessions. Animals who received BBB disruption and Doxil had a median survival time of 34.5 days, which was significantly longer than that found in control animals which is 16, 18.5, 21 days who received no treatment, BBB disruption only and Doxil only respectively. This work demonstrates that FUS technique has promise in overcoming barriers to drug delivery, which are particularly stark in the brain due to the BBB.

4:06PM D42.00007 Insights into protein – DNA interactions, stability and allosteric communications: A computational study of MutS-DNA recognition complexes¹, LACRAMIOARA NEGUREANU, FREDDIE SALSBURY, Wake Forest University — DNA mismatch repair proteins (MMR) maintain genetic stability by recognizing and repairing mismatched bases and insertion/deletion loops mistakenly incorporated during DNA replication, and initiate cellular response to certain types of DNA damage. The most abundant MMR mismatch-binding factor in eukaryotes, MutS, recognizes and initiates the repair of base-base mismatches and small insertion/deletions. We performed molecular dynamics simulations on mismatched and damaged MutS-DNA complexes. A comprehensive DNA binding site analysis of relevant conformations shows that MutS proteins recognize the mismatched and platinum cross-linked DNA substrates in significantly different modes. Distinctive conformational changes associated with MutS binding to mismatched and damaged DNA have been identified and they provide insight into the involvement of MMR proteins in DNA-repair and DNA-damage pathways. Stability and allosteric interactions at the heterodimer interface associated with the mismatch and damage recognition step allow for prediction of key residues in MMR cancer-causing mutations. A rigorous hydrogen bonding analysis for ADP molecules at the ATPase binding sites is also presented. A large number of known MMR cancer causing mutations among the residues were found.

¹ Acknowledge support from the NIH NCI.

4:18PM D42.00008 Glycoprotein Mucin Molecular Brush on Cancer Cells and its Correlation with Resistance Against Drug Delivery, XIN WANG, AALOK SHAH, ROBERT CAMPBELL, KAI-TAK WAN, Northeastern University — Uptake of cytotoxic drugs by typical tumor cells is limited by the dense dendritic network of oligosaccharide mucin chains that forms a mechanical barrier. Atomic force microscopy is used to directly measure the force needed to pierce the mucin layer to reach the cell surface. Measurements are analyzed by deGennes' steric repulsion theory. Multi-drug resistant ovarian tumor cells shows significantly larger penetration load compared to the wild type. A pool of pancreatic, lung, colorectal, and breast cells are also characterized. The chemotherapeutic agent, benzyl- α -GalNAc, for inhibiting glycosylation is shown to be effective in reducing the mechanical barrier.

4:30PM D42.00009 Bcl-2 apoptosis proteins, mitochondrial membrane curvature, and cancer, GHEE HWEE LAI, NATHAN SCHMIDT, Physics, UIUC, LORI SANDERS, Materials Science and Engineering, UIUC, ABHIJIT MISHRA, GERARD WONG, Bioengineering, UCLA, OLENA IVASHYNA, ERIC CHRISTENSON, PAUL SCHLESINGER, Cell Biology and Physiology, WUSTL Sch. of Medicine, KIYOTAKA AKABORI, CHRISTIAN SANTANGELO, Physics, U. of Massachusetts — Critical interactions between Bcl-2 family proteins permeabilize the outer mitochondrial membrane, a common decision point early in the intrinsic apoptotic pathway that irreversibly commits the cell to death. However, a unified picture integrating the essential non-passive role of lipid membranes with the contested dynamics of Bcl-2 regulation remains unresolved. Correlating results between synchrotron x-ray diffraction and microscopy in cell-free assays, we report activation of pro-apoptotic Bax induces strong pure negative Gaussian membrane curvature topologically necessary for pore formation and membrane remodeling events. Strikingly, Bcl-xL suppresses not only Bax-induced pore formation, but also membrane remodeling by disparate systems including cell penetrating, antimicrobial or viral fusion peptides, and bacterial toxin, none of which have BH3 allosteric domains to mediate direct binding. We propose a parallel mode of Bcl-2 pore regulation in which Bax and Bcl-xL induce antagonistic and mutually interacting Gaussian membrane curvatures. The universal nature of curvature-mediated interactions allows synergy with direct binding mechanisms, and potentially accounts for the Bcl-2 family modulation of mitochondrial fission/fusion dynamics.

4:42PM D42.00010 Drift, draft, waves, and ratcheting: evolutionary models of cancer progression, CHRISTOPHER MCFARLAND¹, Harvard University, KIRILL KOROLEV², LEONID MIRNY³, MIT — Recent evidence has found that many mutations are detrimental to tumor growth in cancer. These mutations, called *passenger mutations*, are distinguished from the better known cancer-causing *driver mutations*, which increase a tumor cell's proliferative capacity. How passenger mutations arise, despite selection against them, is not well understood nor fully explained by existing theory. Here, we extend several population genetics models to explain their accumulation in a precancerous population of cells and compare our findings against stochastic simulations. We find that passenger mutations alter and can avert progression to cancer. The probability of cancer depended heavily, and non-monotonically, on both the deleteriousness and rate of mutations. Counter-intuitively, high mutation rates decrease the likelihood of cancer—a finding recently corroborated by clinical data[1]. Our models suggest that therapies exploiting passenger mutations can avert cancer and may be more effective than targeting driver mutations.

1. Birkbak, N.J., et al., *Paradoxical relationship between chromosomal instability and survival outcome in cancer*. Cancer Res, 2011. **71**(10): p. 3447-52.

¹PhD Candidate in Biophysics

²Pappalardo Fellow in Physics

³Professor of Health Sciences and Technology and Physics; Broad Institute Associate Member

Monday, February 27, 2012 2:30PM - 5:30PM –

Session D43 DCMP GSNP: Invited Session: Recent Advances in the Physics of Fractures 157AB

2:30PM D43.00001 Failure of molecules, bones, and the Earth itself, SINAN KETEN, Northwestern University — Materials fail by recurring rupture and shearing of interatomic bonds at microscopic, molecular scales, leading to disintegration of matter at macroscale, and a loss of function. In this talk, the state-of-the-art of investigations on failure mechanisms in materials will be presented, in particular focusing on atomistic origin of deformation and fracture, and the relationships between molecular mechanics and macroscale behavior. Simple examples of fracture phenomena are used to illustrate the significance and impact of material failure on our daily lives. Based on case studies, mechanisms of failure of a wide range of materials are discussed, ranging from tectonic plates to rupture of single molecules, and an explanation on how atomistic simulation can be used to complement experimental studies and theory to provide a novel viewpoint in the analysis of complex systems is provided. Biological protein materials are used to illustrate how extraordinary properties are achieved through the utilization of intricate structures where the interplay of weak and strong chemical bonds, size and confinement effects, and hierarchical features play a fundamental role. This leads to a discussion of how even the most robust biological material systems fail, leading to diseases that arise from structural and mechanical alterations at molecular, cellular, and tissue levels. New research directions in the field of materials failure and materials science are discussed and the impact of improving the current understanding of materials failure for applications in nanotechnology, biotechnology, medicine as well as the built environment.

3:06PM D43.00002 Fast fracture in slow motion: Dynamic fracture and the effect of near-tip elastic nonlinearities in brittle gels, JAY FINEBERG, The Racah Institute of Physics, The Hebrew University of Jerusalem — We present recent results of fracture experiments in poly-acrylamide gels [1]. These gels are soft polymers in which the characteristic sound speeds are on the order of a few meters/sec - thereby slowing down fracture dynamics by 3 orders of magnitude. We first show that the dynamics of rapid cracks are universal; the fracture of gels exhibits characteristic features that are identical with those seen in "classic" materials such as glass. These include:

- Excellent quantitative agreement with the two different equations of motion for single dynamic cracks predicted by Linear Elastic Fracture Mechanics (LEFM) – each for different classes of loading conditions.
- The same branching instabilities, localized waves confined to the crack front, and the characteristic structure formed on the resulting fracture surface as observed in "standard" amorphous brittle materials, such as soda-lime glass.

We utilize the "slow motion" inherent in the fracture of gels to experimentally and theoretically investigate the structure of the deformation fields that surround the tip of highly dynamic cracks. We find that:

- The singular fields predicted by LEFM change their structure due to nonlinear elastic effects that dominate the near-tip region [3].
- This non-linear elastic region provides a quantitative explanation for the oscillatory instability of cracks [2,4] as their speed approaches the Rayleigh wave speed.

These results provide a quantitative first-principles description of how elastic nonlinearity influences the rapid dynamics of a crack.

[1] A. Livne, G. Cohen, and J. Fineberg, Physical Rev. Lett. **94**, 224301 (2005); T. Goldman, A. Livne, and J. Fineberg, Physical Rev. Lett. **104**, 11430 (2010).

[2] A. Livne, O. Ben-David, and J. Fineberg, Phys. Rev. Lett., **98**, 124301 (2007).

[3] A. Livne, E. Bouchbinder, and J. Fineberg, Phys. Rev. Lett. **101**, 264301 (2008); E. Bouchbinder, A. Livne, and J. Fineberg, Phys. Rev. Lett. **101**, 264302 (2008); A. Livne, E. Bouchbinder, I. Svetlizky, and J. Fineberg, Science **327**, 1359 (2010).

[4] E. Bouchbinder, Phys. Rev. Lett. **103**, 164301 (2009).

3:42PM D43.00003 Shapes formed by interacting cracks, KAREN DANIELS, Dept. of Physics, North Carolina State University — Brittle failure through multiple cracks occurs in a wide variety of contexts, from microscopic failures in dental enamel and cleaved silicon to geological faults and planetary ice crusts. In each of these situations, with complicated stress geometries and different microscopic mechanisms, pairwise interactions between approaching cracks nonetheless produce characteristically curved fracture paths. We investigate the origins of this widely observed “en passant” crack pattern by fracturing a rectangular slab which is notched on each long side and subjected to quasi-static uniaxial strain from the short side. The two cracks propagate along approximately straight paths until they pass each other, after which they curve and release a lens-shaped fragment. We find that, for materials with diverse mechanical properties, each curve has an approximately square-root shape, and that the length of each fragment is twice its width. We are able to explain the origins of this universal shape with a simple geometrical model.

4:18PM D43.00004 Fracture Statistics: Universality vs. Nucleation¹, ASHVINI SHEKHAWAT, Cornell University — We reexamine several common assumptions about fracture strength, utilizing large-scale simulations of a fuse network model and applying both renormalization-group and nucleation theory methods. Statistical distributions of fracture strengths are believed to be universal and material independent. The universal Weibull and Gumbel distributions emerge as a consequence of the “weakest-link hypothesis” and have been studied in the classical theory of extreme value statistics. These distributions are also the fixed points of a renormalization group (RG) flow. However, the engineering community often ignores the Gumbel distribution and uses the Weibull form almost exclusively to fit experimental data. Further, such fits are often extrapolated beyond the available data to estimate the probability of rare events in a variety of applications ranging from structural reliability to insurance pricing. Our recent studies of the random fuse network model raises doubts about most of these practices. We find that the emergent distribution of fracture strengths is the Gumbel distribution. However, the extremely slow convergence to the universal Gumbel form renders it unusable at least in this case. On the other hand, we show that a non-universal distribution derived by using a Griffiths type nucleation theory (due to Duxbury et al.) converges rapidly even for moderate system sizes. We find that while extrapolating the RG based universal Gumbel distribution is perilous and gives wildly incorrect predictions, the nucleation based non-universal results can be extrapolated with confidence. It is entertaining that fracture provides wonderful examples of the statistical mechanics tools developed to study both continuous as well as abrupt phase transitions.

¹This research was partially supported by DOE-BES DE-FG02-07ER-46393

4:54PM D43.00005 Avalanches in crack front propagation¹, STEFANO ZAPPERI, National Research Council of Italy CNR — We study avalanches in a model for a planar crack propagating in a disordered medium. Due to long-range interactions, avalanches are formed by a set of spatially disconnected local clusters, the sizes of which are distributed according to a power law. We derive a scaling relation between the local cluster and the global avalanche distributions. For length scales above a crossover length proportional to the Larkin length, the aspect ratio of the local clusters scales with the roughness exponent of the line model. For smaller lengthscales we observe multiscaling in the crack line correlations. Our analysis provides an explanation for experimental results on planar crack avalanches in Plexiglas plates, but the results are applicable also to other systems with long-range interactions such as Barkhausen avalanches in ferromagnetic thin films.

¹in collaboration with L. Laurson, S. Santucci and G. Durin

Monday, February 27, 2012 2:30PM - 5:30PM —
Session D44 GQI DCMP: Invited Session: Topological Quantum Computing with Majorana Fermions 157C

2:30PM D44.00001 Non-abelian anyons and topological quantum information processing in 1D wire networks, JASON ALICEA, UC Irvine — Topological quantum computation provides an elegant solution to decoherence, circumventing this infamous problem at the hardware level. The most basic requirement in this approach is the ability to stabilize and manipulate particles exhibiting non-Abelian exchange statistics – Majorana fermions being the simplest example. Curiously, Majorana fermions have been predicted to arise both in 2D systems, where non-Abelian statistics is well established, and in 1D, where exchange statistics of any type is ill-defined. An important question then arises: do Majorana fermions in 1D hold the same technological promise as their 2D counterparts? In this talk I will answer this question in the affirmative, describing how one can indeed manipulate and harness the non-Abelian statistics of Majoranas in a remarkably simple fashion using networks formed by quantum wires or topological insulator edges.

3:06PM D44.00002 Realization and detection of Majorana modes at generic spin-orbit coupled semiconductor/s-wave superconductor interfaces¹, JAY SAU, Department of Physics, Harvard University, Cambridge, MA 02138 — Majorana fermions are hitherto unobserved particles that have been theoretically predicted to have non-Abelian statistics that may be used for Topological Quantum Computation. For over a decade the only candidate systems for observing Majorana fermions were the non-Abelian $\nu = 5/2$ fractional quantum Hall state and chiral p-wave superconductors. More recently, motivated by developments in the area of topological insulators it was realized that a more general class of topological superconductors, some of which may be as simple as the interface of InAs and Al, should support such excitations. This talk will start by explaining why superconductors are a natural host for Majorana fermions. Following this, it will be argued that Majorana fermions should exist in generic semiconductor/superconductor interfaces, both in 1D and 2D, the crucial ingredients being s-wave superconductivity, spin-orbit coupling, and Zeeman splitting. Such Majorana fermions at the end of a nanowire appear as a magnetic-field tunable zero-bias peak in the STM spectrum with quantized conductance. Following this experimental challenges *en route* to realizing Majorana fermions in these structures such as disorder and the required tuning of the chemical potential of the semiconductor, will be discussed. Finally, we will conclude by showing how the spin-orbit coupled nanowires motivate a class of intrinsically number conserving microscopic models for topological superconductor with end Majorana fermions. The bosonization approach used to study this one-dimensional model, directly connects the Majorana fermions, which are typically described as Bogoliubov quasiparticles in mean-field theory, to an emergent Ising order in the one-dimensional nanowire model. The robustness of the topological degeneracy to weak local perturbations can be explicitly demonstrated.

¹Work done at CMTc, UMD in collaboration with Sankar Das Sarma, Sumanta Tewari, Roman Lutchyn and supported by DARPA QuEST, JQI-NSF-PFC, and Microsoft Q. Bosonization work was done in collaboration with B. I. Halperin and K. Flensberg.

3:42PM D44.00003 The Search for Majorana Fermions in Semiconductor Nanowires, LEO KOUWEN-HOVEN, Kavli Institute of NanoScience, Delft, The Netherlands — Majorana Fermions can arise as quasi-particles in specially designed nanoscale, electronic devices. Our approach is to use semiconductor nanowires with strong spin-orbit interaction (InAs or InSb). We induce superconductivity in the nanowires and control the electron density through a nearby gate. Several properties are measured such as the spin-orbit strength (including the dependence on the magnetic field direction), the induced superconducting gap (including magnetic field dependence) and the flow of supercurrents. For the determined experimental values we estimate the temperature scale to be ~ 2 Kelvin as the transition temperature for the reaching the phase of a topological superconductor. Majorana Fermions should be detectable as special features in the tunneling conductance or in the periodicity of an interferometer setup (SQUID geometry).

4:18PM D44.00004 Manipulation of Majorana fermions using superconducting qubits, ANTON AKHMEROV, Leiden University — Majorana fermions are special particles, predicted to appear in certain superconductors. They are extremely useful for quantum computation, due to the possibility to store quantum information in the degenerate ground state of the system. Moreover braiding Majorana fermions around each other allows to implement certain quantum gates in a fault-tolerant manner. I introduce a scheme of quantum computation with Majorana fermions which relies on interplay of charging and Josephson energy to measure, controllably couple, and braid Majorana fermions. The advantage of this scheme is that it fully relies on control elements usual for superconducting circuitry and does not require fine tuning on the scale of Fermi wavelength.

4:54PM D44.00005 Disorder effects in topological quantum wires, and alternative platforms for Majorana Fermion realization, PIET BROUWER, Freie Universitaet Berlin — Spinless p-wave superconducting wires can be in a topological phase in which they harbor Majorana bound states at their ends. Although there are no known spinless p-wave superconductors in nature, several routes to the artificial creation of such systems have been proposed. In this talk, I will discuss how non-idealities in some of the proposed routes, such as potential disorder and deviations from a strict one-dimensional limit, affect the topological phase. In particular, I'll discuss how the topological phase can persist at weak disorder or for multichannel wires, although some of the signatures of the presence of Majorana fermions are obscured.

Monday, February 27, 2012 2:30PM - 5:30PM —

Session D51 DCMP DFD: Liquid Crystals: Chromonics and Nematics Boston Convention Center 154

2:30PM D51.00001 Lyotropic chromonic liquid crystals in the biphasic region, XUXIA YAO, Georgia Institute of Technology, ALEJANDRO REY, McGill University, JUNG PARK, MOHAN SRINIVASARAO, Georgia Institute of Technology — Lyotropic chromonic liquid crystals have a wide coexistence temperature range where the isotropic and nematic phases are in equilibrium. Negative tactoids (isotropic droplets in the nematic medium) or positive tactoids (nematic droplets in the isotropic medium) form and grow as the nuclei of the new phases in the biphasic region. We studied the growth of tactoids as a function of temperature, the prolate shape of tactoids as well as their thermal fluctuation, based on which the viscoelastic properties of chromonic liquid crystals were obtained.

2:42PM D51.00002 Order Parameter measurements of Chromonic Liquid Crystal Benzopurpurin 4B using polarized Raman scattering¹, KARTHIK NAYANI, JUNG OK PARK, MOHAN SRINIVASARAO, Georgia Institute of Technology — Benzopurpurin 4B (BPP4B), a commonly used textile dye, is known to form chromonic liquid crystal phases in aqueous solutions at fairly low concentrations (<0.5 wt%) in comparison with other chromonic liquid crystals. Also the aggregation properties and the structure of the aggregates in aqueous solutions of BPP4B are not well understood. Recently McKitterick et al. reported a study on the aggregation and phase behavior of BPP4B in water.² Further understanding of the behavior of BPP4B in aqueous solutions can be gained by studying how the order parameter of its liquid crystalline phase varies with some relevant parameters. Planar monodomains of BPP4B were obtained using a flat rectangular capillary. Thermal evolution of the order parameter of these aligned monodomains was carried out using polarized Raman scattering measurements. Further, the concentration dependence and the effect of salt on the order parameter were studied. The variation of the order parameter with the above parameters was correlated to the structure of the aggregates using the UV-Vis absorption data.

¹This study was partially supported by NSF (DMR-0706235) and PSE fellowship (Georgia Institute of Technology).

²C. B. McKitterick, N. L. Erb-Satullo, N. D. LaRacune, A. J. Dickson, P. J. Collings. *J. Phys. Chem. B.* **2010.** 114, 1888.

2:54PM D51.00003 Textural transformations in lyotropic chromonic liquid crystals under confinement¹, ALIREZA SHAMS, Department of Chemical Engineering, McGill University, Montreal, Quebec H3A 2B2, Canada, XUXIA YAO, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA, ALEJANDRO D. REY², Department of Chemical Engineering, McGill University, Montreal, Quebec H3A 2B2, Canada, JUNG OK PARK³, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA, MOHAN SRINIVASARAO⁴, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332, USA — Lyotropic chromonic liquid crystals under capillary confinement display textural transformations between planar radial and planar polar modes, in which a +1 disclination branches into two +1/2 lines. The texture transformation is characterized by the nature and kinematics of the branch point, the aperture angle, and the shape of the lines. This work presents and validates a model of these four phenomena, which yield the viscoelastic moduli of these novel mesophases.

¹This work is partially supported by a grant from the U.S. Office of Basic Energy Sciences, Department of Energy; grant DE-SC0001412 and McGill Engineering Doctorate Award.

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⁴School of Materials Science and Engineering and Center for Advanced Research on Optical Microscopy, Georgia Institute of Technology, Atlanta, GA 30332, USA

3:06PM D51.00004 Molecular Aggregation in Disodium Cromoglycate¹, GAUTAM SINGH, D. AGRA-KOOIJMAN, Kent State University, P.J. COLLINGS, Swarthmore College, SATYENDRA KUMAR, Kent State University — Details of molecular aggregation in the mesophases of the anti-asthmatic drug disodium cromoglycate (DSCG) have been studied using x-ray synchrotron scattering. The results show two reflections, one at wide angles corresponding to $\pi - \pi$ stacking (3.32 Å) of molecules, and the other at small angles which is perpendicular to the direction of molecular stacking and corresponds to the distance between the molecular aggregates. The latter varies from 35 - 41 Å in the nematic (N) phase and 27 - 32 Å in the columnar (M) phase. The temperature evolution of the stack height, positional order correlations in the lateral direction, and orientation order parameter were determined in the N, M, and biphasic regions. The structure of the N and M phases and the nature of the molecular aggregation, together with their dependence on temperature and concentration, will be presented.

¹Work supported by NSF grant DMR-0806991.

3:18PM D51.00005 Flexopolydispersity of Nematic Liquid Crystals¹, YUE SHI, DONG CHEN, Department of Physics and Liquid Crystal Material Research Center, University of Colorado-Boulder, RIZWAN MAHMOOD, Department of Physics, Slippery Rock University, NOEL CLARK, Department of Physics and Liquid Crystal Material Research Center, University of Colorado-Boulder — Flexopolydispersity is the coupling of gradients in the director field $\mathbf{n}(\mathbf{r})$ of a nematic phase made from a polydisperse mixture of anisotropic particles in solution to the spatial change in variables describing the local mean particle shape, size, and concentration: In solutions of sufficiently polydisperse plates this coupling can lead to a nematic phase with a “blue-phase” like array of +1 defect lines. Such a structure has been observed in the lyotropic nematic phase of solutions of graphene oxide sheets.

¹Supported by NSF MRSEC Grant DMR-0820579.

3:30PM D51.00006 Nematic order in toroidal and higher-genus droplets¹, EKAPOP PAIRAM, JAYA LAKSHMI, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology, GEORGIA TECH TEAM — We generate toroidal and higher-genus droplets filled with nematic liquid crystal which are stabilized inside viscoelastic fluid with a non-zero yield stress. The work presented here is the preliminary observations of our experiments.

¹Georgia Institute of Technology, NSF Career

3:42PM D51.00007 Seeing and Sculpting Nematic Liquid Crystal Textures with the Thom construction, BRYAN CHEN, University of Pennsylvania, GARETH ALEXANDER, University of Warwick — Nematic liquid crystals are the foundation for modern display technology and also exhibit topological defects that can readily be seen under a microscope. Recently, experimentalists have been able to create and control several new families of interesting defect textures, including reconfigurably knotted defect lines around colloids (Ljubljana) and the “toron,” a pair of hedgehogs bound together with a ring of double-twist between them (CU Boulder). We apply the Thom construction from algebraic topology to visualize 3 dimensional molecular orientation fields as certain colored surfaces in the sample. These surfaces turn out to be a generalization to 3 dimensions of the dark brushes seen in Schlieren textures of two-dimensional samples of nematics. Manipulations of these surfaces correspond to deformations of the nematic orientation fields, giving a hands-on way to classify liquid crystal textures which is also easily computable from data and robust to noise.

3:54PM D51.00008 Patterned Liquid Crystal Droplets, JAKUB KOLACZ, ANDREW KONYA, Kent State University Liquid Crystal Institute, JULIO AVILA, California State University, FENG WANG, QI-HUO WEI, Kent State University Liquid Crystal Institute — Geometrical confinement has a significant influence on the structure and properties of liquid crystals. Prior research in this area is mainly on polymer-dispersed liquid crystals and liquid crystals in porous media where the liquid crystal droplets are usually non-uniform in size. Here we use microfabrication techniques to pattern liquid crystals into droplets of different geometrical shapes and sizes, and study the liquid crystal ordering in these liquid crystal droplets. The experimental observations will be compared with simulation results.

4:06PM D51.00009 The mechanism of controlling liquid crystal surface pretilt angle on plasma beam sputtered films¹, RU-PIN PAN, National Chiao Tung University, MENG-CHIOU HUANG, Institute of Atomic and Molecular Sciences, Academia Sinica, WEI-TA WU, CHENG-WEI LAI, HSIN-YING WU, National Chiao Tung University — In liquid crystal (LC) devices, the surface alignment is essential. The polyimide (PI) film is commonly used to make LC molecules parallel to the surface. A rubbing process is usually applied to choose a particular direction on the surface. A pretilt angle is also induced, which is useful but usually very small. In previous works, we have found out that the sputtered ion-oxide films can give a homeotropic alignment to LC, i.e., the LC molecules are perpendicular to the surface. In this work, we combine these two effects by sputtering the ion-oxide particles onto the PI coated glasses. By adjusting the sputtering conditions, the LC alignment are controlled. A wide range of pretilt angles have been achieved, while the rubbing process is no longer required. A thorough study by varying the sputtering conditions, such as voltage, current, and time duration, and observing the pretilt angles is carried out. The sputtered surfaces are examined with scanning electron microscope to see the coverage. By considering the charge distribution and electric field within the sputter, a quantitative model is then developed, which explains how the sputtering conditions affect the pretilt angles almost perfectly.

¹Supported by National Science Council, ROC, under grand number 96-2221-E-009-131-MY3 and Academia Sinica AS-98-TP-A10.

4:18PM D51.00010 Transient Splitting of Conoscopic Isogyres of a Uniaxial Nematic¹, YOUNG-KI KIM, BOHDAN SENUK, LUANA TORTORA, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, Kent, OH, USA, SAMUEL SPRUNT, Physics Department, Kent State University, Kent, OH, USA, MATTHIAS LEHMANN, Institute of Chemistry, Chemnitz University of Technology, Chemnitz, Germany, OLEG D. LAVRENTOVICH, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, Kent, OH, USA — The phase identification is often based on conoscopic observations of homeotropic cells: A uniaxial nematic produces a pattern with crossed isogyres, while the biaxial nematic shows a split of isogyres. We demonstrate that the splitting of isogyres occurs even when the material remains in the uniaxial nematic phase. In particular, in the bent core material J35, splitting of isogyres is caused by change of the temperature. The effect is transient and the isogyres return to a uniaxial (crossed) configuration after a certain time that depends on sample thickness, temperature, and rate of temperature change; the time varies from a few seconds to tens of hours. The transient splitting is caused by the temperature-induced material flow that triggers a (uniaxial) director tilt in the cell. The flows and the director tilt are demonstrated by the CARS microscopy and fluorescent confocal polarizing microscopy (FCPM). This transient effect is general and can be observed even in E7 and 5CB. The effect should be considered in textural identifications of potential biaxial nematic materials.

¹The work was supported by DOE grant DE-FG02-06ER46331 and by SEC.

4:30PM D51.00011 A comparison between “cybotactic” groups in bent-core and rod-like nematic liquid crystals, SAONTI CHAKRABORTY, NICHOLAS DIORIO, WILL CARR, JAMES GLEESON, ANTAL JAKLI, SAMUEL SPRUNT, Kent State University — It is becoming increasingly clear that short-range smectic-CP order is the basis for some of the unusual macroscopic properties of bent-core nematic (BCN) liquid crystals. By analyzing small angle X-ray diffraction patterns taken on a bent-core and a chemically related calamitic (rod-like) nematic, we have attempted to clarify the nature of the “cybotactic groups” (or molecular clusters) contributing to this short-range order in BCNs, and to distinguish their signature from the scattering due to smectic fluctuations normally observed above a nematic to smectic transition. We find that persistent, finite-sized, tilted smectic clusters, with short, temperature-independent correlation lengths, account for the scattering observed from the BCN, while the calamitic material provides a remarkably clear example of temperature-dependent fluctuations in smectic order observed even far above a smectic-C phase. Supported by NSF DMR-0964765

4:42PM D51.00012 Optimizing liquid crystalline properties for bio-sensing at aqueous interfaces¹, WILDER IGLESIAS, Kent State University, NICHOLAS L. ABBOTT, University of Wisconsin, ELIZABETH K. MANN, ANTAL JÁKLI, Kent State University — Recent studies show that surfactant or phospholipid assemblies can be monitored at interfaces between aqueous solutions and thermotropic liquid crystals. The capability of these liquid crystals to change birefringence with the reordering induced by the decorated surface allows to study and characterize dynamical phenomena happening at the interfaces. In this work we tune the surface anchoring and the viscoelastic properties of the liquid crystal mesogens in order to increase sensitivity and optimize the response to events at the surface.

¹This Work was supported by NSF DMR-0907055.

4:54PM D51.00013 Competing Ordering Processes at Liquid Crystal Surfaces Laden with Semifluorinated Alkane Molecules, XUNDA FENG, Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, D-37077 Göttingen, Germany, AHMED MOURRAN, MARTIN MOELLER, DWI an der RWTH Aachen e.V. and Institute for Technical and Macromolecular Chemistry, RWTH Aachen, Forckenbeckstr. 50, D-52056 Aachen, Germany, CHRISTIAN BAHR, Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, D-37077 Göttingen, Germany — Ellipsometric measurements elucidate the interplay between the surface order at the isotropic liquid crystal/air interface and a structural phase transition in a Gibbs film on the same interface. Gibbs films formed by the semifluorinated alkane C18H37–C12F25 exhibit a sharp transition from a dilute state at higher temperatures to a dense state at lower temperatures. The transition temperature can be tuned by controlling the C18H37–C12F25 concentration in the bulk liquid crystal phase. When the transition takes place in the temperature range in which a molecular thin smectic or nematic film exists at the isotropic liquid crystal/air interface, the smectic surface order is destroyed while the nematic surface order is affected by a change of the orientation of the liquid crystal molecules. The ellipsometric data indicate that both behaviors result from a change of the anchoring condition of the liquid crystal molecules in contact with the Gibbs film.

5:06PM D51.00014 Revealing the inner arrangement of cholesteric liquid crystals confined in polymeric electrospun fibers¹, GIUSY SCALIA, Seoul National University, EVA ENZ, MLU Halle-Wittenberg, VERA LA FERRARA, ORONZO CALÓ, ENEA C.R. Portici, JAN LAGERWALL, Seoul National University — Cholesteric liquid crystals, like other types of LCs, can be confined inside polymeric fibers by coaxial electrospinning. In this way the interesting optical properties of cholesterics could be transferred to very long fibers that can form flexible or rigid mats according to the outer sheath material. Selective reflection was easily detected from polymeric fibers with cholesteric LC core. Despite the uniformity of the external morphology of the fibers, evaluated by SEM, defects in the optical texture could be observed in some locations as well as differences in the wavelength of the reflected light. The reason for such differences needs to be clarified in order to achieve a uniform, controlled optical texture. The understanding was achieved by direct observation of the cross section of the LC-filled fibers by cutting and sectioning the fibers by Focused Ion Beam (FIB). This revealed differences in dimensions of the inner cavity correlating them to the observed wavelengths of the selectively reflected light, but also changes in shape, in some parts with strongly varying width that accounts for the defect lines observed. We could also visualize the effect of flow instability of the jet during spinning, inducing the formation of chains of LC droplets.

¹Research supported by grants from the AICT (SNU, Korea) and NRF (Korea)

5:18PM D51.00015 Macroscopic torsional strain and induced molecular conformational deracemization, RAJRATAN BASU, JOEL PENDERY, ROLFE PETSCHKE, Case Western Reserve University, ROBERT LEMIEUX, Queen's University, CHARLES ROSENBLATT, Case Western Reserve University — A macroscopic helical twist is imposed on an achiral nematic liquid crystal by controlling the azimuthal alignment directions at the two substrates. On application of an electric field the director rotates in the substrate plane. This electroclinic effect, which requires the presence of chirality, is strongest at the two substrates and increases with increasing imposed twist distortion. We present a simple model involving a tradeoff among bulk elastic energy, surface anchoring energy, and deracemization entropy that suggests the large equilibrium director rotation at the surfaces induces a deracemization of chiral conformations in the molecules, quantitatively consistent with experiment.

Monday, February 27, 2012 2:30PM - 5:30PM —

Session D52 GSNP: General Statistical and Nonlinear Physics and GSNP Student Prize Talks

153C

2:30PM D52.00001 Dynamic phase transition in the classical anisotropic XY model on a square lattice¹, WILLIAM BAEZ, The Ohio State University, TRINANJAN DATTA, Augusta State University — Ginzburg-Landau analysis of the anisotropic XY model in a spatially homogeneous oscillating magnetic field on a square lattice suggests the existence of several dynamical phases - Ising symmetry restoring order (Ising SRO), Ising symmetry breaking order (SBO), XY symmetry restoring order (XY SRO), and XY symmetry breaking order (XY SBO). We investigate the presence of these phases and the dynamic phase transition (DPT) between these phases using classical Monte Carlo simulation techniques. We explore the system for a range of values for the external field amplitude, field frequency, and anisotropy parameter. Utilizing the period-averaged magnetization (in both the x- and y- component) as the dynamic order parameter we confirm the presence of multiple DPT transitions in the model. We also construct the probability density histograms of the dynamic order parameter to validate the existence of the four DPT phases.

¹Cottrell College Science Awards (RCSA Award #20073)

2:42PM D52.00002 Non-universal local critical exponents at a non-equilibrium phase transition¹, MICHEL PLEIMLING, HYUNHANG PARK, Virginia Tech — We study the dynamic phase transition in the two-dimensional semi-infinite kinetic Ising model in an oscillating field. We focus on the critical regime where the competition between the half-period of the oscillating field $t_{1/2}$ and the metastable lifetime $\langle \tau \rangle$ is most pronounced. We focus on layer-dependent quantities, such as the period-averaged magnetization per layer $Q(z)$ and the layer susceptibility $\chi_Q(z)$, and determine surface critical exponents through finite size scaling. We find that the values of these non-equilibrium exponents are non-universal as they depend on the strength of the surface couplings. Results for the three-dimensional model are also briefly discussed and compared to the two-dimensional case.

¹Supported in part by the US National Science Foundation through Grant DMR-0904999.

2:54PM D52.00003 ABSTRACT WITHDRAWN —

3:06PM D52.00004 Extremal Optimization for p-Spin Models¹ , STEFAN FALKNER, STEFAN BOETTCHER,

Emory University — It was shown recently that finding ground states in the 3-spin model on a 2d dimensional triangular lattice poses an NP-hard problem [1]. We use the extremal optimization (EO) heuristic [2] to explore ground state energies and finite-size scaling corrections [3]. EO predicts the thermodynamic ground state energy with high accuracy, based on the observation that finite size corrections appear to decay purely with system size. Just as found in 3-spin models on r -regular graphs, there are no noticeable anomalous corrections to these energies. Interestingly, the results are sufficiently accurate to detect alternating patterns in the energies when the lattice size L is divisible by 6. Although ground states seem very prolific and might seem easy to obtain with simple greedy algorithms, our tests show significant improvement in the data with EO.

[1] PRE 83 (2011) 046709,

[2] PRL 86 (2001) 5211,

[3] S. Boettcher and S. Falkner (in preparation).

¹Supported by NSF-DMR grant #0812204.

3:18PM D52.00005 A novel Kinetic Monte Carlo algorithm for Non-Equilibrium Simulations

, PRATEEK JHA, Northwestern University, VLADIMIR KUZOVKOV, University of Latvia, BARTOSZ GRZYBOWSKI, MONICA OLVERA DE LA CRUZ, Northwestern University — We have developed an off-lattice kinetic Monte Carlo simulation scheme for reaction-diffusion problems in soft matter systems. The definition of transition probabilities in the Monte Carlo scheme are taken identical to the transition rates in a renormalized master equation of the diffusion process and match that of the Glauber dynamics of Ising model. Our scheme provides several advantages over the Brownian dynamics technique for non-equilibrium simulations. Since particle displacements are accepted/rejected in a Monte Carlo fashion as opposed to moving particles following a stochastic equation of motion, nonphysical movements (e.g., violation of a hard core assumption) are not possible (these moves have zero acceptance). Further, the absence of a stochastic “noise” term resolves the computational difficulties associated with generating statistically independent trajectories with definitive mean properties. Finally, since the timestep is independent of the magnitude of the interaction forces, much longer time-steps can be employed than Brownian dynamics. We discuss the applications of this scheme for dynamic self-assembly of photo-switchable nanoparticles and dynamical problems in polymeric systems.

3:30PM D52.00006 How an aggregation process helps us understanding solid fragmentation ,

VLEDOUTS ALEXANDRE, NICOLAS VANDENBERGHE, EMMANUEL VILLERMAUX, IRPHE — We report on an experiment intended to understand the fragmentation of a ring composed of cohesive solid spheres (magnets in dipolar interaction). At initial time, the ring is forced to expand radially and the spheres separate from each other. Because of the dipolar attractive force between the spheres, their uniform angular distribution is unstable and the spheres aggregate with each other to form fragments. We record the full dynamics of the spheres assembly and we show that the final fragment size distribution is the signature of the aggregation process giving birth to it. In particular, we introduce a Weber number We , based on the radial velocity of the ring, the density of the spheres and their magnetization. We find that the final mean fragment size scales like $We^{-1/3}$ and that the standard deviation of the fragments distribution is proportional to it. We will also discuss the relation between our findings and the fragmentation of elastic rings studied by Sir N. Mott.

3:42PM D52.00007 Thermodynamic limit, quasi-stationary states and the range of pair inter-

actions , ANDREA GABRIELLI, Istituto dei Sistemi Complessi - CNR (Rome, Italy), MICHAEL JOYCE, LPNHE - Université Paris 6 (France), BRUNO MARCOS, Lab. J.A. Dieudonné, UMR 6621, Université de Nice (France) — “Quasi-stationary” states are approximately time-independent out of equilibrium states which have been observed in a variety of systems of particles interacting by long-range interactions. We investigate here the conditions of their occurrence for a generic pair interaction $V(r \rightarrow \infty) \sim 1/r^\gamma$ with $\gamma > 0$, in $d > 1$ dimensions. We generalize analytic calculations known for gravity in $d = 3$ to determine the scaling parametric dependences of their relaxation rates due to two body collisions, and report extensive numerical simulations testing their validity. Our results lead to the conclusion that, for $\gamma < d - 1$, the existence of quasi-stationary states is ensured by the large distance behavior of the interaction alone, while for $\gamma > d - 1$ it is conditioned on the short distance properties of the interaction, requiring the presence of a sufficiently large soft-core in the interaction potential.

3:54PM D52.00008 ABSTRACT WITHDRAWN —

4:06PM D52.00009 Numerical study of Potts models with aperiodic modulations: influence

on first-order transitions¹ , NILTON BRANCO, Departamento de Fisica, Universidade Federal de Santa Catarina, Florianopolis, SC, Brazil, DANIEL GIRARDI, National Institute of Science and Technology for Complex Systems, Universidade Federal Fluminense, Volta Redonda, RJ, Brazil — We perform a numerical study of Potts models on a rectangular lattice with aperiodic interactions along one spatial direction. The number of states q is such that the transition is a first-order one for the uniform model. The Wolff algorithm is employed, for many lattice sizes, allowing for a finite-size scaling analyses to be carried out. Three different self-dual aperiodic sequences are employed, such that the exact critical temperature is known: this leads to precise results for the exponents. We analyze models with $q = 6$ and 15 and show that the Harris-Luck criterion, originally introduced in the study of continuous transitions, is obeyed also for first-order ones. The new universality class that emerges for relevant aperiodic modulations depends on the number of states of the Potts model, as obtained elsewhere for random disorder, and on the aperiodic sequence. We determine the occurrence of log-periodic behavior, as expected for models with aperiodic modulated interactions.

¹We acknowledge financial support from Brazilian Agencies FAPESC, CNPq, and CAPES.

4:18PM D52.00010 BREAK —

4:30PM D52.00011 Boundaries Matter for Confined Colloidal Glasses , GARY HUNTER, Emory University,

KAZEM V. EDMOND, New York University, ERIC R. WEEKS, Emory University — We confine dense colloidal suspensions within emulsion droplets to examine how confinement and properties of the confining medium affect the colloidal glass transition. Samples are imaged via fast confocal microscopy. By observing a wide range of droplet sizes and varying the viscosity of the external continuous phase, we separate finite size and boundary effects on particle motions within the droplet. Suspensions are composed of binary PMMA spheres in organic solvents while the external phases are simple mixtures of water and glycerol. In analogy with molecular super-cooled liquids and thin-film polymers, we find that confinement effects in colloidal systems are not merely functions of the finite size of the system, but are strongly dependent on the viscosity of the confining medium and interactions between particles and the interface of the two phases.

4:42PM D52.00012 Dynamics near shear-jamming for a dense granular system¹, JIE REN, JOSHUA DIJKSMAN, ROBERT BEHRINGER, Duke University — This talk will present several systematic experimental studies of a two-dimensional, frictional dense granular system subjected to simple shear deformation. The first experiment consists of linear shear for densities smaller than the isotropic jamming point, and examines both the evolution of the average stress and the evolution of force network. These measures reveal three distinguishable regimes of the granular system with increasing shear strain: unjammed, fragile, and shear-jammed regimes. The second experiment uses small amplitude cyclic shear to probe the dynamical response of the states from the first experiment. For fragile or jammed regimes, cyclic shear drives the system through transient states that evolve towards relatively stable forces networks and system-averaged stress. The timescale of the transient increases rapidly as the system moves deeper into the fragile, or shear-jammed regimes. These experiments also involve particle tracking (displacements and rotations) to search for and characterize non-affine motion and spatial heterogeneity. There is a clear increase in particle diffusion with increasing density and shear strain amplitude, even when the system is still unjammed and experiences only minimal stress. When the system is fragile or jammed, the heterogeneity of particle displacements reveals subtle correlations with the force network.

¹This work is funded by NSF grants: DMR0906908, DMS0835571, NASA grant NNX10AU01G and ARO grant W911NF-11-1-0110.

4:54PM D52.00013 Elasticity of adherent active cells on a compliant substrate¹, SHILADITYA BANERJEE, Department of Physics, Syracuse University, AARON F. MERTZ, ERIC R. DUFRESNE², Department of Physics, Yale University, M. CRISTINA MARCHETTI, Department of Physics and Syracuse Biomaterials Institute, Syracuse University — We present a continuum mechanical model of rigidity sensing by living cells adhering to a compliant substrate. The cell or cell colony is modeled as an elastic active gel, adapting recently developed continuum theories of active viscoelastic fluids. The coupling to the substrate enters as a boundary condition that relates the cell's deformation field to local stress gradients. In the presence of activity, the substrate induces spatially inhomogeneous contractile stresses and deformations, with a power law dependence of the total traction forces on cell or colony size. This is in agreement with recent experiments on keratinocyte colonies adhered to fibronectin coated surfaces. In the presence of actomyosin activity, the substrate also enhances the cell polarization, breaking the cell's front-rear symmetry. Maximal polarization is observed when the substrate stiffness matches that of the cell, in agreement with experiments on stem cells.

¹This work was supported by NSF grants to MCM (DMR-0806511 and DMR-1004789) and ERD (DBI-0619674) and NSF graduate fellowship to AFM.

²Additional Affiliations: Department of Mechanical Engineering and Materials Science, Department of Chemical and Environmental Engineering, Department of Cell Biology, Yale University.

5:06PM D52.00014 Differential geometry of the space of Ising models, BENJAMIN MACHTA, RICKY CHACHRA, Department of Physics, Cornell University, MARK TRANSTRUM, Department of Bioinformatics and Computational Biology at the MD Anderson Cancer Center, JAMES SETHNA, Department of Physics, Cornell University — We use information geometry to understand the emergence of simple effective theories, using an Ising model perturbed with terms coupling non-nearest-neighbor spins as an example. The Fisher information is a natural metric of distinguishability for a parameterized space of probability distributions, applicable to models in statistical physics. Near critical points both the metric components (four-point susceptibilities) and the scalar curvature diverge with corresponding critical exponents. However, connections to Renormalization Group (RG) ideas have remained elusive. Here, rather than looking at RG flows of parameters, we consider the reparameterization-invariant flow of the manifold itself. To do this we numerically calculate the metric in the original parameters, taking care to use only information available after coarse-graining. We show that under coarse-graining the metric contracts very anisotropically, leading to a “sloppy” spectrum with the metric's Eigenvalues spanning many orders of magnitude. Our results give a qualitative explanation for the success of simple models: most directions in parameter space become fundamentally indistinguishable after coarse-graining.

5:18PM D52.00015 Seeing and Sculpting Nematic Liquid Crystal Textures with the Thom construction, BRYAN CHEN, University of Pennsylvania, GARETH ALEXANDER, University of Warwick — Nematic liquid crystals are the foundation for modern display technology and also exhibit topological defects that can readily be seen under a microscope. Recently, experimentalists have been able to create and control several new families of interesting defect textures, including reconfigurably knotted defect lines around colloids (Ljubljana) and the “toron,” a pair of hedgehogs bound together with a ring of double-twist between them (CU Boulder). We apply the Thom construction from algebraic topology to visualize 3 dimensional molecular orientation fields as certain colored surfaces in the sample. These surfaces turn out to be a generalization to 3 dimensions of the dark brushes seen in Schlieren textures of two-dimensional samples of nematics. Manipulations of these surfaces correspond to deformations of the nematic orientation fields, giving a hands-on way to classify liquid crystal textures which is also easily computable from data and robust to noise.

Monday, February 27, 2012 2:30PM - 5:30PM –
Session D53 GSNP DFD: Focus Session: Jamming – Nonlinear Acoustics and Vibrational Response 153B

2:30PM D53.00001 Vibrational Modes in Colloidal Crystals, KE CHEN, TIM STILL, Department of Physics and Astronomy, University of Pennsylvania, KEVIN APTOWICZ, Department of Physics, West Chester University, ARJUN YODH, Department of Physics and Astronomy, University of Pennsylvania — We investigate vibrational modes in quasi-two-dimensional colloidal crystals using video microscopy and displacement covariance matrix analysis. Debye scaling in the phonon density of states and the dispersion curve for two-dimensional hexagonal crystals are recovered for both mono-layer and double layer colloidal crystals. Using “soft spots” analysis, low-frequency quasi-localized phonon modes, which were found to coincide with fragile regions in glasses [1] appear to be spatially correlated with structural defects in colloidal crystals. Thus, “soft spots” may be a useful general identifier for defects in both crystalline and amorphous solids. This work is supported by NSF DMR 0804881, MRSEC DMR11-20901, and by NASA NNX08AO0G.

[1] K. Chen et al, Phys. Rev. Lett. 107, 108301 (2011)

2:42PM D53.00002 Acoustic measurement of a granular density of state, ELI OWENS, KAREN DANIELS, North Carolina State University — Measurements of the vibrational density of states $D(\omega)$ in glasses reveal that an excess number of low-frequency modes is associated with a loss of mechanical rigidity. An excess number of such modes has also been observed in both simulations of idealized granular materials near the jamming point, and in experiments on colloids. We experimentally investigate similar features in a jammed, quasi-two-dimensional granular material. We mimic thermal fluctuations using an electromagnetic driver to inject acoustic white noise, while piezoelectric sensors embedded inside a subset of the particles provide measurements of single-particle velocities. By analogy with conventional thermal techniques, we calculate a $D(\omega)$ -like quantity via the spectrum of the velocity autocorrelation function. We measure $D(\omega)$ as a function of the confining pressure and find that the peak in the density of states shifts to higher frequency with system pressure. At low pressure, disordered systems have more low frequency modes than do hexagonally-packed systems.

2:54PM D53.00003 Elastic weakening of a dense granular medium by acoustic fluidization, XIAOPING JIA, JEROME LAURENT, Université Paris-Est, SIET WILDENBERG, MARTIN VAN HECKE, Universiteit Leiden, LPMDI TEAM, ONNES LAB TEAM — Elastic waves propagating through a dense granular pack provide a unique probe of the elastic properties and internal dissipation of the medium [1], and also allow investigating the irreversible rearrangement of the contact network at large vibration amplitude. In this talk, we describe two distinct types of nonlinearity, i.e. hertzian and frictional, at the grain contact by sound amplitude and velocity measurements, respectively, under different confining pressure [2]. Beyond certain wave amplitude, the sound-matter interaction becomes irreversible, leaving the medium in a weakened and slightly compacted state. A slow recovery of the initial elastic modulus is observed after acoustic perturbation, revealing the plastic creep growth of microcontacts. The cross-correlation function of configuration-specific acoustic speckles highlights the relationship between the macroscopic elastic weakening and the local change of the contact networks, induced by strong sound vibration, in the absence of appreciable grain motion. We show that the softening of elastic modulus is much more pronounced with the shear wave (up to 20%) than with the compressional wave (to 10%).

[1] Th. Brunet, X. Jia and P. Mills, Phys. Rev. Lett **101**, 138001 (2008)

[2] Th. Brunet, X. Jia and P. Johnson, Geophys. Res. Lett **35**, L19308 (2008); X. Jia, Th. Brunet and J. Laurent, Phys. Rev. E **00**, 000300(R) (2011)

3:06PM D53.00004 Nonharmonicity in vibrated granular solids, CARL SCHRECK, Yale University — We have shown that granular packings composed of frictionless particles with repulsive contact interactions are strongly nonharmonic. When infinitesimally perturbed along linear response eigenmodes of the static packing, energy leaks from the original mode of vibration to a continuum of frequencies due solely to contact breaking even when the system is under significant compression. Further, vibrated packings possess well-defined equilibrium positions that are different than those of the unperturbed packing. The vibrational density of states obtained using the displacement matrix and velocity autocorrelation function methods exhibit an increase in the number of low-frequency modes over that obtained from linear response of the static packing. The form of the density of states in vibrated granular packings is reminiscent of the low-frequency behavior of the vibrational density of states in fluid systems. We also investigate the effects of inter-particle friction, dissipation, particle shape, and degree of positional order on the density of states and thermal transport properties in driven granular packings.

3:42PM D53.00005 Irreversible Incremental Behavior in a Granular Material¹, LUIGI LA RAGIONE, Cornell University, VANESSA MAGNANIMO, MSM, CTW, University of Twente, 7500EA Enschede (NL), JAMES JENKINS, Cornell University, HERNAN MAKSE, City College New York — We test the elasticity of dense, isotropic, compressed aggregates of frictional spheres using cyclic increments of shear and volume strain in a numerical simulation. For both types of increments, we measure irreversibility in relative displacements and contact forces that is stronger for the increments in shear. The strength of the irreversibility increases as the average number of contacts per particle (the coordination number) decreases. This irreversibility may be associated with the opening of contacts in an increment of loading, pointed out in a recent paper of Schreck et al. (PRL, 2011); such contact opening could lead to irreversible rearrangement of the contact network when the increment is relaxed.

¹Office of Naval Research, Global

3:54PM D53.00006 Experimental Measurements of Force Propagation in Vibrated Photoelastic Disks¹, ALINE HUBARD, MARK SHATTUCK, CUNY Graduate Center and the Benjamin Levich Institute and Physics Department of The City College of New York — We measure and analyze the propagation forces in vibrated disks under constant pressure with different amplitudes and frequencies. We use photoelastic particles to visualize the stress within each particle using a high-speed video camera. From the images we can extract the time dependent force at each contact to determine how force propagates through the contact network. Using mono-disperse particles we focus on force propagation during the phase transition from an ordered solid-like state to a disordered fluid-like state as we change the vibration amplitude. With bi-disperse particles we compare with the transition to a disordered solid-like state.

¹Supported by NSF PREM (DMR-0934206).

4:06PM D53.00007 Nonlinear acoustics of glass bead packings at vanishing static pressures¹, VINCENT TOURNAT, LAUM, CNRS, Université du Maine, Le Mans, France, VITALYI GUSEV, LPEC, CNRS, Université du Maine, Le Mans, France — We present here a set of recent results obtained in three experimental configurations: linear and nonlinear acoustic probing of a granular slab at different compacities, surface acoustic waves in granular layers submitted to gravity, resonances of a granular layer with an in-depth elasticity gradient. We succeeded to overcome the experimental issues associated to the dramatic increase of acoustic wave attenuation when the confining pressure diminishes. Interpretations reveal that the manifestations of nonlinear effects (self-demodulation, nonlinear resonance, second harmonic or subharmonic generation...) allow to isolate the different types of nonlinearities involved (Hertz, clapping, stick-slip, hysteresis...). Also, some discrepancies are observed for the extracted linear elastic parameters scaling laws as a function of vanishing pressure (lower than 100 Pa typically) between the different developed experimental configurations and the theoretical predictions. Explanations for these discrepancies are given. We show that under some conditions, it is necessary to take into account the coupling of grain motion with that of the saturating air. Application of these results to the probing of granular layers under destabilization will be presented.

¹This work is supported by ANR contract “Stabingram” ANR-2010-BLAN-0927-03.

4:18PM D53.00008 Acoustic Echoes in Model Glasses, JUSTIN BURTON, SIDNEY NAGEL, The University of Chicago — At low temperatures, glasses and crystals behave in qualitatively different ways. In particular, glasses have a great many more low-energy excitations that have traditionally been explained in terms of a distribution of dilute, two-level quantum states that are created by clusters of particles tunneling between two nearly degenerate ground states. Strong evidence for this model has come from the saturation effects and acoustic echoes [1] observed in these excitations. We show that, in contrast to conventional wisdom, the quasi-localized, strongly anharmonic, normal modes of jammed systems [2] can produce acoustic echoes due to the shift in the mode frequency with increasing amplitude. We observe this both in jammed packings of spherical particles with finite-range, Hertzian repulsions, and in model glasses interacting with a Lennard-Jones potential. In contrast to pulse echoes in two-level systems, a distinguishing feature of these “anharmonic echoes” is the appearance of multiple echoes after two excitation pulses, a feature also observed in experiments [1].

[1] B. Golding and J. E. Graebner. Phys. Rev. Lett. **37**, 852 (1976).

[2] N. Xu, V. Vitelli, A. J. Liu, and S. R. Nagel. Europhys. Lett. **90**, 56001 (2010).

4:30PM D53.00009 Extreme Physics and Rearrangements near Jamming, MARTIN VAN HECKE, Leiden University, ZORANA ZERAVCIC, Harvard University, ALEX SIEMENS, JOHANNES SIMON, DANIEL GELEN, Leiden University — Near jamming, linear response becomes irrelevant. I briefly discuss how this gives rise to a range of intrinsically nonlinear, even extreme, phenomena. Moreover, reversibility also breaks down, and I will discuss the nature of rearrangements near jamming.

4:42PM D53.00010 Formation, Propagation, and Attenuation of Shocks Waves in Jammed Matter, LEOPOLDO GOMEZ, Leiden University - Universidad Nacional del Sur - CONICET, VINCENZO VITELLI, Leiden University — We study the formation and propagation of fully non-linear waves in jammed granular media. Close to the jamming point, an arbitrary initial distortion of the media will induce the formation of non-linear finite amplitude waves. There are two regimes in the evolution of these waves. At early times non-linear interactions dominate the propagation, leading to a temporal evolution strongly dependent on the initial distortion. At long times the propagation is characterized by a new universal regime, dominated by hydrodynamical attenuation. Here the non-linear waves evolve in a self-similar fashion, characterized by a power law attenuation whose exponent is weakly dependent on the initial pressure of the system.

4:54PM D53.00011 Jamming of soft spheres at finite temperature : a granular experiment, CORENTIN COULAIS, CEA Saclay, OLIVIER DAUCHOT, ESPCI, ROBERT BEHRINGER, Duke University, GIT - SPEC - CEA SACLAY TEAM, ESPCI TEAM¹, GIT-SPEC-CEA SACLAY / BEHRINGER'S GROUP AT DUKE COLLABORATION — At large packing fraction, disordered packings of particles with repulsive contact interactions jam into a rigid state where they withstand finite shear stresses before yielding. For frictionless particles and at zero temperature, the jamming transition coincides with the onset of iso-staticity and many geometrical and mechanical properties scale with the distance to the jamming point. What are the vestige of jamming at finite temperature and how jamming impacts the thermodynamics of glasses remain open issues. We address these questions experimentally by investigating the dynamics of both the density field and the force network of an horizontally shaken bi-disperse packing of photo-elastic disks. The average number of contact clearly displays an abrupt transition which we interpret as the jamming transition. Besides, dynamical heterogeneities are observed and their amplitude exhibits a maximum, which, in turn, signs a dynamical transition. We discuss in detail the interplay between these two transitions and how they depend on the particle softness and amplitude of the horizontal vibration.

¹The Team is in Saclay and Olivier Dauchot has recently move to ESPCI

5:06PM D53.00012 Density of vibrational modes in partially crystalline granular packings¹, THIBAUT BERTRAND, Yale University, Dpt of Mechanical Engineering, CARL F. SCHRECK, Yale University, Dpt of Physics, MARK SHATTUCK, Benjamin Levich Institute and Physics Department, The City College of the City University of New York, COREY S. O'HERN, Yale University, Dpt of Mechanical Engineering, O'HERN GROUP, YALE UNIVERSITY TEAM — Numerous numerical results have shown that systems of monodisperse frictionless disks crystallize readily and that disordered mechanically stable packings are rarely obtained. We numerically investigate the dependence of the cluster size distribution on system size and quench rate. We also investigate the effect of crystallization on the vibrational response outside the linear response regime. We study changes in the density of vibrational modes due to changes in the average crystallite size and perturbation amplitude in partially crystalline granular packings. In particular we determine how the number of contacts (above the isostatic value) affects anharmonic response in granular packings.

¹Acknowledgement: NSF CBET-0967262, CBET-0968013

5:18PM D53.00013 Studying the low-frequency quasilocalized modes in disordered colloidal systems, LEI XU, PENG TAN, Physic Dept., The Chinese University of Hong Kong, NING XU, Physic Dept., The University of Science and Technology of China, ANDREW SCHOFIELD, Physic Dept., University of Edinburgh — In disordered colloidal systems, we experimentally measure the normal modes with covariance matrix method, and clarify the origin of low-frequency quasilocalization at single-particle level. We observe important features from both jamming and glass simulations: there is a plateau in the density of states which is suppressed upon ompression, as predicted by jamming; within the same systems, we also find that the low-frequency quasilocalization originates from the coupling between large vibrations of defective structures and transverse excitations, consistent with recent glass simulation. The coexistence of these features demonstrates an experimental link between jamming and glass. Extensive simulations further show that such structural origin of quasilocalization is universally valid for various temperatures and volume fractions.

Monday, February 27, 2012 2:30PM - 5:30PM —
Session D54 GSNP: Focus Session: Complex and co-evolving networks - Foundations in Complex Networks 152

2:30PM D54.00001 Dynamics of Random Graphs with Bounded Degrees, ELI BEN-NAIM, Los Alamos National Laboratory, PAUL KRAPIVSKY, Boston University — We investigate the dynamic formation of regular random graphs. In our model, we pick a pair of nodes at random and connect them with a link if both of their degrees are smaller than d . Starting with a set of isolated nodes, we repeat this linking step until a regular random graph, where all nodes have degree d , forms. We view this process as a multivariate aggregation process, and formally solve the evolution equations using the Hamilton-Jacobi formalism. We calculate the nontrivial percolation thresholds for the emergence of the giant component when $d \geq 3$. Also, we estimate the number of steps until the giant component spans the entire system and the total number of steps until the regular random graph forms. These quantities are non self-averaging, namely, they fluctuate from realization to realization even in the thermodynamic limit.

2:42PM D54.00002 Influence of Boundary Conditions on Metastable Lifetimes for The Ising Model on the Hyperbolic Plane¹, HOWARD L. RICHARDS, Physics, Marshall University, DIPENDRA SHARMA CHAPAGAIN, Physics, Berea College, JAMES MOLCHANOFF, Math, West Virginia Wesleyan University — Some corals grow in shapes that resemble 3D models of the hyperbolic plane, since this allows them to have greater area for a given growth radius. Each polyp could be represented by an Ising site, with "feeding" = "up" and "retracted" = "down". The mechanisms of metastable decay could be interpreted as how the coral as a whole reacts to changing conditions of food availability or predation. Previous studies have shown that there is a spinodal field for the Ising model on a regular lattice in the hyperbolic plane if it is infinite or has periodic or mean-field boundary conditions. This happens because the size of the boundary grows asymptotically at the same rate as the droplet volume, in clear contrast with droplets in the Euclidean plane. Our simulations show, however, that the spinodal field disappears if more physically relevant open boundary conditions are used instead.

¹This research was conducted as part of Marshall University's REU in Scientific Computing, supported by NSF grant OCI-1005117. For more information see www.marshall.edu/reu.

2:54PM D54.00003 Quantifying the complexity of random Boolean networks¹, XINWEI GONG, JOSHUA E.S. SOCOLAR, Department of Physics, Duke University — We study two measures of the complexity of spatially extended systems in the context of random Boolean networks. A measure defined by Shalizi et al. for cellular automata, based on a criterion for optimal statistical prediction [1], does not distinguish between the spatial inhomogeneity of the ordered phase and the dynamical inhomogeneity of the disordered phase. A modification in which complexities of individual nodes are calculated yields vanishing complexity values for networks in the ordered and critical regimes and for highly disordered networks, peaking somewhere in the disordered regime. Individual nodes with high complexity are the ones that pass the most information from the past to the future, a quantity that depends in a nontrivial way on both its own Boolean function and the location of the node within the network.

[1] C. R. Shalizi, K. L. Shalizi, and R. Haslinger, Phys. Rev. Lett. 93, 118701 (2004).

¹This research is supported by the Duke Network Analysis Center

3:06PM D54.00004 Synchronization in Noisy Networks with Multiple Time Delays¹, DAVID HUNT, GYORGY KORNISS, BOLESŁAW SZYMANSKI, Rensselaer Polytechnic Institute — We expand our previous work of uniform time delays in stochastic, linearly-coupled synchronization problems² by including descriptions of networks with multiple delays. Non-uniform time delays can arise when there are multiple sources of delay, e.g. the time to transmit and the time to process information. In this particular two-delay case³, the primary limitation on the network to synchronize without any centralized direction does not come from restrictions in the transmission of a node's state to its neighbors; rather it depends on the ability for each node to process and respond to the information about itself in the context of its local environment. Furthermore, given a network's structure, there are optimal transmission delays for which the network remains synchronizable for longer processing delays. As a result, synchronization is not always improved—and in some cases it can be totally destroyed—by minimizing the transmission delays. For special cases we also study the scaling function that quantifies the synchronization of the system. This shows the limitation of synchronization in a noisy network

¹This research has been supported in part by DTRA and ONR.

²D. Hunt, G. Korniss, B.K. Szymanski, Phys. Rev. Lett. **105**, 068701 (2010)

³D. Hunt, G. Korniss, B.K. Szymanski, Phys. Lett. A **375**, 880 (2011)

3:18PM D54.00005 Continuous Percolation by Discontinuities, JAN NAGLER, MPI DS, Goettingen — In the very recent article [Science **333**, 322 (2011)], O. Riordan and L. Warnke, state that (i) *any rule based on picking a fixed number of random vertices gives a continuous transition*, and (ii) that therefore *explosive percolation is continuous*. It is equally true that certain percolation processes based on picking a fixed number of random vertices are discontinuous. Here we resolve this seeming paradox. We exemplify this by studying an extremal case of a process that is continuous in the sense of Riordan and Warnke but still exhibits infinitely many discontinuous jumps in arbitrary vicinity of the onset of the continuous phase transition. Moreover, we demonstrate analytically that continuity at the phase transition and discontinuity of the percolation process are compatible and generic for certain competitive percolation systems.

3:30PM D54.00006 Random Transverse Ising Model on Annealed Complex Networks, GINESTRA BIANCONI, Northeastern University — In order to shed light on critical phenomena on cuprates, here we propose a stylized model capturing the essential characteristics of the superconducting-insulator transition of a highly dynamical, heterogenous granular material: the Disordered Quantum Transverse Ising Model (DQTIM) on Annealed Complex Network. We show that when the networks encode for high heterogeneity of the expected degrees described by a power law distribution, the critical temperature for the onset of the superconducting phase diverges to infinity as the power-law exponent γ of the expected degree distribution is less than 3, i.e. $\gamma < 3$. Moreover we investigate the case in which the critical state of the electronic background is triggered by an external parameter g that determines an exponential cutoff in the power law expected degree distribution characterized by an exponent γ . We find that for $g = g_c$ the critical temperature for the superconductor-insulator transition has a maximum if $\gamma > 3$ and diverges if $\gamma < 3$.

3:42PM D54.00007 Dynamical Instability in Boolean Networks as a Percolation Problem, SHANE SQUIRES, MICHELLE GIRVAN, EDWARD OTT, University of Maryland – College Park — Boolean networks, a widely used model of gene regulatory networks, exhibit a phase transition between a stable regime, in which small perturbations die out, and an unstable regime, in which small perturbations grow exponentially. We show that this phase transition can be mapped onto a static percolation problem which predicts the critical point and the long-time Hamming distance between perturbed and unperturbed systems. The results, which apply to Boolean networks with a broad class of topologies and update functions, are confirmed by numerical simulations.

3:54PM D54.00008 Critical Behavior of the Ising Model on Small-world Hanoi Networks¹, TRENT BRUNSON, STEFAN BOETTCHER, Emory University — The addition of small-world bonds on hierarchical lattices changes a typical Ising model ferromagnetic phase transition to one of infinite order, referred to as the inverted-Berezinski-Kosterlitz-Thouless transition. We study this shift in phase behavior on Hanoi networks, which are one-dimensional Ising chains connected by small-world bonds that are self-similar and hierarchical in structure [1]. The phase behavior of the Ising model near T_c on Hanoi networks is studied using an exact renormalization group and Monte Carlo techniques. We show that compared to the Migdal-Kadanoff hierarchical lattice, Hanoi networks possess characteristics in their thermodynamic densities that are more physical. These densities are studied in detail and the behavior of their critical exponents near T_c is described. By introducing a continuous parameter which regulates the strength of small-world bonds in the Hanoi networks, we begin to uncover the essential small-world properties that dictate this change in phase behavior from second- to infinite-order.

[1] S. Boettcher and C.T. Brunson, Phys. Rev. E, **83**, 021103 (2011)

¹Funded under NSF grant #0812204.

4:06PM D54.00009 Popularity versus similarity in growing networks, DMITRI KRIOUKOV, University of California San Diego, FRAGISKOS PAPADOPOULOS, Cyprus University of Technology, MAKSIM KITSACK, University of California San Diego, MARIANGELES SERRANO, MARIAN BOGUNA, University of Barcelona — Preferential attachment is a powerful mechanism explaining the emergence of scaling in growing networks. If new connections are established preferentially to more popular nodes in a network, then the network is scale-free. Here we show that not only popularity but also similarity is a strong force shaping the network structure and dynamics. We develop a framework where new connections, instead of preferring popular nodes, optimize certain trade-offs between popularity and similarity. The framework admits a geometric interpretation, in which preferential attachment emerges from local optimization processes. As opposed to preferential attachment, the optimization framework accurately describes large-scale evolution of technological (Internet), social (web of trust), and biological (E.coli metabolic) networks, predicting the probability of new links in them with a remarkable precision. The developed framework can thus be used for predicting new links in evolving networks, and provides a different perspective on preferential attachment as an emergent phenomenon.

4:18PM D54.00010 Is it really a small world after all , BARUCH BARZEL, ALBERT-LASZLO BARABASI, Northeastern University, THE CENTER FOR COMPLEX NETWORK RESEARCH TEAM — One of the most intriguing revelations in the study of complex networks is the ubiquitous appearance of small worlds, that is networks exhibiting a small, and sometimes even ultra-small, average path length. This suggests that these networks feature globally connected dynamics, where all nodes are affected by all other nodes, given the short distance between them. Nevertheless, empirical data on the dynamics of such networks shows that in practice, such global connectedness is rarely observed. To address this gap between the topology and the observed dynamics of networks we developed the network correlation function method, a framework in which we obtain the patterns of influence between nodes in the network. In simple words we complement the topological description of *who is connected to whom*, by the dynamical description of *who is affected by whom*. Strikingly, using this method, we find that small world topology tends to avoid global dynamics, while non-small worlds could potentially support it. We test our results on a set of networks from various fields, ranging from social to biological networks, and discuss the implications on the dynamical stability of these systems.

4:30PM D54.00011 Metric Structure of Bipartite Networks , MAKSIM KITSACK, UCSD, FRAGKISKOS PADOPOULOS, Cyprus University of Technology., DMITRI KRIOUKOV, UCSD — Many social, biological and technological systems can be conveniently represented as bipartite networks, consisting of two disjoint sets of elements along with edges connecting only elements from different sets. Many of such systems are characterized by high values of bipartite clustering coefficient. We also find that pairs of elements in these bipartite systems tend to have many common neighbors. We present a natural interpretation of these observations. We suggest that elements of the above bipartite systems exist in underlying metric spaces, such that the observed high clustering is a topological reflection of the triangle inequality, the key property of metric space. We propose a simple stochastic mechanism of formation of bipartite networks embedded in metric spaces. We prove that this mechanism is able to reproduce the observed topological properties of bipartite networks. We also discuss the possibility of constructive embedding of real bipartite systems into metric spaces. In my talk I will overview the concept of hidden metric spaces with respect to both unipartite and bipartite networks. I will also discuss existing methods used to infer hidden metric spaces in real networks and possible applications for bipartite networks.

4:42PM D54.00012 Topological features of a fractal model for complex networks , LIN BO, HERNAN MAKSE, Levich Institute and Physics Department, the City College of New York — We study the construction and topological features of fractal and non-fractal hierarchical tree-like models generated through an inverse-renormalization growth mechanism with various parameters. These complex networks are characterized by scale-free distribution of connections, clustering coefficient, modular structure, degree correlation and a set of fractal dimensions. We compare the results with analytic expressions and show the dependence of topological properties on growing parameters. Networks with different tendency of hub-hub repulsion are produced and classified in terms of degree correlations. Interloops and intraloops are introduced into growing process to test robustness and stability of networks under attack.

4:54PM D54.00013 Control Centrality and Hierarchical Structure in Complex Networks , YANG-YU LIU, Northeastern University, JEAN-JACQUES SLOTINE, Massachusetts Institute of Technology, ALBERT-LASZLO BARABASI, Northeastern University — We introduce the concept of control centrality (C_c) to quantify the ability of a single node to control a directed weighted network. We map the control centrality into a combinatorial optimization problem. We calculate the distribution of control centrality for several real networks and find that it is mainly determined by the network's degree distribution. We show that the underlying hierarchical structure of a general directed network plays an important role in determining the distribution of control controllability. We rigorously prove that in directed acyclic graphs, i.e. directed networks without loops, a node's control centrality is uniquely determined by its topological position in the underlying hierarchical structure of the network. Our finding on the relation between control centrality and the hierarchical structure inspires us to design an effective random attack strategy against the controllability of malicious networks, without requiring the detailed knowledge of the network structure. We test our random attack strategy on several real networks and find it is indeed effective and even comparable to those targeted attacks which rely on the detailed knowledge of the network structure.

5:06PM D54.00014 A community detection approach to image segmentation and its phases , DANDAN HU, PETER RONHOVDE, ZOHAR NUSSINOV, Department of Physics, Washington University in St. Louis — In this talk, I will discuss "unsupervised" image segmentation that relies on phase diagram structure of the community detection method. Specifically, we apply a replica-inference-based community detection method. "Community detection" describes the general problem of partitioning a complex system involving many elements into optimally decoupled communities of such elements. In our image segmentation analysis, we invoke a multi-resolution community detection variant to ascertain the overall structure of the image at different resolutions. Information based measures (e.g., the normalized mutual information) are used to determine the significant structures at which "replicas" of the systems are strongly correlated. We report on the "easy", "hard", and "unsolvable" phases of the corresponding Potts model at both zero and finite temperatures. The optimal image segmentations are obtained by choosing parameters at the easy phase of the Potts model. The determination of the phase diagram in the analysis of the image segmentation is proved to be highly efficient. We demonstrate in a detailed study of various test cases that our method is fast and accurate and to be especially suited to the detection of camouflaged images.

5:18PM D54.00015 Ordinary Percolation with Discontinuous Transitions¹ , VIJAY SINGH, STEFAN BOETTCHER, Dept. of Physics, Emory University, Atlanta, GA 30322 USA — We study percolation on hierarchical networks using generating functions and renormalization group techniques. Our exact results show the presence of novel features in these networks including the existence of non-trivial critical points, three distinct regimes in the phase diagram and, most importantly, a discontinuity in the formation of the extensive cluster at a critical point $p_c < 1$. At p_c , the order parameter P_∞ describing the probability of any node to be a part of the largest cluster, jumps instantly to a finite value. We present simple examples of small-world networks with various hierarchies of long range bonds, indicating that the presence of discontinuous transitions is generic.

[1] S. Boettcher, V. Singh, and R.M. Ziff. Ordinary Percolation with Discontinuous Transitions. Arxiv preprint arXiv:1110.4288 (2):25, 2011.

¹Supported by NSF grant # 0812204.

Monday, February 27, 2012 5:45PM - 6:45PM —
Session E1 APS Prizes and Awards Ceremonial Session 253AB

5:45PM E1.00001 AWARD PRESENTATIONS —

Monday, February 27, 2012 6:45PM - 8:00PM —
Session F1 APS Welcome Reception Ballroom East

6:45PM F1.00001 WELCOME RECEPTION —

Monday, February 27, 2012 8:00PM - 9:30PM – Session G1 DCMP: Physics Community Outreach: The Kitchen as a Lab 253AB

8:00PM G1.00001 The Kitchen as a Lab, FERRAN ADRIA, JOSE ANDRES, World-famous Chef, MICHAEL P. BRENNER, Harvard University — Provocative world-famous Chef Ferran Adria, often associated with originating the modernist cuisine movement, and Washington DC chef Jose Andres, credited with bring the “small plates” movement to North America, will discuss their views on the creative preparation of food with unexpected contrasts of flavor, temperature, and texture. Their discussion will be followed by a talk by Michael P. Brenner, a professor of applied mathematics, who (along with physics professor David A. Weitz) teaches a course at Harvard University on science and cooking. Come learn about the science and the art of food preparation!

Tuesday, February 28, 2012 8:00AM - 11:00AM – Session H1 GIMS: Focus Session: Advances in Scanned Probe Microscopy I: Novel Approaches to Complex Systems 203

8:00AM H1.00001 Hybrid STM/AFM study of half-metallic surface states in cobaltates¹, ALEX W. CONTRYMAN, FRANCIS NIESTEMSKI, MING RUE D. THIAN, CAROLINA PARRA, YULIN CHEN, Stanford University, THORSTEN HESJEDAL, Oxford University, Z.X. SHEN, HARI C. MANOHARAN, Stanford University — Na_xCoO_2 is a well-known compound that has been studied at various Na concentrations, and has drawn much attention for its unconventional superconductivity and antiferromagnetic phase. In its stoichiometric concentration, NaCoO_2 has recently been proposed as a system for observing topological superconductivity when mixed with a superconductor's electronic states through the proximity effect. We examine NaCoO_2 using an ultrahigh-vacuum low-temperature hybrid scanning tunneling and atomic force microscope at 4 K. We use the tuning-fork AFM mode to study the topography of this bulk insulating material when no tunneling is possible, and utilize a special electrical contact scheme to access the electronic surface states for spectroscopy.

¹Supported by DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under contract DE-AC02-76SF00515. Alex W. Contryman is supported by a Dr. Robert M. Noyce Stanford Graduate Fellowship.

8:12AM H1.00002 Trend and novel challenges in spectroscopic imaging scanning tunneling microscopy for correlated electron materials research, JHINHWAN LEE, JIMIN KIM, SEOK HWAN CHOI, CHANHEE KIM, KAIST, HWANSOO SUH, Samsung Advanced Institute of Technology, KAZUHIRO FUJITA, Cornell University, SHIN-ICHI UCHIDA, University of Tokyo, J.C. SEAMUS DAVIS, Cornell University, Brookhaven National Lab — In this presentation we would like to discuss the recent progress of the spectroscopic imaging scanning tunneling microscopy (SI-STM) and how the real- and momentum-space sensitive spectroscopic tool is evolving into a more robust quantum theoretical tool for the phase transition study of the correlated electron materials.

- [1] Jhinhwan Lee, et al., Science 325, 1099 (2009).
- [2] Michael J. Lawler, et al., Nature 466, 374 (2010).
- [3] Colin V. Parker, et al., Nature 468, 677 (2010).
- [4] Ilija Zeljkovic, et al., arXiv:1104.4342v1 (2011).

8:24AM H1.00003 Unique vortex states on nanosize superconducting islands observed by LT-STM, TAKAKI SAKAMOTO, TAKAAKI TOMINAGA, Inst. Solid State Phys., Univ. Tokyo, TAKAHIRO NISHIO, RIKEN, TOYOAKI EGUCHI, JST-ERATO/Keio Univ., YASUO YOSHIDA, YUKIO HASEGAWA, Inst. Solid State Phys., Univ. Tokyo — With rapid progress of fabrication methods for nano-size superconductors, many novel properties of their superconductivity have been studied. Several vortex states unique to the nano superconductors, such as, vortex clustering, giant vortex, and anti-vortex, have been reported/predicted on specific size and shape of the islands. In this study we used Pb island structures with atomically flat surface formed on the Si(111) substrate under ultrahigh vacuum conditions as the superconducting sample. We investigate vortex states formed on the Pb islands under magnetic fields using low-temperature scanning tunneling microscopy (LT-STM), which enable us to observe the surface topograph and the superconducting gap (DOS) at atomic scale spatial resolutions simultaneously in real space. We performed precise tunneling spectroscopy on the Pb islands to take two dimensional DOS mapping at the Fermi level and succeeded in observing several kinds of vortex states (ex. multi vortex state and giant vortex state) in real space. The details will be discussed in the presentation.

8:36AM H1.00004 Scanning SQUID microscopy: A powerful tool for probing magnetism and superconductivity in complex oxides, JULIE A. BERT, Stanford Institute for Materials and Energy Science, Stanford University — Magnetic measurements are useful in investigating novel materials because they probe the behavior of electrons and their interactions. Superconducting Quantum Interference Devices (SQUIDS) are ultra-sensitive flux magnetometers and, when used in imaging mode, they become a powerful tool for mapping magnetic fields above a sample. This talk will outline the basics of scanning SQUID microscopy and highlight our recent measurements on a new material system: complex oxide interfaces. Our scanning SQUID technique uncovered the coexistence of superconductivity and magnetism in the LAO/STO oxide system. These measurements highlight many key benefits of the scanning SQUID technique including a 3 micron imaging kernel, excellent flux sensitivity, and an on-chip field coil to simultaneously measure both the intrinsic magnetism and the sample's response to an applied magnetic field.

9:12AM H1.00005 Spatial Dependence of Kondo Screening and Magnetic Anisotropy on Saturated Copper Nitride Islands, M. REYES CALVO, London Centre for Nanotechnology, UCL, London, UK, JENNY C. OBERG, London Centre for Nanotechnology, Dept. of Physics and Astronomy, UCL, London, UK, F. DELGADO, JOAQUIN FERNANDEZ-ROSSIER, International Iberian Nanotechnology Laboratory, Braga, Portugal, CYRUS F. HIRJIBEHEDIN, London Centre for Nanotechnology, Dept. of Physics and Astronomy, Dept. of Chemistry, UCL, London, UK — Co adatoms on a copper nitride surface constitute a unique system for studying the interplay between Kondo physics and anisotropy in a high spin atom ($S=3/2$). By using scanning tunneling spectroscopy techniques, we can determine both the energy scales of the Kondo screening and the spin excitations on a single atom. Here we study the case of Co adatoms on large nitride islands that form as the copper surface is saturated with nitrogen. These islands present a rich spatial variation of their electronic structure. We observe how changes in the electronic structure of the insulator result in dramatic changes in the spectroscopy of the cobalt adatoms: a considerable increase of the anisotropy energy occurs as the Kondo resonance disappears. These results allow us to explore in detail the interplay between these two phenomena.

9:24AM H1.00006 Evolution of the Kondo Resonance for Screened Atoms on Metals and Thin Insulators , JENNY C. OBERG, London Centre for Nanotechnology, UCL, UK; Department of Physics & Astronomy, UCL, UK, M. REYES CALVO, London Centre for Nanotechnology, UCL, UK, CYRUS F. HIRJIBEHEDIN, London Centre for Nanotechnology, UCL, UK; Department of Physics & Astronomy, UCL, UK; Department of Chemistry, UCL, UK — We study the magnetic anisotropy and the Kondo screening of the spin of Co atoms deposited on Cu₂N using scanning tunneling microscopy and spectroscopy. We find that for Co atoms placed on Cu₂N islands the Kondo screening is weaker when the atom is very close to the edge and at the same time has significant changes in the magnetic anisotropy. Furthermore we observe that Co atoms that are placed on the Cu surface but near the Cu₂N islands still show anisotropy and an unusually small Kondo temperature. At larger distances from the Cu₂N islands the usual large Kondo temperature recovers. We examine possible causes for these dramatic changes in the Kondo screening and magnetic anisotropy, including a possible extension of the electronic properties of the Cu₂N islands compared to the topographic influence.

9:36AM H1.00007 Atomic force microscopy as nano-stethoscope to study living organisms, insects , IGOR SOKOLOV, MAXIM DOKUKIN, NATALIYA GUZ, Clarkson University — Atomic force microscopy (AFM) is a known method to study various surfaces. Here we report on the use of AFM to study surface oscillations (coming from the work of internal organs) of living organisms, like insects. As an example, ladybird beetles (*Hippodamia convergens*) measured in different parts of the insect at picometer level. This allows us to record a much broader spectral range of possible surface vibrations (up to several kHz) than the previously studied oscillations due to breathing, heartbeat cycles, coelopulses, etc. (up to 5 -10 Hz). The used here AFM method allows collecting signal from the area as small as ~100nm² (0.0001μm²) with an example of noise level of (2±0.2)×10⁻³ nm r.m.s. at the range of frequencies >50Hz (potentially, up to a MHz). Application of this method to humans is discussed. The method, being a relatively non-invasive technique providing a new type of information, may be useful in developing of what could be called “nanophysiology.”

9:48AM H1.00008 Scanning tunneling microscopy study of the assembly and structure of filamentous virus M13 bound to graphite , PRASHANT SHARMA, Department of Physics, Suffolk University, Boston, MA 02114 — Viruses are an important class of biomaterials used for placing nano particles on inorganic substrates. To accomplish greater control over viral assembly on a substrate it is important to determine the in situ nanoscale structure of the viral protein coat. Scanning tunneling microscopy offers the unique potential for determining the structure and arrangement of the proteins of a virus adsorbed on a conducting substrate. In this work, I develop an experimental technique for isolating and studying M13 viruses that bind to graphite. Using scanning tunneling microscopy in ambient conditions I obtain the correct lateral dimension of the virus and the periodicity of its protein structure when it is bound to graphite. I also analyze the tunneling conductance fluctuations in these measurements and introduce a simple model for tunneling through an assembly of proteins to obtain an accurate estimation of the vertical dimension of a virus bound to a conducting substrate. I discuss broader implications of this scanning tunneling microscopy study for the in situ structure determination of other biomolecules.

10:00AM H1.00009 Nanomechanics of Murine Articular Cartilage Reveals the Effects of Chondroadherin Knockouts¹ , MICHAEL BATISTA, ALAN GRODZINSKY, MIT, CHRISTINE ORTIZ, Massachusetts Institute of Technology, DICK HEINEGÅRD, Lund University, LIN HAN, Massachusetts Institute of Technology — With high resolution nanotechnology tools, quantification of cartilage biomechanical properties provides important insights into the role of low abundance matrix molecules on cartilage function and pathology. In this study, the role of chondroadherin (CHAD) on cartilage mechanical properties was assessed via atomic force microscopy-based nanoindentation (0.1-10 μm/s z-piezo displacement rates) of murine knee cartilage from wild type (WT) and CHAD knockout (KO) animals ages 1 year, 4 month, and 11 weeks (n≥4 joints/age-group). A significant increase in indentation modulus, E, with indentation rate in all specimens (p<0.05, Friedman) suggested poro-viscoelastic behavior. For all age groups, CHAD KO significantly reduced E at all indentation rates (p<0.05, 2-way ANOVA); e.g., at 1-year, E was 0.77±/-0.1 MPa for WT (mean±/-SEM 1μm/s rate) and 0.25±/-0.07 MPa for CHAD KO cartilage. Lack of CHAD appears to delay development of load bearing extracellular matrix. This could affect the effective cross-link density of the tissue network and, hence, decrease local osmotic swelling while increasing the hydraulic permeability of the aggrecan-filled network. Ongoing studies are investigating the biochemical properties and nanostructure of CHAD KO joints.

¹This work was supported by the National Science Foundation MIT Center for Materials Science and Engineering (DMR-0819762), and the National Security Science 400 and Engineering Faculty Fellowship (N00244-09-1-0064) and by the Swedish Research Council.

10:12AM H1.00010 Nanoindenter Stiffness Measurements on a MEMS Sound Sensor¹ , R. DOWNEY, L. BREWER, G. KARUNASIRI, Naval Postgraduate School — We demonstrate a novel technique to extract the various components of the stiffness (or compliance) measured along the surface of a MEMS directional sound sensor. Because the sensor comprises a cantilever beam mounted on torsion springs, the overall stiffness consists of various compliance components added in series. Stiffness measurements made using a nanoindenter are found to agree with an analytical model and a finite element model (FEM) of the sensor. Moreover, by exploiting the differing power-law characteristics of the individual compliance components, we demonstrate extraction of the separate components from a logarithmic plot of the overall stiffness. Finally, we measure the ultimate (failure) strength of the sensor, from which we obtain the maximum acoustic intensity the sensor can tolerate.

¹Supported by NSF

10:24AM H1.00011 Primary electron beam generation in Near-Field-Emission SEM , DANILO ANDREA ZANIN, HUGO CABRERA, LORENZO GIUSEPPE DE PIETRO, URS RAMSPERGER, DANILO PESCIA, Laboratory for Solid State Physics, ETH Zurich, Switzerland — Due to low electron energies used in Near-Field-Emission SEM (NFESSEM), the understanding of the physical phenomena governing the primary electron beam generation is of fundamental relevance. The geometry and the chemical composition of the ultra-sharp field emitter have been therefore investigated by using different well-known electron microscopy techniques. The last hundreds of nanometers of such a field emitter, produced by electrochemical etching of a tungsten wire, can be macroscopically approximated by a cone with angle of aperture of about 6° ± 1°. The shape of the very apex is strongly dependent on the preparation conditions. Moreover, the only remaining contamination after the annealing procedure of the tungsten tips is a tungsten-oxide coating, uniformly distributed on the surface.

10:36AM H1.00012 Chemical contrast in Near-Field-Emission SEM , LORENZO GIUSEPPE DE PIETRO, MANFRED THALMANN, HUGO CABRERA, DANILO ANDREA ZANIN, URS RAMSPERGER, DANILO PESCIA, Laboratory for Solid State Physics, ETH Zurich, Switzerland — In Near-Field-Emission SEM the primary electron beam, of some tens of eV, is generated by cold field emission from a polycrystalline W-tip. Recently, topography images have been obtained by scanning a W(110) sample with a tip at constant height, typically of tens of nm, recording the secondary electron yield and the emission current. We report on the observation of a chemical contrast of a W(110) surface covered by submonolayer of Fe achieved with the NFESSEM technique. The chemical contrast is caused by a significant lower secondary electron yield for Fe with respect to W. The Fe islands with a diameter of 2 nm to 5 nm are clearly distinguishable, giving a direct indication of the microscope lateral resolution. The adsorbate position, size and shape are confirmed by STM. Moreover, this technique shows the presence of Fe growing along the step edges of the substrate, which can not be identified with STM.

10:48AM H1.00013 Electrostatic characterization of Near-Field-Emission SEM, HUGO CABRERA, DANILO ANDREA ZANIN, LORENZO GIUSEPPE DE PIETRO, URS RAMSPERGER, DANILO PESCIA, Laboratory for Solid State Physics, ETH Zurich, Switzerland — The properties of the primary electron beam in Near-Field-Emission SEM (NFEM) are uniquely determined by the actual geometry and position of the conducting components in the experimental apparatus. The reciprocal dependence of the accessible quantities, namely the voltage applied to the emitting tip with respect to the conducting sample surface (V), the relative distance between the tip and the sample (d) and the field-emission current (I), has been thoroughly characterized. In particular, the voltage V needed to produce a given current I has been measured as a function of d ; the values of I have been chosen in the range from 0.05 nA to 1.5 nA, while d has been varied from 4 to 1500 nm. For values of d smaller than a certain threshold $\bar{d}$, dependent on the tip, V turns out to be directly proportional to the distance between the tip and the sample surface. At larger distances, $d > \bar{d}$, we found $V \propto I^a \cdot d^b$, with a and b generally varying from one tip to the another. These results are supported by preliminary theoretical calculations which assume electrostatic geometries directly inspired by the NFEM setup, such as an hyperboloid-shaped emitter with a conduction plane lying at a generic d .

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H2 FPS FEd: Invited Session: Novel and Proven Methods of Communicating Science to the Public 204AB

8:00AM H2.00001 Creating Catalytic Collaborations between Theater Artists, Scientists, and Research Institutions¹, DEBRA WISE, Catalyst Collaborative @ MIT — Catalyst Collaborative@MIT (CC@MIT) is a collaboration between MIT and Underground Railway Theater (URT), a company with 30 years experience creating theater through interdisciplinary inquiry and engaging community. CC@MIT is dedicated to creating and presenting plays that deepen public understanding about science, while simultaneously providing artistic and emotional experiences not available in other forms of dialogue about science. CC@MIT engages audiences in thinking about themes in science of social and ethical concern; provides insight into the culture of science and the impact of that culture on society; and examines the human condition through the lens of science that intersects our lives and the lives of scientists. Original productions range from Einstein's Dreams to From Orchids to Octopi – an evolutionary love story; classics re-framed include The Life of Galileo and Breaking the Code (about Alan Turing). CC@MIT commissions playwrights and scientists to create plays; engages audiences with scientists; performs at MIT and a professional venue near the campus; collaborates with the Cambridge Science Festival and MIT Museum; engages MIT students, as well as youth and children. Artistic Director Debra Wise will address how the collaboration developed, what opportunities are provided by collaborations between theaters and scientific research institutions, and lessons learned of value to the field.

¹Would like to acknowledge support from both MIT and Underground Railway Theater.

8:36AM H2.00002 Using Cartoons to Communicate Science, ODD TODD, Odd Todd Studios — No abstract available.

9:12AM H2.00003 Drawing at the Speed of Talk: doodling complex discussions in real-time to create animated “Conversation Portraits”, FLASH ROSENBERG, Artist in Residence for LIVE from the New York Public Library — What does your research look like as a drawing? Imagine the guy who delivered your pizza understanding the latest paper you delivered. Flash Rosenberg will describe how she “live-draws” discussions between prominent authors and scientists to create lucid animations. She will offer strategies for how to translate the impenetrable into the understandable, convert equations into sensations, and enable everyone to appreciate issues in physics as relevant, intriguing fun. View sample “Conversation Portraits” at <http://vimeo.com/flashrosenberg/videos>

9:48AM H2.00004 The New Wave of Science Festivals and their Establishment, JOHN DURANT, Director of MIT Museum and the Cambridge Science Festival — No abstract available.

10:24AM H2.00005 Celebrating 24 years of Public Outreach of Science and Engineering in Portland Oregon, TERRY BRISTOL, President, Institute for Science, Engineering and Public Policy — There have been several core strategies in our highly successful 24-year Science, Technology and Society outreach program. However, the strategy for each season is also dynamic, requiring innovation and novel coalitions. As Bob Dylan put it so succinctly, “He not busy being born is busy dying.” Public outreach programs - as the Chautauquas of the past - should be positioned in the cultural milieu along with the opera, symphony and theatre. Support for the enterprise needs to be a broad and diverse coalition, based ideally on the creative formation of win-win relationship. You want people to see your success as their success: “Together we can enhance the intellectual environment in ways that none of us could do alone.” Being multi-disciplinary presents challenges but has considerable advantages. For instance, enlightened managers of established organizations recognize the value of exposing their employees to a diversity of problem solving approaches. Instead of inviting speakers for one large lecture we now invite them to be Resident Scholars for two-three days and develop a range of additional smaller public engagements. Science and engineering topics must be relevant - placed in the broader Science, Technology and Society framework. We avoid “gee-whiz” in favor of what stimulates reflection on who we are, where we came from, and our role in the universe. I will briefly review how we have survived and thrived and, finally, what I see as future trends and opportunities.

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H3 DCMF: Invited Session: Electronic Properties of the Pseudogap Phase in Cuprates 205AB

8:00AM H3.00001 Extremely Correlated Fermi Liquids¹, SRIRAM SHASTRY, University of California Santa Cruz — A new framework is reported for calculating the properties of extremely correlated electronic systems with eliminated double occupancy. Based on Schwinger's approach to field theory, it avoids using auxiliary variables, and leads to a low (particle) density expansion with equations that approximately double the complexity of the standard theory for interacting electrons. Concrete results for the one electron spectral function of the t - J model in 2-dimensions are presented to lowest non trivial order in density. These already show considerable promise in the context of cuprate superconductors. A distinguishing characteristic of this theory is the low energy long wavelength asymmetry between adding holes and particles. Prospects for the experimental observation of this asymmetry are discussed.

[1] “Extremely Correlated Fermi Liquids,” B. S. Shastry, arXiv:1102.2858 (2011), Phys. Rev. Letts. 107, 056403 (2011).

[2] “Dynamical Particle Hole Asymmetry in Cuprate Superconductors,” B. S. Shastry, arXiv: 1110.1032 (2011)

¹This work was supported by DOE under Grant No. FG02-06ER46319

8:36AM H3.00002 The new extremely correlated electron perspective of the normal state of high temperature superconductors, GEY-HONG GWEON, UC Santa Cruz — In this talk, two recent angle resolved photoelectron spectroscopy (ARPES) studies on high temperature superconductors are discussed. These studies show the importance of the “extreme electron correlation” a la t-J model. First, we will discuss the normal state single particle spectral function, which has been considered both anomalous and crucial to understand. Here, we report [1] an unprecedented success of applying the new t-J model based “extremely correlated Fermi liquid theory” by Shastry, to describe both laser ARPES data and conventional synchrotron ARPES data on $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ and synchrotron ARPES data on $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$. It fits all data sets with the same physical parameter values, satisfies the particle sum rule and successfully addresses two widely discussed kink anomalies in the dispersion. Second, new ARPES investigation [2] of the Fermi surface geometry of $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$ from underdoping to overdoping shows that the “weak correlation” Luttinger sum rule, based on Fermi surface only, clearly breaks down in the underdoped case. We note that a t-J model based theory by Yang, Rice and Zhang provides an alternative “extreme correlation” Luttinger sum rule, based on both Fermi surface and “Luttinger surface.” This extreme correlation Luttinger sum rule offers much more natural explanation for the observed ARPES data. These two studies imply that the extreme correlation as embodied in the t-J model is essential for understanding high temperature superconductors over a wide doping range.

[1] Gweon, Shastry, and Gu, Phys. Rev. Lett. 107, 056404 (2011).

[2] Meng, Gweon et al., Phys. Rev. B 84, 060513(R) (2011).

9:12AM H3.00003 A Phenomenological Theory of the Anomalous Pseudogap Phase in Underdoped Cuprates, T. MAURICE RICE, Theoretical Physics, ETH Zurich, CH 8093 Zurich Switzerland — A consistent theoretical description of the many anomalous properties that characterize the pseudogap phase in the underdoped region of the cuprate phase diagram has proved challenging. The continuous progress in spectroscopic and other experiments suggests a phenomenological approach. An ansatz based on analogies to the transition to Mott localization at weak coupling in lower dimensional systems, has been proposed by Yang, Rice and Zhang some years back [1]. This ansatz has had success in describing a wide range of experiments [2]. The motivation underlying this ansatz will be described and some of the comparisons to experiment reviewed. The implications for a more microscopic theory will be discussed together with the relation to microscopic theories that start directly from strongly coupled Hamiltonians.

[1] K-Y. Yang, T. M. Rice & F. C. Zhang, Phys. Rev. B73,174501 (2006)

[2] T. M. Rice, K.-Y. Yang & F. C. Zhang, arXiv 1109.0632

9:48AM H3.00004 Fermi pockets and the pseudogap in underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8^1}$, HONGBO YANG, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory — The Fermi surface topologies of underdoped samples of the high T_c superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ have been measured with angle resolved photoemission. By examining thermally excited states above the Fermi level, we show that the observed Fermi surfaces in the pseudogap phase are actually components of enclosed hole-pockets. The spectral weight of these pockets is vanishingly small at the magnetic zone boundary, creating the illusion of Fermi “arc”. The area of the pockets as measured in this study is consistent with the doping level, and hence carrier density, of the samples measured. Furthermore, the shape and area of the pockets is well reproduced by phenomenological models of the pseudogap phase as a spin liquid. The demonstration that the pseudogap in the anti-nodal region is a gap symmetric about the chemical potential is a clear indication that singlet pairing takes place in the normal state.

¹The work at Brookhaven is supported in part by the U.S. DOE under Contract No. DE-AC02-98CH10886 and in part by the Center for Emergent Superconductivity (CES), an Energy Frontier Research Center funded by the U.S. DOE, Office of Basic Energy Sciences.

10:24AM H3.00005 Nodal-antinodal dichotomy in underdoped cuprates: a cluster-dynamical mean-field theory perspective., ANTOINE GEORGES, College de France — A distinctive feature of the normal state of underdoped cuprates is the strong dichotomy between nodal and antinodal regions. The nodal regions display well-defined quasiparticle excitations. In contrast, single-particle lineshapes are very broad near the antinodes, where a pseudogap opens. Cluster extensions of dynamical mean-field theory provide an understanding of this phenomenon as a momentum-selective Mott transition. This will be reviewed in this talk and confronted to experiments and to other theoretical approaches.

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H4 DAMOP: Spin-orbit Coupling in Ultracold Gases 205C

8:00AM H4.00001 Topological phase transitions in ultra-cold Fermi superfluids: the evolution from BCS to BEC under artificial spin-orbit fields, LI HAN, KANGJUN SEO, CARLOS A.R. SA DE MELO, School of Physics, Georgia Institute of Technology — We discuss topological phase transitions in ultra-cold Fermi superfluids induced by interactions and artificial spin orbit fields. We construct the phase diagram for population imbalanced systems at zero and finite temperatures, and analyze spectroscopic and thermodynamic properties to characterize various phase transitions. For balanced systems, the evolution from BCS to BEC superfluids in the presence of spin-orbit effects is only a crossover as the system remains fully gapped, even though a triplet component of the order parameter emerges. However, for imbalanced populations, spin-orbit fields induce a triplet component in the order parameter that produces nodes in the quasi-particle excitation spectrum leading to bulk topological phase transitions of the Lifshitz type. Additionally a fully gapped phase exists, where a crossover from indirect to direct gap occurs, but a topological transition to a gapped phase possessing Majorana fermions edge states does not occur.

8:12AM H4.00002 BCS-BEC Crossover and Topological Phase Transition in 3D Spin-Orbit Coupled Degenerate Fermi Gases, MING GONG, Department of Physics and Astronomy, Washington State University, Pullman, Washington, 99164, USA, SUMANTA TEWARI, Department of Physics and Astronomy, Clemson University, Clemson, South Carolina 29634, USA, CHUANWEI ZHANG, Department of Physics and Astronomy, Washington State University, Pullman, Washington, 99164, USA, CHUANWEI ZHANG TEAM, SUMANTA TEWARI COLLABORATION — We investigate the BCS-BEC crossover in three-dimensional degenerate Fermi gases in the presence of spin-orbit coupling (SOC) and Zeeman field. We show that the superfluid order parameter destroyed by a large Zeeman field can be restored by the SOC. With increasing strengths of the Zeeman field, there is a series of topological quantum phase transitions from a nontopological superfluid state with fully gapped fermionic spectrum to a topological superfluid state with four topologically protected Fermi points (i.e., nodes in the quasiparticle excitation gap) and then to a second topological superfluid state with only two Fermi points. The quasiparticle excitations near the Fermi points realize the long-sought low-temperature analog of Weyl fermions of particle physics. We show that the topological phase transitions can be probed using the experimentally realized momentum-resolved photoemission spectroscopy. Phys. Rev. Lett. 107, 195303 (2011).

8:24AM H4.00003 BCS-BEC crossover in 2D spin-orbit coupled degenerate Fermi gases¹, CHUANWEI ZHANG, GANG CHEN, MING GONG, Department of Physics and Astronomy, Washington State University, Pullman, WA 99164 — The recent experimental realization of spin-orbit coupling for ultra-cold atoms has generated much interest in the physics of spin-orbit coupled degenerate Fermi gases. Although recently the BCS-BEC crossover in 3D spin-orbit coupled Fermi gases has been intensively studied, the corresponding 2D crossover physics has remained unexplored. In this talk, we discuss the BCS-BEC crossover physics in 2D degenerate Fermi gases in the presence of spin-orbit coupling. We derive the zero temperature mean field gap and atom number equations suitable for the 2D spin-orbit coupled Fermi gases, from which the dependence of the ground state properties (pairing gap, chemical potential, etc.) on the system parameters (e.g., binding energy, spin-orbit coupling strength) is obtained, both numerically and analytically. We characterize the dependence of the BKT transition temperature as well as the vortex-antivortex lattice melting temperature on the spin-orbit coupling strength and the external Zeeman field.

¹This work is supported by DARPA-YFA, ARO, NSF, and AFOSR

8:36AM H4.00004 One-dimensional Ultracold Fermi Gases with Spin-orbit Coupling, YINGFEI GU, HUI ZHAI, Institute for Advanced Study, Tsinghua Univ., Beijing 100084 — We study one-dimensional ultracold Fermi gases with spin-orbit coupling. We use the Bogoliubov-de Gennes equations to determine pairing order parameter, and find out new phases in addition to fully polarized normal phase, fully paired BCS phase and the FFLO phase. We complete the phase diagram in terms of polarization, interaction parameter and strength of spin-orbit coupling.

8:48AM H4.00005 Who is the Lord of the Rings in the Zeeman-spin-orbit Saga: Majorana, Dirac or Lifshitz?¹, CARLOS SA DE MELO, KANGJUN SEO, LI HAN, Georgia Institute of Technology — Zeeman, spin-orbit fields and interactions can be tuned in the context of ultra-cold atoms and allow for the visitation of several different phases. For systems with zero Zeeman field, the evolution from BCS to BEC superfluidity in the presence of spin-orbit effects is only a crossover [1]. In contrast, for finite Zeeman fields, spin-orbit coupling induces a triplet component in the order parameter that produces nodes in the quasiparticle excitation spectrum leading to bulk topological phase transitions of the Lifshitz type [2]. A fully gapped phase also exists, where a crossover from indirect to direct gap occurs. For spin-orbit couplings with equal Rashba and Dresselhaus strengths the nodal quasi-particles are Dirac fermions that live at and in the vicinity of rings of nodes. Transitions from and to nodal phases can occur via the emergence of zero-mode Majorana fermions at phase boundaries, where rings of nodes of Dirac fermions annihilate [3]. Lastly, we characterize different phases via spectroscopic and thermodynamic properties and conclude that Lifshitz is the “Lord of the Rings.”

[1] Li Han, C. A. R. Sa de Melo, arXiv:1106.3613v1.

[2] Kangjun Seo, Li Han and C. A. R. Sa de Melo, arXiv:1108.4068v2.

[3] Kangjun Seo, Li Han and C. A. R. Sa de Melo, arXiv:1110.6364v1.

¹We thank the Army Research Office (W911NF-09-1-0220) for support.

9:00AM H4.00006 Quantum phases of atomic Fermi gases with spin-orbit coupling¹, MENDERES ISKIN, Koc University, LEVENT SUBASI, Istanbul Technical University — We consider a general anisotropic spin-orbit coupling and analyze the phase diagrams of both balanced and imbalanced Fermi gases for the entire BCS-BEC evolution. First we use the self-consistent mean-field theory at zero temperature, and show that the topological structure of the ground-state phase diagrams is quite robust against the effects of anisotropy. Then we go beyond the mean-field description, and investigate the effects of Gaussian fluctuations near the critical temperature. This allows us to derive the time-dependent Ginzburg-Landau theory, from which we extract the effective mass of the Cooper pairs and their critical condensation temperature in the molecular BEC limit.

¹Supported by Marie Curie IRG FP7-PEOPLE-IRG-2010-268239; TUBITAK Career 3501-110T839, and TUBA-GEBIP grants.

9:12AM H4.00007 Low-density molecular gas of tightly-bound Rashba-Dresselhaus fermions, SO TAKEI, CHIEN-HUNG LIN, Condensed Matter Theory Center, The University of Maryland College Park, BRANDON ANDERSON, National Institute for Standards and Technology, VICTOR GALITSKI, Joint Quantum Institute and Physics Department, University of Maryland — We study interacting Rashba-Dresselhaus fermions in two spatial dimensions. First, we present a new exact solution to the two-particle pairing problem of spin-orbit-coupled fermions for arbitrary Rashba and Dresselhaus spin-orbit interactions. An exact molecular wave function and the Green function are explicitly derived along with the binding energy and the spectrum of the molecular state. In the second part, we consider a thermal Boltzmann gas of fermionic molecules and compute the time-of-flight velocity and spin distributions for a single fermion in the gas. We show that the pairing signatures can be observed already in the first-moment expectation values, such as time-of-flight density and spin profiles.

9:24AM H4.00008 Order by Disorder in Spin-Orbit Coupled Bose-Einstein Condensates, RYAN BARNETT, STEPHEN POWELL, Joint Quantum Institute and Condensed Matter Theory Center, University of Maryland, TOBIAS GRASS, ICREA-Institutio Catalana de Recerca i Estudis Avancats, MACIEJ LEWENSTEIN, ICREA-Institutio Catalana de Recerca i Estudis Avancats and ICFO, SANKAR DAS SARMA, Joint Quantum Institute and Condensed Matter Theory Center, University of Maryland — Motivated by recent experiments, we investigate the system of isotropically-interacting bosons with Rashba spin-orbit coupling. At the non-interacting level, there is a macroscopic ground-state degeneracy due to the many ways bosons can occupy the Rashba spectrum. Interactions treated at the mean-field level restrict the possible ground-state configurations, but there remains an accidental degeneracy not corresponding to any symmetry of the Hamiltonian, indicating the importance of fluctuations. By finding analytical expressions for the collective excitations in the long-wavelength limit and through numerical solution of the full Bogoliubov-de Gennes equations, we show that the system condenses into a single momentum state of the Rashba spectrum via the mechanism of order by disorder. We show that in 3D the quantum depletion for this system is small, while the thermal depletion has an infrared logarithmic divergence, which is removed for finite-size systems. In 2D, on the other hand, thermal fluctuations destabilize the system. This work is supported in part by JQI-PFC.

9:36AM H4.00009 Exotic 3D Spin-Orbit Couplings, BRANDON ANDERSON, JQI, NIST and the University of Maryland, GEDIMINAS JUZELIUNAS, Institute of Theoretical Physics and Astronomy and Vilnius University, IAN SPIELMAN, VICTOR GALITSKI, JQI, NIST and the University of Maryland — We describe a scheme for creating an isotropic three-dimensional spin-orbit coupling, dubbed Weyl spin-orbit coupling, in systems of ultracold atoms. This coupling is induced by Raman transitions that link four internal atomic states with a tetrahedral geometry. This spin-orbit coupling gives rise to a Dirac point that is robust against environmental perturbations. We then propose a general procedure for generating exotic three-dimensional spin-orbit couplings with degenerate ground states on more complex manifolds. The procedure is applied to produce a spin-orbit coupling with a toroidal ground state manifold. Finally, we discuss the many-body implications of the exotic spin-orbit couplings.

9:48AM H4.00010 Cold-atom systems with synthetic SU(3) spin-orbit coupling¹, GREG BOYD, RYAN BARNETT, VICTOR GALITSKI, University of Maryland — Recently, the ability to create and control artificial gauge fields in cold gases has been experimentally demonstrated. Here, we propose a scheme to realize synthetic SU(3) spin-orbit interactions and derive an effective single-particle Hamiltonian, parameterized by the Gell-Mann matrices. We then investigate a many-body system of SU(3)-spin-orbit-coupled bosons and derive and analyze numerically the Gross-Pitaevskii equation to describe the effect of interaction on the possible ground states. The time-of-flight density profiles to probe various many-body states in the rich phase diagram of the system are calculated.

¹This research is supported by ARO's atomtronics MURI (G.B. and V.G.) and JQI-PFC (R.B.)

10:00AM H4.00011 Superfluidity of Bosons in Optical lattices with Spin-Orbit coupling¹, QINQIN LU, DANIEL SHEEHY, Louisiana State University — Recent experimental and theoretical work has explored artificial spin-orbit coupling induced among two species of boson. Here we examine superfluidity of a cold gas of bosons with spin-orbit coupling in a periodic optical lattice, in the presence of additional short-range interactions. We compute the density distribution after free expansion from the lattice as a probe of superfluidity, and phase transitions, of the trapped gas.

¹This work has been supported by the Louisiana Board of Regents, under grant LEQSF (2008-11)-RD-A-10.

10:12AM H4.00012 Spinor Bose-Einstein Condensates Under Synthetic Gauge Field¹, XIAO-QIANG XU, JUNG HOON HAN, Department of Physics and BK21 Physics Research Division, Sungkyunkwan University, Suwon 440-746, Korea — Due to the recent popularity of synthetic gauge field in ultracold atoms, I will talk about the combined effects of Rashba spin-orbit coupling (SOC) and rotation in spin -1/2 condensates [X.-Q. Xu et al, Phys. Rev. Lett. 107, 200401 (2011)]. Novel features appear in the ground state wave function, such as the existence of a half-quantum vortex or giant vortex, domains of stripe-like phase, suppressed Skyrmion order. Additionally, I will talk about the interesting mapping between pure Rashba BECs and chiral magnets with Dzyaloshinskii-Moriya (DM) interaction.

¹We are supported by the Mid-career Researcher (No. 2010-0008529) and acknowledge helpful interactions with Hui Zhai.

10:24AM H4.00013 BCS-BEC crossover induced by a synthetic non-Abelian gauge field¹, VIJAY B. SHENOY, JAYANTHA P. VYASANAKERE, Indian Institute of Science, S. ZHANG, Ohio State University — We investigate the ground state of interacting spin-*half* fermions(3D) at a finite density ($\rho \sim k_F^3$) in the presence of a uniform non-Abelian gauge field (with magnitude λ) that generates a generalized Rashba spin-orbit interaction. For a weak attractive interaction in the singlet channel described by a small negative scattering length ($k_F|a_s| \lesssim 1$), the ground state in the absence of the gauge field ($\lambda = 0$) is a BCS superfluid with large overlapping pairs. With increasing λ , a non-Abelian gauge field engenders a crossover of this BCS ground state to a BEC ground state of bosons even with a weak attractive interaction. For large gauge couplings ($\lambda/k_F \gg 1$), the BEC attained is a condensate of bosons whose properties are solely determined by the gauge field (and not by the scattering length); we call these bosons "rashbons." In the absence of interactions ($a_s = 0^-$), the shape of the Fermi surface of the system undergoes a topological transition at a critical gauge coupling λ_T . For high symmetry gauge field configurations we show that the crossover from the BCS superfluid to the rashbon BEC occurs in the regime of λ near λ_T .

¹Supported by DST and DAE, India

10:36AM H4.00014 Trapped fermions in a synthetic non-Abelian gauge field¹, SUDEEP KUAMAR GHOSH, JAYANTHA P. VYASANAKERE, VIJAY B. SHENOY, Indian Institute of Science Bangalore — On increasing the coupling strength (λ) of a non-Abelian gauge field that induces a generalized Rashba spin-orbit coupling, the topology of the Fermi surface of a homogeneous gas of non-interacting fermions of density $\rho \sim k_F^3$ undergoes a change at a critical value, $\lambda_T \approx k_F$ [PRB 84, 014512 (2011)]. We analyze how this affects the size/shape of a cloud of fermions trapped in a harmonic potential. We develop an adiabatic formulation, with Pancharatnam-Berry phase terms, for the one particle states in a trap with the gauge field. Local density approximation reveals that the cloud shrinks in a *characteristic fashion with increasing* λ and predicts a spherical cloud for all gauge field configurations. We show, via a calculation of the cloud shape using exact eigenstates, that for certain gauge fields there is systematic anisotropy in the cloud shape that increases with increasing gauge coupling λ . An important spin-off of our adiabatic formulation is that it reveals exciting possibilities for the cold-atom realization of interesting Hamiltonians (eg. quantum hall spherical geometry) by using a non-Abelian gauge field in conjunction with another potential.

¹Supported by DST and DAE, India

10:48AM H4.00015 Effects of the interplay between spin-orbit coupling and interaction on bosons, QI ZHOU, The Chinese University of Hong Kong, XIAOLING CUI, Institute for Advanced Study, Tsinghua University — We show that spin-orbit coupling drastically changes the properties of bosons. The interplay between the spin-orbit coupling and interaction determines the fate of Bose-Einstein condensate, which may even not exist in the presence of isotropic spin-orbit coupling. For anisotropic spin-orbit coupling, condensates survive and are characterized by anisotropic energy spectrum, with a slower sound velocity along the direction of weaker spin-orbit coupling. The spectrum can also be used to distinguish the plane wave phase and the tripe phase.

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H5 DMP: Focus Session: Interfaces in Complex Oxides - Polar Interfaces and Ferro-electrics 206A

8:00AM H5.00001 First-principles study of intermixing and polarization at the DyScO₃/SrTiO₃ interface, KOUROSH RAHMANIZADEH, GUSTAV BIHLMAYER, STEFAN BLÜGEL, Peter Gruenberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Juelich and JARA, 52425 Juelich, Germany, MARTINA LUYSEBERG, Peter Gruenberg Institut (PGI-5) & Ernst Ruska Centre, Forschungszentrum Juelich and JARA, 52425 Juelich, Germany — Exploring oxide interfaces is an attractive challenge, due to the emerging novel behaviors which don't exist in the corresponding parent bulk compounds. E. g. joining two simple band insulators LaAlO₃ and SrTiO₃ with different polarity can induce conductivity at the interface. We carried out density functional theory (DFT) calculations based on the full potential linearized augmented planewave (FLAPW) method as implemented in the FLEUR code (www.flapw.de) for studying the polar to non-polar interface of DyScO₃ and SrTiO₃. Due to the polar discontinuity, arising from nominally charged DyO or ScO₂ layers, sharp interfaces induce a strong ferroelectric-like polarization in the SrTiO₃, while in off-stoichiometric interfaces this discontinuity is avoided and no such polarization can be found. In both scenarios the interface remains insulating with only a small reduction of the bandgap. Our calculations show that chemically mixed interfaces are energetically more favorable than sharp ones. Our DFT calculations explore also different configurations of the Dy and Sr atoms within the mixed interface plane. The calculated ground state configuration is confirmed by experimental observations.

8:12AM H5.00002 Growth and transport properties of fractionally δ -doped oxide superlattices¹, HO NYUNG LEE, WOO SEOK CHOI, Oak Ridge National Laboratory, SUYOUN LEE, Korea Institute of Science and Technology, VALENTINO COOPER, Oak Ridge National Laboratory — LaTiO₃/SrTiO₃ (LTO/STO) heterostructures are interesting as they show an intriguing 2D conduction, and their bulk counterpart, La_xSr_{1-x}TiO₃ (LSTO), exhibits a filling-controlled insulator-metal transition (IMT). In this study, we investigated the filling controlled IMT in 2D geometry by fabricating monolayer-thick fractionally δ -doped LSTO/STO superlattices (SLs), in order to find ways to enhancing the carrier mobility of two dimensional electron gas (2DEG). Fractional layers of LSTO have been grown in between STO using advanced PLD. It is found that the SLs' transport properties are governed by a multichannel conduction with at least two distinctly different carriers: (1) High-density-low-mobility carriers presenting at the LSTO interface layer and (2) low-density-high-mobility carriers residing in the STO layers away from the δ -doped layer. By optimizing x , we could tune the effective mass and carrier density to enhance the carrier mobility by about an order of magnitude, selectively for the high-density-low-mobility carriers. This proves that the fractional δ -doping is an effective way to controlling the filling controlled IMT, resulting in highly improved transport properties

¹The work was supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

8:24AM H5.00003 Characterization of extreme-concentration 2DEGs at the SrTiO₃/GdTiO₃ interface, CLAYTON JACKSON, POUYA MOETAKEF, TYLER CAIN, UC Santa Barbara, SIDDHARTH RAJAN, Ohio State University, JAMES ALLEN, SUSANNE STEMMER, UC Santa Barbara — Heterostructures of Mott and band insulators exhibit unique interface properties, including two-dimensional electron gases (2DEGs) with extremely high sheet carrier densities due to the polarization discontinuity at the interface. Of paramount importance for the properties is the location, spatial extent and confinement of the 2DEG. Here, we study the 2DEG with carrier densities of $3 \times 10^{14} \text{ cm}^{-2}$ formed at GdTiO₃/SrTiO₃ interfaces grown by MBE. Using a self-consistent Schrödinger-Poisson solver, we estimate the majority of the carriers are confined in a narrow region ($< 3 \text{ nm}$) at the SrTiO₃-side of the interface. Given the large and rapid spatial variation in charge density, experiments are needed to verify the assumptions underlying such models. We measure the admittance as a function of frequency at different fixed DC bias. To extract the carrier distribution in the depletion approximation, a distributed model is used to account for loss and series resistance effects. The resulting CV profile corresponds to a p-type layer. This is explained with a highly conductive space charge layer, resulting in significant depletion only in the p-type GdTiO₃. We report on the carrier distribution near the interface.

8:36AM H5.00004 Dynamical conductivity of the extreme concentration 2DEGs in GdTiO₃/SrTiO₃ heterostructures, DANIEL OUELLETTE, Dept. of Physics, University of CA, Santa Barbara, POUYA MOETAKEF, Materials Dept., University of CA, Santa Barbara, CHRISTOPHER MORRIS, Dept. of Physics and Astronomy, John Hopkins University, MARK SHERWIN, Dept. of Physics and Institute for Terahertz Science and Technology, University of CA, Santa Barbara, S. JAMES ALLEN, Dept. of Physics, University of CA, Santa Barbara, SUSANNE STEMMER, Materials Department, University of CA, Santa Barbara — Metallic conductivity with extremely high 2D carrier concentration is observed at the interface between the Mott insulator GdTiO₃ and the band insulator SrTiO₃. Irrespective of layer thickness or repeats, MBE-grown GdTiO₃/SrTiO₃ heterostructures have carrier density of approximately $1/2$ electron per interface unit cell, or $3 \times 10^{14} \text{ cm}^{-2}$ per interface, in excellent agreement with the polar discontinuity model. To probe the orbital character, confinement, and correlations of carriers in this system we have measured the static (dc) and dynamical conductivity of a variety of heterostructures, using a combination of THz time-domain and FTIR spectroscopies. Samples with SrTiO₃ layers exceeding $\sim 10 \text{ nm}$ thickness exhibit a Drude conductivity that may arise from d_{xz} and d_{yz} electric subbands at the interface. A discrepancy between the measured dynamical and dc conductivity measurements indicates the presence of a few additional carriers with very low scattering rate. By contrast, the Drude response of samples with thinner SrTiO₃ layers shows an increased scattering rate with excellent agreement between the dc and THz frequency dynamical conductivity.

8:48AM H5.00005 Electrostatic carrier doping of GdTiO₃/SrTiO₃ heterostructures, POUYA MOETAKEF, TYLER CAIN, Materials Department, University of California Santa Barbara, DANIEL OUELLETTE, Physics Department, University of California Santa Barbara, JACK ZHANG, CLAYTON JACKSON, Materials Department, University of California Santa Barbara, SIDDHARTH RAJAN, Department of Electrical and Computer Engineering, Ohio State University, JAMES ALLEN, Physics Department, University of California Santa Barbara, SUSANNE STEMMER, Materials Department, University of California Santa Barbara — Two-dimensional electron gases (2DEGs) at interfaces between Mott insulators and band insulators have attracted significant attention because they can exhibit unique properties, such as strong electron correlations, superconductivity and magnetism. At interfaces between SrTiO₃ and the rare earth titanates (Mott insulators) an interfacial fixed polar charge arises due to a polarization discontinuity, which can be compensated by a 2DEG, residing in the bands of the Mott/band insulator. In this presentation, we report on intrinsic electronic reconstructions at a Mott/band insulator interface between stoichiometric GdTiO₃ and SrTiO₃ that were grown using molecular beam epitaxy. The sheet carrier densities of all GdTiO₃/SrTiO₃ heterostructures containing more than one unit cell of SrTiO₃ are approximately $1/2$ electron per unit cell, independent of layer thickness and growth sequence. These carrier densities closely meet the electrostatic requirements for compensating the fixed charge at these polar interfaces. Based on the experimental measurements, insights into the location and confinement of the charge and the influence of different electrostatic boundary conditions are obtained.

9:00AM H5.00006 High mobility electron gas in the surface vicinity of the cubic-perovskite KTaO₃ via Ar⁺-irradiation, SATOSHI HARASHIMA, SLAC National Accelerator Laboratory, The University of Tokyo, CHRIS BELL, YASUYUKI HIKITA, SLAC National Accelerator Laboratory, HAROLD Y. HWANG, SLAC National Accelerator Laboratory, Stanford University — KTaO₃ (KTO), like SrTiO₃ (STO), can be doped to create a high mobility perovskite oxide semiconductor. However, while the low dimensional electronic states of STO have attracted intense interest via spectroscopic [1,2] and transport [3] studies, analogous investigations in KTO have been limited. Of particular interest is the fact that the cubic crystal symmetry in KTO is preserved at low temperatures, in contrast to STO. Here we electron dope KTO via oxygen-vacancy formation by Ar⁺-irradiation [4]. Below $T = 10$ K, the Hall mobility ($> 10^4$ cm²/Vs) of the electrons is significantly higher than in previous studies of STO [4]. The angular dependence of the Shubnikov-de Haas oscillations indicates a Fermi surface without cubic symmetry, in contrast to that expected for bulk KTO. We discuss the possible origins of these data, including the formation of quantum well structures, the coexistence of surface and bulk electrons, and the suppression of cyclotron motion by finite size effects.

[1] A. F. Santander-Syro *et al.*, Nature **469**, 189 (2011).

[2] W. Meevasana *et al.*, Nat. Mater. **10**, 114 (2011).

[3] Y. Kozuka *et al.*, Nature **462**, 487 (2009).

[4] J. H. Ngai *et al.*, Phys. Rev. B **81**, 241307 (2010).

9:12AM H5.00007 Memristive behavior of ferroelectric tunnel junctions¹, ALEXEI GRUVERMAN, University of Nebraska-Lincoln — Employment of polarization reversal in ultrathin ferroelectric layers opens new possibilities for development of electronic devices with novel functional properties not available in conventional systems. A particularly promising aspect is realization of resistive switching in the ferroelectric tunnel junctions (FTJ), which can be used as non-charge based logical switches in nonvolatile memory devices. Functionality of FTJs is intrinsically linked to a relationship between polarization orientation and tunneling resistance, which brings about a problem of ferroelectric switching and polarization retention in ultrathin ferroelectric barriers. Here, we demonstrate a giant resistive switching effect of more than 105% at room temperature in the FTJ device structure composed of an epitaxial BaTiO₃ ferroelectric barrier sandwiched between bottom and top electrodes. We provide experimental evidence of the memristive behavior of these FTJs where both the low- and high-resistance states can be tuned by the external voltage by several orders of magnitude. The mechanism of the memristive behavior in our junctions is discussed in terms of the modifications of the tunneling potential profile driven by the charge accumulation in the BaTiO₃ layer.

¹This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering (DOE grant DE-SC0004876).

9:48AM H5.00008 Exploring and alleviating detrimental interface dipole effects in ultra-thin all-oxide metal-ferroelectric-metal heterostructures, XIAOHUI LIU, YONG WANG, PAVEL LUKASHEV, J.D. BURTON, EVGENY TSYMBAL, Department of Physics and Astronomy, University of Nebraska-Lincoln — Ultrathin-film metal-ferroelectric-metal heterostructures present an exciting prospect for switchable nanoelectronic memories and devices such as ferroelectric tunnel junctions. The main challenge is to realize ferroelectricity in ultrathin-films where detrimental interface effects become increasingly more pronounced as ferroelectric film thicknesses approach the nanoscale. We studied the ferroelectric polarization of BaTiO₃ in epitaxial SrRuO₃/BaTiO₃/SrRuO₃ junctions by first-principles density functional theory and phenomenological modeling. The calculations show that the presence of a RuO₂/BaO termination sequence at the SrRuO₃/BaTiO₃ interface leads to a pinned interface dipole and is therefore detrimental to the stability of ferroelectricity, leading to the disappearance of switchable polarization under a certain thickness. Here, we propose to alleviate this behavior by depositing a thin layer of SrTiO₃ at this interface to suppress the RuO₂/BaO interface termination sequence, thereby eliminating the associated unfavorable pinned interface dipole. By doing this we find, and experiments confirm, that a switchable ferroelectric state can be stabilized in much thinner heterostructures.

10:00AM H5.00009 ABSTRACT WITHDRAWN —

10:12AM H5.00010 Domains and Electrostatic Coupling in Ferroelectric Superlattices, PAVLO ZUBKO, NOEMIE JECKLIN, CELINE LICHTENSTEIGER, University of Geneva, ALMUDENA TORRES-PARDO, ALEX GLOTER, Université Paris-Sud, PABLO AGUADO-PUENTE, JAVIER JUNQUERA, Universidad de Cantabria, ODILE STEPHAN, Université Paris-Sud, JEAN-MARC TRISCONE, University of Geneva — Superlattices composed of ferroelectric and paraelectric oxides have been the subject of numerous studies, delving into fundamental questions about ferroelectric size effects, revealing novel interfacial phenomena, and opening new possibilities for tailoring the functional properties of these artificially layered ferroelectrics. Here we examine the role of periodic 180 degree ferroelectric nanodomains on the structural and electrical properties of PbTiO₃/SrTiO₃ superlattices. Using a combination of X-ray diffraction and electrical measurements, nanoscale motion of domain walls under applied field has been detected and linked to the large enhancement of the dielectric response. Electrostatic interactions between the ferroelectric layers have been studied in detail, revealing an unexpected decoupling of the ferroelectric layers once the paraelectric layer thickness exceeds just a few perovskite unit cells. Recent advances in transmission electron microscopy allowed us to map out the local structural distortions across the superlattice using electron energy loss spectroscopy with unit-cell resolution, revealing highly inhomogeneous polarization profiles near the interfaces and giving new microscopic insight into the behavior of these fascinating materials.

10:24AM H5.00011 In situ x-ray study of oxide superlattice growth in reactive molecular-beam epitaxy, JUNE HYUK LEE, X-ray Science Division, Argonne National Lab, SEO HYOONG CHANG, Materials Science Division, Argonne National Lab, I-CHENG TUNG, Department of Materials Science and Engineering, Northwestern University, JEFF EASTMAN, DILLON FONG, Materials Science Division, Argonne National Lab, JOHN FREELAND, HAWOONG HONG, X-ray Science Division, Argonne National Lab — Improper ferroelectricity found in ultrashort period PbTiO₃/SrTiO₃ superlattices has attracted interests as one of new 'interfacially engineered' materials.[1] At the interface of PbTiO₃/SrTiO₃ superlattices, the coupling between the ferroelectric mode and antiferrodistortive rotations of oxygen octahedra creates improper ferroelectricity with a large dielectric constant. PbTiO₃/SrTiO₃ superlattices were grown using reactive molecular-beam epitaxy in a chamber with in situ x-ray diffraction capability at the Advanced Photon Source. The use of in situ surface x-ray diffraction allows one to study the evolution of oxide heterostructures. Here we present initial studies of PbTiO₃ and SrTiO₃ single layers as well as superlattices. [1] E. Bousquet, M. Dawber, N. Stucki, C. Lichtensteiger, P. Hermet, S. Gariglio, J.-M. Triscone, and P. Ghosez, Nature 452, 732 (2008).

10:36AM H5.00012 ABSTRACT WITHDRAWN —

10:48AM H5.00013 The memristive magnetic tunnel junction as a nanoscopic synapse-neuron system¹ , ANDY THOMAS, PATRYK KRZYSTECZKO, JANA MÜNCHENBERGER, GÜNTER REISS, MARKUS SCHÄFERS, Physics department, Bielefeld University — Memristors cover a gap in the capabilities of basic electronic components by remembering the history of the applied electric potentials, and are considered to bring neuromorphic computers closer by imitating the performance of synapses. We used memristive magnetic tunnel junctions based on MgO to demonstrate that the synaptic functionality is complemented by neuron-like behavior in these nanoscopic devices. The synaptic functionality originates in a resistance change caused by a voltage-driven oxygen vacancy motion within the MgO layer. The additional functionality provided by magnetic electrodes enabled a current-driven resistance modulation due to spin-transfer torque. We report on memristive magnetic tunnel junctions characterized by the simultaneous occurrence of resistive switching and tunnel magnetoresistance. Since resistivity provides a natural measure of the synaptic strength, and because of the bipolar nature of the resistance change, long term potentiation and long term depression were emulated. Furthermore, we show that the flux is a good variable for describing voltage-induced resistance variation, which provides the scope for the emulation of spike timing dependent plasticity as well.

¹This work was supported by the MIWF of the NRW state government.

Tuesday, February 28, 2012 8:00AM - 10:48AM —
Session H6 DMP: Focus Session: van der Waals Bonding in Advanced Material - Methods and Application to Water and Ice 206B

8:00AM H6.00001 van der Waals interactions in water and ice from density functional theory simulations: improvements and challenges¹ , MARIVI FERNANDEZ-SERRA², Stony Brook University — Accounting for long range van der Waals (vdW) type correlations in the description of water and ice has proven to be one of the most important improvements in density functional theory (DFT)-based simulations of water. I will show how our understanding of the network structure in liquid water has changed with the newly available vdW density functionals, derived from the original version of Dion et al. [Phys. Rev. Lett. 92, 246401 (2004)]. In particular I will focus on the links between the density of water and the interplay between the hydrogen bonds and the so called vdW-bonds, easily identifiable in the liquid. These new vdW-DFs have also proven to be very important in the description of ice. In particular I will show how they are capable of accurately describing the anomalous nuclear quantum effects in ice, bringing DFT simulations and experimental results very close together. Our results show that current vdW-DFs are capable of correctly describing the subtle interplay between inter-molecular libration modes and intra-molecular stretching modes in ice, thus reproducing the experimental results once the zero point of these modes is accounted for in the simulations.

¹Work supported by DOE award numbers DE-FG02-08ER46550 and DE-SC0003871

²Betul Pamuk (Stony Brook University), Phillip B. Allen (Stony Brook University), Jose M. Soler (Universidad Autonoma Madrid)

8:36AM H6.00002 The Effect of van der Waals Interactions on the Structure of Liquid Water.¹ , ROBERT DISTASIO JR., ZHAOFENG LI, ROBERTO CAR, Princeton University — In this work, we demonstrate the importance of including van der Waals (vdW) interactions in the theoretical prediction of the structure of liquid water. These effects are investigated by computing and analyzing the oxygen-oxygen, oxygen-hydrogen, and hydrogen-hydrogen radial distribution functions (RDFs) obtained from highly accurate *ab initio* molecular dynamic simulations that explicitly account for vdW interactions. In particular, we utilize an efficient order(N) algorithmic implementation of the self-consistent energy and analytical forces of the density functional based vdW correction proposed by Tkatchenko and Scheffler (PRL 102, 073005 (2009)) to demonstrate the importance of vdW interactions in obtaining RDFs that are in close agreement with experiment. In addition, we also provide an analysis of finite size effects in vdW-based liquid water simulations as well as a comparison to several other competitive theoretical methods for treating vdW interactions.

¹NSF CHE-0956500; DOE-DE-SC0005180

8:48AM H6.00003 Van der Waals interactions and vibrational effects in ice from first principles¹ , EAMONN MURRAY, GIULIA GALLI, University of California, Davis — We present a comparative study of the equation of state and of the electronic and vibrational properties of ice XI and VIII, as obtained with *ab-initio* calculations using semi-local (PBE) and nonlocal, van der Waals functionals. The two functionals yield similar electronic properties for both phases, however they perform very differently in describing their vibrational properties, and the transition pressure from the low to the high pressure phase. The latter is overestimated by a factor of about 6 when using PBE and in agreement with experiment when dispersion forces are taken into account. The inclusion of zero point energy contributions does not affect the computed transition pressure, while it substantially affects structural properties, including equilibrium volumes and bulk moduli, especially for the high pressure phase.

¹This work is supported by SciDAC-e grant number DE-FC02-06ER25777

9:00AM H6.00004 Hydrogen Bonds and van der Waals Forces in Ice at Ambient and High Pressures , BISWAJIT SANTRA, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany, JIŘÍ KLIMEŠ, London Centre for Nanotechnology and Department of Chemistry, University College London, London, UK, DARIO ALFÈ, Department of Earth Sciences, University College London, London, UK, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany, BEN SLATER, Department of Chemistry, University College London, London, UK, ANGELOS MICHAELIDES, London Centre for Nanotechnology and Department of Chemistry, University College London, London, UK, ROBERTO CAR, Department of Chemistry, Princeton University, Princeton, USA, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — The balance between van der Waals (vdW) forces and hydrogen bonding in ambient and high pressure phases of ice has been examined with the first principles approaches, density-functional theory (DFT) and quantum Monte Carlo. At higher pressure, the contribution to the lattice energy from vdW increases and that from hydrogen bonding decreases, leading vdW to have a substantial effect on the transition pressures between the crystalline ice phases. An important consequence, likely to be of relevance to molecular crystals in general, is that the transition pressures obtained from DFT functionals which neglect vdW forces are greatly overestimated [Phys. Rev. Lett. 107, 185701 (2011)].

9:12AM H6.00005 ABSTRACT HAS BEEN MOVED TO Q35.00010 —

9:24AM H6.00006 Higher-order van der Waals coefficients from static multipole polarizability¹

JIANMIN TAO, JOHN PERDEW, ADRIENN RUZSINSZKY, Tulane University — van der Waals interaction is a long-range nonlocal correlation arising from instantaneous charge fluctuations on each fragment. Though very weak, it considerably affects the properties of molecules and solids. Evaluation of van der Waals coefficients is of strong current interest. In this work, we have derived a general expression for these coefficients in terms of static multipole polarizability only. Applications of the present theory to atom as well as molecular pair interactions have been made.

¹This material is based upon work supported by the National Science Foundation under the NSF Cooperative Agreement No. EPS-1003897 with additional support from the Louisiana Board of Regents.

9:36AM H6.00007 Quantum Monte Carlo Simulation of condensed van der Waals Systems¹

ANOUAR BENALI, Argonne National Laboratory, LUKE SHULENBURGER, Sandia National Laboratories, NICHOLS A. ROMERO, Argonne National Laboratory, JEONGNIM KIM, Oak Ridge National Laboratory, O. ANATOLE VON LILIENTFELD, Argonne National Laboratory — Van der Waals forces are as ubiquitous as infamous. While post-Hartree-Fock methods enable accurate estimates of these forces in molecules and clusters, they remain elusive for dealing with many-electron condensed phase systems. We present Quantum Monte Carlo [1,2] results for condensed van der Waals systems. Interatomic many-body contributions to cohesive energies and bulk modulus will be discussed. Numerical evidence is presented for crystals of rare gas atoms, and compared to experiments and methods [3]. Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DoE's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

[1] J. Kim, K. Esler, J. McMinis and D. Ceperley, SciDAC 2010, J. of Physics: Conference series, Chattanooga, Tennessee, July 11 2011

[2] QMCPACK simulation suite, <http://qmcpack.cmscc.org> (unpublished)

[3] O. A. von Lilientfeld and A. Tkatchenko, J. Chem. Phys. 132 234109 (2010)

¹This research used resources of the Argonne Leadership Computing Facility at Argonne National Laboratory, which is supported by the Office of Science of the U.S. DoE under contract DE-AC02-06CH1135.

9:48AM H6.00008 Van der Waals interactions based on maximally localized Wannier functions

in ABINIT, CAMILO ESPEJO, CINVESTAV-Unidad Querétaro, Universidad Jorge Tadeo Lozano, TONATIUH RANGEL, Université Catholique de Louvain, YANN POUILLON, Nano-Bio Spectroscopy Group - ETSF, ALDO ROMERO, CINVESTAV-Unidad Querétaro, XAVIER GONZE, Université Catholique de Louvain — We review the recent implementation¹ of the method to evaluate van der Waals (vdW) interactions based on maximally localized Wannier functions^{2,3} in the DFT software ABINIT⁴. The implementation allows for the evaluation of vdW interaction energies for molecular and periodic systems on the same grounds and at a low additional computational cost as compared with a normal DFT calculation. Some results on test systems such as Ar₂, benzene dimer and graphene bilayer show both its reliability and performance. Discussion of new defined variables controlling the calculation and guide lines for the user will be presented along with an application to MoS₂ structure.

¹C. Espejo et al. Computer Phys. Comm. In press (2011), doi:10.1016/j.cpc.2011.11.003

²P. L. Silvestrelli. Phys. Rev. B., **100**, 053002 (2008)

³P. L. Silvestrelli. J. Phys. Chem. A., **113**, 5224 (2009)

⁴X. Gonze et al. Computer Phys. Comm. **180**, 2582 (2009)

10:00AM H6.00009 Density-Functional Theory with Screened van der Waals Interactions for the Modeling of Hybrid Inorganic/Organic Systems¹

VICTOR G. RUIZ, WEI LIU, Fritz-Haber-Institut der MPG, EGBERT ZOJER, Institute of Solid State Physics, Graz University of Technology, MATTHIAS SCHEFFLER, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG — The electronic properties and the function of hybrid inorganic/organic systems (HIOS) are intimately linked to their geometry, with van der Waals (vdW) interactions playing an essential role for the latter. Here we show that the inclusion of the many-body collective response of the substrate electrons inside the inorganic bulk enables us to reliably predict the HIOS geometries and energies. Specifically, dispersion-corrected density-functional theory (the DFT+vdW approach) [*PRL* **102**, 073005 (2009)], is combined with the Lifshitz-Zaremba-Kohn theory [*PRB* **13**, 2270 (1976)] for the non-local Coulomb screening within the bulk. Our method (DFT+vdW^{surf}) includes both image-plane and interface polarization effects. We show that DFT+vdW^{surf} yields geometries in remarkable agreement (≈ 0.1 Å) with normal incidence x-ray standing wave measurements for the 3,4,9,10-perylene-tetracarboxylic acid dianhydride (C₂₄H₈O₆, PTCD) molecule on Cu(111), Ag(111), and Au(111). Similarly accurate results are obtained for xenon and benzene adsorbed on metal surfaces.

¹FP7 Marie Curie Actions of the European Commission, via the Initial Training Network SMALL (MCITN-238804)

10:12AM H6.00010 Stress and Vibrational Properties of non-local van der Waals exchange-correlation functionals

RICCARDO SABATINI, International School for Advanced Studies (SISSA), via Bonomea 265, 34136 Trieste, Italy, STEFANO DE GIRONCOLI, International School for Advanced Studies (SISSA) and CNR-IOM DEMOCRITOS Simulation Center, via Bonomea 265, 34136 Trieste, Italy — Van der Waals interaction is an essential component in the description of soft matter and plays an important role in many other systems, from adsorbates to water interaction. Within the framework of Density Functional Theory in the last years a great effort has been made to overcome the limitations of LDA or GGA functionals, and a new class of non-local functionals is now filling the gap giving interesting results. We present here several new improvements in this field, and some selected applications. In particular, i) we worked out the theoretical formalism needed to define both the stress tensor and the phonon vibrations associated to the non-local functional form proposed by Dion[1], and ii) we developed and implemented in the Quantum ESPRESSO simulation package a new functional inspired by the work of Vydrov and Van Voorhis[2], simple to compute efficiently in plane wave approach and with great performances on the S22 set. Finally we present some results obtained on aminoacid crystal and other simple molecules where these new tools are benchmarked and compared with experimental results and other theoretical approaches.

[1] M. Dion, B. I. Lundqvist et al., Phys. Rev. Lett. **92**, 246401 (2004);

[2] Oleg A. Vydrov and Troy Van Voorhis, Phys. Rev. Lett. **103**, 06300

10:24AM H6.00011 Dispersion interactions in Density Functional Theory, LAMPROS ANDRINOPOULOS, NICHOLAS HINE, ARASH MOSTOFI, Imperial College London — Semilocal functionals in Density Functional Theory (DFT) achieve high accuracy simulating a wide range of systems, but miss the effect of dispersion (vdW) interactions, important in weakly bound systems. We study two different methods to include vdW in DFT: First, we investigate a recent approach [1] to evaluate the vdW contribution to the total energy using maximally-localized Wannier functions. Using a set of simple dimers, we show that it has a number of shortcomings that hamper its predictive power; we then develop and implement a series of improvements [2] and obtain binding energies and equilibrium geometries in closer agreement to quantum-chemical coupled-cluster calculations. Second, we implement the vdW-DF functional [3], using Soler's method [4], within ONETEP [5], a linear-scaling DFT code, and apply it to a range of systems. This method within a linear-scaling DFT code allows the simulation of weakly bound systems of larger scale, such as organic/inorganic interfaces, biological systems and implicit solvation models. [1] P. Silvestrelli, JPC A 113, 5224 (2009). [2] L. Andrinopoulos et al, JCP 135, 154105 (2011). [3] M. Dion et al, PRL 92, 246401 (2004). [4] G. Román-Pérez, J.M. Soler, PRL 103, 096102 (2009). [5] C. Skylaris et al, JCP 122, 084119 (2005).

10:36AM H6.00012 A Qbox Implementation of van der Waals Density Functionals with Applications¹, JUN WU, Graduate Group in Applied Science, University of California Davis, Davis CA 95616, FRANCOIS GYGI, Department of Computer Science, University of California Davis, Davis CA 95616 — We present an implementation of the non-local van der Waals correlation functional proposed by Dion et al. [1] in the Qbox code [2]. We develop a simple approach to remove the logarithmic singularity in the kernel function, and derive the non-local potential needed for self-consistent calculations of energies, ionic forces and stress for simulations in arbitrary-shaped unit cells. We compare the performance of five different van der Waals functionals in applications to the benzene-water dimer, the benzene crystal and other organic molecular crystals.

[1] M. Dion et al. Phys. Rev. Lett. 92, 246401 (2004)

[2] <http://eslab.ucdavis.edu/software/qbox>

¹Supported by NSF OCI 60000572 and DOE SciDAC DE-FC02-06ER25794

Tuesday, February 28, 2012 8:00AM - 11:00AM — Session H7 DMP: Focus Session: Carbon Nanotube Sensing 207

8:00AM H7.00001 Selective, Reversible Near-Infrared Fluorescence Quenching of Boronic Acid–Single-Walled Carbon Nanotube Complexes in Response to Glucose, KYUNGSUK YUM, JIN-HO AHN, THOMAS MCNICHOLAS, PAUL BARONE, BIN MU, JONG-HO KIM, RISHABH JAIN, MICHAEL STRANO, Massachusetts Institute of Technology — We present the high throughput screening of a library of 30 boronic acid derivatives to form complexes with sodium cholate suspended single-walled carbon nanotubes (SWNTs) to screen for their ability to reversibly report glucose binding via a change in SWNT fluorescence. The screening identifies 4-cyanophenylboronic acid which uniquely causes a reversible wavelength red-shift in SWNT emission. The results also identify 4-chlorophenylboronic acid which demonstrates a turn-on fluorescence response when complexed with SWNTs upon glucose binding in the physiological range of glucose concentration (0 to 30 mM). The mechanism of fluorescence modulation in both of these cases is revealed to be a photo-induced excited-state electron transfer that can be disrupted by boronate ion formation upon glucose binding. This “turn-on” sensing scheme that uses the reversible fluorescence quenching and wavelength shift of the BA–SWNT complex offers a new approach for nIR optical sensing of glucose.

8:12AM H7.00002 The transduction mechanism of carbon nanotube transistors monitoring single molecule protein dynamics, PATRICK C. SIMS, YONGKI CHOI, TIVOLI J. OLSEN, GREGORY A. WEISS, PHILIP G. COLLINS, Depts. of Physics and Astronomy, Chemistry, and Molecular Biology, Univ. of California at Irvine, Irvine, CA 92697 — Recently we have demonstrated high resolution, real-time monitoring of single molecule chemistry using molecules attached to a single-walled carbon nanotube (SWCNT) transistor. The transduction mechanism of SWCNT sensing is often claimed to be due to charge transfer, but here we clearly show the entire effect to be electrostatic. In this study, the chemical system of interest is lysozyme and its enzymatic processing of its binding substrate, peptidoglycan. We investigate the interaction of a lysozyme molecule with the SWCNT conductivity by building devices out of eight different lysozyme variants synthesized by mutagenesis. Each lysozyme variant has a different sequence of surface charges near the SWCNT attachment site, providing a calibrated method of looking at the electrostatic interactions. We observe that positively- and negatively-charged amino acids induce signals of opposite magnitude, while quasi-neutral amino acids like alanine induce little signal at all. The results indicate that careful consideration and manipulation of the charge environment near the attachment site may enhance the signal-to-noise of SWCNT sensors for studying single molecule interactions.

8:24AM H7.00003 Electrical Detection of Resonance in a Helically Coiled Carbon Nanowire, DOYL DICKEL, DEEPIKA SAINI, BALU PILLAI, HERBERT BEHLOW, MALCOLM SKOVE, APPARAO RAO, Clemson University — Helically coiled Carbon Nanowires (HCNWs) are promising elements, both for their promise as components for NEMS devices as well as for fundamental research. This is due primarily to their exotic geometry. We present here the electrostatic excitation of a HCNW cantilever to resonance and an entirely electrical measurement of the same using harmonic detection of resonance (HDR). The correlation between the directly observed resonance and the electrical signal is shown and, in addition to calculating a lateral spring constant from the observed resonance frequency, we examine the nonlinear behavior of the HCNW when driven to large amplitudes of vibration. Specifically, elliptical oscillation is visually evident and we have measured the electrical response of the corresponding combination mode.

8:36AM H7.00004 Arrays of Versatile DNA-Carbon Nanotube Hybrid Chemical Sensor for Vapor Analyte Detection, NICHOLAS KYBERT, MITCHELL LERNER, ZHENGQING JOHN QI, A.T. CHARLIE JOHNSON, University of Pennsylvania, Department of Physics and Astronomy — Large arrays of nanoscale sensors were fabricated for the detection of small molecules based on single-stranded DNA (ssDNA) for chemical recognition and single-walled carbon nanotube field effect transistors (SWNT FETs) for electronic read-out. These versatile sensors are capable of detecting very low concentrations of molecules ranging from volatile organic compounds, whose detection could provide a method for detection or identification of individuals, to noxious compounds designed to harm them. In this work, we deposited enriched semiconducting SWNTs on Si/SiO₂ with an APTES adhesion layer. Photolithographically defined contacts resulted in high yield, high performance arrays of SWNT FETs, which were then individually coated in different ssDNA. The arrays of devices were then simultaneously exposed to analytes down to ppb concentrations. The sensing response of a single device is both analyte and ssDNA sequence dependant. The response and recovery to baseline are both fast (seconds) and repeatable without need for refreshing. By using large arrays of differently functionalized devices, we distinguished similar analytes and established electronic signatures indicative of their presence, paving the way for incorporation of ssDNA/SWNT FET arrays in “electronic nose”-type systems.

8:48AM H7.00005 Environmental Charge Noise in Suspended Carbon Nanotube Biosensors

, TAL SHARF, Oregon State University, JOSHUA W. KEVEK, Cornell University, ETHAN D. MINOT, Oregon State University — Carbon nanotube field effect transistors (CNT FETs) are a promising platform for probing biological systems at nanometer length scales. The sensitivity of a CNT FET sensor is ultimately limited by intrinsic fluctuations in the conductance of the sensor. Our work aims to understand the mechanisms responsible for these conductance fluctuations, and therefore understand the fundamental detection limits of charge-sensitive biosensors. We have measured conductance fluctuations in both surface-bound CNTs and suspended CNTs. Experiments are performed in physiological buffers — the typical environment for real-time biosensing. We compare our measurements to a charge noise model and the Hooke model. We find good agreement with the charge noise model, and find that charge noise is reduced by 10 –fold when CNTs are suspended rather than surface-bound. By measuring conductance fluctuations in a variety of liquid buffers we uncover new clues about the origins of charge noise in electrolyte environments.

9:00AM H7.00006 Generalized Protein Attachment Chemistry for Highly Sensitive Carbon

Nanotube-Based Biosensors, MITCHELL LERNER, Univ. of Pennsylvania, Dept. of Physics and Astronomy, TATIANA PAZINA, MATTHEW ROBINSON, Fox Chase Cancer Center, A.T. CHARLIE JOHNSON, Univ. of Pennsylvania, Dept. of Physics and Astronomy — We developed a label free covalent functionalization procedure for attaching proteins to carbon nanotube field effect transistors (CNTFETs). Biomarker proteins are becoming increasingly useful for early diagnosis of disease, ranging from cancer to arthritis to stress. Current clinical immunoassays for measuring patient protein levels are costly and require significant processing time. Using diazonium salts followed by stabilization of carboxylic acid groups, we can attach a variety of proteins to carbon nanotubes as confirmed by atomic force microscopy. Proteins maintain the integrity of their epitope and bind to their corresponding complementary proteins. Carbon nanotube transistors are superior readout elements for such protein binding events due to their speed and comparable scale. Resulting changes in the electronic transport properties of CNTFETs demonstrate a concentration-dependent response. Binding of osteopontin (OPN), a biomarker for prostate cancer, to its complementary single chain variable fragment (scFv) can be detected down to 1 pg/mL with these methods. Moreover, these devices exhibit selectivity for OPN. Such high sensitivity biosensors could be used in parallel to test a single small volume patient sample for any number of potentially ominous biomarker proteins.

9:12AM H7.00007 Detection of carbon nanotubes in plant roots through microwave-induced

heating, FAHMIDA IRIN, Department of Chemical Engineering, Texas Tech University, BABINA SHRESTHA, JACLYN CANAS, The Institute of Environmental and Human Health, Texas Tech University, MOHAMMAD SAED, Department of Electrical and Computer Engineering, Texas Tech University, MICAH GREEN, Department of Chemical Engineering, Texas Tech University — We demonstrate a novel technique for quantitative detection of CNTs in biological samples by utilizing the thermal response of CNTs under microwave irradiation. In particular, rapid heating of CNTs due to microwave absorption was employed to quantify the amount of CNTs present in alfalfa plant roots. Alfalfa roots were prepared by injecting a known amount of CNTs (single walled and multi walled) and exposed to 30-50 W microwave power to generate calibration curves (temperature rise vs. CNT mass). These calibration curves serve as a characterization tool to determine the unknown amount of CNTs absorbed by alfalfa plant roots grown in CNT-laden soil with superior accuracy and sensitivity. Moreover, the threshold for detectable CNT concentration is much lower than common analytical methods of detecting nanomaterials, such as scanning electron microscopy (SEM), transmission electron microscopy (TEM), and Raman spectroscopy. Considering the lack of effective detection methods for CNT uptake in plants, this method is not only unique but also practical, as it addresses a major problem in the field of nanotoxicology risk assessment.

9:24AM H7.00008 Adsorption of noble gases on individual suspended single-walled carbon

nanotubes, HAO-CHUN LEE, ZENGHUI WANG¹, RICHARD ROY, ERIK FREDRICKSON, OSCAR VILCHES, DAVID COBDEN, Department of Physics, University of Washington — Suspended single-walled carbon nanotubes can act as nanomechanical resonators, offering the ability to detect an adsorbed substance with very high sensitivity via the frequency shift due to the adsorbed mass. By measuring the resonance frequency electrically in the presence of vapors at controlled temperature and pressure we have obtained isotherms for 4He, Ar, Kr and Xe, on multiple nanotubes. The behavior resembles that on graphite but with notable differences, including weaker binding energies. The lower binding allows access to behavior at lower 2D chemical potential than on conventional substrates. For 4He the binding energy is reduced by as much as a factor of two. For Ar the derived two-dimensional phase diagram is similar to that on conventional substrates. For Kr there is variation between nanotubes which may be related to commensurability and area per site on the surface of a cylinder. Work supported by NSF DMR 0907690.

¹Zenghui Wang had graduated from UW.

9:36AM H7.00009 Conductance isotherms for adsorption of noble gases on individual single-walled carbon nanotubes¹

, BORIS DZYUBENKO, HAO-CHUN LEE, OSCAR VILCHES, DAVID COBDEN, University of Washington — Using transistors made from suspended carbon nanotubes allows one to probe the interaction of adsorbed atoms and molecules with the carbon substrate electrons. We have studied the effects of adsorbing He, Ne, Ar, Kr, Xe, and other gases on the electrical properties of individual suspended single-walled nanotubes, as a function of pressure and temperature. The conductance changes measurably, and sometimes dramatically, as a monolayer forms and undergoes phase transitions. It yields complementary information to the coverage, which is obtained from the mass shift in the natural vibrational frequency of the nanotube. For example, measurements below the 2D critical point show nonmonotonic features and fluctuations heralding the first-order phase transition. Conductance changes can be measured on a timescale of milliseconds, permitting studies of the dynamics of the monolayer. In the nonlinear regime we observe features in the I-V characteristics as phase transitions are induced by the current and nonequilibrium stationary states occur.

¹Supported by NSF grant DMR 0907690

9:48AM H7.00010 Dependence of adsorption kinetics on the geometry of substrate¹

, DINESH RAWAT, SAIKAT TALAPATRA, VAIVA KRUNGLEVICIUTE, ALDO MIGONE, Department of Physics, Southern Illinois University at Carbondale, IL-62901, USA, DEPARTMENT OF PHYSICS, SOUTHERN ILLINOIS UNIVERSITY AT CARBONDALE, IL-62901, USA TEAM — We report on the results of an adsorption kinetics study of linear alkanes on planar graphite and on aligned multiwalled carbon nanotubes. The kinetics study was performed by monitoring the equilibration times for methane, butane and pentane adsorbed on these two substrates as a function of fractional coverage. For methane, the time required to reach equilibration was found to decrease as the surface coverage increased. However, for butane and pentane, a systematic increase in the equilibration time with increasing fractional coverage was observed. Although similar results were found for both substrates, the waiting times for longer alkanes adsorbed on multiwalled carbon nanotubes, were found to be longer than the ones obtained for planar graphite. We speculate that the observed increase in the equilibration time with coverage for the longer alkanes is due to the rearrangement of the adsorbed molecules. Results of the current study will also be compared to our previous study of adsorption kinetics of linear alkanes on single-walled carbon nanotubes.

¹Aldo Migone would like to acknowledge support provided for this study by the National Science Foundation through Grant No. DMR-0705077

10:00AM H7.00011 New concepts in molecular and energy transport within carbon nanotubes: thermopower waves and stochastically resonant ion channels, MICHAEL STRANO, MIT — Our laboratory has been interested in how carbon nanotubes can be utilized to illustrate new concepts in molecular and energy transfer. In the first example, we predict and demonstrate the concept of thermopower waves for energy generation [1]. Coupling an exothermic chemical reaction with a thermally conductive CNT creates a self-propagating reactive wave driven along its length. We realize such waves in MWNT and show that they produce concomitant electrical pulses of high specific power >7 kW/kg. Such waves of high power density may find uses as unique energy sources. In the second system, we fabricate and study SWNT ion channels for the first time [2] and show that the longest, highest aspect ratio, and smallest diameter synthetic nanopore examined to date, a $500\text{ }\mu\text{m}$ SWNT, demonstrates oscillations in electro-osmotic current at specific ranges of electric field, that are the signatures of coherence resonance, yielding self-generated rhythmic and frequency locked transport. The observed oscillations in the current occur due to a coupling between stochastic pore blocking and a diffusion limitation that develops at the pore mouth during proton transport.

[1] Choi W, Hong S, Abrahamson JT, Han JH, Song C, Nair N, Baik S, **Strano MS**: Chemically driven carbon-nanotube-guided thermopower waves. NATURE MATERIALS, 9 (2010) 423-429.

[2] Lee, CY, Choi W, Han, JH, **Strano MS**: Coherence Resonance in a Single-Walled Carbon Nanotube Ion Channel. SCIENCE, 239

10:36AM H7.00012 Neon adsorption on oxidized single-walled carbon nanohorns¹, VAIVA KRUNGLEVICIUTE, ALDO MIGONE, Southern Illinois University Carbondale, MASAKO YUDASAKA, National Institute of Advanced Industrial Science and Technology, Nanotube Research Center, Japan, SUMIO IJIMA, National Institute of Advanced Industrial Science and Technology, Nanotube Research Center; Fundamental Research Laboratory, NEC Corporation, Japan — We will present the results of a study of neon adsorption on oxidized single-walled carbon nanohorns. Our adsorption isotherm measurements were conducted at temperatures below 24.5 K, the triple point for Ne. Results for the effective specific surface area and for the effective pore volume of the nanohorn aggregates will be presented. We will also report on the sorbent-loading dependence of the isosteric heat of neon on the nanohorns, and on the binding energy. Our results for this system will be compared with those obtained for Ne on a sample of dahlia-like nanohorns annealed at 520 K.

¹This work is supported by the NSF through grant DMR-1006428.

10:48AM H7.00013 Carbon dioxide adsorption on open single walled carbon nanohorn aggregates¹, SHREE BANJARA, VAIVA KRUNGLEVICIUTE, ALDO MIGONE, Southern Illinois University Carbondale, MASAKO YUDASAKA, National Institute of Advanced Industrial Science and Technology, Nanotube Research Center, Japan, SUMIO IJIMA, National Institute of Advanced Industrial Science and Technology, Nanotube Research Center; Fundamental Research Laboratory, NEC Corporation, Japan — The adsorption of carbon dioxide was measured on aggregates of single-walled carbon nanohorns treated with H₂O₂. Volumetric adsorption isotherms were conducted at several temperatures between 162 and 212 K (below the triple point for CO₂). Results on adsorption equilibration times, on the substrate-loading dependence of the isosteric heat, and on the binding energy will be presented. The effective specific surface area values obtained in this study will be compared with the ones obtained for other carbon nanohorn samples.

¹This work is supported by the NSF through grant DMR-1006428.

Tuesday, February 28, 2012 8:00AM - 11:00AM — Session H8 DMP GMAG: Focus Session: Frustrated Magnetism - Kagome I 208

8:00AM H8.00001 Confinement transitions of Z2 spin liquids on the kagome lattice¹, MATTHIAS PUNK, Harvard University — Motivated by numerical evidence of a Z₂ spin liquid ground state of the Heisenberg model on the kagome lattice and indications of a proximate valence bond solid (VBS) phase (see S. Yan et al, Science 332, 1173 (2011)), we study quantum phase transitions between Z₂ spin liquids and VBS states, in which the space group of the kagome lattice is broken. These confinement transitions are driven by the condensation of elementary vortex excitations of the Z₂ spin liquid, so called visons. In this talk I will show how a projective symmetry group (PSG) analysis of effective models for the visons can be used to construct quantum field theories for such confinement transitions, which in turn allow for a classification of the spatial symmetries of possible VBS states. Interestingly, the kagome lattice is unique in the sense that the critical properties at the confinement transition are seemingly not described by the Wilson-Fisher fixed point, as is the case for other lattice geometries.

¹Support by the National Science Foundation (DMR-0757145), AFOSR as well as the Austrian Science Fund (J3077-N16) is gratefully acknowledged.

8:36AM H8.00002 NMR study of the spin-1/2 near-kagome system Vesignieite, JEFFREY QUILLIAM, FABRICE BERT, Laboratoire de Physique des Solides, Universite Paris-Sud, ROSS COLMAN, DAVID BOLDRIN, ANDREW WILLS, Department of Chemistry, University College London, PHILIPPE MENDELS, Laboratoire de Physique des Solides, Universite Paris-Sud — The spin-1/2 kagome lattice antiferromagnet is understood to be an ideal setting in which to find novel quantum spin liquid physics. Here, ⁵¹V NMR results are presented on the quantum spin system Vesignieite, which closely approximates such an antiferromagnetic kagome model, possessing a minute 0.7% length difference between inequivalent Cu-Cu bonds. We obtain a measure of the intrinsic magnetic susceptibility of the near-kagome lattice, which shows commonalities with other kagome systems, in particular Herbertsmithite. Meanwhile, the system is found to undergo partial spin freezing at a surprisingly high temperature of $T_C = 9\text{ K} \simeq J/6$. Through a loss of NMR intensity and detailed analysis of the spectral linewidth, we infer a heterogeneous ground state in which 50% of the spins are very weakly frozen, with a moment of $\sim 0.2\text{ }\mu_B$ and the remaining 50% remain dynamic down to very low temperatures. These results are found to be highly consistent with μ SR studies, which find a similar frozen fraction and small size of magnetic moment. We propose that the elevated transition temperature and weakly frozen ground state are explained by the Dzyaloshinskii-Moriya interaction and a proximity to the resulting quantum phase transition.

8:48AM H8.00003 Magnetization Process of Spatially Anisotropic Kagome Heisenberg Model, RYUI KANEKO, TAKAHIRO MISAWA, YUHEI YAMAJI, Department of Applied Physics, University of Tokyo, HIROKI NAKANO, Graduate School of Material Science, University of Hyogo, MASATOSHI IMADA, Department of Applied Physics, University of Tokyo — Motivated by recent experiments on volborthite, a typical spin-1/2 antiferromagnet with a kagome lattice structure, we study magnetization process of a Heisenberg model on a kagome lattice with a spatial anisotropy in applied magnetic fields. First, for the classical Heisenberg model, by using the Monte Carlo method, we find a magnetization step due to the anisotropy at low temperatures and low magnetic fields. The magnetization step signals a first-order transition, between two phases distinguished by distinct and well-developed short-range spin correlations, one characterized by a local 120° structure and the other by a partially spin-flopped structure. These states are also evident in magnon dispersions based on a classical spin configuration for each phase. Then, to clarify how quantum fluctuations affect the magnetization process, we calculate the sublattice magnetization by using the exact diagonalization method. We find that the sublattice magnetization process of the quantum model looks qualitatively similar to that of the classical model, which indicates that the spin structure observed in the classical model also appears in the quantum model. Finally, we point out the relevance of our results to the magnetization steps observed in volborthite.

9:00AM H8.00004 Investigation of fermi-liquid-like specific heat and spin-density-wave signatures in the distorted kagome compound Volborthite, $\text{Cu}_3\text{V}_2\text{O}_7(\text{OH})_2 \cdot 2\text{H}_2\text{O}$, TYLER DODDS, YONG BAEK KIM, University of Toronto — The distorted kagome compound Volborthite shows signatures of spin-density-wave magnetic order and Fermi-liquid specific heat at low temperatures and magnetic fields. A recent density functional study [O. Janson *et al.*, Phys. Rev. B **82**, 104434 (2010)] suggests that Volborthite can be viewed as coupled frustrated Heisenberg spin chains, a model we approach using a slave-fermion representation of the spins. For a certain range of couplings, our mean-field theory finds a Fermi surface of spinons, a portion of which contains nesting. We investigate whether the coexistence of a U(1) spin liquid with a spinon Fermi surface, along with a spinon spin-density-wave, may describe the aforementioned features of the low-field phase. Furthermore, at higher fields, conventional magnetically ordered states are found. We examine if higher magnetic fields can lead to the destruction of the fermi surface, prompting a spinon confinement transition into such a conventionally magnetically ordered state.

9:12AM H8.00005 Experimental signatures of spin liquid physics on the $S=1/2$ kagomé lattice¹, YOUNG LEE, Massachusetts Institute of Technology — I will describe our recent experimental progress on the quest to study novel ground states in frustrated magnets. New states of matter may be produced if quantum effects and frustration conspire to prevent the ground state from achieving classical order. Materials based on the kagomé lattice appear to be ideal hosts for the possibility of a quantum spin liquid ground state in two-dimensions. I will discuss our work which includes single crystal growth, bulk characterization, and neutron scattering measurements of the $S=1/2$ kagomé lattice material $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$ (also known as herbertsmithite). Recent susceptibility measurements on single crystals yield valuable information on the additional terms in the spin Hamiltonian beyond nearest neighbor Heisenberg exchange, and anomalous x-ray diffraction yields detailed information on the presence of a small amount of atomic impurities. Most interestingly, inelastic neutron scattering measurements of the spin correlations in a single crystal sample reveal a continuum of spinon excitations in this two-dimensional insulating magnet. We will discuss our results in relation to recent theories for spin liquid physics on the $S=1/2$ kagomé lattice.

¹This work was supported by the Department of Energy under Grant No. DE-FG0207ER46134.

9:48AM H8.00006 Spin cluster operator theory for the kagome lattice antiferromagnet¹, KWON PARK, KIAS, KYUSUNG HWANG, Seoul National Univ. and KIAS, YONG BAEK KIM, Univ. of Toronto and KIAS, JAEJUN YU, Seoul National Univ. — The spin-1/2 quantum antiferromagnet on the kagome lattice provides a quintessential example in the strongly correlated electron physics where both effects of geometric frustration and quantum fluctuation are pushed to their limit. Among possible non-magnetic ground states, the valence bond solid (VBS) with a 36-site unit cell is one of the most promising candidates. Improving the bond operator theory, we propose a new approach dubbed as the spin cluster operator theory in which extended clusters of spin are treated as fundamental building blocks of the system. As a result, it is shown that the lowest spin excitation has a gap much lower than the previous value obtained by the bond operator theory, narrowing the difference against exact diagonalization results.

¹National Research Foundation of Korea grant under the Quantum Metamaterials Research Center (K.P.) and the ARP (J.Y.), NSERC of Canada, Canada Research Chair Program, and CIFAR (Y.B.K.)

10:00AM H8.00007 Low Energy Spectrum and Correlation Functions of the $S = 1/2$ Kagome Antiferromagnet, ANDREAS LAUCHLI, Theoretische Physik, University of Innsbruck, Austria, RAINER JOHANNI, Computing Center of the Max Planck Society, Garching, Germany — We report a large scale Exact Diagonalization study of the $S = 1/2$ Heisenberg antiferromagnet on samples of up to 48 sites. The singlet spectrum at low energies involves only energy levels at the Gamma point, indicating the probable absence of spontaneous translation symmetry breaking in the thermodynamic limit. The spin-spin correlations are short ranged as expected, and the dimer-dimer correlation functions reveal traces of diamond-like resonances. We discuss the compatibility of our results with different theoretical proposals for the ground state of the Kagome antiferromagnet.

10:12AM H8.00008 Valence bond crystals in the kagome spin-1/2 Heisenberg antiferromagnet: Symmetry classification and projected wave function study, YASIR IQBAL, Laboratoire de Physique Theorique UMR-5152, CNRS and Universite' de Toulouse, FEDERICO BECCA, CNR Officina dei Materiali and SISSA, DIDIER POILBLANC, Laboratoire de Physique Theorique UMR-5152, CNRS and Universite' de Toulouse — We present a hierarchical group theoretical classification and representation of Valence bond crystal (VBC) phases on the kagome lattice. Starting from the most symmetric parent VBC, we enumerate and give the ansatz for all 6, 12, and 36-site unit cell VBC's in order of increasing number of broken point group symmetry elements. We treat the VBC's within the class of Gutzwiller projected fermionic variational wave functions, which are optimized using a sophisticated implementation of the stochastic reconfiguration method. In particular, for the spin-1/2 quantum Heisenberg antiferromagnetic model, we show that the U(1) Dirac spin liquid is remarkably stable (locally and globally) with respect to all possible VBC patterns enumerated. However, upon addition of a small ferromagnetic next-nearest-neighbor coupling we find that the lowest energy state is a non-trivial generalized 36-site VBC, which can be regarded as being continuously connected to a uniform RVB spin liquid. We also communicate the ground state energy on the kagome 48 site cluster for the nearest-neighbor spin-1/2 quantum Heisenberg antiferromagnetic model, using the technique of application of a few Lanczos steps (within a variational Monte carlo scheme) on the U(1) Dirac spin liquid and the uniform RVB wave function.

10:24AM H8.00009 Neutron Scattering and Thermodynamic Studies of Low Spin Kagome Magnets¹, ROBIN CHISNELL, DANNA FREEDMAN, MIT, JOEL HELTON, NIST Center for Neutron Research, CHRIS STOCK, FRANZ DEMMEL, ISIS Facility - Rutherford Appleton Laboratory, DANIEL NOCERA, YOUNG LEE, MIT — Materials containing low quantum number spins arranged on a kagome lattice are some of the most promising candidates to display spin liquid ground states due to the high degree of geometric frustration. $\text{Cu}(1,3\text{-bdc})$ is a hybrid organometallic compound featuring antiferromagnetically coupled $S=\frac{1}{2}$ Cu^{2+} ions on a kagome lattice. Below $T=1.8$ K the magnetic moments enter a quasi-static phase with no long range magnetic order but extremely slow spin fluctuations. Application of a magnetic field quickly leads to a competing magnetic phase, with a 1 Tesla field able to completely polarize the magnetization below $T=2$ K. We present inelastic neutron scattering measurements of $\text{Cu}(1,3\text{-bdc})$ and note the emergence of low-energy modes in the quasi-static phase. We also present new thermodynamic data on the compound $\text{BaNi}_3(\text{OH})_2(\text{VO}_4)_2$, recently synthesized by our group, which features $S=1$ Ni^{2+} ions on a kagome lattice.

¹This work was supported by the US Department of Energy under Grant No. DE-FG02-07ER46134

10:36AM H8.00010 Magnetic studies of $S=1/2$ kagomé lattice single crystals, TIANHENG HAN, SHAOYAN CHU, MIT, YASU TAKANO, University of Florida, JOSE RODRIGUEZ-RIVERA, NCNR NIST, COLLIN BROHOLM, John Hopkins University, DANIEL NOCERA, YOUNG LEE, MIT — Herbertsmithite $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$ —one of the most promising quantum spin liquid candidates—presents a promising system for studies of frustrated magnetism on an $S=1/2$ kagomé lattice. Following our recent success in crystal growth, we have measured anisotropies in the magnetic susceptibility and specific heat. The implication on the Hamiltonian will be discussed. Specific heat has been measured at dilution fridge temperatures up to 18 T on a single crystal sample which gives further information on the low temperature phases. In addition, inelastic neutron scattering has been performed and the broad continuum observed is consistent with deconfined 2D spinons which lends further support of herbertsmithite's quantum spin liquid candidacy.

10:48AM H8.00011 Single Crystal NMR Study of Frustrated Spin-Liquid in $S = 1/2$ Kagome Lattice $ZnCu_3(OD)_6Cl_2$, MINGXUAN FU, DAVID. A. TORCHETTI, Department of Physics and Astronomy, McMaster University, Hamilton, ON L8S 4M1, CAN, TAKASHI IMAI, Department of Physics and Astronomy, McMaster University, Hamilton, ON L8S 4M1, CAN; Canadian Institute for Advanced Research, Toronto M5G 1Z8, CAN, TIANHENG HAN, YOUNG. S. LEE, Department of Physics, MIT, Cambridge, Massachusetts 02139, USA — Herbertsmithite $ZnCu_3(OD)_6Cl_2$ is one of the most promising examples for a quantum spin liquid state. Despite the remarkable absence of long range magnetic order down to at least 50mK, understanding the magnetic properties of $ZnCu_3(OD)_6Cl_2$ remains a challenge. This is mainly due to the difficulty in locating the defects, and in understanding the possible role of defects in the physical properties of this material. We have investigated the local magnetic and lattice environment of $ZnCu_3(OD)_6Cl_2$ single crystals¹ using NMR techniques². With successful identification of ^2D NMR signals arising from the nearest neighbors of Cu^{2+} defects substituting Zn, we find that 14(2)% of Zn sites are occupied by these weakly interacting Cu^{2+} defect spins, which contribute to the large Curie-Weiss enhancement of bulk susceptibility at low temperatures. We then discuss the key aspects of nuclear spin-lattice relaxation rate $1/T_1$ measured near the defect and intrinsic sites.

¹T. H. Han *et al.*, Phys. Rev. B **83**, 100402(R) (2011)

²T. Imai *et al.*, Phys. Rev. B **84**, 020411(R) (2011); see also Phys. Rev. Lett. **100**, 077203 (2008)

Tuesday, February 28, 2012 8:00AM - 11:00AM – Session H9 DMP GMAG: Focus Session: Complex Bulk Oxides: Ruthenates 209

8:00AM H9.00001 Nonlinear conduction phenomena in the Mott insulator Ca_2RuO_4 , RYUJI OKAZAKI, YASUO NISHINA, YUKIO YASUI, ICHIRO TERASAKI, Department of Physics, Nagoya University, FUMIHIKO NAKAMURA, YUSAKU KIMURA, MARIKO SAKAKI, TAKASHI SUZUKI, ADMS, Hiroshima University — The 4d-electron Mott insulator Ca_2RuO_4 has attracted considerable attention because of its rich electronic states dramatically varied by temperature change, pressure, and isovalent Sr substitution. Recently, Nakamura *et al.* reported an intriguing result of current-voltage characteristics in Ca_2RuO_4 and found an E -induced insulator-to-metal transition caused by relatively low electric field $E \sim 50$ V/cm [1]. In this study we investigate the nonlinear conduction phenomena in the Mott insulating phase of Ca_2RuO_4 with a proper evaluation for self-heating effects. By utilizing a non-contact infrared thermometer, sample temperature was accurately determined even in the presence of large Joule heating. The resistivity shows a typical insulating behavior featured by thermal activation with an energy gap, but clearly depends on the applied currents. The result is highlighted by a strong suppression of the energy gap by the electrical currents. A striking similarity to the current dependence of charge-order gap in organic insulators is discussed in terms of the nonequilibrium phase transition.

[1] F. Nakamura *et al.*, (submitted).

8:12AM H9.00002 Emergent electronic and magnetic state in $Ca_3Ru_2O_7$ induced by Ti doping, XIANGLIN KE, Oak Ridge National Laboratory, J. PENG, Tulane University, D.J. SINGH, T. HONG, W. TIAN, C.R. DELA CRUZ, Oak Ridge National Laboratory, Z.Q. MAO, Tulane University — We report an emergent electronic and magnetic state in the bilayer ruthenate $Ca_3Ru_2O_7$ upon doping with a small concentration of Ti on the Ru sites. In contrast to a quasi-two-dimensional metallic state in $Ca_3Ru_2O_7$, which has an antiferromagnetic state formed by ferromagnetic bilayers stacked antiferromagnetically along the c-axis [1,2], we find an insulating state with a “G”-type nearest neighbor antiferromagnetic order in $Ca_3(Ru_{1-x}Ti_x)_2O_7$ for $x \geq 0.03$ [3]. The close proximity of these two distinct electronic and magnetic states demonstrates unique competing magnetic interactions in $Ca_3Ru_2O_7$, which provides a rare opportunity to investigate the interplay between correlated metal physics and Mott physics. Work supported by U.S. DOE.

[1] W. Bao *et al.*, Phys. Rev. Lett. **100**, 247203 (2008).

[2] X. Ke *et al.*, Phys. Rev. B **84**, 014422 (2011).

[3] X. Ke *et al.*, Phys. Rev. B **84**, 201102 (R) (2011).

8:24AM H9.00003 From quasi-2D metal with ferromagnetic bilayers to Mott insulator with G-type antiferromagnetic order in $Ca_3(Ru_{1-x}Ti_x)_2O_7$, JIN PENG, GAOCHAO WANG, Department of Physics and Engineering Physics, Tulane University, New Orleans, LA 70118, XIANGLIN KE, TAO HONG, Neutron Scattering Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, ZHIQIANG MAO, Department of Physics and Engineering Physics, Tulane University, New Orleans, LA 70118 — $Ca_3Ru_2O_7$ exhibits unique electronic and magnetic properties, such as giant magnetoresistance, a quasi-2D metallic ground state, and antiferromagnetic (AFM) order comprising of ferromagnetic bilayers coupled antiferromagnetically along the c-axis [1-3]. In this talk, we will show that only a few percent of Ti-doping at Ru sites can tune the ground state to a Mott-insulating state with “G”-type, nearest neighbor AFM order [4]. We have established the electronic and magnetic phase diagram of this doped system to address the underlying physics of such a Mott-transition. We find that a strong scattering effect due to the Ti ions’ empty 3d orbital significantly reduces electrons’ itinerancy, playing a pivotal role in the suppression of the bilayer ferromagnetism and inducing the Mott transition. These findings imply that $Ca_3Ru_2O_7$ involves competition between the antiferromagnetism due to the Mott transition and the itinerant ferromagnetism due to a Stoner instability. [1] X.N. Lin *et al.*, Phys. Rev. Lett. **95**, 017203(2005). [2] W. Bao *et al.*, Phys. Rev. Lett. **100**, 247203 (2008). [3] Y. Yoshida *et al.*, Phys. Rev. B **69**, 220411 (R) (2004). [4] X. Ke *et al.*, Phys. Rev. B **84**, 201102 (R) (2011).

¹This work is supported by DOD ARO under Grant No. W911NF0910530 and the LA-SiGMA program.

8:36AM H9.00004 Orbital selective phase transition¹, YU-ZHONG ZHANG, Physics Department, Tongji University, Shanghai 200092, P.R. China, HUNPYO LEE, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Frankfurt am Main 60438, Germany, HAI-QING LIN, Beijing Computational Science Research Center, Beijing 100089, China, CHANG-QIN WU, Department of Physics and State Key Laboratory of Surface Physics, Fudan University, Shanghai 200433, China, HARALD JESCHKE, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Frankfurt am Main 60438, Germany — Orbital selective phase transition (OSPT), proposed to be responsible for the coexistence of localized and itinerant electrons, has attracted extensive interest from both experimentalists and theoreticians, since the observation of an anomalous behavior with a Curie-Weiss-like local spin in the metallic phase of $Ca_{2-x}Sr_xRuO_4$ at $0.2 \leq x \leq 0.5$. Recently, even more attentions have been paid to OSPT since the coexistence of localized and itinerant electrons may reconcile the strong debates on how to understand the origin of magnetism in various iron-based superconductors. Here, various mechanisms for OSPT are reviewed and a new mechanism will be proposed. The distinct band dispersion of different orbitals, which should be generally satisfied in various materials, is identified to be the crucial point for OSPT with magnetic order. Such an OSPT are not sensitive to the strength of Hund’s rule coupling. Heavy doping favors collinear antiferromagnetic state over the OSPT. Discussions are made related to the pnictides.

¹Sponsored by 11PJ1409900 and NSFC11174219

8:48AM H9.00005 Magnetic order arising from chemical chaos in A_2MnRuO_6 ($A = Sr, Ca$) double perovskites, ROHAN MISHRA, PATRICK WOODWARD, WOLFGANG WINDL, The Ohio State University — Experimentally Sr_2MnRuO_6 is observed to be a c-type antiferromagnetic insulator with a tetragonal structure, while Ca_2MnRuO_6 is found to be a metallic ferrimagnet with an orthorhombic structure. Both compounds display magnetic ordering even in the absence of any recognizable chemical ordering of Mn and Ru ions. In this work, we present first principles calculations to show that the change in properties of the two compounds is only a consequence of pressure and hence can be tuned either by epitaxial growth or by alloying at A-site with Sr^{2+} or Ca^{2+} ions. We find that the Mn e_g -states are highly sensitive to pressure. Compression raises their energy in Sr_2MnRuO_6 , accompanied by a transfer of electrons from the eg states to the Ru-Mn hybridized t_{2g} -states. This results in a transition from c-type antiferromagnetism to ferrimagnetism. Ferrimagnetic ordering in-turn allows for greater delocalization of the up-spin Ru t_{2g} -electrons, hence increasing the conductivity. We also show that in the presence of disorder, the Mn_{Ru} antisites couple ferromagnetically with their neighboring Mn_{Mn} sites. This allows for the interesting possibility of preserving highly spin-polarized conduction even in the absence of chemical ordering.

9:00AM H9.00006 Surface dynamics and electronic properties of parent and Mn doped $Sr_3Ru_2O_7$ ¹, JING TENG, CHEN CHEN, BIAO HU, JIANDI ZHANG, RONGYING JIN, WARD PLUMMER, Louisiana State University — High resolution Electron Energy Loss Spectroscopy has been utilized to measure the temperature dependence of the low energy excitations at the surface of cleaved $Sr_3(Ru_{1-x}Mn_x)_2O_7$ single crystals ($x = 0, 0.16$). Four loss peaks are observed and assigned as the $A_{1g}(2)$, $A_{2u}(3)$, $A_{2u}(2)$, and $A_{1g}(1)$ vibration modes. The continuous electronic excitation spectra, Drude tail, shows that the parent compound is metallic at all temperatures investigated (80K to RT). But the $A_{1g}(1)$ mode splits into two peaks between 145K and 210K indicating a structural transition at the surface. For the 16% Mn doped samples the bulk is insulating and antiferromagnetic below 160K. In contrast, the surface is always metallic. Upon cooling from RT the $A_{1g}(1)$ mode hardens with its width broadening from RT to 160K, and then softens and narrows quickly until 80K. The Drude tail exhibits similar behavior. Evidently the presence of the surface suppresses AF ordering and kills the insulating phase.

¹Supported by NSF DMR-1002622

9:12AM H9.00007 The Physics of Hunds metals and its relevance for ruthenades, iron pnictides and chalcogenides, KRISTJAN HAULE, Rutgers The State University of New Jersey — I will discuss the physics of Hund's metals. In these systems the Coulomb interaction among the electrons is not strong enough to fully localize them, but it significantly slows them down, such that low-energy emerging quasiparticles have a substantially enhanced mass. This enhanced mass emerges not because of the Hubbard interaction U , but because of the Hund's rule interactions J that tend to align electrons with the same spin but different orbital quantum numbers when they find themselves on the same atom. I will show a few examples of such Hund's metals, including Sr_2RuO_4 , iron pnictides and iron chalcogenides materials. The electronic structure, computed by the Dynamical Mean Field Theory in combination with Density Functional Theory, successfully reproduces several experimental results and explains the key properties of these material: such as the mass renormalizations and anisotropy of quasiparticles, the crossover into an incoherent regime above a low temperature scale, the magnetic moments in iron compounds, etc. While at very low temperature our simulations predict these materials to be Fermi liquids, at finite temperature they strongly deviate from Fermi liquid prediction and can be characterized by self-energy which follows a powerlaw, with non-integer exponents. The origin of this non-Fermi liquid fixed point will be discussed.

9:48AM H9.00008 Anomalous E -type Antiferromagnetism in the ground state of Mn-substituted $Sr_3Ru_2O_7$ ¹, DALGIS MESA, Dept. of Physics, Louisiana State University, Baton Rouge, LA 70802, FENG YE, SONGXUE CHI, JAIME A. FERNANDEZ-BACA, V.O. GARLEA, Neutron Scattering Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, BIAO HU, RONGYING JIN, E.W. PLUMMER, JIANDI ZHANG, Dept. of Physics, Louisiana State University, Baton Rouge, LA 70802 — The bi-layer perovskite, $Sr_3Ru_2O_7$, has sparked a lot of interest because of the quantum critical behavior—related to a metamagnetic (magnetic field-tuned) phase transition. One of the key issues is related to the magnetism in the system. Here we report an investigation of the effects on magnetism resulting from chemical substitution in this compound. Our neutron scattering investigation reveals an unusual E -type antiferromagnetic (AFM) structure induced by Mn-substitution in the ground state of $Sr_3(Ru_{1-x}Mn_x)_2O_7$ ($x = 0.16$). The AFM structure exhibits a long-range order in ab -plane but almost only a single bilayer-thickness correlation along the c -direction, thus characterizing the system as a quasi-two-dimensional antiferromagnet while the AFM order parameter shows almost three-dimensional-like scaling character as T approaches T_N (~ 82 K). The magnetic moments are aligned along the c -axis with an upper limit of $\sim 0.70 \mu_B$ /Ru site. The induced AFM order most likely results from the enhancement of super-exchange interactions rather than from structural distortions or from freezing of electronic instabilities due to the nesting character of Fermi surface in the parent compound.

¹Supported NSF DMR1005562. DM supported by NSF LS-LAMP, DOE ESPCoR.

10:00AM H9.00009 Anisotropy of magnetoresistivities in $Sr_3Ru_2O_7$: Evidence for orbital-dependent metamagnetism¹, D. FOBES, G.C. WANG, Z.Q. MAO, Department of Physics and Engineering Physics, Tulane University, New Orleans, LA — $Sr_3Ru_2O_7$ has been studied extensively due to its rich electronic and magnetic ground state properties, such as its quantum criticality and electronic nematic phase [1,2]. In this talk we will present the results of in-plane angle-resolved directional magnetotransport anisotropy measurements, a technique we used previously to elucidate the orbital-selective nature of the itinerant metamagnetism in $Sr_4Ru_3O_{10}$ [3]. We find that the c -axis magnetoresistivity anisotropy undergoes a drastic change in symmetry from fourfold to twofold through the metamagnetic transition, consistent with the behavior expected for the strong spin polarization. In contrast, the in-plane magnetoresistivity anisotropy remains fourfold through the transition accompanied by only a gradual shift in phase, and only trends towards twofold symmetry at fields well above the transition. These findings suggest the $d_{xz,yz}$ bands, should play a pivotal role in the metamagnetic transition.

[1] S. Grigera *et al.*, Science **294**, 329 (2001)

[2] R. Borzi *et al.*, Science **315**, 214 (2007)

[3] D. Fobes *et al.*, Phys. Rev. B **81**, 172402 (2010)

¹This work is supported by the NSF under Grant No. DMR-0645305.

10:12AM H9.00010 Study of an electronic nematic with precise control of the applied magnetic field vector, JAN BRUIN, SUPA, University of St Andrews, RODOLFO BORZI, Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas and Departamento de Física, IFLP, UNLP, ANDREAS ROST, SUPA, University of St Andrews, ROBIN PERRY, SUPA, University of Edinburgh, SANTIAGO GRIGERA, Instituto de Física de líquidos y sistemas biológicos, UNLP and SUPA, University of St Andrews, ANDREW MACKENZIE, SUPA, University of St Andrews — The layered perovskite metal $\text{Sr}_3\text{Ru}_2\text{O}_7$ has gained considerable interest since the discovery of its field tuned quantum criticality [1] and the subsequent discovery of a new electronic phase with a high magnetoresistive anisotropy, consistent with the existence of an electronic nematic fluid [2]. This anisotropy may be oriented by applying a moderate field (H_{ab}) in the plane of the RuO layers. The study of the behaviour of the electronic nematic state requires precise control over both the magnitude and direction of H_{ab} . For this purpose, we operate a 3-axis 9/1/1 tesla vector magnet, which offers full control of the magnetic field vector with a high degree of precision. Here, we present recent magnetotransport data for $\text{Sr}_3\text{Ru}_2\text{O}_7$ measured in the vector magnet. We confirm the two-fold to four-fold rotational symmetry breaking and show that it occurs even in the limit of small values of H_{ab} . Additionally, we address pinning of the anisotropy underlying crystal lattice. Finally, we show the dependence of the anisotropy on magnetic field and temperature, which may help explain its origin at the microscopic scale.

[1] S. A. Grigera *et al.*, *Science* **294**, 329 (2001) [2] R. A. Borzi *et al.*, *Science* **315**, 214 (2007)

10:24AM H9.00011 Optical Polarization Microscopy of the Electron Nematic Phase in $\text{Sr}_3\text{Ru}_2\text{O}_7$, COLIN HEIKES, DAVID MACNEILL, Cornell University, SAIKAT GHOSH, S N Bose National Centre for Basic Sciences, R. PERRY, J.F. MERCURE, St. Andrews University, E.A. KIM, Cornell University, A. MACKENZIE, St. Andrews University, D.C. RALPH, Cornell University — We report the implementation of a fiber-based optical microscope, capable of operating at temperatures below 100 mK and in magnetic fields in excess of 9 Tesla, with sub-micron spatial resolution. This microscope is integrated into the bore of a dilution refrigerator with an optical fiber coupling light to an external optical table. Bench-top optical elements allow for polarization analysis of the reflected light from a surface and thus the detection of magnetic or other polarization-sensitive properties of mater at low temperature and high fields. As a first application of the instrument, we are studying the proposed electron nematic phase of the $n=2$ Ruddlesden-Popper material $\text{Sr}_3\text{Ru}_2\text{O}_7$, which exhibits a low-temperature phase transition in the form of an in-plane conduction anisotropy. We plan to detect this phase optically by analyzing the polarization rotation of the reflected light through the phase boundary, with the aim of imaging domain structure in the nematic phase.

10:36AM H9.00012 Suppression of An Antiferromagnetic Insulating Phase in $\text{Sr}_3(\text{Ru}_{1-x}\text{Mn}_x)_2\text{O}_7$ by Magnetic Field¹, BIAO HU, E.W. PLUMMER, R. JIN, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803 — Double-layered $\text{Sr}_3\text{Ru}_2\text{O}_7$ is a paramagnetic metal. The partial substitution of Mn for Ru results in metal-insulator transition at T_{MIT} and antiferromagnetic ordering at T_M in $\text{Sr}_3(\text{Ru}_{1-x}\text{Mn}_x)_2\text{O}_7$. Interestingly, both T_{MIT} and T_M can be easily suppressed by the application of magnetic field, especially for low-doping compounds ($x < 0.1$). This behavior can be explained as Mn-doping-induced antiferromagnetic-insulating domains below T_{MIT} . The application of magnetic field suppresses the antiferromagnetic coupling, thus converting the insulating domains back to metallic.

¹Support by NSF under grant Nos. DMR-1002622 and DMR-1122603.

10:48AM H9.00013 The Orbital-Selected Mott Phase of the Nondegenerate Two-Orbital Hubbard Model¹, YUN SONG, Department of Physics, Beijing Normal University — We use the dynamical mean-field theory to study the optical conductivity and orbital susceptibility of the nondegenerate two-orbital Hubbard model in the orbital-selective Mott phase. The optical conductivity of the wide band presents expectedly a nonzero Drude peak, while the localization character is observed for the optical conductivity of the narrow band. Particularly, a rapidly reverse shape in the orbital susceptibility emerges right at Fermi surface, implying the coexistence of the orbital ordering with the orbital-selected Mott phase. We also find that the orbital-selected Mott transition can be suppressed by the negative crystal field splitting. Applying the present findings to compound $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$, we demonstrate that the orbital-selected Mott phase can not survive in wide doping region from $x=0.2$ to 2.0.

¹The National Basic Research Program of China

Tuesday, February 28, 2012 8:00AM - 11:00AM – Session H10 DAMOP: Invited Session: Strongly Interacting Photons 210A

8:00AM H10.00001 Strong photon-photon interaction in a coupled quantum dot- photonic crystal nanocavity¹, JELENA VUCKOVIC, Stanford University — Quantum dots (QDs) in photonic crystal nanocavities are interesting both as a testbed for fundamental cavity quantum electrodynamics (QED) experiments, as well as a platform for classical and quantum information processing. In addition to providing a scalable, on-chip, semiconductor platform, this system also enables very large dipole-field interaction strengths, as a result of the field localization inside of sub-cubic wavelength volumes (vacuum Rabi frequency is in the range of 10's of GHz). We have demonstrated controlled amplitude and phase modulation between two continuous wave (CW) optical beams at the single photon level (power less than a photon per cavity photon lifetime) interacting via a strongly coupled quantum dot - photonic crystal cavity system, and have subsequently extended this experiment to weak time-varying control field and a CW signal field. Recently, we have performed all-optical switching at the single photon level between two pulsed, resonant optical beams (with 40ps pulses and 80MHz repetition rate). In this experiment, we have measured transmission through the strongly coupled QD-cavity system as a function of delay between the two pulses, and have demonstrated a 22% increase in the transmission at zero delay. The increase in the transmission is a result of the saturation of the strongly coupled QD-cavity system. We have also studied the effects of the photon blockade and photon induced tunneling which result from the anharmonicity of the ladder of dressed states in a strongly coupled QD-nanocavity system. These effects lead to dramatic changes in the transmitted photon statistics, which can be varied from sub-Poissonian to super-Poissonian, and can be employed to generate nonclassical states of light (such as Fock or NOON states) with high efficiency.

¹This work has been supported by the ONR (PECASE Award), DARPA, and ARO.

8:36AM H10.00002 Single-photon nonlinearity¹, VLADAN VULETIC, MIT — Optical nonlinearity at the level of single photons will enable a variety of novel effects and applications, including the possibility of quantum gates between individual photons. We generate such a nonlinearity in an atomic ensemble by replacing the strong (classical) coupling field of electromagnetically induced transparency by the mode of an optical resonator. Then the resonant transmission of light through the atomic ensemble can be substantially altered even by the cavity vacuum. The vacuum induces a group delay of the optical pulse that corresponds to a group velocity of 1600 m/s. We also discuss possibilities for implementing a single-photon switch.

¹DARPA, NSF

9:12AM H10.00003 Strongly nonlinear optics with plasmonics, PARK HONGKUN, Harvard University — No abstract available.

9:48AM H10.00004 Slow-light polaritons in Rydberg gases, MICHAEL FLEISCHHAUER, Dept. of Physics, University of Kaiserslautern — Slow-light polaritons are quasi-particles generated in the interaction of photons with laser-driven atoms with a Λ - or ladder-type coupling scheme under conditions of electromagnetically induced transparency (EIT). They are a superposition of electromagnetic and collective spin excitations. If one of the states making up the atomic spin is a high lying Rydberg level, the polaritons are subject to a strong and non-local interaction mediated by a dipole-dipole or van-der Waals coupling between excited Rydberg atoms. I will present and discuss an effective many-body model for these Rydberg polaritons. Depending on the detuning of the control laser the interaction potential between the polaritons can be repulsive or attractive and can have a large imaginary component for distances less than the so-called blockade radius. The non-local effective interaction gives rise to interesting many-body phenomena such as the generation of photons with an avoided volume, visible in strongly suppressed two-particle correlations inside the blockade volume. Moreover the long-range, power-law scaling of the interaction can in the repulsive case give rise to the formation of quasi-crystalline structures of photons. In a one dimensional system the low-energy dynamics of the polaritons can be described in terms of a Luttinger liquid. Using DMRG simulations the Luttinger K parameter is calculated and conditions for the formation of a quasi-crystal are derived. When confined to a two-dimensional geometry, e.g. using a resonator with quasi-degenerate transversal mode spectrum, Rydberg polaritons are an interesting candidate to study the bosonic fractional quantum Hall effect. I will argue that the formation of photons with an avoided volume is essential for explaining recent experiments on stationary EIT in Rydberg gases [1,2].

[1] J.D. Pritchard et al., Phys. Rev. Lett. 105, 193603 (2010).

[2] D. Petrosyan, J. Otterbach, and M. Fleischhauer, arXiv:1106.1360

10:24AM H10.00005 Fast optical control of atom-light interactions using quantum dots coupled to photonic crystal cavities, EDO WAKS, University of Maryland — Quantum dots (QDs) are stable, bright, semiconductor based light emitters that exhibit a quantized energy spectrum. For these reasons they are excellent candidates for development of lasers, optoelectronic components, and could serve as basic building blocks for future quantum information technology. By coupling these nanostructures to optical cavities the interaction strength between QDs and light can be significantly increased. Photonic crystals (materials with a periodic index of refraction) are particularly promising for enhancing these interactions due to their ability to guide and confine light on the size scale of an optical wavelength. Photonic crystal based optical cavities have already been shown to enable the strong coupling regime of cavity quantum electrodynamics (cQED). In this regime a significant modification of both the QD emission spectrum and cavity reflectivity can be observed due to quantum mechanical mixing of atom-photon states. Control of QD-photon interactions on fast timescales is an important capability that enables strong nonlinear optical effects, opening up the door for a new class of opto-electronic devices at ultra-low light levels. It could also provide a promising route towards quantum information processing using photons and QDs to store and transmit quantum coherence. Here we describe a method to achieve fast all-optical control of atom-light interactions using indium arsenide (InAs) QDs coupled to photonic crystal cavities. We show that a QD strongly coupled to a photonic crystal cavity can exhibit very large optical Stark shifts due to resonant cavity enhancement of the electromagnetic field. Stark shifts as large as 20 GHz are demonstrated with as few as 10 photons in the cavity. These shifts can be used to control the QD resonant frequency on fast time scales, and therefore modify its interactions with the optical cavity through resonant detuning. Using this approach we demonstrate the ability to perform all optical switching with control pulse energies as small as 400 photons and switching times as fast as 140 ps. The approach can be improved through better cavity coupling methods to approach nonlinear optics near the single photon level.

Tuesday, February 28, 2012 8:00AM - 10:48AM —
Session H11 DMP: Focus Session: Graphene Structure, Stacking, Interactions: Interfaces and Adsorbates 210B

8:00AM H11.00001 Confinement of organic solvents by wet transfer of graphene, GREGORY DOIDGE, JOSHUA WOOD, ERIC POP, JOSEPH LYDING, University of Illinois — Transfer of graphene grown by chemical vapor deposition (CVD) on Cu requires a polymer support for the graphene and wet-etching of the Cu growth substrate. After etching, the polymer/graphene film must go through several solvent baths to remove contaminants. Water is commonly used for this cleaning due to its capability as a solvent and its ability to support the polymer/graphene film through high surface tension. By contrast, common organic solvents have lower surface tension, causing the film to tear and fold within the liquid. To bypass this challenge, we have implemented a polymer-bound truss to reinforce the polymer/graphene film, which avoids the need of proper solvent surface tension. We have transferred graphene grown on Cu using common organic solvents like methanol, isopropanol, ethylene glycol, and dimethyl sulfoxide for the final transfer liquids. This process traps the solvents between the graphene and the final substrate. Confinement effects are determined via optical microscopy, atomic force microscopy, and Raman spectroscopy for both the trapped solvent molecules and the graphene. Our procedure opens up the possibility of confining biological materials suspended in organic solvents under graphene.

8:12AM H11.00002 Photo-assisted polymerization of one-dimensional molecular arrays on epitaxial graphene, TEYU CHIEN, APARNA DESHPANDE¹, CHUN-HONG SHAM, JUSTICE ALABOSON, MARK C. HERSAM², Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208 — Self-assembled monolayers provide opportunities to tailor the materials properties of graphene and template subsequent chemical functionalization at molecular length scales. In particular, 10,12 pentacosadiynoic acid (PCA) is found to assemble into one-dimensional arrays on epitaxial graphene on SiC(0001) as revealed by ultra-high vacuum scanning tunneling microscopy (UHV-STM). Furthermore, UV-triggered polymerization of PCA in UHV is achieved, leading to distinct conformational changes at the molecular scale. The sub-5 nm widths of these one-dimensional polymers make them promising candidates for templating the formation of graphene nanoribbons with significant band gaps. Molecular resolution UHV STM characterization of the structure and electronic properties of this nanostructured chemical functionalization strategy will be presented.

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8:24AM H11.00003 Chemical reactivity imprint lithography on graphene: Controlling the substrate influence on electron transfer reactions, QING HUA WANG, ZHONG JIN, KI KANG KIM, ANDREW HILMER, GERALDINE PAULUS, CHIH-JEN SHIH, Massachusetts Institute of Technology, MOON-HO HAM, Gwangju Institute of Science and Technology, JAVIER SANCHEZ-YAMAGISHI, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, JING KONG, PABLO JARILLO-HERRERO, MICHAEL STRANO, Massachusetts Institute of Technology — The chemical functionalization of graphene enables control over electronic properties and interactions with other materials. Graphene's chemical reactivity is strongly influenced by the underlying substrate. In this paper, we show a stark difference in the rate of electron transfer chemistry with aryl diazonium salts on monolayer graphene supported on a broad range of substrates. Reactions proceed rapidly when graphene is on SiO₂ and Al₂O₃ (sapphire), but negligibly on alkyl-terminated and hexagonal boron nitride (hBN) surfaces. The effect cannot be explained by the overall graphene doping levels alone, and can instead be described using a reactivity model accounting for substrate-induced electron-hole puddles in graphene. Raman spectroscopic mapping is used to characterize the effect of the substrates on graphene. Reactivity imprint lithography (RIL) is demonstrated as a technique for spatially patterning chemical groups on graphene by patterning the underlying substrate, and is applied to the covalent tethering of proteins on graphene.

8:36AM H11.00004 Graphene on Metals: Interface Structure and Defects, LYUDMYLA ADAMSKA, RAFIK Q. ADDOU, MATTHIAS BATZILL, IVAN I. OLEYNIK, University of South Florida — The epitaxial growth of graphene on metal substrates is one of the major methods of graphene production for electronic applications. Therefore, the metal/graphene interface interactions as well as the graphene defects appeared during the growth affect in a substantial way the electronic properties of both graphene and graphene/metal contacts, which are both important for device applications. Structural and electronic properties of simple and complex graphene/metal as well as graphene/metal-alloy interfaces were investigated using first principles density functional theory. The point defect structures in graphene on metal substrate were studied and compared with those in free standing graphene.

8:48AM H11.00005 Topologically Frustrated Bonding in Dual-sided Adsorption to an Atomically Thin Membrane, CHENG-ING CHIA, VINCENT CRESPI, Department of Physics, Pennsylvania State University — A seamless sp^2 atomically thin layer cuts space in half, and prevents penetration of atoms through the sheet, while still allowing cross-sheet charge transfer. This geometrical frustration separates charge donating (e.g. alkali) and charge accepting (e.g. halogen) ions in opposite subspaces and generates a collective planar dipole. In this unusual geometry we observe new physics and chemistry. For graphene layer the uncompensated Coulomb interactions generate a system with multiple nearly degenerate structures which are either metallic or small-gap semiconductors, in contrast to the insulating behavior of unfrustrated salt crystals. When the layer is changed to h-BN, the collective dipole imposes a large Stark effect on the halogen and alkali-derived valence and conduction bands, resulting in a large band gap tuning with areal adsorbate density.

9:00AM H11.00006 Correlation between adatom adsorption properties and growth morphology of metal on graphene¹, XIAOJIE LIU, Ames Laboratory, Iowa State University and Jilin University, China, C.Z. WANG, M. HUPALO, Ames Laboratory, Iowa State University, WEN-CAI LU, Jilin University, China, Y.X. YAO, P.A. THIEL, K.M. HO, M.C. TRINGIDES, Ames Laboratory, Iowa State University, AMES LABORATORY, IOWA STATE UNIVERSITY TEAM, JILIN UNIVERSITY, CHINA COLLABORATION — We present a systematic study of various metal adatom adsorption on graphene by *ab initio* calculations. The correlation between the adatom adsorption properties and the growth morphology of the metals on graphene is investigated. We show that the growth morphology is related to the ratio of the adsorption energy to the bulk cohesive energy (E_a/E_c) of the metals and the diffusion barrier (ΔE) of the metal adatom on graphene. The growth morphology is also affected by the strain induced by metal adsorption on graphene. We also show that most of the metal nanostructures on graphene are thermally stable against coarsening. The first-principles calculations are consistent well with the observations from recent experiments.

¹Supported by DOE-BES under Contract No. DE-AC02-07CH11358

9:12AM H11.00007 Lithium Intercalation Induced Decoupling of Epitaxial Graphene on SiC(0001): Electronic Property and Dynamic Process, YUANCHANG LI, GANG ZHOU, Department of Physics, Tsinghua University, Beijing, JIA LI, Institute of Advanced Materials, Graduate School at Shenzhen, Tsinghua University, Shenzhen, JIAN WU, BING-LIN GU, WENHUI DUAN, Department of Physics, Tsinghua University, Beijing, CMT TEAM — This work presents first-principles investigations of the dynamic process of lithium (Li) penetration through the buffer layer on 6H-SiC(0001) surface, as well as the Li-insertion induced change of electronic structure. It is found that the penetration is kinetically forbidden for perfect buffer layer, because of the size confinement of its honeycomb structure. From the analysis of rate coefficient under the experimental conditions, topological defects no smaller than 8-membered ring are predicted to be essential for Li intercalation. Along with the Li insertion, the electronic property of the buffer layer is changed from n-type doping (Li-adsorption) to that of quasi-free-standing graphene (Li-intercalation). It is the electron injection by Li that results in the dissociation of the Si-C bonds and the decoupling of Li-intercalated buffer layer from the substrate. Moreover, we demonstrate the influence of such topological defects on the electronic property of epitaxial graphene, which provides some useful hints for understanding the observed gap and midgap state behavior.

9:24AM H11.00008 Single atom doping of graphene – A theoretical study, AMIR NATAN, Department of Physical Electronics, Tel-Aviv University, 69978 Tel-Aviv, Israel, TAMAR SEIDEMAN, Department of Chemistry, Northwestern University, Evanston IL 60208-3113, USA — We present first principles results and analysis for the electronic structure of chemically modified graphene. We show the relationship between different physical parameters and the electronic band structure of the modified material and its doping level. Finally, we discuss the possible effects of a substrate and of charge transfer patterns for device applications.

9:36AM H11.00009 Hydrogen adsorption induced structural and electronic changes in graphene grown on metal substrate, SRIVATS RAJASEKARAN, SARP KAYA, TOYLI ANNIYEV, HIROHITO OGASAWARA, ANDERS NILSSON, Stanford Synchrotron Radiation Lightsource, FAN YANG, DARIO STACCHIOLA, Chemistry Department, Brookhaven National Laboratory, FRANK-ABILD PEDERSON, JENS NORSKOV, SUNCAT, STANFORD SYNCHROTRON RADIATION LIGHTSOURCE TEAM, CHEMISTRY DEPARTMENT, BROOKHAVEN NATIONAL LABORATORY COLLABORATION, SUNCAT COLLABORATION — Graphene hydrogenation proposed to open a band gap has also been shown to be the case for graphene on metal substrates. Our carbon specific soft x-ray (photoelectron, absorption, emission) spectroscopy studies on single and few layer graphene on Pt(111) do not indicate band opening due to hydrogenation. The graphene layer is weakly interacting with the Pt(111) substrate but hydrogenation induces structural changes which lead to observation of density of states at the Fermi level (contrary to band opening hypothesis) due to strong hybridization with substrate. Hydrogenation observed to occur only on the surface atoms of few layers of graphene induces interlayer carbon-carbon bonding due to structural distortions initiated at the surface, i.e. propagation of sp^3 hybridization to underneath carbon layers. This structure is stabilized due to hybridization of the carbon atoms in the bottom layer with the Pt(111) substrate.

9:48AM H11.00010 Vibrational Spectrum of “Crystalline Graphane”, A.I. KOLESNIKOV, Oak Ridge National Laboratory, Oak Ridge, TN, USA, V.E. ANTONOV, I.O. BASHKIN, V.S. EFIMCHENKO, Ins. Solid State Physics RAS, Chernogolovka, Russia, G.E. GRANROTH, Oak Ridge National Laboratory, Oak Ridge, TN, USA, V.I. KULAKOV, Ins. Solid State Physics RAS, Chernogolovka, Russia, T. SHERLINE, Oak Ridge National Laboratory, Oak Ridge, TN, USA, ORNL TEAM, ISSP RAS TEAM — Since the discovery of graphene, a flat monolayer of carbon atoms, a great interest was attracted to synthesis of chemically modified carbon sheets. In particular, it was proposed that graphane, representing a graphene sheet saturated by hydrogen adsorbed from both sides, would be stable [1], and this prediction was confirmed by TEM [2]. Recently, hydrogenated graphite with a composition close to CH has been synthesized by exposing the graphite to gaseous hydrogen at $P=2$ to 7 GPa and $T=350$ to 450°C [3]. The formation of hydrographite is accompanied by a 40% increase in the c -parameter of the unit cell. The IR spectrum shows a strong band near 2850 cm^{-1} due to stretching vibrations of the C-H covalent bonds. In the present work, we studied the vibrational spectrum of hydrographite by inelastic neutron scattering. The obtained spectrum is very similar to that calculated for a single graphane plane [4]. This suggests a weak interaction between the graphane layers in hydrographite, so it could be considered as a “crystalline graphane” material. 1. J.O. Sofo et al., PRB **75**, 153401 (2007). 2. D.C. Elias et al., Sci. **323**, 610 (2009). 3. I.O. Bashkin et al., Int. Symp. Metal-Hydr. Syst., Reykjavik, Iceland, 2008. 4. G. Savini et al., PRL **105**, 037002 (2010).

10:00AM H11.00011 Direct determination of the dominant scatterer in graphene on silicon oxide¹, JYOTI KATOCH, MASA ISHIGAMI, Department of Physics and Nanoscience Technology Center, University of Central Florida, Orlando, FL — Previously the density of native scatterers in graphene on silicon oxide was shown to be proportional to the number of adsorption sites for atomic hydrogen [1]. However, this study provided limited information about the sites in graphene with affinity to atomic hydrogen. We employed a detailed temperature programmed desorption study on hydrogen-dosed graphene sheets. The determined desorption energy is used to reveal the nature of the dominant scatterer in graphene on silicon oxide.

[1] J. Katoch, J.H. Chen, R.Tsuchikawa, C.W. Smith, E.R. Mucciolo, and M. Ishigami, *Uncovering the dominant scatterer in graphene sheets on SiO₂*, Physical Review B Rapid Communications, 82, 081417 (2010).

¹This work is based upon research supported by the National Science Foundation under Grant No. 0955625

10:12AM H11.00012 Electron Heat Capacity of Nitrogen Doped Graphene in Low Temperature, DI LUO, WANG-CHUANG KUO, None — We calculate the electron heat capacity of nitrogen doped graphene with a simple method. There are four kinds of bonds to be considered, the pi and anti-pi bonds of C-C and C-N. And the extra electrons are treated as free constituents. We found a small amount of difference in the electron heat capacity between a pure graphene and a thin film CN_x. Nevertheless, with a precise measurement on the electron heat capacity of the thin film or layer structure of CN_x, we can determine the doping concentration of nitrogen.

10:24AM H11.00013 Chemical reactions and thermal stability of oxygen impurities on graphene¹, BIN WANG, Department of Physics and Astronomy, Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University and ORNL — Oxygen as an impurity is known to degrade conductivity in graphene, but annealing at moderate temperature reverses the effect. Here we report first-principles calculations of oxygen binding and reactions on graphene that elucidate the underlying physics. We find that two O atoms can form an O dimer that can desorb from graphene with an overall activation barrier of 1.3 eV. Oxygen can also be removed in a more complicated reaction in which C atoms in graphene are consumed. We find that structural defects such as Stone-Wales defect and grain boundaries show enhanced binding to O atoms due to the local strain, facilitating the O reaction. If H atoms coexist, an O atom can bind to an H atom forming an OH group, which can also be removed by thermal annealing due to the weak binding, resulting in defect-free graphene.

¹This work was supported by DTRA Grant No. HDTRA1-10-1-0016 and the William A. and Nancy F. McMinn Endowment at Vanderbilt University. The calculations were performed at Air Force Research Laboratory DoD Supercomputing Resource Center.

10:36AM H11.00014 Efficient adsorbate transport on graphene by electromigration, KIRILL VELIZHANIN, Los Alamos National Laboratory, DMITRY SOLENOV, Naval Research Laboratory — Chemical functionalization of the surface of graphene holds promise for various applications ranging from nanoelectronics to surface catalysis and nano-assembling. In many practical situations it would be beneficial to be able to propel adsorbates along the graphene sheet in a controlled manner. We propose to use electromigration as an efficient means to transport adsorbates along the graphene surface. Within the tight-binding approximation for graphene, parametrized by density functional theory calculations, we estimate the contributions of the direct force and the electron wind force to the drift velocity of electromigration and demonstrate that the electromigration can be rather efficient. In particular, we show that the drift velocity of atomic oxygen covalently bound to graphene can reach up to 4 cm/s for realistic graphene samples. Further, we discuss ways to dynamically, i.e., during experiment, control the efficiency of electromigration by charging and/or local heating of graphene.

Tuesday, February 28, 2012 8:00AM - 11:00AM —

Session H12 DMP DCMP: Chemical Doping of Graphene and Applications: Solar Cells, Sensors

210C

8:00AM H12.00001 I-V characteristics of organic molecules coated graphene, SEUNG JAE BAEK, YUNG WOO PARK, Seoul National University — Thin layers of organic molecules, OTS and DMF, are coated on top of graphene which was extracted by the exfoliation. I-V characteristics of the organic molecules coated graphene were investigated at low temperature by varying the gate voltage. P-doping with slight enhancement of mobility was observed with the OTS coating. On the other hand, n-doping with relatively higher enhancement of mobility was obtained with the DMF coating. CNT is nested on top of the organic molecules coated graphene by dielectrophoresis and Coulomb blockade was observed in the sandwich device.

8:12AM H12.00002 Investigation of Electrochemical Gate Controlled Charge Transport in Large Area Boron-Nitrogen Doped Graphene, SUJOY GHOSH, Southern Illinois University, Carbondale, SWASTIK KAR, Northeastern University, Boston, ZHENG LIU, ROBERT VAJTAI, PULICKEL AJAYAN, Rice University, Houston, SAIKAT TALAPATRA, Southern Illinois University, Carbondale, SOUTHERN ILLINOIS UNIVERSITY COLLABORATION, NORTHEASTERN UNIVERSITY COLLABORATION, RICE UNIVERSITY COLLABORATION — We report on the investigation of charge transport measurements of B and N doped graphene C (B,N) under the influence of an electrochemical gate. These C (B,N) systems are expected to have unique electronic properties due to the combination of impurities including both atomistically separated B and N species, as well as hexagonal boron nitride (*h*-BN) units within the graphitic C lattice. Investigations were performed on large area BN doped graphene devices fabricated with different BN doping levels. The electrochemically gate controlled interfacial capacitance and quantum capacitance of BN doped graphene devices were measured. The effect of doping on the quantum capacitance and electron mobility will be discussed.

8:24AM H12.00003 Stable Chemical Doping of Graphene for Low Electrical Resistance and High Optical Transparency, KARA BERKE¹, SEFAATTIN TONGAY², MAX LEMAITRE³, ZAHRA NASROLLAHI⁴, DAVID TANNER⁵, BILL APPLETON⁶, ARTHUR HEBARD⁷, University of Florida — Since becoming experimentally available, graphene has been used in various devices such as field effect transistors (FETs), solar cells and sensing applications. Although graphene based devices with modest characteristics have been reported, in some device geometries a lower graphene resistance with different Fermi level values is still desired. Here, we describe our use of a hydrophobic organic dopant with strong electronegativity, environmental stability and high optical transmittance which is spin cast onto CVD-grown graphene films. We observe a typical 70% reduction in resistance upon chemical modification of the graphene. Magnetoresistance measurements imply that the modified graphene is hole doped, and time-dependent resistance measurements show excellent stability. Using Raman spectroscopy we confirm the doping of graphene sheets from the shifts in G and 2D peak positions and intensity ratios. We show transmittance and SEM characteristics of the graphene sheets before and after doping. These results may serve as a guide for modification of graphene's properties as desired for various applications.

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8:36AM H12.00004 Reversible and Robust Carrier Doping in Graphene *via* Mechanical Actuation of Tethered Azobenzene, PHONG NGUYEN, VIKAS BERRY, NIHAR MOHANTY, KABEER JASUJA, Kansas State University, VIVEK SHENOY COLLABORATION — machines – molecules capable of responding to external stimuli - have gained great interest due to their applications in molecular actuation nanodevices. In this talk, we demonstrate that ultrathin graphene exhibits high-sensitivity to orientation, surface-vicinity, electronegativity, and density-of-states of interfaced molecules. This enables the realization of reversible doping of graphene *via* molecular mechanics on its surface. Here, few-layer-graphene (FLG) sheets were functionalized with electronegative and isomerizable azobenzene-molecules. The optical transformation of these azo-molecules from their *trans* conformation to *cis* conformation dopes 7.5×10^3 holes/ μm^2 in the underlying graphene. This corresponds to ~ 20 azobenzene molecules producing 1 hole (hole-mobility of $301 \mu\text{m}^2/\text{V/s}$) in the azobenzene-FLG (AFLG) device. Further, we demonstrate the facile fabrication of the AFLG device and the mechanism of electrical modulation due to molecular mechanics. We also compare the response of the AFLG device with an FLG device directly doped with electronegative perylene tetracarboxylic acid, which led to ~ 3 fold increase in the hole density. -abstract-

8:48AM H12.00005 Tuning the Electrical Properties of Large Area Graphene through Boron-Nitrogen Co-Doping, BALEESWARAIAH MUCHHARLA, ARJUN PATHAK, Southern Illinois University, Carbondale, ZHENG LIU, LI SONG, Rice University, SWASTIK KAR, Northeastern University, Boston, ROBERT VAJTAI, PULICKEL AJAYAN, Rice University, Houston, SAIKAT TALAPATRA, NAUSHAD ALI, Southern Illinois University, Carbondale, SOUTHERN ILLINOIS UNIVERSITY, CARBONDALE TEAM, RICE UNIVERSITY, HOUSTON COLLABORATION, NORTHEASTERN UNIVERSITY, BOSTON COLLABORATION — We report on investigation of low temperature electrical transport measurements of B and N co-doped graphene layers C (B, N). We find that the temperature dependence of resistance ($5\text{K} < T < 400\text{K}$) of pure graphene shows a metallic behavior, whereas the C (B, N) samples show an increasingly semiconducting behavior with increasing doping levels. Within the studied temperature range, at higher temperatures, the doped samples showed a band-gap dominated Arrhenius-like temperature dependence. At the lowest temperatures, the temperature dependence deviates from an activated behavior, and presents evidence for a conduction mechanism that is consistent with Mott's 2D-Variable Range Hopping (2D-VRH).

9:00AM H12.00006 Raman studies of ultra-clean graphene on hexagonal boron nitride with controlled doping, YILEI LI, INANC MERIC, KIN FAI MAK, LEANDRO MALARD, CORY DEAN, PHILIP KIM, KENNETH SHEPARD, TONY HEINZ, Columbia University — Graphene prepared by exfoliation on hexagonal boron nitride (h-BN) provides an ideal platform for studies of the intrinsic properties of Dirac electrons because of its unprecedented charge homogeneity. With this system, many of the fascinating phenomena hidden by charge inhomogeneity in conventional graphene samples have recently been revealed. Here we describe progress in examining both electron-phonon and electron-electron interactions by means of Raman scattering by the G- and the 2D-modes. In our studies, we were able to observe a symmetric energy shift in the Raman 2D peak at low doping levels when the Fermi level was tuned from the electron side to the hole side. This shift is understood as a change in the double-resonance condition induced by the renormalization of the electron and phonon band structures. At the same time, the 2D peak is broadened under electron or hole doping. Additionally, we observed very weak doping dependence of the G peak (both position and width) at Fermi energies less than half of the phonon energy and the subsequent usual removal of non-adiabatic Kohn anomaly with increased doping, which reflects again the extremely homogeneous charge distribution in our samples.

9:12AM H12.00007 Scanning Tunneling Microscope (STM) Study of B-doped Monolayer Graphene, LIUYAN ZHAO, Columbia University, MARK LEVENDORF, Cornell University, CHRISTOPHER GUTIERREZ, THEANNE SCHIRO, GEORGE FLYNN, Columbia University, JIWOONG PARK, Cornell University, ABHAY PASUPATHY, Columbia University, COLUMBIA UNIVERSITY COLLABORATION, CORNELL UNIVERSITY COLLABORATION — Chemical doping is a promising technique to tailor the electronic properties of graphene. Here we focus on an atomic scale characterization of Boron-doped monolayer graphene sheets using primarily STM, assisted by Raman Spectroscopy and X-ray Absorption Spectroscopy (XAS). We will show in topography that there are two major structures that result from B-doping, and in spectroscopy that each of these structures plays different roles in modifying the electronic properties of graphene. Raman Spectroscopy and XAS provide complementary information about the nature of the B-C bonds in the sample.

9:24AM H12.00008 Substituent Effects for the Control of Covalent Electronic Doping of CVD Graphene, GERALDINE L.C. PAULUS, Massachusetts Institute of Technology, MOON-HO HAM, Kyungwon University, QING HUA WANG, ANDREW J. HILMER, KI KANG KIM, CHIH-JEN SHIH, ZACHARY ULISSI, JING KONG, MICHAEL S. STRANO, Massachusetts Institute of Technology — Controlling the electrical properties of graphene is of particular interest for future electronic, optoelectronics and sensing applications. We investigate the doping effect of different chemical functional groups covalently attached to CVD-grown graphene devices with a polymer electrolyte top-gate. The covalent reaction is based on a diazonium chemistry, specifically the type and degree of doping for a diazonium salt with a nitro group, a bromo group or an alkyne group attached are investigated. We use three different approaches to inspect various aspect of the doping in graphene: Gaussian calculations, Raman measurements and transfer-characteristics. The transfer curves show that nitro groups induce p-doping while the bromo- and alkyne groups induce n-doping. A new model that takes into account both coulombic and resonant scattering as well as a asymmetric electron and hole transport is developed to fit the transfer-curves. The graphene transistors are very robust and reproducible, suggesting this is a simple and facile way to control the electronic properties of graphene.

9:36AM H12.00009 Charge transfer and density of states modifications of graphene upon molecular adsorption - Implications for gas and molecular sensors, DAVID CAREY, ALEXANDER SAMUELS, University of Surrey — The adsorption of molecules on single layer graphene can result in significant modifications to the band structure and density of states near the Dirac point and can result in the introduction of scattering centres which can modify the carrier mobility. Understanding how the competing interactions of increased carrier density and density of scattering centres is therefore an important consideration in the description of the properties of graphene. We have used ab initio methods to explore the degree of charge transfer, modification to the band structure and density of states associated with the adsorption of a range of open and closed shell molecules, organometallic molecules and planar organic molecules. We show how the charge transfer can be related to the position of the molecule related energy levels on adsorption relative to the Dirac point. We find low levels ($<0.05e$) of charge transfer for NH_3 , NO and NO_2 molecules but larger values for cobaltocene (n-type, 0.31 e/molecule) and about 0.3 e/molecule for the organic molecules TDAE (n-type) and DDQ (p-type) respectively. These molecules open up ways to dope graphene to high levels and are important considerations in sensing. We also discuss the factors that control the charge transfer.

9:48AM H12.00010 Biochemical Sensing in Solution Gated Graphene Field Effect Transistors¹, MAURICIO D. BEDOYA, JAN SCRIMGEOUR, School of Physics and Petit Institute for Bioengineering and Bioscience, Georgia Institute of Technology Atlanta, GA 30332 (USA), JAMES PALMER, W.A. DEHEER, School of Physics, Georgia Institute of Technology Atlanta, GA 30332 (USA), C. BERGER, School of Physics, Georgia Institute of Technology Atlanta, GA 30332 (USA) and CNRS-Institut Neel, BP 166, 38042 Grenoble, Cedex 9, France, J.E. CURTIS, School of Physics and Petit Institute for Bioengineering and Bioscience, Georgia Institute of Technology Atlanta, GA 30332 (USA) — Epitaxial graphene is a promising material for the construction of label-free chemical and biochemical sensors. In this work, graphene of few-layers is used as a sensor for pH and ionic strength in a solution gated field effect transistor (SGFET). In order to improve the sensitivity of the SGFET to pH and ionic changes the transistor is connected in a four-point (van der Pauw) configuration. Results for the shift in the Dirac point when the pH or ionic strength is changed are shown.

¹This work is supported by the National Science Foundation under Grant No. DMR-0820382

10:00AM H12.00011 Combined transport-Scanning Probe Microscopy study of reduced graphene oxide sensors, CHRISTOPHER KEHAYIAS, JOSEPH RAHAMIM, Physics and Astronomy, Tufts University, SAMUEL MAC-NAUGHTON, SAMEER SONKUSALE, Electrical and Computer Engineering, Tufts University, CRISTIAN STAIL, Physics and Astronomy, Tufts University — We present an in-depth study of the sensing properties of chemically reduced graphene oxide (rGO) based devices. Graphene oxide is an electronically hybrid material that can be controllably tuned from an insulator to a semiconductor material via reduction chemistry. Due to their chemical structure and large surface to volume ratio rGO sensors can detect gas adsorption at very low concentrations. rGO devices are created by dielectrophoretic assembly of rGO platelets onto interdigitated electrode arrays, which are lithographically pre-patterned on top of SiO_2/Si wafers. The gas sensing properties of these devices are characterized using novel combined transport-Scanning Kelvin Probe Microscopy and transport-Electrostatic Force Microscopy measurements in the presence of different gas analytes. These measurements show unique, very sensitive and repeatable responses to various volatile organic compounds and other gases. Maps of the electrostatic potential and charge distribution across these circuits are used to model the dynamics of electronic transport through the rGO system.

10:12AM H12.00012 Biomimetic graphene sensors: functionalizing graphene with peptides¹, MASA ISHIGAMI, Department of Physics and Nanoscience Technology Center, University of Central Florida, Orlando, FL, SANG NYON KIM, RAJESH NAIK, Materials and Manufacturing Directorate, Air Force Research Laboratory, Wright-Patterson Air Force Base, OH 45433, SUREN A. TATULIAN, Department of Physics, University of Central Florida, Orlando, FL, 32816-2385, JYOTI KATOCH, Department of Physics and Nanoscience Technology Center, University of Central Florida, Orlando, FL — Non-covalent biomimetic functionalization of graphene using peptides is one of more promising methods for producing novel sensors with high sensitivity and selectivity. Here we combine atomic force microscopy, Raman spectroscopy, and attenuated total reflection Fourier transform infrared spectroscopy to investigate peptide binding to graphene and graphite. We choose to study a dodecamer peptide identified with phage display to possess affinities for graphite and we find that the peptide forms a complex mesh-like structure upon adsorption on graphene. Moreover, optical spectroscopy reveals that the peptide binds non-covalently to graphene and possesses an optical signature of an α -helical conformation on graphene.

¹This work is based upon research supported by the National Science Foundation under Grant No. 0955625

10:24AM H12.00013 Solution-gated graphene field-effect transistors as local pH sensors in microfluidic systems, WAN LI, Department of Physics, Cornell University, HÉCTOR D. ABRUÑA, Department of Chemistry and Chemical Biology, Cornell University, DANIEL C. RALPH, Department of Physics, Cornell University — We report a study of solution-gated graphene field-effect transistors (SGGFETs) as high-performance local pH sensors in microfluidic devices. Previous experiments have shown that SGGFETs can function as pH sensors for bulk volumes of solutions, and a response of 20 mV/(unit pH) shift in the Dirac point was typically observed. In our study, we investigated SGGFETs micro-fabricated out of CVD graphene grown on copper foil and found a robust pH sensitivity of 50 mV/(unit pH). This value is close to the thermodynamically allowed maximum value, i.e., the Nernst value of 59 mV/(unit pH) at room temperature. We further integrated the SGGFETs into microfluidic systems for lab-on-chip applications. We found the SGGFETs are capable of real-time detection of local pH changes in microfluidic channels, thus providing reliable measurement of the local pH for small volumes of liquids (a few nL). Possible applications of this microfluidic detection system, for example, in monitoring chemical diffusion and reactions in microfluidic channels, will be discussed.

10:36AM H12.00014 A low cost construction method for Graphene based resistive chemical sensors¹, SILPA KONA, CINDY K. HARNETT, University of Louisville — Graphene is a 2D material with distinctive properties and a large surface area that can be exposed to surface adsorbates from a target gas, making it attractive as a sensing material. This enables studies on the interaction of gas molecules with the graphene surface and subsequent changes in its properties. Due to its high electron mobility at room temperature, graphene exhibits high sensitivity, making it a good candidate for environmental and industrial sensing applications. Several models of graphene based sensors have been put forth previously based on high-resolution lithographic techniques and for individual electrode attachment to the sensing film with e-beam lithography. These techniques can produce small numbers of devices that explore the limits of molecular scale sensing, but the methods are currently impractical for large scale production of low cost sensors. We present our graphene based sensor with the focus on designing small, cost effective and reliable sensors with high sensitivity towards the target gas, detailing the assembly of graphene/acrylic devices, their characterization and investigation of their performance as resistive chemical sensors using differential voltage measurements.

¹NSF GRANT AWARD # 0644511

10:48AM H12.00015 Finite temperature quantum transport in nanosensors based on graphene nanoribbons¹, KIRTI KANT PAULLA, AMIR FARAJIAN, Department of Mechanical and Materials Engineering, Wright State University — We study finite temperature quantum conductance of nanosensors based on graphene nanoribbons exposed to carbon and nitrogen oxides. Using ab-initio-based Green's function formalism, the quantum conductance of the nanoribbon with and without adsorbed oxide molecules is calculated. We investigate the effects of molecular vibrations and electron-vibron coupling on conductance modulation. The implication of the results concerning nanosensor functionality under desired environmental temperatures, and the differences with the low-temperature cases, are discussed

¹This research is supported by the National Science Foundation Grant ECCS- 0925939.

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H13 DMP GMAG: Focus Session: Low-Dimensional and Molecular Magnetism - Magnetism and Transport of Isolated Molecular Magnets - Molecular spintronics 211

8:00AM H13.00001 Manipulating Molecular Kondo Effect by Chemical Reactions, HOWON KIM, Department of Physics, Korea University, YUNHEE CHANG, Graduate School of Nanoscience and Technology (WCU), KAIST, MIN HUI CHANG, Department of Physics, Korea University, YONG-HYUN KIM, Graduate School of Nanoscience and Technology (WCU), KAIST, SE-JONG KAHNG, Department of Physics, Korea University — Motivated by spintronic applications, the control of Kondo effect arising from spin exchange interaction between isolated spins and conduction electrons of non-magnetic metals, has been explored. A method to control the molecular Kondo effect is demonstrated via chemical reactions. A spontaneous binding between molecules was exploited to control the molecular Kondo effect on Au(111). The Kondo effect was switched back on using local scanning tunneling microscope manipulation. This method relies on the hybridized pairing of unpaired spins two molecules, as supported by our density functional theory calculation results.

8:12AM H13.00002 Electronic readout of a single nuclear spin using a molecular spin transistor, R. VINCENT, Institut Neel, CNRS, Grenoble, S. KLYASTSKAYA, M. RUBEN, INT and KIT, Karlsruhe, Germany, W. WERNSDORFER, F. BALESTRO, Institut Neel, CNRS, Grenoble — Quantum control of individual spins in condensed matter devices is an emerging field with a wide range of applications ranging from nanospintronics to quantum computing [1,2]. The electron, with its spin and orbital degrees of freedom, is conventionally used as carrier of the quantum information in the devices proposed so far. However, electrons exhibit a strong coupling to the environment leading to reduced relaxation and coherence times. Indeed quantum coherence and stable entanglement of electron spins are extremely difficult to achieve. We propose a new approach using the nuclear spin of an individual metal atom embedded in a single-molecule magnet (SMM). In order to perform the readout of the nuclear spin, the quantum tunneling of the magnetization (QTM) of the magnetic moment of the SMM in a transistor-like set-up is electronically detected. Long spin lifetimes of an individual nuclear spin were observed and the relaxation characteristics were studied. The manipulation of the nuclear spin state of individual atoms embedded in magnetic molecules opens a completely new world, where quantum logic may be integrated.

[1] L. Bogani, W. Wernsdorfer, Nature Mat. 7, 179 (2008).

[2] M. Urdampilleta, S. Klyatskaya, J.P. Cleuziou, M. Ruben, W. Wernsdorfer, Nature Mat. 10, 502 (2011).

8:24AM H13.00003 DFT calculations of the charged states of N@C60 and {Fe4} single molecule magnets investigated in tunneling spectroscopy, JAVIER NOSSA, FHOKRUL ISLAM, CARLO CANALI, Linnaeus University, Kalmar, Sweden, MARK PEDERSON, Naval Research Laboratory, Washington, USA — For device applications of single molecule magnets (SMMs) in high-density information storage and quantum-state control it is essential that the magnetic properties of the molecules remain stable under the influence of metallic contacts or surface environment. Recent tunneling experiments [1, 2] on N@C60 and {Fe4} SMM have shown that these molecules preserve their magnetic characteristics when they are used as the central island of single-electron transistors. Although quantum spin models have been used extensively to study theoretically tunneling spectroscopy of SMMs, it has been shown recently that the orbital degrees of freedom, which is absent in spin models, can significantly affect the tunneling conductance [3]. In this work we present first-principles calculations of the neutral and charged states of N@C60 and {Fe4} SMMs, and discuss a strategy to include their properties into a theory of quantum transport. We also present results of the magnetic anisotropy for the different charge states of Fe4 and discuss their relevance for experiments [2] in the sequential tunneling and cotunneling regimes.

[1]. N. Roch et al., Phys. Rev. B 83, 081407 (2011).

[2]. A.S. Zyazin et al., Nano Lett. 10, 3307 (2010).

[3]. L. Michalak et al., Phys. Rev. Lett. 104, 017202 (2010).

8:36AM H13.00004 Beller Lectureship: Single Molecular Magnets on Conductive Surfaces¹, ROBERTA SESSOLI, Department of Chemistry & INSTM, University of Florence — For more than a decade molecules showing magnetic bistability, generally known as Single Molecule Magnets, have represented a playground to study quantum effects that appear in magnetism when the nanometer scale is attained. The field is now mature to investigate more complex nanostructures where the interplay between transport and magnetism at the molecular scale can be exploited. The first step along this direction requires to organize SMMs on surfaces rather than as bulk phases. Pursuing this apparently straight forward task has already encountered many difficulties because of the complex nature and fragility of SMMs and of the peculiar origin of their magnetic bistability. Also robust SMMs based on lanthanide ions and phthalocyanine lose most of their SMM properties when the crystalline phase is abandoned. Thanks to a collaboration with Prof. Cornia in Modena, Italy, and Prof. Saintavrit in Paris, France, we have carried out a very low temperature synchrotron investigation showing that a polynuclear SMM cluster, based on a propeller-like tetranuclear iron(III) core, Fe4, retains the typical hysteresis also when the molecules are chemically grafted to a gold surface. The tailoring of the anchoring ligand has allowed the control of the orientation of the molecules on the substrate and has given the possibility to observe the resonant quantum tunneling of the magnetization. Preliminary investigations on Fe4 SMMs thermally evaporated in UHV conditions on a conducting ferromagnetic oxide like Lanthanum Strontium Manganite, have shown an unprecedented phenomenon. While the reported studies of paramagnetic molecules on magnetic substrates have in general shown a sizeable magnetic interaction with the substrate but no evidences of SMM behavior, in our investigation the magnetic hysteresis of Fe4 exceeds in coercive field that of the substrate, recorded at the Mn L3 edge. More interestingly, the zero field step of the hysteresis, typical of quantum tunneling of magnetization that characterizes Fe4 SMMs, disappears when deposited on LSMO, opening the perspective of a novel hybrid magnetism at the nanoscale.

¹The support of the European Research Council through the Advanced Grant MolNanoMaS is acknowledged.

9:12AM H13.00005 Theoretical study of hysteresis in electron transport through spin-crossover molecules, KRISTEN BROWN, KYUNGWHA PARK, Dept. of Physics, Virginia Tech, Blacksburg, VA 24061 — Recent advances in nanoscale molecular systems stimulate experimental studies of electron transport across molecular junctions formed by single molecules or nanoparticles bridged between electrodes, or molecular monolayers adsorbed onto surfaces, using three-terminal set-ups or scanning tunneling microscope. Among them, spin-crossover molecular systems draw attention due to their unusual coupling between spin degrees of freedom and external stimuli. Spin magnetic moments of these molecular systems increase with increasing temperature or pressure, or shining light, and their magnetization shows hysteresis behavior with temperature, pressure, or light. Recent transport measurements across nanoparticles made of such spin-crossover molecules reveal hysteresis behavior in current-voltage characteristics, driven by voltage at a given temperature. In this talk, we present our work on understanding of hysteresis in electron transport through a nanoparticle consisting of Fe-based spin-crossover molecules, using a model-Hamiltonian approach and insight obtained from density functional theory.

9:24AM H13.00006 Individual Magnetic Molecules on Ultrathin Insulating Surfaces, FADI EL HALLAK, London Centre for Nanotechnology, UCL, London, UK, BEN WARNER, London Centre for Nanotechnology, UCL, London, UK; Department of Physics & Astronomy, UCL, London, UK, CYRUS HIRJIBEHDIN, London Centre for Nanotechnology, UCL, London, UK; Department of Physics & Astronomy, UCL, London, UK; Department of Chemistry, UCL, London, UK — Single molecule magnets have attracted ample interest because of their exciting magnetic and quantum properties. Recent studies have demonstrated that some of these molecules can be evaporated on surfaces without losing their magnetic properties [M. Mannini *et al.*, *Nature* 468, 417, (2010)]. This remarkable progress enhances the chances of real world applications for these molecules. We present STM imaging and spectroscopy data on iron phthalocyanine molecules deposited on Cu(100) and on a Cu₂N ultrathin insulating surface. These molecules have been shown to display a large magnetic anisotropy on another thin insulating surface, oxidized Cu(110) [N. Tsukahara *et al.*, *Phys. Rev. Lett.* 102, 167203 (2009)]. By using a combination of elastic and inelastic electron tunnelling spectroscopy, we investigate the binding of the molecules to the surface and the impact that the surface has on their electronic and magnetic properties.

9:36AM H13.00007 Interfacial Electronic and Magnetic Coupling in Organic-metal System Studied by Scanning Tunneling Microscopy, YU-HSUN CHU, C.H. HSU, P.J. HSU, W.J. HSIEH, C.I. LU, S.W. CHEN, C.J. BUTLER, Department of Physics, National Taiwan University, 10617 Taipei, Taiwan, CHAO-CHENG KAUN, Research Center for Applied Sciences, Academia Sinica, Taipei 106, Taiwan, MINN-TSONG LIN, Department of Physics, National Taiwan University, 10617 Taipei, Taiwan — Organic materials have drawn much attention in spintronics studies because of their tunable properties by functional groups and potential to achieve molecular magnets. An important factor influencing these properties is the interfacial effect. In organic-metal systems, different interfaces lead to strong modulation of electronic structures and even magnetic behaviors like spin coupling. In our study, Mn-phthalocyanine (MnPc) deposited on Cu(111) surface have been measured by scanning tunneling microscopy (STM) and spectroscopy (STS) at 4.5 K. With different deposition amount, MnPc are adsorbed as isolated molecules or in an ordered assembled structure. From STS curves, assembled MnPc possess a broadened state near the onset of Cu(111) surface state comparing to isolated ones. According to ab initio calculation, distance between the central Mn atom and the substrate in assembled molecules is reduced due to intermolecular interaction and affects the electronic structures. Magnetic behaviors of MnPc on ferromagnetic metal substrate are further investigated by spin-polarized STM (SP-STM). Spin contrast of isolated molecules on Co nanoislands on Cu(111) is found near the Fermi level in STS maps, which is considered to be ferromagnetic coupling between MnPc and Co islands.

9:48AM H13.00008 The Kondo effect in molecular magnets from first principles, DAVID JACOB, Max Planck Institute of Microstructure Physics Halle, MICHAEL KAROLAK, ALEXANDER I. LICHTENSTEIN, University of Hamburg, MARIA SORIANO, JUAN JOSE PALACIOS, Universidad Autonoma de Madrid — When a magnetic molecule is deposited on a metallic substrate or attached to metallic contacts its magnetic moment may actually be screened by the conduction electrons due to the Kondo effect. In view of possible applications of molecular magnets such as nanoscale spintronics and magnetic storage devices, it is important to being able to predict whether the Kondo effect will take place or not in a given system. Also one would like to understand in detail how the Kondo effect emerges in a given situation and how it is controlled by the various parameters such as the molecular conformation and the type of substrate. Using a recently developed ab initio approach for molecular devices [1,2] that explicitly takes into account the strong electronic correlations that give rise to the Kondo effect, we have calculated the electronic structure and transport properties of different magnetic molecules coupled to nanocontacts [3] and surfaces [4]. Our calculations shed light on the complex nature of the Kondo effect in molecular-scale devices. [1] D. Jacob *et al.*, *PRL* 103, 016803 (2009); [2] D. Jacob *et al.*, *PRB* 82, 195115 (2010); [3] M. Karolak *et al.*, *PRL* 107, 146604 (2011); [4] K. J. Franke *et al.*, *Science* 20 940 (2011)

10:00AM H13.00009 ABSTRACT WITHDRAWN —

10:12AM H13.00010 Electronic transport in Co-based valence tautomeric conjugated polymers¹, MARCO BUONGIORNO NARDELLI, YIFENG CHEN, North Carolina State University, ARRIGO CALZOLARI, Istituto Nanoscienze CNR-NANO-S3, WANDERLA SCOPEL, North Carolina State University — Using first principle density functional theory (DFT) methods combined with maximally localized Wannier function (MLWF), real-space basis sets and a Green's function transport scheme within the Landauer ballistic transport regime, we investigated the electronic structures and electronic transport properties of a Co-based valence tautomeric (VT) conjugated backbone polymeric system. We found that GGA+U induced high-spin structure not in satisfactorily agreement with realistic circumstances from the computed Co projected density of states (PDOS). So we instead employed constrained magnetization calculations to induce the low-spin to high-spin magnetic transition computationally. Transport calculations showed that the high-spin structure is two orders of magnitude more conductive than the low-spin structure, thus supporting the vision that this kind of Co-based VT polymer can function as basis for switchable molecular spintronic devices. Finally, we will briefly discuss the chemisorption of this VT system on metallic substrates the spin transport properties of metal-molecule-metal configurations.

¹NSF Center for Chemical Innovation: Center for Molecular Spintronics (CHE-0943975)

10:24AM H13.00011 Dynamical magnetic anisotropy in spin-1 molecular systems¹, DAVID RUIZ-TIJERINA, Ohio University, PABLO CORNAGLIA, CARLOS BALSEIRO, Centro Atomico Bariloche, e Instituto Balseiro, Argentina, SERGIO ULLOA, Ohio University — We study electronic transport through a deformable spin-1 molecular system in a break junction setup, under the influence of a local vibrational mode. Our study shows that the magnetic anisotropy, which arises due to stretching along the transport axis [Science 328 1370 (2010)], is renormalized by the interactions with vibrations. The coupling induces additional spin-asymmetric hybridizations that contribute to the net molecular anisotropy. We show that the low temperature physics of such device can be described by an anisotropic Kondo model ($J_{\perp} > J_{\parallel}$), with a magnetic anisotropy term, $A_{Net} S_z^2$, negative at zero stretching. A quantum phase transition (QPT) is explored by stretching the molecule, driving A_{Net} into positive values, and changing the character of the device from a non-Fermi-liquid (NFL) to a Fermi liquid (FL) ground state. This transition can be directly observed through the zero-bias conductance, which we find to be finite for negative anisotropy, zero for positive anisotropy, and to reach the unitary limit at $A_{Net} \approx 0$. At that point, an underscreened spin-1 Kondo ground state appears due to the restitution of the spin-1 triplet degeneracy.

¹Supported by NSF-PIRE and NSF-MWN/CIAM.

10:36AM H13.00012 Hot electron spin transport in C₆₀ fullerene¹, LUIS EDUARDO HUESO, CIC nanoGUNE AND IKERBASQUE, Basque Foundation for Science, MARCO GOBBI, AMILCAR BEDOYA-PINTO, FEDERICO GOLMAR, ROGER LLOPIS, CIC nanoGUNE, FELIX CASANOVA, CIC nanoGUNE AND IKERBASQUE, Basque Foundation for Science — Carbon-based molecular materials are interesting for spin transport application mainly due to their small sources of spin relaxation [1]. However, spin coherence lengths reported in many molecular films do not exceed a few tens of nanometers [2]. In this work we will present results showing how hot spin-polarized electrons injected well above the Fermi level in C₆₀ fullerene films travel coherently for hundreds of nanometers. We fabricated hot-electron vertical transistors, in which the current created across an Al/Al₂O₃ junction is polarized by a metallic Co/Cu/Py spin valve trilayer and subsequently injected in the molecular thin film. This geometry allows us to determine the energy level alignment at each interface between different materials. Moreover, the collector magnetocurrent excess 85%, even for C₆₀ films thicknesses of 300 nm. We believe these results show the importance of hot spin-polarized electron injection and propagation in molecular materials. [1] V. Dediu, L.E. Hueso, I. Bergenti, C. Taliani, Nature Mater. 8, 707 (2009) [2] M. Gobbi, F. Golmar, R. Llopis, F. Casanova, L.E. Hueso, Adv. Mater. 23, 1609 (2011)

¹We acknowledge funding from the European Research Council (Project 257654 Spintros) and the Spanish MICINN (Project MAT2009-08494)

10:48AM H13.00013 A Copper Nitride Nanotemplate for Individual Magnetic Molecules, BEN WARNER, London Centre for Nanotechnology, Department of Physics & Astronomy, UCL, London, UK, FADI EL HALLAK, London Centre for Nanotechnology, UCL, London, UK, MICHAEL WATERS, School of Chemistry, University of Nottingham, Nottingham, UK, JORIS VAN SLAGEREN, Institut für Physikalische Chemie, Universität Stuttgart, Stuttgart, Germany, CYRUS HIRJIBEHEDIN, London Centre for Nanotechnology, Department of Physics & Astronomy, Department of Chemistry, UCL, London, UK — Molecular magnets hint at a promising future in information technology applications because of their interesting quantum and magnetic properties in the bulk. If these molecules are to be useful for device applications, it may be necessary to place them on surfaces, and work has begun to concentrate in this area. However, the practical issues of isolating and accessing these molecules have yet to be resolved. We present scanning tunnelling microscopy (STM) data on FePc and (DyPc₂) deposited on a (Cu₂N-Cu(100)) surface. (Cu₂N-Cu(100)) forms a quasi-periodic lattice, and has been shown to force porphyrin molecules to sit at specific sites (D. Eciya et al., Appl. Phys. Lett. 92, 223117 (2008)). As with the porphyrins, we find that these molecules sit at the intersection of the copper lines. This spatial separation restrains any potential dipolar or exchange interaction between the molecules, and it allows for individual, independent spins to be addressed. Using data taken with an STM we investigate the properties of these molecules, and furthermore show that the molecules on this surface are immobile up to room temperature.

Tuesday, February 28, 2012 8:00AM - 10:12AM —
Session H14 GMAG DMP FIAP: Focus Session: Spins in Semiconductors - Electrical Spin Injection 212

8:00AM H14.00001 Electrical Spin Injection and Detection in Silicon: Effect of Interface States, JONAS BEARDSLEY, YONG PU, Ohio State University Department of Physics, ADRIAN SWARTZ, PAT ODENTHAL, UC Riverside Department of Physics, ANDREW BERGER, DONGKYUN KO, VIDYA BHALLAMUDI, PETER CHRISTOPHER HAMMEL, Ohio State University Department of Physics, ROLAND KAWAKAMI, UC Riverside Department of Physics, EZEKIEL JOHNSTON-HALPERIN, JON PELZ, Ohio State University Department of Physics — We have observed (using the local Hanle method) electrical spin injection into n and p type Si through a Fe/MgO/Si tunnel, with an effective spin lifetime of ~130ps and an extremely large spin RA product as high as ~0.1 MΩ*μm² at low bias and temperature. Both the spin-RA and the differential resistance decrease exponentially with bias at temperatures below 150K. The effective spin lifetime weakly depends on temperature, decreasing by ~30% from 10K to 300K. We observe the inverse Hanle effect when an external magnetic field is applied parallel to the magnetization, possibly indicating the presence of stray fields near the Si surface. These observations roughly agree with other local Hanle spin injection studies in Silicon and GaAs, but differ strongly from the results expected for injection into bulk Silicon. The two stage tunneling model through localized states (LS) developed by Tran *et al* (PRL 102; p. 036601) can explain the large magnitude of the observed spin RA, and we have developed an extended LS model which can explain the voltage dependence, which will be discussed in another talk.

8:12AM H14.00002 Non-local spin transport and accumulation measurements in Si:AlGaAs with tunable carrier density¹, JENNIFER MISURACA, J.-I. KIM, Florida State University, K.K. MENG, L. CHEN, J. LU, J.H. ZHAO, Institute of Semiconductors, Chinese Academy of Sciences, P. XIONG, S. VON MOLNAR, Florida State University — The spin lifetime in GaAs varies strongly with carrier density near the insulator to metal transition (IMT), possibly peaking at the transition [1]. However, determining the optimal spin lifetime in this material is challenging because many replica samples need to be fabricated and measured. This difficulty can be circumvented by employing Si:Al_{0.3}Ga_{0.7}As, a persistent photoconductor, as the spin transport medium. This material has been characterized and has an effective carrier density which can be tuned *in situ* via photo-excitation from 10¹⁴ to 10¹⁸ cm⁻³ and a critical carrier density for the IMT of 9.0 × 10¹⁶ cm⁻³ at 5K [2]. Heterostructures have been grown by MBE, consisting of 2 μm Si:AlGaAs, a thin epitaxial Fe layer, and an AlGaAs graded junction to create Schottky tunnel barrier contacts. Non-local spin devices have been fabricated and measured. Based on non-local 4 terminal (NL 4T) and local and NL 3T Hanle effect measurements, the initial electrical spin transport and accumulation measurements in this material are reported. The spin lifetimes range from 600 ps to 2.8 ns for multiple carrier densities, ranging from 3.5 × 10¹⁶ to 2.4 × 10¹⁷ cm⁻³. [1] J. M. Kikkawa et al., Phys. Rev. Lett. 80, 4313 (1998). [2] J. Misuraca et al., Phys. Rev. B. 82, 125202 (2010).

¹This work was supported by NSF DMR-0908625 and NSFC 10920101071.

8:24AM H14.00003 Electrical spin injection and detection in Fe/MgO/Si: influence of interface states, YONG PU, JONAS BEARDSLEY, Center for Emergent Materials, The Ohio State University, ADRIAN SWARTZ, PATRICK ODENTHAL, Dept. of Physics and Astronomy, University of California-Riverside, ANDREW BERGER, DONGKYUN KO, VIDYA BHALLAMUDI, CHRIS HAMMEL, Center for Emergent Materials, The Ohio State University, ROLAND KAWAKAMI, Dept. of Physics and Astronomy, University of California-Riverside, EZEKIEL JOHNSTON-HALPERIN, JON PELZ, Center for Emergent Materials, The Ohio State University — We report electrical spin injection and detection in Fe/MgO/Si tunnel diodes using a 3-terminal (3T) geometry. Analysis of our Hanle curves yields an effective spin life-time of ~0.1 ns and a spin-RA product ~1 MΩ * μm², both of which are in rough agreement with previous 3T studies. However, according to our analysis the spin-RA is ~ 6 orders of magnitude larger than expectations for bulk Si, and the 0.1 ns effective spin life-time is much smaller than reported value in Si by ESR or non-local methods. Here we provide a detailed analysis of electrical injection and detection in the 3T geometry. We present an alternative expression for the 3T spin signal than is usually used, and we propose that spin is accumulating in localized states (LS) at the MgO/Si interface rather than just in bulk Si. Incorporating a theory of spin accumulation in LS developed by M. Tran *et al* (PRL 102, 036601), we propose an energy distribution for the density of localized states, and introduce a model that agrees well with our anomalously large spin-RA and can explain the strong bias dependence of both spin and charge transport.

8:36AM H14.00004 Spin accumulation in Fe/MgO/Ge heterostructures, A.T. HANBICKI, S.-F. CHENG, R. GOSWAMI, O.M.J. VAN 'T ERVE, B.T. JONKER, Naval Research Laboratory — We have investigated the injection of spins into n-type Ge(001) from Fe through an MgO tunnel barrier using 3-terminal Hanle measurements. While significant progress has been made in Si, spin research in Ge is still at a nascent stage, due in part to the fact that significant Fermi level pinning at the Ge interface makes it difficult to efficiently inject carriers. We observe here precessional dephasing of the spin accumulation in an applied magnetic field (the Hanle effect) in Fe/MgO/Ge structures for both forward and reverse bias. We determine spin lifetimes and corresponding spin diffusion lengths for injection into Ge substrates of varying carrier concentration and see a trend of increasing spin lifetime with decreasing doping density. At room temperature, spin lifetimes range from $\tau_s = 50$ ps to 123 ps as the carrier concentration is reduced from $n=8 \times 10^{17} \text{ cm}^{-3}$ to $2 \times 10^{16} \text{ cm}^{-3}$. We will discuss the spin-RA product as a function of carrier concentration and the role of interface states. The observed room temperature injection of spins shows that despite persistent Fermi level pinning, spin accumulation is possible in the surface of Ge. This work was supported by core programs at NRL.

8:48AM H14.00005 Spin Transfer from a Ferromagnet into a Semiconductor through an Oxide barrier, CLODOALDO IRINEU LEVARTOSKI DE ARAUJO, MILTON ANDRE TUMELERO, ALEXANDRE DA CAS VIEGAS, Laboratorio de Filmes finos e Superfícies (LFFS), Universidade Federal de Santa catarina, NICOLAS GARCIA, Laboratorio de Fisica de Sistemas Pequenos y Nanotecnología, Consejo Superior de Investigacione Cientificas (CSIC), ANDRE AVELINO PASA, Laboratorio de Filmes finos e Superfícies (LFFS), Universidade Federal de Santa catarina — We present results on the magnetoresistance of the system Ni/Al203/n-doped Si/Al2O3/Ni in fabricated nanostructures. The results at temperature of 14K reveal a 75% magnetoresistance that decreases in value up to approximately 30K where the effect disappears. We observe minimum resistance in the antiparallel configurations of the source and drain of Ni. As a possibility, it seems to indicate the existence of a magnetic state at the Si/oxide interface. The average spin diffusion length obtained is of 650 nm approximately. Results are compared to the window of resistances that seems to exist between the tunnel barrier resistance and two threshold resistances but the spin transfer seems to work in the range and outside the two thresholds.

9:00AM H14.00006 Comparing nonlocal and three terminal Hanle experiments in Silicon, OLAF VAN 'T ERVE, CONNIE LI, AUBREY HANBICKI, PHILLIP THOMPSON, BEREND JONKER, Naval Research Laboratory — We have recently shown electrical spin injection in the technologically important material Si up to 500K and demonstrated a dependence of the spin lifetime with carrier concentration. In previous work on GaAs, we have seen excellent agreement between the spin lifetime derived from Hanle data measured directly at the injector contact using a three terminal measurement and the simultaneously measured nonlocal signal outside of the charge path. Unfortunately, simultaneous measurement of three terminal and nonlocal measurements is impractical on the Silicon devices due to the high resistance of the $6 \times 100 \mu\text{m}^2 \text{ Fe/AlO}_x/2\text{e}18$ n-type Si injector contact. Instead we used a separate $150 \times 100 \mu\text{m}^2 \text{ Fe/AlO}_x/\text{Si}$ contact on the same substrate to do three terminal measurements and nonlocal measurements independently. Lorentzian fits to the data shows a spin lifetime of 280 ps measured directly underneath the spin injecting contact. This data is in excellent agreement with the spin lifetime vs. carrier concentration for NiFe/SiO₂/Si contacts, however it is a factor of 3 lower than the spin lifetime of ~ 1 ns measured at the nonlocal contact. We discuss this observed difference and other properties such as temperature dependence and bias dependence of the three terminal vs. nonlocal experiments.

9:12AM H14.00007 Electrical injection and detection of spin accumulation in Si at 500 K with magnetic metal/SiO₂ contacts, CONNIE H. LI, Naval Research Lab — Electrical spin injection into Si (001) from a ferromagnetic metal through an Al₂O₃ tunnel barrier has been demonstrated.¹ However, the utilization of SiO₂ as the tunnel barrier can have significant impact on the development of Si based spintronics. Here we demonstrate the electrical injection, detection and precession of spin accumulation in Si, via injection from ferromagnetic contacts such as Ni_{0.8}Fe_{0.2} and Co_{0.9}Fe_{0.1} through a SiO₂ tunnel barrier.² The injection of spin-polarized carriers produce a net spin polarization and an imbalance in the spin-dependent electrochemical potential under the contact, which is detected as a voltage at the same contact. The decrease of this voltage with increasing out-of-plane magnetic field due to spin dephasing, i.e., Hanle precession of the electron spin, is observed up to 500 K. We observe Hanle precession of electron spin accumulation in Si for a wide range of bias, and demonstrate that the spin lifetime (extracted from the Lorentzian fit to the Hanle data) varies with Si carrier density. Details of the bias and temperature dependence of the spin lifetime and spin diffusion length will also be presented at the meeting. These results confirm spin accumulation in the Si transport channel up to 500 K rather than trapping in localized interface states, and demonstrate the practical aspect of spin-based semiconductor device technology. Supported by ONR.

¹B. T. Jonker et al., Nature Phys. 3, 542 (2007); S. P. Dash et al., Nature 462, 491 (2009).

²C. H. Li et al., Appl. Phys. Lett. 95, 172102 (2009).

9:48AM H14.00008 Spin-filter effect of quantum dot with spin-orbit interaction in magnetic field, TOMOHIRO YOKOYAMA, MIKIO ETO, Faculty of Science and Technology, Keio University — We theoretically investigate a spin-polarized current generation in a semiconductor quantum dot (QD) with spin-orbit interaction in a magnetic field. In the absence of magnetic field, a spin-polarized current is generated only when the QD is connected to more than two leads.¹ In the presence of magnetic field, on the other hand, we show that the two-terminal QD works as a spin filter due to the spin-orbit interaction even if the Zeeman effect is negligibly small. First, we focus on the vicinity of current peaks of Coulomb oscillation due to the resonant tunneling, considering the two energy levels around the Fermi level in the leads, and obtain an analytical form of spin-dependent current. The spin-polarization of the current is largely enhanced when the spacing between the two levels is smaller than the level broadening due to the tunnel coupling to the leads. Second, we perform a numerical simulation using a realistic model for the confining potential of the QD. We find more than 40% spin-filtering efficiency around some current peaks.

¹M. Eto and T. Yokoyama, J. Phys. Soc. Jpn. **79**, 123711 (2010).

10:00AM H14.00009 Tailoring Chirp in Spin-Lasers, JEONGSU LEE, SUNY at Buffalo, GUILHEM BOERIS, Ecole Polytechnique, KAREL VYBORNÝ, Institute of Physics ASCR, IGOR ZUTIC, SUNY at Buffalo — The interplay of spin injection in lasers and their nonlinear response leads to novel spintronic devices [1]. Such spin-lasers can enable desirable properties including threshold reduction, bandwidth enhancement, and low chirp [1-3]. These lasers can also be viewed as spin-amplifiers, since high circular polarization in the output can be achieved even with nearly spin-unpolarized injection [2,3]. In the present work, we study chirp in spin-lasers and suggest new modulation schemes to improve their performance. Supported by NSF-ECCS, U.S. ONR, AFOSR-DCT, and NSF-NEB 2020.

[1] M. Holub et al., Phys. Rev. Lett. 98, 146603 (2007); J. Rudolph et al., Appl. Phys. Lett. 87, 241117 (2005).

[2] J. Lee, W. Falls, R. Oszwadowski, and I. Žutić, Appl. Phys. Lett. 97, 041116 (2010).

[3] C. Gøthgen, R. Oszwadowski, A. Petrou, and I. Žutić, Appl. Phys. Lett. 93, 042513 (2008).

[4] G. Boeris, J. Lee, K. Výborný, and I. Žutić, preprint (2011).

Tuesday, February 28, 2012 8:00AM - 11:00AM –

Session H15 DMP FIAP GMAG: Focus Session: Spin and Dynamics in Metal, Spin logic and Spin-Based Devices 213

8:00AM H15.00001 A novel three-terminal spintronics device utilizing the spin Hall effect, CHI-FENG PAI, LUQIAO LIU, HSIN-WEI TSENG, YUN LI, School of Applied and Engineering Physics, Cornell University, DANIEL C. RALPH, Department of Physics, Cornell University, ROBERT A. BUHRMAN, School of Applied and Engineering Physics, Cornell University — Previous work¹ has established that the spin Hall effect (SHE) in certain thin film metallic layers can generate a transverse spin current large enough to effect, through spin transfer torque (STT), the reversible magnetic switching of an adjacent ferromagnetic layer having perpendicular magnetic anisotropy. Here we discuss a new three-terminal spintronics device that utilizes the SHE induced STT to efficiently and reversibly switch the magnetic orientation of a thin free layer electrode of an MgO magnetic tunnel junction having in-plane magnetization. The low write currents ($\leq 1\text{mA}$), large output impedance and good thermal stability ($45\text{k}_B\text{T}$) that has been achieved with this SHE three-terminal device approach, which separates the write and read operations in a manner that is relatively straightforward to fabricate, demonstrate an attractive candidate for application in next generation STT MRAM and non-volatile spin logic circuits.

¹Luqiao Liu *et al.*, arXiv:1110.6846 and Luqiao Liu invited presentation this conference (focus topic 10.1.4)

8:12AM H15.00002 Electric field assisted switching in magnetic tunnel junctions¹, WEIGANG WANG, MINGEN LI, STEPHEN HAGEMEN, C. L. CHIEN, Johns Hopkins University — It is of great interest to acquire large effects of electric field on magnetic properties, partly driven by the premise that voltage-controlled magnetization reversal would be far more energy efficient and be compatible with the ubiquitous voltage-controlled semiconductor devices. Normally the effect of electric field in metallic systems is negligible because the electric field can only penetrate into the materials by a few monolayers due to screening by the free electrons. Here we report the pronounced effects of electric field in magnetic tunnel junctions (MTJs) with very thin CoFeB electrodes, where the magnetic anisotropy originates solely from the CoFeB/MgO interfaces. The MTJs have the key structure of Co₄₀Fe₄₀B₂₀(1.2-1.3nm)/MgO(1.2-2nm)/Co₄₀Fe₄₀B₂₀(1.6nm) and the tunneling magnetoresistance in all junctions is in excess of 100%. Due to the redistribution of electrons among the different 3d orbitals of Fe and Co, the perpendicular magnetic anisotropy of the CoFeB electrodes can be significantly modified by an applied electric field. As a result, the coercivity, the magnetic configuration, and the tunneling magnetoresistance of the MTJs can be manipulated by voltage pulses, such that the high and low resistance states of the MTJ can be reversibly controlled by voltages less than 1.5 V in magnitude and with much smaller current densities.

¹W. G. Wang, M. E. Li, S. Hageman and C. L. Chien, Nature Materials, AOP (Nov 13, 2001), DOI: 10.1038/NMAT3171. This work has been supported by the US NSF grant DMR 05-20491

8:24AM H15.00003 Nanomagnetic triangles for a non-volatile logic applications¹, ALEXANDER KOZHANOV, University of California Santa Barbara, S. JAMES ALLEN, University of California at Santa Barbara — Single domain triangular nanomagnet is a base element in the recently proposed non-volatile logic application [1]. Dependent on the triangle shape and dimensions “Y” or “buckle” magnetization alignment ground states are defined by configurational anisotropy. In the “Y” ground state the local magnetization is aligned to point either towards or away from the triangle vertices. The three triangle vertices are used for information storage while switching between different ground states performs logic operations. In this work we study nanomagnetic triangle ground states and switching between them using micromagnetic simulations. We show that triangle shape engineering within the fabrication method tolerance allows maintaining the “Y” ground state despite the shape distortions typical for fabrication process. We correlate the height and profile of the energy barrier between the triangle ground states with the triangle shape and dimensions. We discuss ground state switching mechanisms and assess the triangle use for non-volatile logic and memory applications.

[1] A. Kozhanov, C.J. Palmstrom, S.J Allen “Spin Torque Triad for a non-volatile logic gates” US Patent pending.

¹Supported by Nano Electronics Research Corporation via the Nanoelectronics Research Initiative at the Western Institute of Nanoelectronics Center

8:36AM H15.00004 Ultra low-energy hybrid spintronics and straintronics: multiferroic nanomagnets for memory, logic and ultrafast image processing¹, JAYASIMHA ATULASIMHA², Virginia Commonwealth University — We have theoretically shown that multiferroic nanomagnets (consisting of a piezoelectric and a magnetostrictive layer) could be used to perform computing while dissipating $\sim$ few 100 kT/bit (Appl. Phys. Lett. 97,173105, 2010) at clock rates of $\sim$ 1GHz. They can act as memory elements (Appl. Phys. Lett. 99, 063108, 2011), logic gates (Nanotechnology, 22, 155201, 2011, <http://arxiv.org/abs/1108.5758v1>) and associative memory for higher order computing such as ultrafast image reconstruction and pattern recognition (J. Phys. D: Appl. Phys. 44, 265001 (2011), <http://arxiv.org/abs/1109.6932v1>). This talk will provide an overview of our research in:

1. Theoretical study of stress induced magnetization dynamics in isolated multiferroic nanomagnets (memory) and dipole coupled nanomagnetic arrays laid out in specific geometric patterns to implement a universal logic gate.
2. Monte Carlo simulations of the magnetization trajectories in such systems described by the stochastic Landau-Lifshitz-Gilbert (LLG) equation, that show error-free ($>99.99\%$) fast ($\sim 1\text{GHz}$) switching with very low dissipation (few 100kT/bit/magnet).
3. Demonstrating that multiferroic nanomagnets possessing biaxial anisotropy could be used for four-state logic and perform image processing applications such as image reconstruction and pattern recognition.
4. Experimental fabrication of such devices using e-beam lithography and deposition to create $\sim 100\text{nm}$ diameter elliptical nanostructures and study them with magnetic force microscopy.

¹This work is supported under NSF NEB2020 grant ECCS-1124714, NRI project 2203.001 of SRC and VCU PRIP.

²co-author: Supriyo Bandyopadhyay

9:12AM H15.00005 Reliable switching in MRAM and multiferroic logic , KAMARAM MUNIRA, Charles L. Brown Department of Electrical and Computer Engineering, University of Virginia, SUPRIYO BANDYOPADHYAY, Department of Electrical and Computer Engineering, Virginia Commonwealth University, JAYASIMHA ATULASIMHA, Department of Mechanical Engineering , Virginia Commonwealth University, EUGENE CHEN, Grandis, Inc., AVIK W. GHOSH, Charles L. Brown Department of Electrical and Computer Engineering, University of Virginia — Low reliable writing in spintronic devices limits their applicability in the automotive and defense industries. Coupling stochastic macromagnetic simulator with quantum transport, we show how greater reliable switching can be achieved in MRAM and multiferroic logic. Using a combination of spin-transfer torque and small applied perpendicular field in MRAM, the error rate can be considerably reduced for a given voltage pulse. In multiferroic logic, strain plays the role of the magnetic field. Information is passed along an array of nanomagnets (NM) (magnetostrictive + piezoelectric layers) through dipole coupling with neighboring NMs. A low voltage applied to the piezoelectric element causes the NM's magnetization to switch to its hard axis. Upon releasing the stress, the magnetization of the NM relaxes to the easy axis, with its final orientation determined by the dipolar coupling with the left NM, thus achieving a low power Bennett clocked computation. In the face of stagnation points along the potential energy landscape, the success rate of the straintronic switching can be controlled with by how fast the stress is removed from the NM. (Funding: DARPA, GRANDIS, NSF-NEB).

9:24AM H15.00006 Low-energy information transfer between dipolar-coupled magnetic disks observed by time resolved magnetic soft X-ray microscopy¹ , PETER FISCHER, CXRO/LBNL, HYUNSUNG JUNG, KISUK LEE, DAE-EUN JEONG, YOUNG-SEOK CHOI, YOUNG-SANG YU, DONG-SOO HAN, Dept MSE/Seoul Natl U, ANDREAS VOGEL, LARS BOCKLAGE, GUIDO MEIER, IAP/U Hamburg, MI-YOUNG IM, CXRO/LBNL, SANG-KOOG KIM, Dept MSE/Seoul Natl U — The coupling between oscillators allows to mutually transfer energy and also to propagate information signals. Utilizing the concept of coupled oscillators, we experimentally demonstrated a new mechanism for energy transfer between spatially separated dipolar-coupled magnetic disks by stimulated vortex gyration. Direct experimental evidence was obtained by state-of-the-art experimental time-resolved soft X-ray microscopy probe. The rate of energy transfer from one disk to the other was derived from the two normal modes' frequency splitting caused by dipolar interaction. This mechanism provides tunable energy transfer rates, low-power input signals and negligible energy loss in the case of negligible intrinsic damping. Coupled vortex-state disks might find applications in future information-signal processing. H. Jung, et al., NPG - Scientific Reports 1 59 (2011); M.-W. Yoo, et al., Phys. Rev. B 82, 174437 (2010); H. Jung, et al., Appl. Phys. Lett. 97, 222502 (2010); Y.-S. Choi, et al., Phys. Rev. B 80, 012402 (2009); P. Fischer, et al., Phys Rev B 83 212402 (2011).

¹Supported by Basic Science Research Program (NRF Korea) No. 20110000441, DOE/BES No. DE-AC02-05-CH1123, DFG/SFB 668 and GK 1286 and City of Hamburg

9:36AM H15.00007 Four-state straintronics: Ultra low-power collective nanomagnetic computing using multiferroics with biaxial anisotropy¹ , NOEL D'SOUZA, JAYASIMHA ATULASIMHA, SUPRIYO BANDYOPADHYAY, Virginia Commonwealth University — Two-phase multiferroic nanomagnets, consisting of elastically coupled magnetostrictive/piezoelectric layers, can be endowed with four stable magnetization states by introducing biaxial magnetocrystalline anisotropy in the magnetostrictive layer. These states can encode four logic bits. We show through extensive modeling that dipole coupling between such 4-state magnets, combined with stress sequences that appropriately modulate the energy barriers between the stable states through magnetoelastic coupling, can be used to realize 4-state NOR logic (J. Phys. D: Appl. Phys. 44, 265001 (2011)) as well as unidirectional propagation of logic bits along a "wire" of nanomagnets (arXiv:1105.1818). As very little energy is consumed to "compute" in such a system, this could emerge as an ultra-efficient computing paradigm with high logic density. We show, by solving the Landau-Lifshitz-Gilbert (LLG) equation, that such nanomagnet arrays can be used for ultrafast image reconstruction and pattern recognition that go beyond simple Boolean logic. The image processing attribute is derived from the thermodynamic evolution in time, without involving any software. This work is supported by the NSF under grant ECCS-1124714 and VCU under PRIP.

¹This work is supported by the NSF under grant ECCS-1124714 and Virginia Commonwealth University under PRIP.

9:48AM H15.00008 GMAG Dissertation Award Talk: All Spin Logic – Multimagnet Networks interacting via Spin currents¹ , SRIKANT SRINIVASAN, School of Electrical and Computer Engineering, Purdue University — Digital logic circuits have traditionally been based on storing information as charge on capacitors, and the stored information is transferred by controlling the flow of charge. However, electrons carry both charge and spin, the latter being responsible for magnetic phenomena. In the last few decades, there has been a significant improvement in our ability to control spins and their interaction with magnets. All Spin Logic (ASL) represents a new approach to information processing where spins and magnets now mirror the roles of charges and capacitors in conventional logic circuits. In this talk I first present a model [1] that couples non-collinear spin transport with magnet-dynamics to predict the switching behavior of the basic ASL device. This model is based on established physics and is benchmarked against available experimental data that demonstrate spin-torque switching in lateral structures. Next, the model is extended to simulate multi-magnet networks coupled with spin transport channels. The simulations suggest ASL devices have the essential characteristics for building logic circuits. In particular, (1) the example of an ASL ring oscillator [2, 3] is used to provide a clear signature of directed information transfer in cascaded ASL devices without the need for external control circuitry and (2) a simulated NAND [4] gate with fan-out of 2 suggests that ASL can implement universal logic and drive subsequent stages. Finally I will discuss how ASL based circuits could also have potential use in the design of neuromorphic circuits suitable for hybrid analog/digital information processing because of the natural mapping of ASL devices to neurons [4].

[1] B. Behin-Aein, A. Sarkar, S. Srinivasan, and S. Datta, "Switching Energy-Delay of All-Spin Logic devices," *Appl. Phys. Lett.*, 98, 123510 (2011).

[2] S. Srinivasan, A. Sarkar, B. Behin-Aein, and S. Datta, "All Spin Logic Device with Inbuilt Non-reciprocity," *IEEE Trans. Magn.*, 47, 10 (2011).

[3] S. Srinivasan, A. Sarkar, B. Behin-Aein and S. Datta, "Unidirectional Information transfer with cascaded All Spin Logic devices: A Ring Oscillator," *IEEE Device Research Conference* (2011).

[4] A. Sarkar, S. Srinivasan, B. Behin-Aein and S. Datta, "Multimagnet networks interacting via spin currents" *IEEE International Electron Devices Meeting* 2011. (to appear).

¹This work was supported by the Nanoelectronics Research Initiative (NRI-INDEX) under theme 1463.008. Collaborators: A. Sarkar, Dr. B. Behin-Aein and Prof. S. Datta, Purdue University.

10:24AM H15.00009 "Spin inverter" as building block of All Spin Logic devices¹ , ANGK SARKAR, SRIKANT SRINIVASAN, SUPRIYO DATTA, School of Electrical and Computer Engineering, Purdue University, W. Lafayette, IN, USA — All-spin logic (ASL) represents a new approach to information processing where the roles of charges and capacitors in charge based transistors are played by spins and magnets, without the need for repeated spin-charge conversion. In our past work, we have presented numerical simulations based on a coupled spin transport and Landau Lifshitz Gilbert model showing that ring oscillators and logic circuits with intrinsic directionality [IEEE Trans. Magn. 47,10, 4026, 2011; Proc. IEDM, 2011]] can be implemented by manipulation of spins in magnetic nanostructures. The aim of this talk is (1) to identify a basic ASL unit that can be interconnected to build up spin circuits analogous to the way transistors are interconnected to build conventional circuits and (2) to present a compact model for this basic unit that can be used to design and analyze large scale spin circuits. We will show that this basic ASL unit is a one-magnet "spin inverter" with gain that can be cascaded to accomplish a spin circuit implementation of almost any logic functionality

¹Supported by INDEX, NRI and NSF Centre for Science of Information.

10:36AM H15.00010 Ultra low-power straintronics with multiferroic nanomagnets: magnetization dynamics, universal logic gates and associated energy dissipation, MOHAMMAD SALEHI-FASHAMI, JAYASIMHA ATULASIMHA, SUPRIYO BANDYOPADHYAY, Virginia Commonwealth University — Stress induced magnetization dynamics of dipole coupled multiferroic nanomagnet arrays is modeled by solving the Landau-Lifshitz-Gilbert (LLG) equation. We show that in such multiferroic nanomagnets, consisting of magnetostrictive layers elastically coupled to piezoelectric layers, the single domain magnetization can be rotated by a large angle ($\sim 90^\circ$) in ~ 1 ns if a tiny voltage of a few tens of millivolts is applied across the piezoelectric layer [Nanotechnology, 22, 155201, 2011, Appl. Phys. Lett. 99, 063108, 2011]. Arrays of such multiferroic nanomagnets can be laid out in specific geometric patterns to implement combinational and sequential logic circuits by exploiting inter-magnet dipole coupling and Bennett clocked with specific stress cycles to propagate logic bits and implement dynamic logic. In this work, we theoretically demonstrate logic propagation in and fan-out characteristics of a universal NAND gate and discuss energy dissipation in the magnet and in the external clock. We show that this energy dissipation can be 3 orders of magnitude more energy-efficient than current CMOS technology for a reasonable clock speed of 1 GHz. This work is supported by the NSF under grant ECCS-1124714.

10:48AM H15.00011 Hybrid spintronics and straintronics: A paradigm for ultra-low-energy computing¹, KUNTAL ROY, SUPRIYO BANDYOPADHYAY, Electrical and Computer Engg., Virginia Commonwealth University, Richmond, VA 23284, JAYASIMHA ATULASIMHA, Mechanical and Nuclear Engg., Virginia Commonwealth University, Richmond, VA 23284 — We have shown in the past that the magnetization of a two-phase multiferroic single-domain nanomagnet can be electrically switched (flipped) with very little energy dissipation at low temperatures. This heralds a new energy-efficient magnetic logic and memory technology [Appl. Phys. Lett., 99, 063108, 2011, Phys. Rev. B, 83, 224412, 2011, Nanotechnology, 22, 155201, 2011]. Here, we extend our low-temperature result to room temperature where thermal noise can cause switching failures and increase average energy dissipation and switching delay. Using Monte Carlo simulations of switching trajectories described by the stochastic Landau-Lifshitz-Gilbert (LLG) equation, we show that even at room temperature, nearly error-free fast switching is possible with very low dissipation. The energy dissipated to switch an appropriately designed nanomagnet with $> 99.99\%$ probability at room temperature is only ~ 400 kT for a switching delay of sub-nanosecond. This is enabled by the complex interplay between the in-plane and out-of-plane excursions of the magnetization vector which aids switching. This work is supported by the NSF under grant ECCS-1124714.

¹This work is supported by the NSF under grant ECCS-1124714

Tuesday, February 28, 2012 8:00AM - 11:00AM – Session H16 DCMP DAMOP: Quantum Fluids: Mainly Helium, Vortices, and Solitons 251

8:00AM H16.00001 Weak to strong limits in confined superfluid helium¹, STEPHEN R.D. THOMSON, JUSTIN K. PERRON, FRANCIS M. GASPARINI, The State University of New York University at Buffalo — Experiments with ^4He confined in $(2\ \mu\text{m})^3$ boxes connected via a thin film 33 nm thick have shown that the boxes act as isolated entities when spaced $4\ \mu\text{m}$ edge-to-edge [1], whereas when spaced $2\ \mu\text{m}$ edge-to-edge, they are strongly coupled to each other [2]. To investigate the spatial dependence of this coupling we are currently measuring $(2\ \mu\text{m})^3$ boxes spaced $1\ \mu\text{m}$ edge-to-edge. We report measurements of the specific heat and superfluid density of helium confined in this geometry. These new data will help us to map the transition between fully isolated to fully coupled boxes which, in this limit, should behave like a $2\ \mu\text{m}$ thick film. Questions involving our understanding of the correlation length ξ arise, since it is observed that coupling is manifest over much larger distances than ξ .

[1] Perron J K, Kimball M O, Mooney K P and Gasparini F M 2010 *Nat. Phys.* **6** 499–502

[2] Perron J K, and Gasparini F M 2011 *submitted to PNAS*

¹This work was supported by the NSF grants DMR-0605716 and DMR-1101189 and utilized The Cornell Nanoscale Science and Technology Facility.

8:12AM H16.00002 Critical point coupling in liquid helium and the significance of the correlation length¹, JUSTIN K. PERRON, STEPHEN R.D. THOMSON, FRANCIS M. GASPARINI, The State University of New York, University at Buffalo — Recent measurements of liquid helium confined to $(2\ \mu\text{m})^3$ boxes connected through a 33 nm film have shown coupling effects between boxes spaced distances much larger than the correlation length $\xi(t, L)$ [1,2] and proximity effects on the connecting film [3]. An analysis of data suggests that $\xi(t, L)$ is the relevant parameter in these effects. This dependence on $\xi(t, L)$ is used to argue that the enhancement in the specific heat due to coupling is a reflection of the finite-size correlation length in the boxes and hence its scaling function. All this raises some profound questions about our physical understanding of $\xi(t, L)$.

[1] Perron J K, Kimball M O, Mooney K P and Gasparini F M 2010 *Nat. Phys.* **6** 499–502

[2] Perron J K, and Gasparini F M 2011 *submitted to PNAS*

[3] Perron J K, and Gasparini F M 2011 to be published in *JPCS*

¹This work was supported by the NSF grants DMR-0605716 and DMR-1101189; The Cornell Nanoscale Science and Technology Facility; The Mark Diamond Research Fund of the GSA at the University at Buffalo, and internal funding from the University at Buffalo.

8:24AM H16.00003 Creating Only Isotropic Homogeneous Turbulence in Liquid Helium near Absolute Zero¹, G.G. IHAS, K.J. THOMPSON, G. LABBE, Department of Physics, University of Florida, PO Box 118440, Gainesville, FL 32607, P.V.E. MCCLINTOCK, Department of Physics, Lancaster University, Lancaster LA1 4YB, UK — Flow through a grid is a standard method to produce isotropic, homogeneous turbulence for laboratory study. This technique has been used to generate quantum turbulence (QT) above 1 K in superfluid helium² where QT seems to mimic classical turbulence. Efforts have been made recently³ to make similar measurements near absolute zero, where there is an almost total absence of normal fluid and hence classical viscosity. This presents the difficulty that most motive force devices produce heat which overwhelms the phenomena being investigated. The process of designing and implementing a “dissipation-free” motor for pulling a grid through superfluid helium at millikelvin temperatures has resulted in the development of new techniques which have broad application in low temperature research. Some of these, such as Meissner-affect magnetic drives, capacitive and inductive position sensors, and magnetic centering devices will be described. Heating results for devices which can move in a controlled fashion from very low speed up to 10 cm/s will be presented. Acknowledgement: We thank W.F. Vinen for many useful discussions.

¹Work supported in part by US NSF DMR#0602778 and #1007937.

²S. R. Stalp, L. Skrbek, and R. J. Donnelly, *Phys. Rev. Lett.* **82**, 4831 (1999).

³G. G. Ihas, G. Labbe, S-c. Liu, and K. J. Thompson, *J. Low Temp. Phys.* **150**, 384 (2008).

8:36AM H16.00004 Superfluid Onset and 2D phase transitions of Helium-4 on Lithium and Sodium, ANGEL VELASCO, FAWN HUISMAN, University of California, Irvine, ELI VAN CLEVE, Lawrence Livermore National Laboratory, PETER TABOREK, University of California, Irvine — We have fabricated lithium and sodium films on quartz crystal microbalances (QCM) using in situ low temperature pulsed laser deposition. The frequency shift and dissipation of the QCM was measured as a function of helium pressure and chemical potential and used to construct the phase diagram of helium films on these substrates. Pressure measurement techniques based on an RGA mass spectrometer, which provides accurate measurement below 10^{-8} Torr will be described. Lithium and sodium are predicted to be intermediate strength substrates which are strong enough to be wetted by He-4 but weak enough that solid-like layers do not form, so they are candidates for observing sub-monolayer superfluidity in direct contact with a metallic surface. Helium adsorption isotherms and quenches between 0.5K and 1.6K on both lithium and sodium indicated continuous, sub-monolayer helium film growth and superfluid onsets in sub-monolayer films. Features below 1K indicate a collision between a classical 2D liquid/vapor phase transition and the Kosterlitz-Thouless superfluid phase transition. We see no evidence for the pre-wetting step instability predicted for helium on sodium.

8:48AM H16.00005 ABSTRACT WITHDRAWN —

9:00AM H16.00006 Discrepancies Between Theory and Experiment for Field-Dependence and f -wave Interactions in Superfluid $^3\text{He-B}$, C.A. COLLETT, J. POLLANEN, JIA LI, W.J. GANNON, W.P. HALPERIN, Department of Physics and Astronomy, Northwestern University — We have performed transverse acoustics experiments in superfluid $^3\text{He-B}$, exploring the magnetic field splitting of the imaginary squashing mode (ISQ), a collective mode of the order parameter labelled by its total angular momentum $J = 2$. We have compared theoretical calculations¹ of the Zeeman splitting, g_2 , and its dependence on the strength of f -wave pairing interactions, x_3^{-1} , with our recent experimental data, showing unexpected discrepancies. We suggest that the origin of these discrepancies can be traced to limits on the applicability of the theoretical calculations at high magnetic field and at frequencies some distance from the order parameter collective mode. We discuss the analysis done by Davis *et al.* in light of those limitations.² This work was supported by the National Science Foundation DMR-1103625.

¹J.A. Sauls and J.W. Serene, Phys. Rev. Lett. **49**, 1183 (1982).

²J.P. Davis *et al.*, Phys. Rev. Lett. **100**, 015301 (2008).

9:12AM H16.00007 Role of the order parameter manifold on surface Majorana fermions and spin susceptibility of superfluid $^3\text{He-B}$, TAKESHI MIZUSHIMA, Dept. of Phys., Okayama University, MASATOSHI SATO, ISSP, The University of Tokyo, KAZUSHIGE MACHIDA, Dept. of Phys., Okayama University — Here, we theoretically investigate surface Andreev bound states (SABS) in superfluid $^3\text{He-B}$ confined to a slab geometry. It is known that the Majorana property gives rise to the Ising anisotropy of spin susceptibility on the surface, which reflects the assumption that the order parameter manifold of the B-phase is restricted to the subspace. In this talk, we first demonstrate that the $\text{SO}(3)$ manifold, which describes the relative rotation of spin and orbital, plays a critical role on the various properties associated with the SABS, such as the Majorana nature, gapless dispersion, topological invariant, and spin susceptibility. Then, based on the quasiclassical Eilenberger theory which takes account of the dipole interaction, we quantitatively discuss thermodynamics and the Majorana property of the SABS in superfluid $^3\text{He-B}$ under a magnetic field, where the Majorana property and spin susceptibility is determined by the interplay of the magnetic field and dipole interaction.

9:24AM H16.00008 Macroscopic quantum tunneling of a single vortex in a rotating Bose-Einstein condensate¹, KINJAL DASBISWAS, ALAN T. DORSEY, Department of Physics, University of Florida — A vortex can be created in a metastable state near the center of a harmonically trapped Bose condensate when it is rotated with suitable velocities. This state has a finite lifetime before which the vortex tunnels outwards to the edge of the trap. We estimate this tunneling rate semiclassically with the vortex treated as a point particle. This is followed by a more exact treatment incorporating the dynamics and mass of the vortex. The calculation is based on a Thomas-Fermi approximation, relevant to the typically large atomic densities used in experiments, but we also analyze the low density limit in a “weakly nonlinear” perturbative framework. We discuss the feasibility of detecting this effect with currently achievable experiments.

¹This work is supported by the NSF

9:36AM H16.00009 Expansion Dynamics of a Ring Bose-Einstein Condensate¹, MARK EDWARDS, Georgia Southern University and NIST, HADAYAT SEDDIQI, MICHAEL KRYGIER, BRANDON BENTON, Georgia Southern University, CHARLES CLARK, Joint Quantum Institute and NIST — We studied the dynamics of BECs when released from a ring trap under conditions similar to those that obtained in a recent experiment done at NIST. In that experiment a ring-shaped BEC was formed in an all-optical trap created by intersecting a horizontal light sheet and a vertical Laguerre-Gaussian beam. Condensates were created in these traps and then “stirred” by applying Raman pulses having orbital angular momentum (OAM). We modeled the dynamics of condensates formed under these conditions by first solving the 2D time-dependent Gross-Pitaevskii equation (GPE) in imaginary time to obtain the initial condensate shape. We accounted for the OAM by applying a phase imprint to this wave function and then propagated it using the GPE in real time with the trap off. We found that, after release, the condensate expands both inward and outward. When no OAM was applied, this inward expansion causes the hole in the ring to close up entirely in turn causing a buildup of atom density there. Inflow and outflow of atoms from the center caused expanding interference rings to form. With non-zero applied initial OAM similar behavior was observed except that the central hole never closes with hole size increasing with increasing initial OAM. We compare our results with the NIST experiment.

¹Work supported by NSF grant numbers PHY-0758111 and PHY-1068761

9:48AM H16.00010 Quantum Dynamics of a Bose Superfluid Vortex¹, LARA THOMPSON, Massachusetts Institute of Technology, PHILIP STAMP, University of British Columbia, Pacific Institute of Theoretical Physics — Quantum vortex dynamics remain poorly understood despite decades of theoretical investigation. The vortex is a topological soliton, arising from the same medium as the quasiparticles with which it interacts. Hence the coupling between the vortex “zero mode” and the quasiparticles has no term linear in the quasiparticle variables – the lowest order coupling is quadratic. We present a fully quantum-mechanical derivation of the vortex equation of motion valid at low temperatures where the normal fluid density is small. The resulting equation of motion is naturally expressed as a function of the dimensionless frequency $\tilde{\Omega} = \hbar\Omega/k_B T$. The usual Hall-Vinen/Iordanskii equations are valid when $\tilde{\Omega} \ll 1$ (the “classical regime”), but elsewhere, the equations are strongly memory dependent. We will discuss the experimental implications of this frequency dependence in Bose superfluids and cold atomic gases.

¹This work was supported by NSERC, CIFAR, PITP, and by a Killam fellowship.

10:00AM H16.00011 Fragmented Many-Body states of definite angular momentum and stability of attractive 3D Condensates , MARIOS C. TSATSOS, ALEXEJ I. STRELTISOV, OFIR E. ALON, LORENZ S. CEDERBAUM, Heidelberg University — We consider a 3D Bose-Einstein Condensate (BEC), with attractive interparticle interactions, embedded in a harmonic, spherically symmetric trap. This system is metastable only if the total number of bosons N and the interaction strength λa_0 do not exceed some critical values. Otherwise the system collapses. Gross-Pitaevskii (GP) theory predicts the maximum (critical) number of bosons N_{cr}^{GP} that, for a given λ_0 , can be loaded to the system, without its collapse. But, what happens to the excited states? To investigate the structure and stability of these states we must go beyond GP theory; these states have definite values of angular momentum (AM) L , are highly fragmented and can support number of bosons much greater than N_{cr}^{GP} . Secondly, we investigate the impact of external rotation of the trap to the AM and stability of the gas. We find that, for all allowed values of rotation frequency no significant stabilization occurs. The symmetry of the ground state does not change and no AM is transferred to the gas. This behaviour is attributed to the attractive nature of the interparticle interaction.

10:12AM H16.00012 Origins of bright soliton transparency to Bogoliubov quasi-particles¹ , ZAIJONG HWANG, MAXIM OLSHANII, University of Massachusetts Boston — Bogoliubov quasi-particles can pass through a one-dimensional bright soliton without reflection at all energies.² Reflectionless properties of this kind usually originate from a supersymmetric structure of the corresponding Hamiltonian.^{3,4} However, we give a strong indication that in this case¹, the mathematical mechanism enabling full spectrum transparency of a scattering object does not fall into any of the conventional paradigms.

¹Supported by NSF, ONR, and IFRAF

²D. J. Kaup, Phys. Rev. A **42**, 5689 (1990).

³E. Witten, Nucl. Phys. B **188**, 513 (1981).

⁴C. V. Sukumar, J. Phys. A **18**, 2917 (1985).

10:24AM H16.00013 Supersymmetric Structure of two Families of Solitons¹ , ANDREW KOLLER, MAXIM OLSHANII, University of Massachusetts Boston — Solitons have generated considerable interest in the cold atoms and condensed matter communities. We demonstrate that two families of n -soliton solutions (with n an integer) – one for the attractive nonlinear Schrödinger (NLS) equation, and one for the sine-Gordon (sG) equation – originate from a quantum-mechanical supersymmetric (QM-SUSY) chain connecting a set of reflectionless operators $\hat{H}_n$. The families consist of breather-type solitons for NLS² and multi-(anti)kink solitons with specific velocities for sG. The operators $\hat{H}_n$, which we refer to as Akulin's Hamiltonians³, form reflectionless direct-scattering initial conditions for the inverse scattering method. Such a QM-SUSY chain is analogous to the known connection between QM-SUSY chains of Pöschl-Teller potentials and solitons of the Korteweg-de Vries (KdV) equation⁴. The existence of QM-SUSY chains connecting soliton solutions, now for three different integrable nonlinear equations, sheds light on the underlying mechanisms responsible for soliton generation.

¹supported by NSF and ONR

²D. Schrader, IEEE J. Quantum Electron. **31**, 2221 (1995).

³V. M. Akulin, Coherent Dynamics of Complex Quantum Systems (Springer, Heidelberg, 2006).

⁴Sukumar, J. Phys. A **19**, 2297 (1986)

10:36AM H16.00014 From Dark Solitons to Vortex Clusters in Bose-Einstein Condensates , PANAYOTIS KEVREKIDIS, University of Massachusetts, Amherst — In this talk, we'll start by considering the experimental, theoretical and numerical dynamical properties of dark solitons in quasi-one-dimensional trapped Bose-Einstein condensates. We will identify the oscillations and interactions of such coherent structures and we will then aim towards generalizing the corresponding notions to quasi-two-dimensional vortex states. In the latter setting, we will use two approaches: one from the linear limit of the underlying system that will permit us to identify the bifurcations of multi-vortex cluster states, while the second in the large density limit will enable our consideration of the vortices as precessing and interacting particles within the condensate. We will corroborate our analytical predictions within these limits and numerical results bridging the limits with experimental observations for the dynamics of few-vortex clusters.

10:48AM H16.00015 Multifractals in Soliton sea on Fibonacci Lattice¹ , MASAHIRO TAKAHASHI, HOSHO KATSURA, Department of Physics, Gakushuin University, MAHITO KOHMOTO, The Institute for Solid State Physics, The University of Tokyo, TOHRU KOMA, Department of Physics, Gakushuin University — Systems exhibiting Bose-Einstein condensation are suitable for fabricating artificially designed structures, e.g., the bichromatic potentials have attracted much attention. More exotic structures also appear to be experimentally feasible in the optical imaging system with high resolution. We consider one of exotic structures, Fibonacci potential, which is quasiperiodic. On the Fibonacci potential without nonlinear interaction, it is known that the spectrum is singular continuous and all the eigenvectors are called a critical state, in which multifractal states are included. On the other hand, the physical properties of the Bose-Einstein condensates confined in a optical lattice can be described in terms of the Schrödinger equation with nonlinear term via particle-particle interactions. We numerically and mathematically investigated nonlinear Schrödinger equation on Fibonacci potential focusing on the competition between nonlinear fluctuation and criticality [M. Takahashi *et al.*, arXiv:1110.6328]. The conclusion is that the critical states with the spectrum in the Cantor set retains their profile irrespective of the strength of the nonlinearity. The spectrum for the critical states is in a sea of "stationary solitons" which appear as a result of nonlinear effects.

¹This work was supported by Grant-in-Aid for Research Activity Start-up (23840034) and Grant-in-Aid for Young Scientists (B) (23740298).

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H17 DMP GERA FIAP: Focus Session: Thermoelectrics - Characterization/Molecular junctions/Magnetic and Low Temp 252A

8:00AM H17.00001 Strategies for developing optimal thermoelectric metrology protocols , JOSHUA MARTIN, National Institute of Standards and Technology — The Seebeck coefficient is an essential physical property routinely measured to evaluate the potential performance of new thermoelectric materials. These materials facilitate the inter-conversion of thermal and electrical energy and are useful in power generation or solid-state refrigeration applications. However, the diversity in Seebeck coefficient measurement techniques, conditions, and probe arrangements has resulted in conflicting materials data, further complicating the inter-laboratory confirmation of reported higher efficiency thermoelectric materials. In an effort to identify optimal thermoelectric measurement protocols, we have developed a complimentary strategy to both evaluate and compare these different probe arrangements and measurement methodologies: first, through the design of an innovative experimental apparatus, and second, through error modeling of Seebeck coefficient measurements using finite element analysis. This talk will include a discussion of key measurement challenges, example diagnostics, and recommended practices to effectively manage uncertainty in Seebeck coefficient measurements.

8:12AM H17.00002 Experimental Determination of the Lorenz Number¹, KEVIN LUKAS, WEISHU LIU, ZHIFENG REN, Boston College, GANG CHEN, MIT, CYRIL P. OPEIL, Boston College — In an effort to improve the dimensionless thermoelectric figure of merit (ZT), thermal conductivity reduction is imperative. Most efforts are made to reduce the lattice portion of the thermal conductivity through nanostructuring. However there is no direct way to measure the lattice contribution and typically the lattice thermal conductivity is approximated by various methods. By experimentally determining the Lorenz number, the lattice thermal conductivity can be directly calculated. A method for determining the Lorenz number of thermoelectric materials $\text{Bi}_2\text{Te}_{2.7}\text{Se}_{0.3}$ and $\text{Bi}_{0.88}\text{Sb}_{0.12}$ will be presented.

¹s3tec Center

8:24AM H17.00003 Anisotropic Two-band Transverse Thermoelectrics in Zero Magnetic Field, CHUANLE ZHOU, Y. TANG, K. HEINSELMANN, M. GRAYSON, EECS Dept., Northwestern University, S. BIRNER, Walter Schottky Institut, Tech. Univ. Munchen — Narrow gap materials with anisotropic electron and hole band conductance are shown to function as anisotropic two-band transverse (A2T) thermoelectrics, whereby longitudinal electrical currents generate transverse Peltier heat flow. Unlike the Ettingshausen effect which requires external magnetic field, a large transverse Seebeck coefficient in A2T thermoelectric results from the anisotropic electron and hole mass tensors without magnetic field. Compared to synthetic transverse thermoelectrics, A2T thermoelectric coolers can be scaled to nanoscale, and the intrinsic nature of this phenomenon is promising for cryogenic applications. With exponentially tapered coolers, arbitrary ΔT can be reached with sufficiently thick layers and a small electric field. Equations for A2T thermoelectric transport from an electron-hole band model yield the optimal orientation to achieve maximum transverse figure of merit $Z_{\perp}T$. The InAs/GaSb type II superlattice is shown to have the appropriate anisotropic band structure, and bandgaps of order kT are calculated to give a competitive $\Delta T = 14$ K at room temperature. Thermal conductivity of the superlattice is 4 W/m-K at 300 K using 3ω method. Preliminary data on in-plane Seebeck coefficient will also be presented.

8:36AM H17.00004 Magnetotransport in thermoelectric materials.¹, MONA ZEBARJADI, MIT, KEVIN LUKAS, CYRIL OPEIL, Boston College, GANG CHEN, MILDRED DRESSELHAUS, MIT, S3TEC TEAM² — The mechanisms behind the magnetic field and temperature dependent thermoelectric effects that have recently been found experimentally in the electrical resistivity, thermopower and thermal conductivity of nanocomposite samples of Bi_2Te_3 and related compounds is studied. Large deviations in the transport coefficients in the presence of an applied magnetic field, both when the magnetic field is parallel and perpendicular to the transport direction has been observed in Bi_2Te_3 compounds, despite the small electronic mean free paths in these materials. An accurate analysis of the experimentally measured data leads to the estimation of electron mean free path and extraction of lattice thermal conductivity contribution from the total thermal conductivity. We will apply a Boltzmann transport equation based formalism to analyze the experimental data and improve the accuracy of the estimation of electronic and lattice part of the thermal conductivity. A particular attention will be paid to the analysis of the anisotropic effects in these samples.

¹This article is based upon work supported as part of the MIT S3TEC, an Energy Frontier Research Center funded by the U.S. Department of Energy

²an Energy Frontier Research Center funded by the U.S. Department of Energy

8:48AM H17.00005 Separation of Joule Heating and Peltier Cooling via Time-Resolved X-Ray Diffraction in Si/SiGe Superlattice¹, MICHAEL KOZINA, MATTHIAS FUCHS, JIAN CHEN, MASON JIANG, Stanford University PULSE Institute, PICE CHEN, PAUL EVANS, University of Wisconsin-Madison Department of Materials Science and Engineering, BJORN VERMEERSCH, JE-HYEONG BAHK, ALI SHAKOURI, University of California-Santa Cruz Department of Electrical Engineering, DALE BREWE, Argonne National Lab, DAVID REIS, Stanford University PULSE Institute — We present detailed measurements of the thermal profile in a pulsed current SiGe-based thermoelectric micro-cooler. The evolution of heat flow in thermoelectric materials has been previously studied using time-domain thermoreflectance imaging; however, such methods are typically only sensitive to the surface temperature of the device, and the heat flow into the material remains hidden. Using time-resolved x-ray diffraction, we probe the transient temperature change in both the surface gold electrode and the underlying Si/SiGe superlattice using the shift in diffraction pattern caused by thermal expansion. We are also able to resolve Joule heating vs. Peltier cooling taking place in the gold through separation of timescales made possible by the relatively short duration (100ps) of the Advanced Photon Source.

¹This research is supported in part by the DOE Office of Science Graduate Fellowship Program (DOE SCGF), made possible in part by the American Recovery and Reinvestment Act of 2009, administered by ORISE-ORAU under contract no. DE-AC05-06OR23100.

9:00AM H17.00006 Reassessment of the carrier concentration in GeTe-based thermoelectric materials by ¹²⁵Te NMR, E.M. LEVIN, J.D. ACTON, K. SCHMIDT-ROHR, Ames Laboratory US DOE and Iowa State University — $\text{Ge}_{1-x}\text{Ag}_x/2\text{Sb}_{x/2}\text{Te}$ *p*-type thermoelectric materials ("TAGS-*n*") were studied extensively in the 1970s and then again recently. They exhibit an unusual combination of large thermopower, *S*, and high hole concentration, *p*, reported based on the Hall effect data, which has not been explained. To solve this puzzle, we have synthesized GeTe, GeTe:Bi, and TAGS-*n* with *n*= 97, 94, 90, and 85 and studied XRD, thermopower, electrical resistivity, thermal conductivity, and ¹²⁵Te NMR. Most importantly, we have determined the carrier concentrations using ¹²⁵Te NMR spin-lattice relaxation and Knight shift. In GeTe and GeTe:Bi, we found that carrier concentrations generally agree with the values reported from Hall effect. In TAGS-*n*, they are much lower but agree better with the values expected from *S* vs. *p* for GeTe-based materials, solving the puzzle partially. The NMR vs. Hall effect discrepancy in TAGS-*n* can be due to the presence not only of holes but also electrons generated by Sb atoms, which results in artificially high hole concentration from Hall effect. Even though the true hole concentration is lower than reported, the thermopower of TAGS-*n* is still significantly larger than that of GeTe and GeTe:Bi at similar carrier concentration. This can be explained by energy filtering enhanced by potential barriers formed due to Ag-Sb pairs in the TAGS-*n* lattice.

9:12AM H17.00007 Charge and Energy Transport in Molecular Junctions, PRAMOD REDDY, University of Michigan — Charge and energy transport in molecular junctions, created by trapping short organic molecules (~1nm) between inorganic electrodes, is expected to be fundamentally different from transport in bulk materials due to their discrete electronic structure. In fact, numerous computational studies have suggested that it may be possible to utilize the novel thermoelectric and thermal transport phenomenon in nanoscale molecular junctions to create efficient energy conversion devices (e.g. thermoelectric devices). However, a large number of these effects remain to be experimentally verified. We will describe our experimental studies where thermoelectric properties of junctions were studied at the single/few molecule level enabling novel insights into the relationship between molecular structure and the thermoelectric properties of junctions. We will also present our recent experimental efforts to probe thermal transport in nanoscale molecular junctions and point contacts. In order to accomplish this goal, it is necessary to accurately measure heat currents as small as 10 picowatts. Towards this goal, we will present a novel device developed by us that is capable of resolving heat currents as small as 4 picowatts.

9:48AM H17.00008 The impact of electron-vibration interactions on the thermoelectric efficiency of molecular junctions, BAILEY HSU, JI-WEI JIANG, YU-CHANG CHEN, Department of Electrophysics, National Chiao-Tung University — From first-principles approaches, we investigate the thermoelectric efficiency of a molecular junction where a benzene molecule is connected directly to the platinum electrodes. We calculate thermoelectric figure of merits ZT in the presence of electron-vibration interactions with and without local heating under two scenarios: linear response (zero bias) and finite bias (non-zero bias) regimes. In the linear response regime, ZT saturates around the electrode temperature $T_e = 25$ K in the elastic case, while in the inelastic case we observe a non-saturated and a much larger ZT beyond $T_e = 25$ K attributed to the tail of the Fermi-Dirac distribution. In the finite bias regime, the inelastic effects reveal the signatures of the molecular vibrations in the low temperature regime. The normal modes exhibiting structures in the inelastic profile are characterized by large components of atomic vibrations along the current density direction on top of each individual atom. In all cases, the inclusion of local heating leads to a higher wire temperature T_w and thus magnifies further the influence of the electron-vibration interactions due to the increased number of local phonons.

10:00AM H17.00009 Interfacial Interactions in Polymer-Nanocrystal Thermoelectric Composites Provide a Novel Route for Power Factor Enhancement, NELSON E. COATES, Lawrence Berkeley National Laboratory, SHANNON K. YEE, Mechanical Engineering, University of California, Berkeley, BORIS RUSS, Department of Chemical and Biomolecular Engineering, University of California, Berkeley, JEFFREY J. URBAN, Lawrence Berkeley National Laboratory, RACHEL A. SEGALMAN, Department of Chemical and Biomolecular Engineering, University of California, Berkeley — The highest performing thermoelectric materials currently available are fabricated via expensive high-temperature vacuum processing techniques. Recently, there has been an increasing interest in the thermoelectric properties of solution-processable materials, which have the potential to dramatically reduce module fabrication costs. These solution-processed materials however often exhibit poor transport properties, which undermines their competitive advantage over the more traditional expensive thermoelectric materials. Here, we present the thermoelectric transport properties of a new class of solution-processable conducting-polymer/inorganic composite materials as a function of nanocrystal loading. In the Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) and Tellurium nanowire composite devices fabricated for this study, the thermoelectric performance of the composite exceeds that of either pure organic or inorganic component alone. This result suggests an interface-driven mechanism for this enhanced performance and provides an exciting route for improving the power factors of organic-inorganic hybrid thermoelectrics.

10:12AM H17.00010 Nernst-Ettingshausen Effect in Elemental Rare-Earth Single Crystals¹, AUDREY CHAMOIRE, JOSEPH HEREMANS, The Ohio State University, THERMAL MATERIALS LABORATORY TEAM — The transverse Nernst-Ettingshausen (N-E) coefficient N measurements of the elemental rare-earth (R-E) single-crystal are for the first time presented from 80 to 420 K. Since they have mainly hexagonal symmetry at room temperature, measurements are given with the heat flux along the [100] and the [001] axes. Due to their complex band structure and Fermi surface, their small thermopower (S) and their multicarrier systems involving electron (e) and hole (h) pockets, their N are expected to be large. Indeed, for such systems, both S and N can be expressed as¹ $S = (S_e\sigma_e + S_h\sigma_h)/(\sigma_e + \sigma_h)$ while $N = [(N_e\sigma_e + N_h\sigma_h)/(\sigma_e + \sigma_h) + (S_h - S_e)(R_Hh\sigma_h - R_He\sigma_e)\sigma_e\sigma_h]/(\sigma_e + \sigma_h)^2$, where σ is the electrical conductivity and R_H the Hall coefficient and the subscript correspond to either carriers. Since $S_h > 0$ and $S_e < 0$, the resulting S should be low thus leading to a large N . These solids are useful in single-material thermoelectric N-E coolers. They create a large temperature differences using thermomagnetic effects, without having to be cascaded. This would resolve the problem of contact resistances of actual multi-stage Peltier coolers, especially in the cryogenic temperature range. The dimensionless figure of merit of N-E coolers is $zT_N = B^2 N^2 \sigma(B) T / \kappa(B)$, with B is the magnetic field, T the absolute temperature and κ the thermal conductivity. a.E.H. Putley, *The Hall Effect and Semiconductor Physics*, New York: Dover publication, 1968.

¹Work supported by DOE-BES Energy Frontier Research Center on Revolutionary Materials for Solid State Energy Conversion, 61-3212B

10:24AM H17.00011 Giant Bipolar Nernst Effect in the Quasi-One-Dimensional Metal, $\text{Li}_{0.9}\text{Mo}_6\text{O}_{17}$, JOSHUA L. COHN, University of Miami, BENJAMIN D. WHITE, Montana State University, CARLOS A. M. DOS SANTOS, Escola de Engenharia de Lorena - USP, Brazil, JOHN J. NEUMEIER, Montana State University — The Nernst coefficient for the quasi-one-dimensional metal, $\text{Li}_{0.9}\text{Mo}_6\text{O}_{17}$, is found to be among the largest known for metals ($\nu \simeq 500 \mu\text{V/KT}$ at $T \sim 20$ K), and is enhanced in a broad range of temperature by orders of magnitude over the value expected from Boltzmann theory for carrier diffusion. A comparatively small Seebeck coefficient implies that $\text{Li}_{0.9}\text{Mo}_6\text{O}_{17}$ is bipolar with large, partial Seebeck coefficients of opposite sign. A very large thermomagnetic figure of merit, $ZT \sim 0.5$, is found at high field in the range $T \approx 35 - 50$ K.

¹This material is based upon work supported by an award from Research Corporation (Univ. Miami), the National Science Foundation under grant DMR-0907036 (Mont. St. Univ.), and in Lorena by the CNPq (301334/2007-2) and FAPESP (2009/14524-6).

10:36AM H17.00012 Cryogenic Thermoelectric Properties of the Bismuth-Magnesium and Bismuth-Antimony-Magnesium Systems¹, CHRISTINE OROVETS, HYUNGYU JIN, Department of Mechanical and Aerospace Engineering, The Ohio State University, BARTLOMIEJ WIENDLOCHA, AGH University of Science and Technology, Krakow, Poland, JOSEPH P. HEREMANS, Department of Mechanical and Aerospace Engineering, The Ohio State University — There is a need to increase the Figure of Merit of thermoelectric materials used in low temperature cooling applications. Band structure calculations show that substitutional magnesium in bismuth can form sharp density of states peaks, suggesting the presence of a resonant level. Single crystal samples of $(\text{Bi}_{1-x}\text{Sb}_x)_{1-y}\text{Mg}_y$ ($0 \leq x \leq 12\%$ and $0 \leq y \leq 0.7\%$ nominally) were synthesized in evacuated ampoules. The composition of each ingot was analyzed using x-ray diffraction, and transport properties were measured using a Thermal Transport Option (TTO) in a Physical Properties Measurement System (PPMS) from 300K to 2K. It is apparent that the addition of magnesium strongly influences thermopower; the data for $\text{Bi}_{90}\text{Sb}_{10}\text{Mg}_{0.7}$ shows a second minimum in thermopower at 20K, in addition to the expected minimum at approximately 50-60K. This could be due to the resonant scattering at the cryogenic temperatures which arises from the excess density of states. The addition of magnesium also appears to decrease thermal conductivity below 30K. We present systematic experimental approaches and the results to elucidate the role of magnesium in bismuth and bismuth-antimony systems.

¹Work supported by AFOSR MURI "Cryogenic Peltier Cooling," contract FA9550-10-1-0533

10:48AM H17.00013 Low Temperature Electronic and Magnetic Properties of CePd_3M_x ¹, STEPHEN BOONA, DONALD MORELLI, Department of Chemical Engineering and Materials Science, Michigan State University — The intermediate valence compound CePd_3 is a strong candidate for low temperature thermoelectric applications due to its unusually large Seebeck coefficient which peaks at approximately $115 \mu\text{V/K}$ near 125K. This phenomenon results from a sharp peak in the density of states near the Fermi level due to the hybridization of conduction electrons with those in the partially occupied cerium f-shell, thus making the system highly sensitive to changes in the average cerium valence state. We have systematically studied the structural and thermoelectric properties of various CePd_3M_x compounds, where M is an s- or p-block element and $0 < x < 0.1$, in order to explore the effects of such partial filling on the cerium valence. The results of X-ray diffraction, Seebeck coefficient, and magnetic susceptibility measurements are reported. We have found that incorporating M elements of various valence configurations has similar effects on the electronic and magnetic properties as changing the M concentration, thus establishing an effective new mechanism for tailoring the thermoelectric properties of the system.

¹Work partially supported by AFOSR-MURI Cryogenic Peltier Cooling Contract FA9550-10-1-0533.

Tuesday, February 28, 2012 8:00AM - 11:00AM –

Session H18 DMP: Focus Session: Electron, Ion, and Exciton Transport in Nanostructures - Nanowires and Superlattices 252B

8:00AM H18.00001 Energy Transfer of Excitons and Electron-Hole Plasmas between Quasi-two-dimensional Semiconductor Layers¹, S.K. LYO, University of California, Irvine, CA — We study the energy transfer mechanisms of excitons and electron-hole plasmas between two quasi-two dimensional (2D) semiconductor quantum wells. It is shown that dipolar (i.e., Foerster) energy transition (ET) mechanism dominates at a short distance while photon-mediated ET mechanism plays a more important role for transfer over a long distance. The magnitude and the dependence of the transfer rates of plasmas and excitons on the temperature, the well-to-well distance, and the density are compared for both ET mechanisms. The spatial dependence of the 2D-2D transfer rates will be compared with that of the ET rate between two quantum dots.

¹Supported by U.S./DOE/BES under Contract No. DE-AC04-94AL85000.

8:12AM H18.00002 Charge transport physics of individual PbSe Nanowire field effect transistors¹, SOONG JU OH, DAVID KIM, CHERIE KAGAN, University of Pennsylvania — We report the charge transport properties of individual PbSe nanowire (NW) field-effect transistors (FETs) fabricated from single crystalline, PbSe NWs 10 nm in diameter synthesized by wet-chemical methods. PbSe is a particularly interesting semiconductor to study in one-dimension as the diameter of the NWs is smaller than the electron, hole and exciton Bohr radii, allowing study of strongly quantum confined NWs. We investigate the temperature dependent charge transport properties of ambipolar and reversibly, surface, p-doped PbSe NW FETs. We demonstrate that PbSe NW FETs behave as Schottky Barrier (SB) FETs, in which the off current is limited by the SB height and decreases as temperature decreases, while the on current is achieved by gate thinning and increases as temperature decreases. We calculate the SB heights for electron and hole injection in ambipolar and hole injection in p-type PbSe NW FETs. The hole mobility in surface-doped, p-type FETs is temperature dependent, rising monotonically from 200 cm²/Vs at room temperature to 2000 cm²/Vs at 4.5K, without signatures of impurity scattering which commonly limits carrier mobilities at low temperatures in substitutionally doped NWs.

¹This work is supported by NSF Division of Materials Research (NSF DMR-0805155)

8:24AM H18.00003 Electronic transport in individual, vertical, catalyst free GaN/AlN nanowires, CAMELIA MARGINEAN, SANTINO CARNEVALE, PATRICK PHILLIPS, THOMAS KENT, DENIS PELEKHOV, MICHAEL MILLS, ROBERTO MYERS, The Ohio State University — In the recent years, the advances in the THz technology, for example the development of the quantum cascade laser, promotes the possibility to use resonant tunneling diodes (RTD) to enhance such technologies. Coaxial m-plane AlN/GaN nanowire based resonant tunneling diode structures were formed by plasma assisted molecular beam epitaxy (MBE) using a two-step growth method that allows for control of vertical and lateral growth [1]. They are spontaneously formed MBE nanowires and they are integrated in Si (111). We discuss ongoing work on the electronic transport in these individual, vertical nanowires using two nanoprobe to contact the top of the nanowire and the substrate. The IV characteristics reveal a clear negative differential resistance (NDR) at room temperature (RT). The NDR was observed ~ 4V with a peak-to-valley ratio as high as 10. [1] S.D. Carnevale *et al.*, *Nano Letters*, 11, (2), 2011.

8:36AM H18.00004 Correlated study of individual nanowires with electronic transport and scanning tunneling microscopy, SHENGYONG QIN, TAE-HWAN KIM, Oak Ridge National Laboratory, YANNING ZHANG, University of California, Irvine, HANNO H. WEITERING, The University of Tennessee, Knoxville, CHIH-KANG SHIH, The University of Texas at Austin, WENJIE OUYANG, RUQIAN WU, University of California, Irvine, ARTHUR P. BADDORF, AN-PING LI, Oak Ridge National Laboratory — The electronic conductance in quantum wires is often dictated by quantum instabilities and strong localization at the atomic scale. We present a novel nano-transport technique which combines local nano-contacts and four-probe STM. The approach allows for correlated study of electron transport and scanning tunneling spectroscopy in individual nanowires. We first apply it to the GdSi₂ quantum wires, which show that isolated nanowires exhibit a metal-insulator transition upon cooling, driven by the defect-induced localizations, while wire bundles maintain a robust metallic state, stabilized by interwire electronic coupling. We then demonstrate applications of this transport technique with carbon nanotubes and copper wires in situ. The method bridges the gap between the transport and the local electronic and structural properties down to the atomic scale.

8:48AM H18.00005 The influence of excitonic effects on charge separation at hybrid nanoscale interfaces¹, ZHIGANG WU, HUASHAN LI, MARK LUSK, Colorado School of Mines — Efficient charge separation is critical in nanostructured photovoltaic systems, but the accurate prediction of charge separation rates remains an extremely difficult task. Although considerable progress has been made, reliable theoretical schemes to describe the charge-separation mechanisms and to compute the interfacial charge transfer dynamics have not been fully developed. In this work, we embrace the excitonic effects that are of critical importance in nanoscale geometries to derive a criterion for charge separation at hybrid nanoscale interfaces beyond the traditional quasiparticle energy-level alignment. The approach utilizes calculations from many-body perturbation theory with Green functions to accurately account for self-energy and electron-hole interactions. Four representative interfaces between Si quantum dots and small molecules are considered using this approach, in order to demonstrate that both excitonic and Coulomb stabilization effects are essential for correctly predicting charge separation at nanostructured interfaces. Interestingly, our calculations suggest that preemptory exciton transfer across interfaces only suppresses the subsequent charge separation. We also compute charge separation rates using the Marcus theory and other methods, and their accuracy are

¹This research is supported by the Renewable Energy Materials Research Science and Engineering Center (REMERSEC) funded by NSF.

9:00AM H18.00006 QM/EM simulation of Junctionless FinFET, JIE PENG, LINYI MENG, CHIYUNG YAM, GUANHUA CHEN, Department of Chemistry, University of Hong Kong, Hong Kong, China — We present here the simulations of a junctionless transistor. Its source, channel and drain are embedded in a piece of uniformly doped silicon nanowire. In the earlier stage, it has been designed to be a normally “ON” device. Quite reversely, the first experimentally presented junctionless transistor is in the “OFF” state when the applied gate voltage is absent. Simulations show that the depletion occurs between the nanowire and hetero-doped gate. A “P-N junction” is formed in the junctionless transistor, whose direction is perpendicular to the direction of the current flowing. Our simulation considers the depletion effect in the Quantum mechanical calculation. I-V curves of transistors with the gate doped by the same and different type of dopants have been obtained. The results match the experiments.

9:12AM H18.00007 Tuning the hole mobility in InP semiconductor nanowires¹, MARIAMA REBELLO SOUSA DIAS, UFSCar Ohio University, ADALBERTO PICININ, VICTOR LOPEZ-RICHARD, UFSCar, SERGIO E. ULLOA, Ohio University, LEONARDO K. CASTELANO, JOSÉ PEDRO RINO, GILMAR E. MARQUES, UFSCar — Transport properties of holes in InP nanowires were calculated considering the effect of temperature and the presence of realistic strain fields. The mobility of holes is obtained analytically by considering electron-phonon interaction via deformation potential through longitudinal optical (LO) phonons. Using molecular dynamics with realistic force potentials, we simulate nanowire structures and the associated phonon density of states; the structures show effects of LO phonon energy renormalization due to the reduced dimensionality and variation of the phonon lifetimes important for carrier mobility. Our mobility calculations include heavy and light hole subbands in a Luttinger Hamiltonian formalism and consider how the valence band ground state changes between light- and heavy-hole character, as both the strain field configuration and the nanowire size are changed. Depending on the dimensions and characteristics of the nanowire, we find interesting sudden changes in the mobility, which arise with the onset of a resonance between the LO phonon frequencies and the subband separation between the ground and first hole state. We will present the effect of strains and temperature on this resonant behavior and discuss the consequences for carrier mobility in these systems.

¹Supported by FAPESP, CNPq, NSF.

9:24AM H18.00008 First-principles study on metal-TaO_x-metal heterostructures: response to applied bias voltages¹, SATOSHI WATANABE, TAKUYA MATSUMOTO, ARIHIRO TAWARA, Dept. of Materials Engineering, The Univ. of Tokyo, TINGKUN GU, School of Electrical Engineering, Shandong Univ., TOMOFUMI TADA, Dept. of Materials Engineering, The Univ. of Tokyo — Metal-TaO_x-metal heterostructures are promising as a novel nonvolatile memory device [1]. The formation of conduction paths in the TaO_x layer is responsible for the low resistance state and the switching mechanism is understood as the electrochemical redox reaction involved with the bias-voltage application. However, microscopic details of the conduction path and switching mechanism have not been clarified yet. We examine electronic states, and electron and ion transport in Cu-TaO_x (x~2.5)-Pt(or Cu) heterostructures from first principles, focusing on the response to applied bias voltages. We show that Cu interstitials in crystalline Ta₂O₅ enhances electronic conduction considerably [2], while does not in amorphous one. We also show that the potential change due to the bias application is sensitive to the structure of TaO_x layer and/or metal-TaO_x interface: in some case, the potential change may be very small near the Cu/TaO_x interface in the TaO_x layer so that the bias application hardly change the mobility of Cu ions in this region. These results will be discussed in terms of electronic states. [1] T. Sakamoto et al., APL 91 (2007) 092110; [2] T. K. Gu et al., ACS Nano 4 (2010) 6477.

¹This work was supported by CREST-JST, Low Power Electronics Association and Projects, and Grants-in-Aid by MEXT-Japan.

9:36AM H18.00009 Theory of spatially inhomogeneous Bloch oscillations in semiconductor superlattices¹, LUIS BONILLA, MARIANO ALVARO, MANUEL CARRETERO, Universidad Carlos III de Madrid — In a semiconductor superlattice with long scattering times, damping of Bloch oscillations due to scattering is so small that nonlinearities may compensate it and Bloch oscillations persist even in the hydrodynamic regime. To demonstrate this, we propose a Boltzmann-Poisson transport model of miniband superlattices with inelastic collisions and derive hydrodynamic modulation equations for the electron density, the electric field and the complex amplitude of the Bloch oscillations. For appropriate parameter ranges, we solve numerically these equations and show that there are solutions having the form of stable Bloch oscillations with spatially inhomogeneous field, charge, current density and energy density profiles. These Bloch oscillations disappear as scattering times become sufficiently short. For sufficiently low lattice temperatures, Bloch and Gunn type oscillations mediated by electric field, current and energy domains coexist for a range of voltages. For larger lattice temperatures (300 K), there are only Bloch oscillations with stationary amplitude and electric field profiles.

¹Supported by the Spanish Ministry of Science and Innovation under Grant no. FIS2011-28838-C02-01.

9:48AM H18.00010 Stochastic current switching in semiconductor superlattices: observation of non-exponential kinetics¹, YU. BOMZE, Duke University, H.T. GRAHN, R. HEY, Paul-Drude-Institute, Berlin, Germany, S.W. TEITSWORTH, Duke University — We report the experimental measurement of first-passage-time distributions associated with noise-induced current switching in doped, weakly-coupled GaAs/AlAs superlattices, in a regime of nonlinear electronic transport where the static current-voltage ($I - V$) curves exhibit multiple branches and bistability. For applied voltages near the end of each branch, internal shot noise induces switching of measured current to the next branch with a stochastically varying switching time. Switching time distributions are constructed by carrying out up to 10^5 measurements under identical initial conditions. We have implemented a novel, high bandwidth technique that permits measurement of switching times over very large dynamic range of approximately 10^9 , with measured times ranging from 4 ns to 10 s. For relatively small times ($< 10\mu\text{s}$), the switching time distributions show exponential tails, as expected for activated escape from an initial metastable state. However, at larger times ($> 10\mu\text{s}$), the distributions exhibit approximate power law tails that extend over several decades of time, with additional fine structure. A rate equation model indicates the possible role of multiple, nearly degenerate metastable states in producing the long tail behavior.

¹Supported by NSF grant DMR-0804232

10:00AM H18.00011 Pseudospin Transfer Torques in Semiconductor Electron Bilayers¹, YOUNGSEOK KIM, Department of Electrical and Computer Engineering, University of Illinois, Urbana, IL, 61801, ALLAN H. MACDONALD, Department of Physics, University of Texas at Austin, Austin, Texas 78712, MATTHEW J. GILBERT², Department of Electrical and Computer Engineering, University of Illinois, Urbana, IL, 61801, MATTHEW J. GILBERT GROUP COLLABORATION — We use self-consistent quantum transport theory to investigate the influence of interactions on interlayer transport in semiconductor electron bilayers in the absence of an external magnetic field. We conclude that even though spontaneous pseudospin ferromagnetism does not occur at zero field, interaction-enhanced quasiparticle tunneling does alter the resultant interlayer I-V curves. We find that the system exhibits a critical bias voltage that is similar to that of the pseudospin ferromagnetic system, but whose properties depend heavily on the charge imbalance between the two layers and their relative spatial separation. When the bias voltage exceeds the critical value, interlayer current is gradually dropped due to the charge imbalance between the layers until the transport current no longer reaches steady state values.

¹We acknowledge support for the Center for Scientific Computing from the CNSI, MRL: an NSF MRSEC (DMR-1121053) and NSF CNS-0960316 and Hewlett-Packard. MJG is supported by the Army Research Office (ARO). YK is supported by Fulbright Science and Technology

²Corresponding Author

10:12AM H18.00012 Effects of Fermion Flavor on Excitonic Condensation in Double Layer Systems¹, ZACHARY ESTRADA, Department of Electrical and Computer Engineering, University of Illinois, Urbana IL 61801, JOHN SHUMWAY, Department of Physics, Arizona State University, Tempe, AZ 85287, MATTHEW GILBERT, Department of Electrical and Computer Engineering, University of Illinois, Urbana IL 61801 — We perform fermionic path integral quantum Monte Carlo (PIMC) simulations to study the physical properties of dipolar exciton condensates in symmetric double layer systems. Recently, the role of screening of additional fermion flavors has been a source of contention in exciton condensates. A room temperature superfluid state has been predicted in bilayer graphene assuming that the condensate screens out additional fermion flavors.² On the other hand, large-N calculations have resulted in much weaker screening of fermion flavors and have placed the transition temperature far lower, around one millikelvin.³ We demonstrate the effect of added fermion flavor on the Kosterlitz-Thouless transition temperature (T_{KT}) in symmetric electron-hole bilayers by collecting static and dynamic response functions.⁴ We find that the addition of fermion flavors decreases T_{KT} , however, due to strong exciton binding, the decrease we observe is not as drastic as is predicted in the earlier large-N calculations.

¹This work is funded by the Army Research Office under grant number W911NF0910347

²H. K. Min, R. Bistritzer, J. J. Su and A. H. MacDonald, *Phys. Rev. B* **78**, 121401 (2008)

³M. Y. Kharitonov and K. B. Efetov, *Semicond. Sci. Technol.* **25**, 034004 (2010)

⁴J. Shumway and M. J. Gilbert, *arXiv:1108.6107* (2011)

10:24AM H18.00013 Magnetic-Field Modulated Josephson Oscillations in a Planar Semiconductor Microcavity¹, GUOJUN JIN, CHUANYI ZHANG, Nanjing University — An exciton-polariton Josephson junction in a planar semiconductor microcavity is studied by considering an external magnetic field applied normal to its plane [1]. Theoretical results show that there is a competition between the Zeeman energy and the interactions of exciton polaritons, and a critical magnetic field can be determined. Below the critical magnetic field, there are time-independent extrinsic and intrinsic Josephson currents which manifest the dc Josephson effect; while above the critical magnetic field, the ac Josephson effect occurs with the oscillating extrinsic and intrinsic Josephson currents. The oscillation frequency and oscillation amplitude of the Josephson currents are modulated by the magnetic field, and also the spontaneous polarization separation and the macroscopic quantum self-trapping of condensate can be realized under an appropriate magnetic field. The physical origin behind is exposed and the analogy with the Josephson effect in a conventional superconducting Josephson junction is discussed. It is suggested that magnetic fields can be used to facilitate the experimental investigations of the exciton polaritons Josephson effect in semiconductor microcavities.

[1] Chuanyi Zhang and Guojun Jin, *Phys. Rev. B* **84**, 115324 (2011).

¹This research was supported by the PAPD, NSFC (Nos. 60876065, 11074108) and NBRPC (Nos. 2009CB929504, 2011CB922102).

10:36AM H18.00014 Lagrange formalism of memory circuit elements: classical and quantum formulations, GUY COHEN, Department of Physics, University of California, San Diego, YURIY PERSHIN, Department of Physics and Astronomy and USC Nanocenter, University of South Carolina, MASSIMILIANO DI VENTRA, Department of Physics, University of California, San Diego — The general Lagrange-Euler formalism for the three memory circuit elements, namely the memristor, memcapacitor, and meminductor [1,2] is introduced for circuits with voltage or current sources. In addition, *mutual meminductance*, i.e., mutual inductance with a state depending on the past evolution of the system, is introduced. The Lagrange-Euler formalism for a general circuit network and the corresponding work-energy theorem are also obtained. We provide examples of this formalism applied to specific circuits both in the classical and quantum regimes showing under which conditions the quantum excitations of the memory degrees of freedom can be observed experimentally. Work was supported in part by NSF.

[1] M. Di Ventra, Y. V. Pershin, and L. O. Chua, *Proc. IEEE* **97**, 1717 (2009).

[2] Y.V. Pershin and M. Di Ventra, *Advances in Physics* **60**, 145-227 (2011).

10:48AM H18.00015 Electrolyte Gated Transistors based on Solution Processed Mesoporous Tungsten Trioxide Thin Films, CLARA SANTATO, DILEK ISIK, Ecole Polytechnique Genie Physique, FABIO CICOIRA, Ecole Polytechnique Genie Chimique — Tungsten trioxide (WO₃) is an important material for electrochromic displays, gas sensors, and photoelectrochemical cells. Despite intensive research efforts, the charge transport properties of nanostructured WO₃ films, as well as of other metal oxide films, are still largely undiscovered. Electrolyte gating provides a powerful platform to study the charge transport properties of nanostructured WO₃ films permitting to achieve high charge density regimes. In turn, this opens the possibility to improve the film transport properties for a wide range of applications. Here we report on electrolyte gated transistors making use of WO₃ films as the semiconductor and H₂SO₄(aq) 1M as the gate dielectric. WO₃ films, prepared by sol-gel method, were deposited on source and drain patterned ITO substrates. The liquid electrolyte was confined using a PDMS well. Atomic force microscopy and scanning electron microscopy images show a mesoporous film structure where the electrolyte can easily penetrate. The mesoporous structure permits an efficient electrolyte gating compared to bulk WO₃ films because of the higher surface available for electrical double layers, which are the underpinning of the electrolyte gating. Upon application of gate bias in the 0-1 V range, with an applied drain voltage ranging between 0-1 V, we were able to tune the conductivity in the WO₃ transistor channel: electrolyte gating of the films led to clear transistor behaviour. Electrolyte gating of WO₃ electrochromism is presently under investigation.

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H19 DCMP GMAG: Invited Session: Current-Driven Spin Textures 253AB

8:00AM H19.00001 Doppler velocimetry of a current driven spin helix, LUYI YANG, UC Berkeley and Lawrence Berkeley National Lab — We present direct observation of the translational motion of spin helices in GaAs quantum wells under the influence of applied electric fields. Previously, the lifetime of such helices was observed by time-resolving the amplitude of light diffracted from the periodic spin polarization [1]. This technique cannot be applied to tracking the motion of current-driven spin helices because diffraction amplitude is insensitive to translation of the center of mass of a periodic structure. In this talk, we describe a new experimental technique, Doppler spin velocimetry, capable of resolving displacements of spin polarization at the level of 1 nm on a picosecond time scale [2]. This is accomplished through the use of heterodyne detection to measure the optical phase of the diffracted light. We discuss experiments in which this technique is used to measure the motion of spin helices as a function of temperature, in-plane electric field, and photoinduced spin polarization amplitude. Several striking observations will be reported – for example, the spin helix velocity changes sign as a function of wavevector and is zero at the wavevector that yields the largest spin lifetime. Another important observation is that the velocity of spin polarization packets becomes equal to the drift velocity of the high-mobility electron gas in the limit of small spin helix amplitude. Finally, we show that spin helices continue propagate at the same speed as the Fermi sea even when the electron drift velocity exceeds the Fermi velocity of 10^7 cm-s⁻¹. In collaboration with J. D. Koralek and J. Orenstein, UC Berkeley and LBNL, D. R. Tibbetts, J. L. Reno, and M. P. Lilly, SNL. Supported by DOE under Contract No. DE-AC02-05CH11231 and DE-AC04-94AL85000.

[1] J. D. Koralek et al., "Emergency of the persistent spin helix in semiconductor quantum wells," *Nature* **458**, 610-613 (2009).

[2] L. Yang et al, "Doppler velocimetry of spin propagation in a two-dimensional electron gas," to appear in *Nature Physics*.

8:36AM H19.00002 Experimental studies of skyrmion textures and spin torque effects in chiral magnets, ROBERT RITZ, Technical University Munich, Physics Department E21 — Small angle neutron scattering and measurements of a topological Hall signal identify the formation of skyrmion lattices in the non-centrosymmetric B20 compounds MnSi [1], $\text{Mn}_{1-x}\text{Fe}_x\text{Si}$, $\text{Mn}_{1-x}\text{Co}_x\text{Si}$ and the strongly doped semiconductor $\text{Fe}_{1-x}\text{Co}_x\text{Si}$ [2]. This observation has been confirmed by Lorentz force microscopy in thin samples of $\text{Fe}_{1-x}\text{Co}_x\text{Si}$, FeGe and, most recently, MnSi, where even individual skyrmions have been spotted [3]. Because the skyrmion lattices are exceptionally weakly pinned to the crystal lattice, extreme care has to be exercised when studying the precise intrinsic morphology of related spin textures in bulk samples. As a particularly striking property each skyrmion supports precisely one quantum of emergent magnetic flux. This permits a highly efficient coupling between skyrmions and conduction electrons which results in spin torque effects at ultra-low current densities as seen in small angle neutron scattering [4] and the emergent electric field when the skyrmions move [5].

Work in collaboration with: T. Adams, A. Bauer, B. Binz, P. Böni, G. Brandl, R. A. Duine, K. Everschor, C. Franz, M. Garst, R. Georgii, S. Gottlieb-Schönmeyer, W. Heusler, M. Janoschek, F. Jonietz, T. Keller, K. Mittermüller, S. Mühlbauer, W. Münzer, A. Neubauer, P.G. Niklowitz, C. Pfleiderer, A. Rosch, T. Schulz, A. Tschendorf, M. Wagner.

[1] S. Mühlbauer et al., *Science* **323**, 915 (2009); A. Neubauer et al., *Phys. Rev. Lett.* **102**, 186602 (2010); C. Pfleiderer et al., *J. Phys. Cond. Matter* **22**, 164207 (2010); T. Adams et al., *Phys. Rev. Lett.*, in press, arXiv/1107.0993.

[2] W. Münzer et al., *Phys. Rev. B* **81**, 041203(R) (2010).

[3] X. Z. Yu et al., *Nature* **465**, 901 (2010); X. Z. Yu et al., *Nature Materials* **10**, 106 (2010).

[4] F. Jonietz et al., *Science*, **330**, 1648 (2010).

[5] *Emergent electrodynamics of skyrmions in a chiral magnet*, T. Schulz, R. Ritz, A. Bauer, M. Halder, M. Wagner, C. Franz, and C. Pfleiderer, K. Everschor, M. Garst, and A. Rosch, preprint 2011.

9:12AM H19.00003 Current-induced domain wall motion stabilized by Rashba spin-orbit coupling, IOAN MIRON, Catalan Institute of Nanotechnology (ICN-CSIC) — No abstract available.

9:48AM H19.00004 Current-driven spin dynamics in spin-orbit coupled superconductors¹, GIOVANNI VIGNALE, Department of Physics, University of Missouri-Columbia — The study of the interplay between spin-orbit coupling (SOC) and superconductivity in two-dimensional electron gases (2DEG) has recently gained impetus following the discovery of i) 2DEGs in InAs or GaAs semiconductor heterostructures that are proximized by ordinary s-wave superconducting leads — a class of systems which plays a key role in the quest for Majorana fermions — and ii) 2DEGs that form at interfaces between complex oxides such as LaAlO_3 and SrTiO_3 , which display tunable SOC and, under appropriate conditions, superconductivity. Motivated by this body of experimental and theoretical literature, we investigate the collective spin dynamics of an archetypical 2DEG model Hamiltonian with Rashba SOC in the presence of *repulsive* electron-electron (e-e) interactions. In the absence of superconductivity a Rashba 2DEG exhibits spin oscillations, which, at long wavelength and for weak repulsive interactions, have a frequency $\approx 2\alpha k_F$, α being the strength of SOC and k_F the usual 2D Fermi wavenumber in the absence of SOC. These oscillations, however, are damped and quickly decay due to the emission of (double) electron-hole pairs, which, in the normal phase, are present at arbitrary low energies. In the presence of superconductivity, collective spin oscillations continue to exist in a wide range of parameters, because the Cooper pairs are mixtures of singlet and triplet components. Further, these excitations are undamped because they lie inside the superconducting gap where no other excitation exists. These spin oscillations can be excited by the application of a magnetic field or a supercurrent and can be used to realize persistent spin oscillators operating in the frequency range of 10 GHz — 1 THz.

Work supported by EU FP7 Programme Grant No. 215368-SEMISPINNET, No. 234970- NANOCTM and No. 248629-SOLID, and by NSF DMR-0705460.

¹A. Agarwal, M. Polini, R. Fazio, and G. Vignale, *Phys. Rev. Lett.* **107**, 077004 (2011).

10:24AM H19.00005 Emergent electrodynamics from moving magnetic whirls in chiral magnets, ACHIM ROSCH, University of Cologne — In chiral magnets a lattice of magnetic whirls — so-called skyrmions — is stabilized in a small temperature and field range by thermal fluctuations [1]. We discuss how electric and spin currents couple to these skyrmions. As the spin of the electrons locally adjusts to the magnetic texture, the electron picks up a Berry phase. The effects of these time-dependent Berry phases are best described by “artificial” electric and magnetic fields of an emergent electrodynamics which couple to the spin and the spin currents. The efficient Berry phase coupling together with a partial cancellation of pinning forces due to the stiffness of the skyrmion lattice allows to explain theoretically experiments [2], which show that skyrmion lattices can be controlled by ultrasmall current densities. Using tiny gradients of temperature or magnetic field it is also possible to induce rotations of the skyrmion lattice. The topologically quantized winding number of the skyrmions induces exactly one quantum of emergent magnetic flux per skyrmion. Therefore one can also determine quantitatively the emergent electric field induced by a moving skyrmion following Faraday’s law of induction as has been measured in recent experiments [3].

[1] *Skyrmion Lattice in a Chiral Magnet*, S. Mühlbauer, B. Binz, F. Jonietz, C. Pfleiderer, A. Rosch, A. Neubauer, R. Georgii, P. Böni, *Science* **323**, 915 (2009).

[2] *Spin Transfer Torques in MnSi at Ultralow Current Densities*, F. Jonietz, S. Mühlbauer, C. Pfleiderer, A. Neubauer, W. Münzer, A. Bauer, T. Adams, R. Georgii, P. Böni, R. A. Duine, K. Everschor, M. Garst, and A. Rosch, *Science* **330**, 1648 (2010).

[3] *Emergent electrodynamics of skyrmions in a chiral magnet*, T. Schulz, R. Ritz, A. Bauer, M. Halder, M. Wagner, C. Franz, and C. Pfleiderer, K. Everschor, M. Garst, and A. Rosch, preprint 2011.

Tuesday, February 28, 2012 8:00AM - 11:00AM —

Session H20 GSNP DFD: Invited Session: Hydrodynamics and Microstructure: From Single Self-Propelled Particles to Active Soft Matter 253C

8:00AM H20.00001 Swimming & Propulsion in Viscoelastic Media¹, PAULO ARRATIA, University of Pennsylvania — Many microorganisms have evolved within complex fluids, which include soil, intestinal fluid, and mucus. The material properties or rheology of such fluids can strongly affect an organism’s swimming behavior. A major challenge is to understand the mechanism of propulsion in media that exhibit both solid- and fluid-like behavior, such as viscoelastic fluids. In this talk, we present experiments that explore the swimming behavior of biological organisms and artificial particles in viscoelastic media. The organism is the nematode *Caenorhabditis elegans*, a roundworm widely used for biological research that swims by generating traveling waves along its body. Overall, we find that fluid elasticity hinders self-propulsion compared to Newtonian fluids due to the enhanced resistance to flow near hyperbolic points for viscoelastic fluids. As fluid elasticity increases, the nematode’s propulsion speed decreases. These results are consistent with recent theoretical models for undulating sheets and cylinders. In order to gain further understanding on propulsion in viscoelastic media, we perform experiments with simple reciprocal artificial ‘swimmers’ (magnetic dumbbell particles) in polymeric and micellar solutions. We find that self-propulsion is possible in viscoelastic media even if the motion is reciprocal.

¹This work is supported by NSF-CAREER-0954084.

8:36AM H20.00002 Assembly and dynamics of synthetic cilia¹, TIM SANCHEZ, Brandeis University, Physics Department — From motility of simple protists to determining the handedness of complex vertebrates, highly conserved eukaryotic cilia and flagella are essential for the reproduction and survival of many biological organisms. Despite extensive studies, the exact mechanism by which individual components coordinate to produce ciliary beating patterns remains unknown. We describe a novel approach towards studying ciliary beating. Instead of deconstructing a fully functional organelle from the top-down, we describe a process by which synthetic cilia-like structures are assembled from the bottom-up. We find that simple mixtures of microtubules, kinesin clusters, and a bundling agent produce spontaneous oscillations in MT bundles, suggesting that self-organized beating may be a generic feature of internally driven bundles. Furthermore, bundles in close proximity spontaneously coordinate their beating to generate metachronal traveling waves, reminiscent of the waves seen in ciliary fields. These findings and future refinements of the system can potentially provide insights into general design principles required for engineering synthetic cilia as well as understanding the biological analogues.

¹Support from Keck and MRSEC (NSF)

9:12AM H20.00003 Polar patterns in active fluids¹, M. CRISTINA MARCHETTI, Physics Department & Syracuse Biomaterials Institute, Syracuse University — Active fluids are a new class of soft materials composed of interacting units that consume energy and collectively generate motion and mechanical stress. Examples include bacterial suspensions, mixtures of cytoskeletal filaments and motor proteins, and migrating epithelial cell layers. Due to their elongated shape, active particles can exhibit orientational order at high concentration and have been likened to “living liquid crystals”, with either nematic or polar symmetry. In this talk I will discuss the spatio-temporal dynamics of continuum models of active fluids in two dimensions, focusing on the case of a system with polar symmetry as relevant to bacterial suspensions. Upon increasing activity, the active fluid displays increasingly complex patterns, including traveling bands, traveling vortices and chaotic behavior. The nonlinear hydrodynamic equations can be mapped onto a diffusion-reaction-convection model, highlighting the connection between the complex dynamics of active system and that of excitable systems.

¹This work was carried out with Luca Giomi and supported by the NSF through grants DMR-0806511 and DMR-1004789.

9:48AM H20.00004 Swimming of Paramecium in confined channels, SUNGHWAN JUNG, Virginia Tech — Many living organisms in nature have developed a few different swimming modes, presumably derived from hydrodynamic advantage. Paramecium is a ciliated protozoan covered by thousands of cilia with a few nanometers in diameter and tens of micro-meters in length and is able to exhibit both ballistic and meandering motions. First, we characterize ballistic swimming behaviors of ciliated microorganisms in glass capillaries of different diameters and explain the trajectories they trace out. We develop a theoretical model of an undulating sheet with a pressure gradient and discuss how it affects the swimming speed. Secondly, investigation into meandering swimmings within rectangular PDMS channels of dimension smaller than Paramecium length. We find that Paramecium executes a body-bend (an elastic buckling) using the cilia while it meanders. By considering an elastic beam model, we estimate and show the universal profile of forces it exerts on the walls. Finally, we discuss a few other locomotion of Paramecium in other extreme environments like gel.

10:24AM H20.00005 Helical swimming in viscoelastic and porous media, BIN LIU, School of Engineering, Brown University — Many bacteria swim by rotating helical flagella. These cells often live in polymer suspensions, which are viscoelastic. Recently there have been several theoretical and experimental studies showing that viscoelasticity can either enhance or suppress propulsion, depending on the details of the microswimmer. To help clarify this situation, we study experimentally the motility of the flagellum using a scaled-up model system - a motorized helical coil that rotates along its axial direction. A free-swimming speed is obtained when the net force on the helix is zero. When the helix is immersed in a viscoelastic (Boger) fluid, we find an increase in the force-free swimming speed as compared with the Newtonian case. The enhancement is maximized at a Deborah number of approximately one, and the magnitude depends not only on the elasticity of the fluid but also on the geometry of the helix. In the second part of my talk, I will discuss how spatial confinements, such as a porous medium, affect the flagellated swimming. For clarity, the porous media are modeled as cylindrical cavities with solid walls. A modified boundary element method allows us to investigate a situation that the helical flagella are very close to the wall, with high spatial resolution and relatively low computational cost. To our surprise, at fixed power consumption, a highly coiled flagellum swims faster in narrower confinements, while an elongated flagellum swims faster in a cavity with a wider opening. We try understanding these effects with simple physical pictures.

Tuesday, February 28, 2012 8:00AM - 11:00AM –

Session H21 DCMP: Superconductivity: Electronic Structure of BSCCO; ARPES and theory
254A

8:00AM H21.00001 Extraction of Normal Electron Self-Energy and Pairing Self-Energy in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ via Laser ARPES, WENTAO ZHANG, Institute of Physics, Chinese Academy of Sciences, Beijing, China, J.M. BOK, J.H. YUN, Dept. of Physics, SungKyunKwan University, Korea, J.F. HE, G.D. LIU, L. ZHAO, H.Y. LIU, J.Q. MENG, X.W. JIA, Y.Y. PENG, D.X. MOU, S.Y. LIU, L. YU, S.L. HE, X.L. DONG, J. ZHANG, Institute of Physics, CAS, Beijing, China, J.S. WEN, Z.J. XU, Brookhaven National Laboratory, USA, G.D. GU, Brookhaven National Laboratory, USA, C.T. CHEN, Z.Y. XU, Technical Institute of Physics and Chemistry, CAS, Beijing, China, H.-Y. CHOI, Dept. of Physics, SungKyunKwan University, Korea, C.M. VARMA, Dept. of Physics and Astronomy, UC Riverside, USA, X.J. ZHOU, Institute of Physics, CAS, Beijing, China — Super-high resolution laser-based angle-resolved photoemission measurements have been performed on a high temperature superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$. The band back-bending characteristic of the Bogoliubov-like quasiparticle dispersion is clearly revealed at low temperature in the superconducting state which gives rise to two peaks in the momentum distribution curves. This makes it possible for the first time to experimentally extract the normal electron self-energy and pairing self-energy in the superconducting state. These information can be used to further determine the Bosonic spectral function that will provide key insight and constraints on the origin of electron pairing in high temperature superconductors.

8:12AM H21.00002 Momentum Dependence of the Self-energy and Fluctuation Spectrum of Bi2212 from High Resolution Laser ARPES, HAN-YONG CHOI, JIN MO BOK, JAE HYUN YUN, SungKyunKwan University, WENTAO ZHANG, X.J. ZHOU, Chinese Academy of Sciences, C.M. VARMA, University of California, Riverside — We report deduction of the Eliashberg function $\alpha^2F(\theta, \omega)$ at energy ω and along momentum cuts at angles θ normal to the Fermi surface from the high resolution laser angle resolved photoemission spectroscopy on slightly underdoped Bi2212 in the normal and superconducting states. Our principle result is that despite the angle dependence of the extracted single-particle self-energy, the Eliashberg function in the normal state collapses onto a single function of ω independent of the angle. It has a peak around 0.05 eV, flattens out above 0.1 eV with the angle dependent cut-off. The cut-off energy is given by the intrinsic value of about 0.4 eV or the energy of the band bottom in direction θ , whichever is lower. These results are consistent only with fluctuation spectra which have the correlation length of the lattice constant or shorter. In the superconducting state, the deduced $\alpha^2F(\theta, \omega)$ exhibits a new peak around 0.015 eV in addition to the 0.05 eV peak and flat spectrum as in the normal state. Both peaks become enhanced as T is lowered or the angle moves away from the nodal direction. The implication of these findings is discussed.

8:24AM H21.00003 Mechanisms for Superconductivity in Cuprates compared with results from the Generalized MacMillan-Rowell Analysis of High Resolution Laser- ARPES, CHANDRA VARMA, University of California, Riverside, CA., HAN-YONG CHOI, Korea Institute for Advanced Study, Seoul 130-722, Korea., WENTAO ZHANG, XINGJIANG ZHOU, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China. — The spectra of fluctuations and their coupling to fermions has been deduced from extensive high resolution laser ARPES in several BISCCO samples and quantitatively analyzed. We ask the question whether some of the theories for superconductivity in Cuprates are consistent or inconsistent with the frequency and the momentum dependence of the deductions. We find that any fluctuation spectra, for example that of Antiferromagnetic Fluctuations, whose frequency dependence depends significantly on momentum dependence are excluded. We consider the quantum-critical spectra of the loop-current order observed in under-doped cuprates and its coupling to fermions and find it consistent with the data.

8:36AM H21.00004 Comparative study of the MDC and two-dimensional analysis of ARPES intensity for Bi2212 bilayer superconductor, JIN MO BOK, HAN-YONG CHOI, SungKyunKwan University, JUNFENG HE, X.J. ZHOU, Chinese Academy of Sciences, C.M. VARMA, University of California — The momentum distribution curve (MDC) analysis is commonly used to analyze the ARPES data. A problem of the MDC analysis, however, is that the matrix elements turn out to be energy dependent. To remedy this we take the two-dimensional (2D) analysis of the ARPES intensity as reported by Meevasana et. al. [1]. We analyze the overdoped Bi2212 superconductor ARPES data by performing both 2D and MDC analysis taking the bilayer splitting into consideration. The deduced self-energy and Eliashberg function from both analysis will be compared and presented.

[1] Meevasana et. al. Phys. Rev. B 77, 104506 (2008).

8:48AM H21.00005 Ultra-High Resolution Time- and Angle-Resolved Photoemission Experiments on High Temperature Superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$, WENTAO ZHANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, CHRIS SMALLWOOD, TRISTAN MILLER, Department of Physics, University of California, Berkeley, CA 94720, USA, CHRIS JOZWIAK, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, HIROSHI EISAKI, Nanoelectronics Research Institute (NeRI), National Institute of Advanced Industrial Science and Technology (AIST) Umezono 1-1-1 Tsukuba, Ibaraki 305, DUNG-HAI LEE, ALESSANDRA LANZARA, Department of Physics, University of California, Berkeley, CA 94720, USA — Ultra-high resolution laser-based time- and angle-resolved photoemission measurements have been carried out on various dopings of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ high temperature superconductor. In this talk, we will report on the study of the dynamical quasiparticle excitation and recombination of the nodal electronic states in cuprate.

9:00AM H21.00006 Momentum-Dependent Ultrafast Quasiparticle Dynamics in Optimally-Doped Bi-2212 Monitored with Time-Resolved ARPES, GEORGI DAKOVSKI, Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park CA, TOMASZ DURAKIEWICZ, Condensed Matter and Magnet Science, Materials Physics and Applications Division, Los Alamos National Laboratory, Los Alamos NM, JIAN-XIN ZHU, Physics of Condensed Matter and Complex Systems, Theoretical Division, Los Alamos National Laboratory, Los Alamos NM, PETER RISEBOROUGH, Department of Physics, Temple University - Philadelphia PA, GENDA GU, Condensed Matter Physics & Materials Science, Brookhaven National Laboratory, Upton NY, STEVE GILBERTSON, GEORGE RODRIGUEZ, Center for Integrated Nanotechnologies, Materials Physics and Applications Division, Los Alamos National Laboratory, Los Alamos NM — We have employed the novel technique of time- and angle-resolved photoelectron spectroscopy (t-ARPES) to investigate the quasiparticle dynamics in photoexcited, optimally-doped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ superconductor across the superconductor-metal transition. In this talk, we will present and analyze the substantially different ultrafast dynamics, tracked in momentum-dependent fashion, by probing the nodal and antinodal regions of the Brillouin zone, on a 35 femtosecond timescale. The consequences of these findings in terms of reentrant superconductivity will be discussed.

9:12AM H21.00007 Tracking Cooper Pair Formation in a Cuprate Superconductor: An Ultra-fast ARPES Study, CHRISTOPHER SMALLWOOD, JAMES HINTON, Department of Physics, UC Berkeley; Materials Science Division, LBNL, CHRIS JOZWIAK, Advanced Light Source, LBNL, WENTAO ZHANG, JAKE KORALEK, Materials Science Division, LBNL, HIROSHI EISAKI, Nanoelectronics Research Institute, National Institute of Advanced Industrial Science and technology, DUNG-HAI LEE, JOSEPH ORENSTEIN, ALESSANDRA LANZARA, Department of Physics, UC Berkeley; Materials Science Division, LBNL — A basic mystery in high temperature superconductivity is the process that drives quasiparticles to form Cooper pairs, the fundamental charge carriers in any superconductor. We use time- and angle-resolved photoemission spectroscopy (TR-ARPES) to measure the relaxation dynamics of low energy excitations in the optimally doped cuprate superconductor Bi-2212. Results are discussed within the context of the Rothwarf-Taylor model of quasiparticle recombination.

9:24AM H21.00008 Nodal Gap of Heavily Under-doped Bi2201 Revealed by VUV Laser ARPES, YINGYING PENG, JIANQIAO MENG, The Institute of Physics, Chinese Academy of Sciences, CHANGTIAN CHEN, ZUYAN XU, Technical Institute of Physics and Chemistry, Chinese Academy of Science, XINGJIANG ZHOU, The Institute of Physics, Chinese Academy of Sciences — We have carried out VUV laser-based angle-resolved photoemission (ARPES) on heavily under-doped $\text{Bi}_2(\text{Sr}_{2-x}\text{La}_x)\text{CuO}_{6+\delta}$ (abbreviated as La-Bi2201) samples with different dopings from antiferromagnetic insulators to superconductors. We find that, along the $(0,0) - (\pi,\pi)$ nodal direction, there is a gap opening that is strongly dependent on the hole doping level. The momentum and temperature dependence of the gap is investigated and the implication of the observations will be discussed.

9:36AM H21.00009 Doping Dependence of Pair-breaking and Pair-forming Processes in BSCCO, THEODORE REBER, NICHOLAS PLUMB¹, YUE CAO, ZHE SUN, STEPHEN PARHAM, QIANG WANG, University of Colorado, HIDEAKI IWASAWA, Hiroshima Synchrotron Radiation Center, Hiroshima University, SHIMPEI ONO, RIKEN, GENDA GU, Brookhaven National Lab, YOSHIHIRO AIURA, AIST, GERALD ARNOLD, DANIEL DESSAU, University of Colorado — Angle resolved photo-emission spectroscopy (ARPES) provides a direct measure of electronic scattering processes in materials. However traditional methods (e.g. MDC widths) of determining the scattering processes from ARPES fail to discriminate between pairing and non-pairing interactions. Our new analysis technique, the ARPES tunneling spectrum (ATS), isolates the pairing channel from all other processes. We will report doping, angle and temperature dependence of both the pair-forming strength and the pair-breaking rate in BSCCO.

¹Now at PSI

9:48AM H21.00010 Momentum dependence of Fermi surface maps in angle-resolved photoemission spectrum of $\text{Bi}_2\text{Sr}_2\text{CuO}_6$ (Bi2201), SUSMITA BASAK, Northeastern U., J. NIEMINEN, M. LINDROOS, Northeastern U. and Tampere U. Tech., Finland, R. S. MARKIEWICZ, A. BANSIL, Northeastern U. — We have investigated the effect of ARPES matrix element on photointensity for emission from the Fermi energy as a function of photon energy in Bi2201 using first-principles as well as tight-binding model calculations. Our results show that as the photon energy increases and photoemitted electrons are spread over a larger area of momentum space, the highest spectral intensities generally remain pinned to the largest momenta probed at any given photon energy. The tight-binding calculations, which involve a three band Hubbard Hamiltonian based on $\text{Cu } d_{x^2-y^2}$ and $\text{O } p_x, p_y$ orbitals, give insight into the role of the ARPES matrix element in shaping the photointensities. A relatively simple formula is derived for the matrix element, showing how much of the zone-to-zone variation of the photointensity is controlled by the structure factor associated with the Bloch wavefunction.

10:00AM H21.00011 Detecting the minimum gap locus in ARPES spectra of Bi2201¹, MAKOTO HASHIMOTO, SSRL, SLAC National Accelerator Lab, RUIHUA HE, Advanced Light Source, Lawrence Berkeley National Lab, Berkeley, ROB MOORE, SIMES, SLAC and GLAM, Departments Departments of Physics and Applied Physics, Stanford University, DONGHUI LU, SSRL, SLAC National Accelerator Lab, YOSHIYUKI YOSHIDA, Nanoelectronics Research Institute, AIST, MOTOYUKI ISHIKADO, Japan Atomic Energy Agency, HIROSHI EISAKI, Nanoelectronics Research Institute, AIST, ZAHID HUSSAIN, Advanced Light Source, Lawrence Berkeley National Lab, Berkeley, TOM DEVEREAUX, ZHI-XUN SHEN, SIMES, SLAC and GLAM, Departments Departments of Physics and Applied Physics, Stanford University — Recent angle-resolved photoemission (ARPES) studies have reported a direct evidence for the competing nature of the pseudogap by showing that the pseudogap dispersion is not tied to Fermi momentum (k_F) [1,2]. In this study, to get more detailed information on how the competing pseudogap evolves across the pseudogap temperature (T^*), we introduce a new analysis method for spectral weight. We found a clear indication that the pseudogap opens at T^* with the minimum gap locus deviating from k_F , which is completely different manner from the gap opening by simple superconductivity, and strongly supports that the pseudogap is another distinct order. [1] M. Hashimoto and R.-H. He *et al.*, Nature Phys. **6**, 14-418 (2010). [2] R.-H. He and M. Hashimoto *et al.*, Science **331**, 1579-1583 (2011).

¹This work is supported by the Department of Energy, Office of Basic Energy Science under contract DE-AC02-76SF00515.

10:12AM H21.00012 Evidence for Charge-Density-Wave in Underdoped Bi2201 from ARPES and LEED, J.A. ROSEN, R. COMIN, G. LEVY, D. FOURNIER, Z.-H. ZHU, B. LUDBROOK, C.N. VEENSTRA, D. WONG, P. DOSANJH, Department of Physics & Astronomy, University of British Columbia, Vancouver, British Columbia V6T 1Z1, Canada, Y. YOSHIDA, H. EISAKI, Superconducting Electronics Group, National Institute of Advanced Industrial Science and Technology, Ibaraki 305-8568, Japan, L. PETACCIA, Sincrotrone Trieste, Strada Statale 14 Km 163.5, 34149 Trieste, Italy, A. DAMASCELLI, Quantum Matter Institute and Department of Physics & Astronomy, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada — While there is mounting evidence for a broken symmetry in the pseudogap state of the high- T_c cuprates, the identification of a specific phase remains elusive. Through the combination of electronic (ARPES) and structural (LEED) probes, we uncover a temperature dependent evolution of the CuO_2 plane band dispersion in highly-ordered Bi2201, which is directly associated with a hitherto-undetected evolution of the incommensurate superstructure. The quasilinear, continuous variation of the modulation wavelength $2\pi/Q_2$ from ~ 66 to $43\text{\AA}$, below a characteristic $T_{Q_2} \simeq 130\text{K}$, provides evidence for an electronically-driven charge-density-wave ordering. This points to a remarkable electron-lattice coupling, in which the footprint of the BiO -layer-induced superstructure is found in the modulated electronic structure of the CuO_2 plane.

10:24AM H21.00013 Electronic Scattering Rates in the High- T_c Superconductor $\text{Bi}_{2.1}\text{Sr}_{1.9}\text{Ca}(\text{Cu}_{1-y}\text{Fe}_y)_2\text{O}_x$, STEPHEN PARHAM, THEODORE REBER, YUE CAO, JUSTIN WAUGH, University of Colorado, GENDA GU, Brookhaven National Laboratory, DANIEL DESSAU, University of Colorado — We investigate the effects of Fe impurities in bi-layer BSCCO. It is known that substituting Fe for Cu in this material reduces T_c , but the mechanism for this decrease is not well understood. We have developed a technique that utilizes ARPES to quantitatively measure the effects of impurities on electronic scattering. Using this technique we investigate the details of how Fe impurities cause an increase in the pair-breaking scattering rate in bi-layer BSCCO.

10:36AM H21.00014 Universal 115meV Feature and High Energy Spectral Weight Transfer in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\Delta}$ Superconductor Revealed by Laser ARPES, JUNFENG HE, XINGJIANG ZHOU, The Institute of Physics, Chinese Academy of Sciences — Quasiparticle dispersion and spectral weight transfer have been investigated by laser-based angle-resolved photoemission spectroscopy in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\Delta}$. A universal energy scale near $\sim 115\text{meV}$ can be clearly identified in superconducting state which is insensitive to momentum and doping levels. A concomitant observation with this energy scale is the spectral weight transfer over a large energy range when the sample goes from the normal state to the superconducting state. The origin and implications of these observations will be discussed.

10:48AM H21.00015 Towards the Standard Model for Fermi Arcs from a Wilsonian Reduction of the Hubbard Model, SEUNGMIN HONG, PHILIP PHILLIPS, University of Illinois, Urbana-Champaign, UNIVERSITY OF ILLINOIS, URBANA-CHAMPAIGN TEAM — Two remarkable features emerge from the exact Wilsonian procedure for integrating out the high-energy scale in the Hubbard model. At low energies, the number of excitations that couple minimally to the electromagnetic gauge is less than the conserved charge, thereby implying a breakdown of Fermi liquid theory. In addition, two charge e excitations emerge in the lower band, the standard projected electron and a composite entity (comprised of a hole and a charge $2e$ bosonic field) which give rise to poles and zeros of the single-particle Green function, respectively. The poles generate spectral weight along an arc centered at $(\pi/2, \pi/2)$ while the zeros kill the spectral intensity on the back-side of the arc. The result is the Fermi arc structure intrinsic to cuprate phenomenology. The presence of composite excitations also produces a broad incoherent pseudogap feature at the $(\pi, 0)$ region of the Brillouin zone, thereby providing a mechanism for the nodal/anti-nodal dichotomy seen in the cuprates.

Tuesday, February 28, 2012 8:00AM - 11:00AM —

Session H22 DMP DCOMP: Focus Session: Fe-based Superconductors - Anisotropic Transport and Anisotropy 254B

8:00AM H22.00001 Temperature-dependent anisotropic resistivity in electron, hole and iso-electron - doped BaFe₂As₂ superconductors¹, M.A. TANATAR, Ames Laboratory USDOE, Ames, Iowa — Anisotropic electrical resistivity, $\rho(T)$, was studied in iron-arsenide superconductors, obtained by doping the parent BaFe₂As₂ compound on three different sites: (1) electron donor transition metal (Co, Ni, Rh, Pd) substitution of Fe [1,2]; (2) hole donor K substitution of Ba [3]; (3) isoelectron P substitution of As. For all three types of dopants a range of T -linear behavior is found at the optimal doping in both the in-plane and the inter-plane $\rho(T)$ above T_c . At some higher temperature this range of T -linear resistivity is capped by a slope-changing anomaly, which, by comparison with NMR, magnetic susceptibility and Hall effect measurements, can be identified with the onset of carrier activation over the pseudogap [1]. The doping-evolution of anisotropic temperature dependent $\rho(T)$ and of the pseudogap are quite different for three types of doping. A three-dimensional $T-H$ phase diagram summarizing our results will be presented. Furthermore, potential correlation of the anisotropic normal state transport and anisotropic superconducting state heat transport will be discussed.

In collaboration with N. Ni, A. Thaler, S.L. Bud'ko, P.C. Canfield, R. Prozorov, Bing Shen, Hai-Hu Wen, K. Hashimoto, S. Kasahara, T. Terashima, T. Shibauchi and Y. Matsuda.

[1] M.A. Tanatar et al. PRB **82**, 134528 (2010)

[2] M.A. Tanatar et al. PRB **84**, 014519 (2011)

[3] M.A. Tanatar et al. arXiv:1106.0533

¹Work at the Ames Laboratory was supported by the Department of Energy-Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

8:36AM H22.00002 Enhanced conductance in the normal state of Fe pnictides & chalcogenides measured by quasiparticle scattering spectroscopy (QPS): evidence of orbital fluctuations, HAMOOD ARHAM, C.R. HUNT, W.K. PARK, L.H. GREENE, U of IL at Urbana, J. GILLET, S.D. DAS, S.E. SEBASTIAN, U. Cambridge, S. RAN, A. THALER, S.L. BUD'KO, P.C. CANFIELD, Ames Lab & ISU, Z.J. XU, J.S. WEN, Z.W. LIN, Q. LI, G. GU, BNL — QPS reveals a conductance enhancement at a temperature, T_{onset} , for RFe₂As₂ (R=Ca, Sr, Ba) and Fe_{1.13}Te. For Ba/Sr Fe₂As₂ and Fe_{1.13}Te the enhancement survives well above the magnetic and structural transition temperatures (Ba: $T_N \sim 132$ K, $T_{onset} \sim 175$ K; Sr: $T_N \sim 192$ K, $T_{onset} \sim 240$ K; Fe_{1.13}Te: $T_N \sim 60$ K, $T_{onset} \sim 75$ K) while for most CaFe₂As₂ junctions it disappears below T_N and T_S (11 junctions tested, only 2 showed weak enhancement above T_N). For Co underdoped BaFe₂As₂ the enhancement coexists with the superconducting Andreev peaks while it is not observed for Co overdoped Ba122. We construct a modified phase diagram for Ba(Fe_{1-x}Co_x)₂As₂ to reflect the presence of this feature for the underdoped regime.¹ We discuss this conductance enhancement in the context of non-Fermi liquid behavior of these compounds due to orbital fluctuations.² This work is supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the US DOE, Office of Science, Award No. DE-AC0298CH1088. Work at Cambridge supported by EPSRC. Work at BNL under DOE Award No. DE-AC0298CH10886. Ames Lab. operated by ISU for the U.S. DOE under Award No. DE-AC02-07CH11358.

¹Arham et. al, arXiv:1108.2749.

²Lee et. al, arXiv:1110.5917.

8:48AM H22.00003 Nematic order in the vicinity of a vortex in superconducting FeSe, DEBANJAN CHOWDHURY, EREZ BERG, SUBIR SACHDEV, Department of Physics, Harvard University — We present a phenomenological theory of the interplay between nematic order and superconductivity in the vicinity of a vortex induced by an applied magnetic field [1]. Nematic order can be strongly enhanced in the vortex core. As a result, the vortex cores become elliptical in shape. For the case where there is weak bulk nematic order at zero magnetic field, the field-induced eccentricity of the vortex core has a slow power-law decay away from the core. Conversely, if the nematic order is field induced, then the eccentricity is confined to the vortex core. We discuss the relevance of our results to recent scanning tunneling microscopy experiments on FeSe [2].

[1] D. Chowdhury, E. Berg and S. Sachdev, to appear in Phys. Rev. B, arXiv: 1109.2600 (2011).

[2] Can- Li Song et al., Science 332, 1410 (2011).

9:00AM H22.00004 T-matrix Impurity Effects on Nematicity in Iron-Based Superconductors, NACHUM PLONKA, ALEXANDER KEMPER, THOMAS DEVEREAUX, Stanford University and SLAC National Accelerator Laboratory — In iron-based superconductors, nematicity has been reported in transport measurements and a broad range of spectroscopies, including angle-resolved photoemission, neutron scattering, and scanning tunneling microscopy. These observed anisotropies of broken tetragonal symmetry have been attributed to pure spin physics or unequal occupation of the iron d-electron orbitals, referred to as orbital ordering. To address this issue, we use realistic multi-orbital tight-binding Hamiltonians and T-matrix formalism to explore the effects of non-magnetic impurities. In particular, we present a detailed examination of the local density of states around impurities, and highlight the interplay of magnetic and orbital degrees of freedom.

9:12AM H22.00005 Surface Structure of Stripe ordered 1x2 phase on (Ba, Ca)(Fe_{1-x}Co_x)₂As₂¹, GUORONG LI, VON BRAUN NASCIMENTO, XIAOBO HE, AMAR B. KARKI, RONGYING JIN, JIANDI ZHANG, WARD PLUMMER, Louisiana State University — Low energy electron diffraction (LEED) and scanning tunneling microscopy/spectroscopy (STM/S) have been utilized to investigate the geometric structure of the stripe 1x2 surface phase of (Ba, Ca)(Fe_{1-x}Co_x)₂As₂ iron pnictides. STM images show that the surface consists of competing ordered and disordered regions. The 1x2 phase appears on the surface of all compounds but coexist with ($\sqrt{2} \times \sqrt{2}$)R45° phase on the surface of Ba122. Quantitative structural analysis of LEED-I(V) using the fractional spots of the 1x2 phase on both parent compounds as well as Ca(Fe_{0.925}Co_{0.075})₂As₂ gives a similar surface structure with a termination layer of 50% Ca/Ba atoms. The surface Ca/Ba layer has a large inward relaxation ~ 0.5 Å and the underneath As-Fe-As layer displays a buckling distortion. The Pendry Rp factor (~ 0.24) obtained in the structural refinement is excellent for all three systems.

¹Research is supported by NSF DMR-1002622

9:24AM H22.00006 Scanning tunneling spectroscopy in Co-doped BaFe₂As₂: what density functional theory can tell us, KLAUS KOEPERNIK, STEVEN JOHNSTON, JEROEN VAN DEN BRINK, IFW Dresden, ERIK VAN HEUMEN, MARK S. GOLDEN, Zeeman Institute, University of Amsterdam, Netherlands — We use density functional theory to simulate the scanning tunneling spectra and topographic images of Co-doped BaFe₂As₂. The matrix element effects are evaluated and the specific contributions of the different surface atoms to the spectra are considered. The results give a better understanding of the measured spectra and assess the resolution of STS measurements in these systems.

9:36AM H22.00007 Scanning tunneling spectroscopic studies of the iron-arsenic superconducting $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ single crystals, M.L. TEAGUE, H. CHU, R. T.-P. WU, N.-C. YEH, Dept. of Physics, Caltech, Pasadena, CA 91125, USA, P. CHEN, B. SHEN, H.-H. WEN, Institute of Physics, Chinese Academy of Sciences, China — Scanning tunneling spectra of $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ ($x=0.06, 0.08, 0.12$) single crystals are studied as a function of temperature (T) and magnetic field (H). For $H = 0$, direct evidence for two-gap superconductivity at energies $\omega = \Delta_\beta$ and $\Delta_{\alpha,\gamma/\delta}$ ($\approx 2\Delta_\beta$) and for magnetic resonance modes at $\Omega \approx \Delta_\beta + \Delta_{\alpha,\gamma/\delta}$ are found for all samples at $T < T_c$. Fourier transformation of the tunneling spectra reveals x - and ω -dependent quasiparticle interference (QPI) wave-vectors $\mathbf{q}_2$ near $(\pm\pi,0)/(0,\pm\pi)$ and $\mathbf{q}_1$ near $(\pm 2\pi,0)/(0,\pm 2\pi)$. The spectral intensity of $\mathbf{q}_2$ exhibits strong ω -dependence, peaking sharply at $\omega = \Delta_\beta, \Delta_{\alpha,\gamma/\delta}$ and Ω . This is in stark contrast to the Bragg diffraction peaks that are independent of ω, T and x . For $H > 0$, additional QPI wave-vector $\mathbf{q}_3$ appears near $(\pm\pi,\pm\pi)$. These findings are consistent with the sign-changing s -wave pairing symmetry. Additionally, for the optimally doped sample, a pseudogap at $\omega \sim \Delta_{\gamma/\delta}$ is found inside the vortex core, possibly due to coexisting superconductivity and spin density waves. This result is in contrast to the zero-bias conductance peaks observed inside the vortex core of $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$, implying asymmetry in the hole and electron-doping of the iron arsenides. This work was supported by NSF DMR-0907251.

9:48AM H22.00008 Examining multiple spectroscopic techniques with multiband Eliashberg theory in $\text{BaCo}_x\text{Fe}_{2-x}\text{As}_2$ ¹, STEVEN JOHNSTON, IFW Dresden, E. VAN HEUMEN, University of Amsterdam, K. KOEPERNIK, IFW Dresden, MASSEE FREEK, J. KAAS, J.B. GOEDKOOP, University of Amsterdam, J. VAN DEN BRINK, IFW Dresden, M.S. GOLDEN, University of Amsterdam — A wealth of experimental data from multiple probes are available for the newly-discovered pnictide superconductors. Here, we exploit this fact and examine a multi-band Eliashberg model for optimal doped $\text{BaCo}_x\text{Fe}_{2-x}\text{As}_2$ assuming a broad spin-fluctuation boson spectrum and retaining the full 3D bandstructure. Our focus is on comparing the model directly with data collected by our group from ARPES, STM and optics experiments performed on samples from the same growth batch. We find that the model captures all of the important aspects of the three probes including the behavior of the gap structure in the dI/dV characteristics and contributions from low-energy interband transitions in the optical conductivity. Our results also indicate the role of matrix elements in establishing the strong particle-hole asymmetry observed in the dI/dV spectra.

¹This work is funded by FOM and the VENI program (both part of NWO).

10:00AM H22.00009 Point-Contact Andreev Reflection Spectroscopy in Pt-Substituted BaFe_2As_2 ¹, STEVEN ZIEMAK, University of Maryland, XIAOHANG ZHANG, National Institute of Standards and Technology, TYLER DRYE, RICHARD GREENE, JOHNPIERRE PAGLIONE, University of Maryland — We have investigated the superconducting order parameter of $\text{BaFe}_{2-x}\text{Pt}_x\text{As}_2$ using point-contact Andreev reflection spectroscopy (PCAR). The samples used were large single crystals with measured Pt concentrations consistent with optimal doping ($x = 0.15$). Junctions were made between gold or lead tips and the c -axis of the superconducting samples. Conductivity spectra were measured over a range of temperatures and fit to curves generated using the Blonder-Tinkham-Klapwijk (BTK) model for two gaps, one isotropic and one angle-dependent gap with nodes.

¹Center for Nanophysics and Advanced Materials, Physics Department, University of Maryland, College Park

10:12AM H22.00010 Scanning tunneling microscopy study of K-doped iron selenide superconductor film by MBE, QI-KUN XUE, WEI LI, HAO DING, PENG DENG, KAI CHANG, SHUIHUA JI, Tsinghua University, KE HE, LILI WANG, XUCUN MA, Chinese Academy of Sciences, JIANG-PING HU, Purdue University, XI CHEN, Tsinghua University — The alkali-doped iron selenide superconductors have generated considerable excitations as well as confusions, regarding the delicate interplay between Fe vacancies, magnetism and superconductivity. We have grown high-quality $\text{K}_x\text{Fe}_{2-y}\text{Se}_2$ thin film with (001) surface orientation on STO substrate by molecular beam epitaxy. The scanning tunneling microscopy (STM) measurement demonstrates that there are two superconducting phases: striped KFe_2Se_2 in adjacent to the phase with $\sqrt{5} \times \sqrt{5}$ Fe vacancy order and doped KFe_2Se_2 with Fe and K vacancies. Both phases have a superconducting gap of 9 meV. These findings elucidate the existing controversies on the role of $\sqrt{5} \times \sqrt{5}$ Fe vacancy order in superconducting $\text{K}_x\text{Fe}_{2-y}\text{Se}_2$. Based on the atomic level information by STM, we will discuss the mechanism of the two different superconducting phases.

10:24AM H22.00011 The Surface Structure of $\text{FeTe}_{1-x}\text{Se}_x$: A LEED/STM Study¹, XIAOBO HE, VON BRAUN NASCIMENTO, GUORONG LI, JIANDI ZHANG, RONGYING JIN, Louisiana State University, Baton Rouge, LA 70803, USA, A.S. SEFAT, M.A. MCGUIRE, B.C. SALES, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, D. MANDRUS, University of Tennessee, Knoxville, TN, 37996, E.W. PLUMMER, Louisiana State University, Baton Rouge, LA 70803, USA — We have utilized low energy electron diffraction (LEED $I - V$) and scanning tunneling microscopy (STM) to investigate the structural properties of $\text{FeTe}_{1-x}\text{Se}_x$ ($x = 0$ and 0.45) surface. The LEED pattern indicates there is no surface reconstruction on both parent and doped compounds. However, the detailed surface structure calculations from LEED $I - V$ show the cleaved surface of FeTe is Te termination with a 0.06 Å compression on the top layer. The STM topography shows the extreme flatness of the FeTe surface with a corrugation of less than 8 pm. The high resolution STM topography indicates that nanoscale chemical phase separation between Te and Se atoms is unambiguously revealed on the surface of $\text{FeTe}_{0.55}\text{Se}_{0.45}$. Chemical phase separation on the nanoscale makes the LEED $I - V$ surface structural analysis of $\text{FeTe}_{1-x}\text{Se}_x$ (001) very challenging. We will discuss the solution of the LEED analysis and the STM observations as a function of x .

¹Supported by NSF DMR-1002622

10:36AM H22.00012 Cryomagnetic Point-Contact Andreev Reflection Spectroscopy on Single Crystal Iron-Chalcogenide Superconductors¹, Y.T. YEN, University of Toronto, RONGWEI HU, C. PETROVIC, Brookhaven National Laboratory, K.W. YEH, M.K. WU, Institute of Physics, Academia Sinica, Taiwan, J.Y.T. WEI, University of Toronto and Canadian Institute for Advanced Research — We report on cryomagnetic point-contact Andreev reflection spectroscopy performed on single crystals of superconducting $\text{FeTe}_{1-x}\text{S}_x$ and $\text{FeTe}_{1-x}\text{Se}_x$. The samples are cleaved in-situ and the measurements are carried out at temperatures down to 4.2K and in a field up to 9T. At base temperature and zero field, we observe a cone-shaped hump at lower voltages in the conductance spectra with no dips at zero bias and a linear background at higher voltages. The spectral evolution of gap size, zero-bias conductance, and excess spectral area are analyzed as a function of temperature and field. Further spectral analysis is carried out using theoretical models of conductance spectra in multiband superconductors [1,2] and of gap symmetry in Fe-based superconductors [3]. The role of interstitial iron is also considered, by comparison with atomically-resolved scanning tunneling spectroscopy data.

[1] V. Lukic and E.J. Nicol, PRB 76, 144508 (2007) [2] A. Golubov *et al.*, PRL 103, 077003 (2009) [3] P.J. Hirschfeld *et al.*, RPP 74, 124508 (2011)

¹Work supported by NSERC, CFI/OIT, CIFAR, Taiwan National Science Council, and part of this work was carried out at BNL, which is operated for the U.S. Department of Energy by Brookhaven Science Associates (Grant No. DE-Ac02-98CH10886)

10:48AM H22.00013 Transport properties of disordered iron-pnictides in case of coexistence between superconducting and spin-density wave order¹, DUSHKO KUZMANOVSKI, MAXIM VAVILOV, University of Wisconsin - Madison — We present a theoretical description of the transport properties of a dirty multi-band superconductor in the case when both superconducting and spin-density wave orders coexist. We focus on differential conductance spectra of normal metal-superconductor junctions. In pure SC phase, we demonstrate that the interband impurity scattering broadens the coherent peak near the superconducting gap and significantly reduces its height even at relatively low scattering rates. This broadening is consistent with a number of recent experiments performed for both tunnel junctions and larger diffusive contacts. We further analyze the effect of the SDW order parameter on the differential conductance and other transport properties in the coexistence phase.

¹Supported by : NSF-DMR 0955500.

Tuesday, February 28, 2012 8:00AM - 11:00AM – Session H23 DCMP: Metals Structural 255

8:00AM H23.00001 Cr based Alloy Cr-Y-Mo-W Oxidation Study from First Principals Molecular Dynamics Simulation, LEI ZHAO, SHIZHONG YANG, EBRAHIM KHOSRAVI, Southern University and A&M College, SHENGMIN GAO, Louisiana State University — First principles molecular dynamics simulations have been performed to study the stability and oxidation progress of Cr based alloys at high temperatures. The bulk phase of cubic Cr-based alloys is investigated with density functional theory (DFT) calculations and *ab initio* molecule dynamic (MD) method. Diffusion of oxygen atoms within different densities of Y, Mo, and W doping and temperatures in Cr-Y systems is studied in this research. The effects of Y, Mo, and W doping are also studied. The properties of the optimized Y, Mo, and W co-doped Cr-based alloys also studied by using *ab initio* MD method. Further improvement of the oxidation resistance and surface corrosion of Cr-based alloys will be discussed.

8:12AM H23.00002 Enhancing mechanical toughness of aluminum surfaces by nanoboron implantation: An *ab initio* study¹, ZHEN ZHU, Michigan State University, DAE-GYEON KWON, YOUNG-KYUN KWON, Kyung Hee University, DAVID TOMANEK, Michigan State University — We use *ab initio* density functional theory to study the formation dynamics and equilibrium atomic arrangement in aluminum surfaces exposed to energetic boron aggregates. Results of our molecular dynamics simulations indicate that after using up their excess kinetic energy to locally melt the aluminum surface, boron atoms prefer to remain in subsurface sites. We perform extensive structure optimization studies to identify the optimum structural arrangement and changes in the electronic structure associated with the formation of strong Al-B bonds, which are responsible for the stability enhancement of the compound. Nano-indentation simulations based on constrained optimization suggest that presence of boron atoms enhances the mechanical hardness and wear-resistance of aluminum surfaces.

¹Supported by the National Science Foundation Cooperative Agreement #EEC-0832785, titled “NSEC: Center for High-rate Nanomanufacturing”.

8:24AM H23.00003 Phase Stability and Deformation Behavior of Mo-Si-B System and effect of alloying¹, OLEG Y. KONTSEVOI, ARTHUR J. FREEMAN, Northwestern University — Molybdenum silicides are promising materials for ultra-high temperature applications above 1300 °C. One of the main drawbacks is their brittleness at low temperatures, which may be improved by additions. We employ first principles calculations with the highly precise FLAPW method to investigate the effect of alloying with 3d, 4d and 5d transition metals on phase stability, cleavage and shear characteristics of the 3-component system Mo – Mo₃Si – Mo₅SiB₂. We determined site preference, phase partitioning of alloying elements, and their effect on shear behavior and preferred deformation modes. We show that in Mo₃Si alloying with 3d transition metals results in a significant reduction of energy barriers to shear deformation (softening effect), while 4d and 5d additions increase shear barriers (hardening effect). In Mo₅SiB₂, 3d transition metals (except for Ti) act as weak softeners, while 4d and 5d show mixed behavior – hardening for early elements and softening for late ones. The softening potency of additions increases with atomic number, but exhibits non-monotonic behavior as a result of a competition between size and electronic effects. The results are discussed in conjunction with possible pathways to ductility enhancement through alloying.

¹Supported by the AFOSR (Grant No. FA 9550-07-1-0174)

8:36AM H23.00004 Structural, elastic and thermal properties of cementite from Modified Embedded Atom Method (MEAM) potential¹, LAALITHA LIYANAGE, Department of physics and astronomy, Mississippi State University, JEFF HOUZE, None, SEONG-GON KIM, Department of physics and Astronomy, Mississippi State University, MARK TSCHOPP, SUNGHO KIM, Center for advanced vehicular systems, Mississippi State University, MIKE BASKES, Los Alamos National Laboratory, MARK HORSTEMEYER, Department of Mechanical Engineering, Mississippi State University — Structural, elastic and thermal properties of cementite were studied using a newly developed MEAM potential for the Fe-C alloy system. The single element potential of C correctly predicts graphite and diamond as the two stable structures. Parameters for the Fe-C alloy potential were constructed based on the structural and elastic properties of elements in the L₁₂ reference structure, calculated from ab-initio simulations. Parameters were further adjusted to reproduce structural properties of cementite and the interstitial energies for Fe correctly. Pair potential parameters were optimized using a method combining Latin hypercube sampling of the N-dimensional parameter space and multi-objective optimization. Elastic constants, surface formation energies, melting temperature and specific heat of cementite were calculated using the potential. The values computed from the Fe-C alloy MEAM potential are in good agreement with DFT calculations and experiments.

¹Department of Energy funded research project

8:48AM H23.00005 High Strain Rate Deformation of BCC Materials: Molecular Dynamics Simulations, CON HEALY, GRAEME ACKLAND, University of Edinburgh — To improve machining processes, a good understanding of plasticity of bulk metals and at high strain rates is required. During machining processes, it is thought that strain rates of $\sim 10^6 \text{s}^{-1}$ are reached. These strain rates are currently not achievable in experimental high strain rate testing techniques. Here we investigate high strain rate deformation of bcc Fe using Molecular Dynamics simulations. Simulations include those of nano-scale single crystal pillars and of a nano-crystalline sample. We show that bcc materials may exhibit different deformation behavior at high strain rates. Under compression at strain rates of $\sim 10^8 \text{s}^{-1}$, nano-scale single crystal pillars may exhibit slip on atypical planes if the direction of maximum resolved shear stress points along that plane. The stress-strain behavior of these pillars is characterized by sudden strain bursts due to slip events. The yield stress required for these slip events can be as high as 2 GPa, much higher than the Peierls stress which is around 25 MPa for an edge dislocation in Fe. The nano-crystalline sample showed stress-strain behavior closer to that of a bulk metal. At high temperatures, pillars exhibit surface premelting. A large portion of the pillar turns amorphous when strained.

9:00AM H23.00006 Effect of lattice vibrations on magnetic phase transition in BCC Iron , JUNQI YIN, MARKUS EISENBACH, AURELIAN RUSANU, DON NICHOLSON, Oak Ridge National Lab — From the first principle calculation of BCC iron, we build a classical Heisenberg model with the interaction coupling as a function of both the distance and local environments (e.g. volume). Using the Johnson potential and Finnis-Sinclair potential, we perform Monte Carlo simulations of BCC iron including the effect of lattice vibrations. The validity of classical Heisenberg model in describing the magnetic phase transition of BCC iron is explained.

9:12AM H23.00007 Phase-Stabilizers in Titanium Alloys , BENGT TEGNER, LINGGANG ZHU, GRAEME ACKLAND, SUPA, School of Physics and Astronomy, The University of Edinburgh — Titanium alloys exhibit three distinct crystal structures: alpha, beta and omega. For various applications alloying elements can be used to stabilize the desired phase. While alloy designers have well established rules of thumb, rigorous theory for non-equilibrium single-phase crystal stability is less well established. Here we tackle this problem using electronic structure calculations. We use two different methods based on density functional theory with pseudopotentials and plane waves, with either explicit atoms or the virtual crystal approximation (VCA). The former is highly reliable, while the latter makes a number of drastic assumptions that typically lead to poor results. Surprisingly, the agreement between the methods is good, showing that the approximations in the VCA are not important in determining the phase stability and elastic properties. This allows us to generalize, showing that the single-phase stability can be related linearly to the number of d-electrons, independent of the actual alloying elements or details of their atomistic-level arrangement. This leads to a quantitative measure of beta-stabilization for each alloying transition metal.

9:24AM H23.00008 Structural properties and phase stability of Ti alloys containing V and Cr by first-principles calculation , LINGGANG ZHU, BENGT TEGNER, GRAEME ACKLAND, SUPA, School of Physics and Astronomy, The University of Edinburgh, QING-MIAO HU, RUI YANG, Shenyang National Laboratory for Materials Sciences, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China — We apply the first-principles plane-wave pseudopotential method and virtual crystal approximation (VCA), to investigate structural properties and phase stability of ternary titanium alloy Ti-V-Cr. The lattice parameters of the alloy vary almost linearly with the number of d electrons in spite of the different ratio of V to Cr, which agrees with the available experimental results. At 0K, we find that an extra 0.4 electrons per atom can stabilise the beta Ti-V-Cr. Debye approximation is used to consider the temperature effect, and it is found that at 973K, with an extra 0.1 d electron per atom, the beta Ti-V-Cr can be stabilised, compared with 0.15-0.20 d electron required experimentally at 973K. It is shown that V and Cr move the Fermi energy to lower values of the density of the states of the beta phase, which accounts for the stabilisation effect.

9:36AM H23.00009 Dynamics of twinning dislocations in Tantalum¹ , LUIS SANDOVAL, MICHAEL SURH, ALEXANDER CHERNOV, DAVID RICHARDS, Condensed Matter and Materials, Physical and Life Science Directorate, Lawrence Livermore National Laboratory — Twinning is one of the major deformation modes of plastic deformation in crystals, being particularly important in systems under extreme conditions of low temperature or high strain rates. Despite decades of work, the nucleation and growth mechanisms of twinning are still poorly understood, especially in bcc metals. Nucleation of twinning dislocations loops on the coherent twin boundary has been considered a principal mechanism of growth of deformation twins. We have used molecular dynamics simulation to study the behavior of twinning dislocations in Tantalum, in particular the dependence of dislocation velocities on shear stress and temperature. The dynamics of edge and screw twinning dislocations is isolated and analyzed. Finally we show how kinetic parameters extracted from these simulations help inform a multiscale strength model for Tantalum that includes both twinning and slip as deformation mechanisms in the regime of high strain rates.

¹This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 (LLNL-ABS-513469).

9:48AM H23.00010 Vacancy Assisted Climb in Continuum Dislocation Dynamics , MATTHEW BIERBAUM, YONG CHEN, WOOSONG CHOI, JAMES SETHNA, Cornell University — Using a mesoscale continuum theory of dislocation dynamics, we study the physical effects of vacancy assisted climb. New physics emerges at high temperatures where dislocations are also able to move in the climb direction due to the absorption and emission of vacancies. We investigate this high temperature behavior using our minimal continuum dislocation dynamics model, which produces fractal cell structures in 2 and 3 dimensions. By coupling the dislocation density to a vacancy field we are able to study the effects of vacancies on diffusion-limited dislocation motion. We calibrate our model using measurements of climb velocities for straight, parallel dislocations and check the limit of no climb by freezing out vacancy motion. We use our model to explore applications of vacancy assisted climb, including dislocation creep and absorption of dislocations at grain boundaries.

10:00AM H23.00011 Stacking-fault energy and anti-Invar effect in FeMn alloys at high temperature , ANDREI REYES-HUAMANTINCO¹, PETER PUSCHNIG, CLAUDIA AMBROSCH-DRAXL, Chair of Atomistic Modelling and Design of Materials, University of Leoben, Austria, OLEG PEIL, I. Institute for Theoretical Physics, Hamburg University, Germany, ANDREI RUBAN, Applied Material Physics, Royal Institute of Technology, Stockholm, Sweden — High-Mn steels (20-30at%Mn, 2-4wt%Si and Al) are of interest for the automotive industry due to their outstanding mechanical properties. Their deformation behavior has been empirically correlated to the stacking-fault energy (SFE), an important quantity in steel design that can be calculated *ab-initio*. Using state-of-the-art methods within density-functional theory together with Monte Carlo simulations, we calculate the free energy of the Fe-22.5at%Mn binary alloy between 300-800 K. Experimentally, the alloy is completely random and in the paramagnetic state, which we model via the coherent potential approximation and the disordered local moment approach, respectively. We treat magnetic excitations by including longitudinal spin-fluctuations and find that the FeMn alloy is an itinerant paramagnet. Our calculations confirm the experimentally observed strong magneto-volume coupling, realized in the anti-Invar behavior. We then obtain the structural stability and the SFE from free energy differences and find very good agreement with measurements. Our results demonstrate that the interplay between magnetic excitations and the thermal lattice expansion is the main factor determining the anti-Invar effect, the *fcc-hcp* martensitic transformation temperature and the SFE.

¹Second Affiliation: Materials Center Leoben, Austria

10:12AM H23.00012 Microstructural and mechanical characterization of 0.2mass% Carbon content steel , SAJJAD TOLLABIMAZRAEHNO, Johannes Kepler University, Altenberger Str. 69, 4040 Linz, Austria, CHRISTIAN COMMENDA, None, GUENTER HESSER, Johannes Kepler University, Altenberger Str. 69, 4040 Linz, Austria, ANDREAS PICHLER, None, KURT HINGERL, Johannes Kepler University, Altenberger Str. 69, 4040 Linz, Austria — The microstructures of low carbon content steel are comprised of bainite, martensite, tempered martensite and retained austenite. These structures are obtained by different heat treatments. The effect of heat treatment on microstructure and mechanical properties were investigated using X-ray diffraction, focused ion beam - scanning electron microscope (FIB-SEM), electron backscatter diffraction (EBSD), and nanoindentation. The experimental misorientation distribution revealed most grain boundaries had misorientation range between 50° and 60°. The lattice relation between bainite and parent austenite is Kurdjumov-Sachs ($\langle 111 \rangle_B \parallel \langle 110 \rangle_A$). FIB-SEM images and nanoindentation were revealed the grain size can influence the hardness.

10:24AM H23.00013 ABSTRACT WITHDRAWN —

10:36AM H23.00014 Ab initio-based interatomic potentials for body-centered cubic refractory metals¹, MICHAEL FELLINGER, HYOUNGKI PARK, JEREMY NICKLAS, JOHN WILKINS, The Ohio State University — A fundamental understanding of transformation and deformation processes in the bcc refractory metals (V, Nb, Ta, Mo, and W) is vital for designing new bcc-based commercial alloys with desired properties. Such an understanding is aided by computational methods capable of reaching length and time scales needed for meaningful simulations of phase transformations and extended defects responsible for plastic deformation. Classical interatomic potentials are indispensable for simulating such phenomena inaccessible to first-principles methods. We develop accurate and robust embedded-atom method (EAM) [1] and modified-EAM (MEAM) [2] potentials for the bcc metals by fitting the model parameters to accurate first-principles data. The potentials are applicable for studying mechanical and thermodynamic properties, yielding excellent agreement with both experiments and first-principles calculations.

[1] M. S. Daw and M. I. Baskes, Phys. Rev. Lett. 50, 1285 (1983).

[2] M. I. Baskes, Phys. Rev. Lett. 59, 2666 (1987).

¹Supported by DOE-Basic Energy Sciences, Division of Materials Sciences (DE-FG02-99ER45795). Computational resources provided by OSC and NERSC.

10:48AM H23.00015 Influence of Nano-Alumina and Micro-Size Copper on Microstructure and Mechanical Properties of Magnesium Alloys AZ31, QUY BAU BOSLEY NGUYEN, SANDAR KHIN TUN, MANOJ GUPTA, National University of Singapore — In this paper, magnesium composites are synthesized through the addition of nano-alumina and micron size copper particulates in AZ31 magnesium alloy using the technique of disintegrated melt deposition. The simultaneous addition of Cu and nano-alumina particulates led to an overall improvement in physical, microstructural characteristics and mechanical response of AZ31. Small size and reasonably distributed second phases were formed. The 0.2% yield strength increased from 180 to 300 MPa (67%), while the ductility increased by almost 24%. The overall tensile properties assessed in terms of work of fracture improved by 66%. An attempt is made to correlate the tensile response of composites with their microstructural characteristics. The results suggest that these alloy composites have significant potential in diverse and wider engineering applications.

Tuesday, February 28, 2012 8:00AM - 11:00AM – Session H24 FIAP: Electrical and Thermal Properties of Semiconductors 256

8:00AM H24.00001 Electrical characterization of SiGeSn grown on Ge substrate using ultra high vacuum chemical vapor deposition, MO AHOUEJJA, University of Dayton, S. KANG, M HAMILTON, Y.K. YEO, Air Force Institute of Technology, ENP, WPAFB, OH, J. KOUVETAKIS, J. MENENDEZ, Arizona State University — There has been recently considerable interest in growing $\text{Si}_y\text{Ge}_{1-x-y}\text{Sn}_x$ alloys for the fabrication of photonic devices that could be integrated with Si technologies. We report temperature dependent Hall (TDH) measurements of the hole concentration and mobility from high quality p-type doped $\text{Si}_{0.08}\text{Ge}_{0.90}\text{Sn}_{0.02}$ layers grown on p-type doped Ge substrates using ultra high vacuum chemical vapor deposition. The TDH measurements show the hole sheet density remains constant at low temperatures before slightly decreasing and dipping at ~ 125 K. It then exponentially increases with temperature due to the activation of shallow acceptors. At temperatures above ~ 450 K, the hole sheet density increases sharply indicating the onset of intrinsic conduction in the SiGeSn and/or Ge layers. To extract the electrical properties of the SiGeSn layer alone, a parametric fit using a multi layer conducting model is applied to the measured hole concentration and mobility data. The analysis yields boron and gallium doping concentrations of $3 \times 10^{17} \text{ cm}^{-3}$ and $1 \times 10^{18} \text{ cm}^{-3}$ with activation energies of 10 meV and 11 meV for the SiGeSn layer and Ge substrate, respectively. Furthermore, a temperature independent hole sheet concentration of $\sim 5 \times 10^{15} \text{ cm}^{-2}$ with a mobility of $\sim 250 \text{ cm}^2/\text{Vs}$, which is believed to be due to an interfacial layer between the SiGeSn layer and the Ge substrate, is also determined.

8:12AM H24.00002 Informatic Strategies for Screening Electron Mobility of Candidate Semiconducting Materials¹, KIM FERRIS, Pacific Northwest National Laboratory, DUMONT JONES, Proximate Technologies, LLC. — While carrier transport properties are critical to semiconductor efficiency, screens for potentially new materials based upon mobility measurements can be problematic. In the early stages of materials development, measured electron mobilities are often unreliable indicators of their eventual performance and serve as a poor basis to assess the longer term potential of candidate materials. In this paper, we describe an information-based approach for estimating an effective upper limit, using the specific case of the II-VI semiconductors. The optical (polaron) electron mobility has been developed as a screening property, supported by informatic estimates of dielectric properties. This mobility represents a practical screen, providing an estimate of the potential bounding value at room temperature. Using this basis, partial screening criteria based on compositional factors can also be constructed.

¹The authors gratefully acknowledge financial support from U.S. Department of Homeland Security under Contract No. HSHQDC-08-X-00872.

8:24AM H24.00003 Measurement of Electron Effective Mass in $\text{GaAs}_{1-x}\text{Bi}_x$ ¹, BRIAN FLUEGEL, RAJEEV KINI², AARON PTAK, DAN BEATON, KIRSTIN ALBERI, ANGELO MASCARENHAS, National Renewable Energy Laboratory — Magnetic field and temperature dependent resistivity measurements on n-type $\text{GaAs}_{1-x}\text{Bi}_x$ epitaxially grown films show clear Shubnikov de Haas oscillations in the range $0 \leq x \leq 0.0088$. An overall decrease in the electron effective mass is observed for this range of compositions. Accounting for the known giant bandgap bowing of $\text{GaAs}_{1-x}\text{Bi}_x$, the measured changes in the electron effective mass are in qualitative agreement with perturbation theory applied to the known bandgap reduction for this alloy, confirming that bismuth mainly perturbs the valence band. The stronger compositional dependence of the measured masses is attributed to effects from the bismuth isolated state.

¹Research supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division under DE-AC36-08GO28308.

²Present address: Indian Institute of Science, Education, and Research, Thiruvananthapuram, Kerala, India

8:36AM H24.00004 Piezo-resistance in n -type $\text{Si}_{1-x}\text{Ge}_x$ alloys as a function of alloy composition and strain¹, FELIPE MURPHY-ARMANDO, STEPHEN FAHY, Tyndall National Institute, University College Cork — We use first-principles electronic structure methods[1,2] to predict the piezoresistance of n -type $\text{Si}_{1-x}\text{Ge}_x$ at various alloy compositions and strain configurations. The gauge factor, $G = d\rho/d\epsilon/\rho$, where ρ is resistivity and ϵ is strain, varies strongly with both composition and strain. Nonlinear changes in resistivity with strain may arise due to changing occupancy of the higher-conductance L valley relative to the lower-conductance Δ valley, coupled to a change in inter-valley alloy and phonon scattering. [1] F. Murphy-Armando and S. Fahy, J. Appl. Phys., accepted for publication (2011). [2] F. Murphy-Armando and S. Fahy, Phys. Rev. Lett., 97, 096606 (2006)

¹Work funded by Science Foundation Ireland

8:48AM H24.00005 Non-diffusive thermal conductivity in semiconductors at room temperature , ALEXEI MAZNEV, JEREMY JOHNSON, JEFFREY ELIASON, KEITH NELSON, AUSTIN MINNICH, KIMBERLEE COLLINS, GANG CHEN, Massachusetts Institute of Technology, JOHN CUFFE, TIMOTHY KEHOE, CLIVIA SOTOMAYOR TORRES, Catalan Institute of Nanotechnology — The “textbook” value of phonon mean free path (MFP) in silicon at room temperature is ~ 40 nm. However, a large contribution to thermal conductivity comes from low-frequency phonons with much longer MFPs. We find that heat transport in semiconductors such as Si and GaAs significantly deviates from the Fourier law at distances much longer than previously thought, ≥ 1 μm at room temperature and above. We use the laser-induced transient thermal grating technique in which absorption of crossed laser pulses in a sample sets up a sinusoidal temperature profile monitored via diffraction of a probe laser beam. By changing the period of the thermal grating we vary the thermal transport distance within the range ~ 1 -10 μm . In measurements performed on thin free-standing Si membranes and on bulk GaAs the thermal grating decay time deviates from the expected quadratic dependence on the grating period, thus providing model-independent evidence of non-diffusive transport. The simplicity of the experimental configuration permits analytical treatment of non-equilibrium phonon transport with the Boltzmann transport equation. Our analysis shows that at small grating periods the effective thermal conductivity is reduced due to diminishing contributions of “ballistic” low-frequency phonons with long MFPs.

9:00AM H24.00006 Thermal conductivity and isotope effect in wide bandgap semiconductors , LUCAS LINDSAY, THOMAS REINECKE, NRL, Washington, DC, ENRICO BELLOTTI, Electrical and Computer Engineering Department, Boston University, DAVID BROIDO, Department of Physics, Boston College — We have calculated the lattice thermal conductivity, k , of wurtzite InN, GaN, and AlN using an exact numerical solution of the phonon Boltzmann transport equation and *ab initio* calculations of interatomic force constants. We find good agreement with experiment for the thermal conductivities around and above room temperature. The large frequency gap between the acoustic and the optic phonon branches in these materials limits anharmonic phonon scattering leading to large enhancements to k with isotopic enrichment. We comment on the roles of various phonon scattering mechanisms on k in these wide bandgap semiconductors.

9:12AM H24.00007 Conductance beyond the Landauer limit and charge pumping in quantum wires driven by linearly polarized radiation , JAY SAU, TAKUYA KITAGAWA, BERTRAND HALPERIN, Department of Physics, Harvard University, Cambridge, MA 02138 — Periodically driven systems, which can be described by Floquet theory, have been proposed to show characteristic behavior that is distinct from static Hamiltonians. Floquet theory proposes to describe such periodically driven systems in terms of states that are indexed by a photon number in addition to the usual Hilbert space of the system. In this work, we propose a way to measure directly this additional state by the measurement of the conductance of a single channel quantum point contact. Specifically, we show that a single channel wire augmented with a grating structure when irradiated with microwave radiation can show a DC conductance above the limit of one conductance quantum set by the Landauer formula. Another interesting feature of the proposed system is that being non-adiabatic in character, it can be used to pump a photo-current even with linearly polarized light. This circumvents the topological restrictions of adiabatic pumping, which necessitate the use of circularly polarized light. J.S. thanks the Harvard Quantum Optics center for support.

9:24AM H24.00008 Positive and Negative Coulomb Drag in a 1D Quantum Circuit , DOMINIQUE LAROCHE, McGill University and Sandia National Laboratories, GUILLAUME GERVAIS, McGill University , MIKE LILLY, JOHN RENO, Sandia National Laboratories — We report Coulomb drag measurements between tunable vertically-coupled quantum wires. The wires are fabricated in a GaAs/AlGaAs double quantum well heterostructure with a 15 nm barrier separating the quantum wells. The Coulomb drag signal is mapped out versus the number of subbands occupied in each wire, and regions of both positive and negative drag are observed (D. Laroche *et. al.* Nature Nanotechnology, doi:10.1038/nnano.2011.182). The observation of negative Coulomb drag at a high one-dimensional electronic density is not predicted by the usual momentum-transfer model for Coulomb drag and shows that the existing picture of the drag effect in one-dimension is incomplete. In order to clarify the origin of this negative signal, temperature dependencies of the Coulomb drag are presented both in the positive and in the negative drag regimes. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:36AM H24.00009 Phonon Mediated Optical Stark Effect for Organic-Semiconductor Heterostructures¹ , QUE HUONG NGUYEN, Marshall University — The system of macroscopic equations of hybrid excitons, photons and phonon is investigated in order to model the optical Stark effect for the hybrid systems with combination of semiconductor and organic materials. The unique properties of the hybrid system will allow tuning the system to get the most preferable outcomes. One of the key points is to study the interaction of different components of the system with each other to get the condition to facilitate the observation of phonon and the phonon-mediated Stark effect.

¹The support from NASA Seed Grant Award 211012 is acknowledged.

9:48AM H24.00010 Electron phonon coupling and carrier lifetimes in III-nitride ternary semiconductors¹ , NANDAN TANDON, P.G. KASSEBAUM, L.R. RAM-MOHAN, Physics Department, Worcester Polytechnic Institute, Worcester, MA, USA — III-nitride semiconductors have a large bandgap and find applications in high power devices, in which the thermal management of energy generated becomes a key issue. The transfer of energy from the energetic carriers to the lattice is determined by the electron-phonon coupling for the crystal. In this work, we present our results on the electron-phonon coupling in ternary and quaternary semiconductors. The full phonon dispersion and electron-phonon coupling is determined using *ab-initio* methods. We then evaluate the carrier lifetimes for the emission of LO phonons by including the full zone and not only the zone center phonons. We expect that the treatment of the electron-phonon coupling effects over the full Brillouin zone could be critical for III-nitride thermal management, and will be directly compared to the results where only the zone center phonons are considered.

¹This work was supported by AFRL/DARPA under contract FA8650-10-1-7046, and by MIT-Lincoln Labs/DARPA.

10:00AM H24.00011 Vibrational structure of defect luminescence bands in GaN from electronic structure calculations , AUDRIUS ALKAUSKAS, CHRIS G. VAN DE WALLE, Materials Department, University of California Santa Barbara, CA 93106-5050 — Optical methods are among the most powerful to characterize defects in materials. The study of optical signatures based on state-of-the-art electronic structure methods is therefore very important. In this work we investigate the vibrational structure of luminescence bands pertaining to deep defect levels in GaN. Since luminescence lineshapes depend sensitively on defect geometries and vibrational frequencies, these should be described accurately. The latter is achieved through the use of hybrid density functionals. Both quasi-localized and bulk phonons are included in our description. In the case of transitions accompanied by very large lattice relaxations, anharmonic effects become sizeable, and these are also accounted for. For the defects studied a very good agreement with available experimental data is achieved. For instance, in the case of wide luminescence bands the resulting line widths are within 0.05 eV of the experimental values. This work was supported by the Swiss NSF and by NSF.

10:12AM H24.00012 Ultrafast Carrier Dynamics in GaAs(110) Studied by Time- and Angle-Resolved Photoelectron Spectroscopy, SHUOLONG YANG, JONATHAN SOBOTA, Stanford University, PATRICK KIRCHMANN, Fritz Haber Institute of the Max Planck Society, ZHI-XUN SHEN, Stanford University — Ultrafast carrier dynamics in GaAs is of particular importance to optoelectronic devices and solar cell technologies. We employ Time- and Angle-Resolved Photoelectron Spectroscopy to elucidate the dynamics of both the occupied and unoccupied states of GaAs(110) upon femtosecond infrared laser excitation. We observe in the conduction band an optically excited population and energy shift, which both decay in ~ 10 ps. The valence band also exhibits energy shifting dynamics which encompasses multiple temporal regimes. More intriguingly, valence band dynamics are also observed for negative pump-probe delays. We explain these observations by a carrier-transport-induced electrostatic potential change within a Drude-like picture.

10:24AM H24.00013 Intraexcitonic Autler-Townes effect in terahertz-driven semiconductor quantum wells, M. WAGNER, D. STEHR, H. SCHNEIDER, S. WINNERL, Helmholtz-Zentrum Dresden-Rossendorf HZDR, Dresden, Germany, A. ANDREWS, S. SCHARTNER, G. STRASSER, TU Vienna, Austria, M. HELM, HZDR — When a two-level system is resonantly driven by intense light non-perturbative phenomena such as Rabi oscillations and their frequency equivalent, the AC Stark or Autler-Townes effect, can be observed. The latter one manifests itself in an absorption line splitting where the magnitude is linear in the light field strength and where the symmetry of the splitting is determined by the detuning from resonance. Known from molecular spectroscopy [1], the effect has also been observed in solid state structures with its much broader line widths, e.g. for intersubband transitions [2]. Here, we present the first unambiguous evidence of this effect in undoped GaAs/AlGaAs quantum wells using the hydrogen atom like intraexcitonic 1s and 2p states of the heavy-hole exciton. These states with a transition energy of 9 meV are resonantly coupled by strong terahertz light from a free-electron laser. For low fields our findings are qualitatively explained by a simple two-level model whereas deviations occur in the 10 kV/cm field range where the rotating-wave approximation of the simplified model breaks down and exciton ionization occurs. Due to the small Rydberg energy we can easily reach a highly non-trivial regime where the Rabi energy and the transition energy become comparable to the photon energy.

[1] S. H. Autler and C. H. Townes, Phys. Rev. 100, 703 (1955).

[2] S. G. Carter et al., Science 310, 651 (2005).

[3] M. Wagner et al., Phys. Rev. Lett. 105, 167401 (2010).

10:36AM H24.00014 Raman Spectroscopy and Scanning Electron Microscopy of the Bismuth Sillenites $\text{Bi}_{25}\text{InO}_{39}$ and $\text{Bi}_{25}\text{FeO}_{39}$ ¹, DANIEL J. ARENAS, THEO JEGOREL, LEV GASPAREOV, University of North Florida, HIDEO KOHNO, Osaka University, CATALIN MARTIN, DAVID B. TANNER, University of Florida, MICHAEL W. LUFASO, University of North Florida — The Raman spectrum of $\text{Bi}_{25}\text{InO}_{39}$, a new type of bismuth sillenite, is reported along with the spectra of $\text{Bi}_{25}\text{FeO}_{39}$. Their spectra are remarkably similar to each other and to other bismuth sillenites reported in the literature. The similarities show that the new samples were successfully grown in the sillenite structure. The parameters of each Raman mode were obtained by fitting the spectra to a Lorentzian oscillator model, and the modes were assigned to symmetry-allowed modes of the I23 space group. The assignments were made by comparison to other materials with the sillenite structure. Scanning Electron Microscope images of the samples are also presented.

¹Work at UNF was supported by NSF under Grant No. DMR-0805073. Work at UF was supported by the US DOE through contract DE-FG02-02ER45984.

10:48AM H24.00015 Two-dimensional Fourier-Transform spectra of PbS semiconductor quantum dots, DENIS KARAISKAJ, PRASENJIT DEY, JASON BYLSMA, Department of physics, University of South Florida — Investigating the correlations of multiple excitons in semiconductor quantum dots is a challenging many-body problem that has drawn considerable experimental and theoretical attention over the last two decades. Nonlinear four-wave mixing experiments have long been known to provide direct probes for the many-body effects in the ultrafast dynamics of excitons in semiconductor nanostructures. With the advent of two-dimensional Fourier-transform (2DFT) spectroscopy many-body contributions can be isolated and identified. 2DFT spectra of colloidal quantum dots will be presented, providing new understanding of the role of many-body interactions in the excitonic decoherence of these nanomaterials.

Tuesday, February 28, 2012 8:00AM - 11:00AM —

Session H25 DCOMP GSCCM DMP: Focus Session: Simulation of Matter at Extreme Conditions - Shock Compression of Metals 257A

8:00AM H25.00001 Invariance of the Dissipative Action at Ultrahigh Strain Rates above the Strong Shock Threshold¹, JONATHAN CROWHURST, MICHAEL ARMSTRONG, KIMBERLY KNIGHT, JOSEPH ZAUG, ELAINE BEHYMER, Lawrence Livermore National Laboratory — We have directly resolved shock structures in pure aluminum in the first few hundred picoseconds subsequent to a dynamic load, at peak stresses up to 43 GPa and strain rates of in excess of 10^{10} s^{-1} . For strong shocks we obtain peak stresses, strain rates, and rise times. From these data, we directly validate¹ the invariance² of the dissipative action in the strong shock regime, and by comparing with data obtained at much lower strain rates show that this invariance is observed over at least 5 orders of magnitude in the strain rate. Over the same range, we similarly validate the fourth-power scaling of strain rate with peak stress (the Swegle-Grady relation). 1. J. C. Crowhurst, M. R. Armstrong, K. B. Knight, J. M. Zaug, E. M. Behymer, Phys. Rev. Lett. 107, 144302 (2011). 2. D. E. Grady, J. Appl. Phys. 107, 013506 (2010). This work was also supported by the EFree, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Grant No. DESC0001057.

¹This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344 with Laboratory directed Research and Development funding (11ERD039)

8:12AM H25.00002 Ultrashort elastic and plastic shock waves in nickel generated by femtosecond laser pulses, NAIL INOGAMOV, Landau Institute for Theoretical Physics, BRIAN DEMASKE, VASILY ZHAKHOVSKY, University of South Florida, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — The structure and evolution of ultrashort shock waves generated by femtosecond laser pulses in thin nickel films were investigated by molecular dynamics and two-temperature hydrodynamics simulations. Ultrafast laser energy deposition results in the formation of a highly-pressurized 100-nm-thick layer below the surface of the film. Relaxation of the stress-confined state leads to the creation of a strong compression wave that later transforms into an ultrashort shock wave. Analysis of experimental data shows that such a shock wave, generated by low absorbed laser fluence, can exhibit a pure elastic structure despite an amplitude exceeding the conventional Hugoniot elastic limit. For absorbed fluences above $\sim 0.6 \text{ J/cm}^2$, two independent processes of elastic and plastic wave breaking are observed with the elastic precursor appearing before formation of the plastic wave. It is found that the amplitude of the elastic precursor is almost independent of the absorbed fluence, but closely related to the pressure at the melting front. The decay rate of the plastic wave amplitude is much higher than that of the elastic wave, which may result in the complete disappearance of the plastic wave within the metal film.

8:24AM H25.00003 Molecular dynamics simulations of steady shock waves in nickel, BRIAN DEMASKE, VASILY ZHAKHOVSKY, University of South Florida, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — Shock waves in single-crystal nickel samples were investigated by molecular dynamics (MD) simulations. Standard piston simulations were used to investigate the elastic-plastic split-shock-wave regime, whereas regimes having a single steady shock-wave structure were studied by a novel moving window (MW-MD) technique. Two distinct regimes were investigated, including the regimes of split elastic and plastic shock waves and the steady two-zone elastic-plastic single wave. Split shock waves were shown to form at moderate piston velocities out of a metastable high-pressure elastic state that decays into a two-wave structure consisting of a slow plastic wave and fast elastic precursor. At higher piston velocities, the plastic wave overtakes the elastic precursor but does not overrun it. Instead, both waves were found to move in tandem with the same average speed while maintaining a finite, and in some cases strongly fluctuating, separation width that may extend to several microns. The dependence of shock wave structure on crystallographic orientation and concentration of defects was investigated.

8:36AM H25.00004 A Molecular dynamics study of a Richtmyer-Meshkov instability¹, FRANK CHERNE, GUY DIMONTE, TIMOTHY GERMANN, VIRGINIE DUPONT, Los Alamos National Laboratory — We simulated a single-mode Richtmyer-Meshkov instability (RMI) using the SPaSM (Scalable Parallel Short-range Molecular-dynamics) code on the RoadRunner supercomputer and its Cerrillos counterpart. The simulations consisted of approximately 60 million atoms shocked along the $\langle 111 \rangle$ direction. The single crystal simulations had a sinusoidal groove with a wavelength of 257 nm. We conclude from the simulations that the RMI interfaces shows an inversion for most of the conditions we studied. For certain amplitudes and stresses, we observe the spike saturating. Simulations have been carried out at shock strengths both above and below the melt transition. A discussion of the spike and bubble characteristics will be discussed.

¹Support for this work was done under US DOE contract DE-AC52-06NA25396.

8:48AM H25.00005 Orientation dependence of shock-induced melting in crystalline aluminum, IVAN OLEYNIK, MIKALAI BUDZEVICH, VASILY ZHAKHOVSKY, University of South Florida, CARTER WHITE, Naval Research Laboratory — The complete evolution of metastable states during shock-induced solid-liquid phase transitions in crystalline aluminum was observed in moving window molecular dynamics simulations. The orientation-dependent transition pathways towards orientation-independent final equilibrium states include both “cold melting” followed by resolidification in $[110]$ - and $[111]$ -oriented shock waves, and crystal overheating followed by melting in $[100]$ shock waves. Such orientation-dependent dynamics of solid-liquid phase transitions takes place within an extended zone up to hundreds of nanometers behind the shock front, which makes it accessible for experimental observation.

9:00AM H25.00006 Strain rate influence on the Hall-Petch effect in Cu, VIRGINIE DUPONT, TIMOTHY C. GERMANN, Los Alamos National Laboratory — The increased strength of materials with a decreasing grain size has been known for several decades as the Hall-Petch effect. This trend is true down to a specific grain size below which the strength starts decreasing again, due to a change in the underlying plasticity mechanisms caused by the increased grain boundary network density. We are interested in the strain rate influence on the Hall-Petch and “reverse Hall-Petch” effects. We use molecular dynamics simulations to study polycrystalline samples of copper of different grain sizes between 5 nm and 30 nm, and under uniaxial compression at a wide range of strain rates (10^8 to 10^{11} s⁻¹). We verify that the yield stress of the material increases with the strain rate, due to the time scale required to generate plasticity. Moreover, we observe that the grain size for which the yield stress is highest depends on the strain rate studied. These results are of particular importance for high strain rate loading conditions, such as shock compression.

9:12AM H25.00007 High Strain Rate and Shock-Induced Deformation in Metals¹, RAMON RAVELO², University of Texas-El Paso — Large-scale non-equilibrium molecular Dynamics (MD) simulations are now commonly used to study material deformation at high strain rates (10^9 - 10^{12} s⁻¹). They can provide detailed information— such as defect morphology, dislocation densities, and temperature and stress profiles, unavailable or hard to measure experimentally. Computational studies of shock-induced plasticity and melting in fcc and bcc single, mono-crystal metals, exhibit generic characteristics: high elastic limits, large directional anisotropies in the yield stress and pre-melting much below the equilibrium melt temperature for shock wave propagation along specific crystallographic directions. These generic features in the response of single crystals subjected to high strain rates of deformation can be explained from the changes in the energy landscape of the uniaxially compressed crystal lattice. For time scales relevant to dynamic shock loading, the directional-dependence of the yield strength in single crystals is shown to be due to the onset of instabilities in elastic-wave propagation velocities. The elastic-plastic transition threshold can accurately be predicted by a wave-propagation stability analysis. These strain-induced instabilities create incipient defect structures, which can be quite different from the ones, which characterize the long-time, asymptotic state of the compressed solid. With increase compression and strain rate, plastic deformation via extended defects gives way to amorphization associated with the loss in shear rigidity along specific deformation paths. The hot amorphous or (super-cooled liquid) metal re-crystallizes at rates, which depend on the temperature difference between the amorphous solid and the equilibrium melt line. This plastic-amorphous transition threshold can be computed from shear-waves stability analyses. Examples from selected fcc and bcc metals will be presented employing semi-empirical potentials of the embedded atom method (EAM) type as well as results from density functional theory calculations.

¹Part of this work was supported by the U.S. Department of Energy under contract DE-AC52-06NA25396.

²Computational Physics Division, Los Alamos National Laboratory

9:48AM H25.00008 Metallurgical Effects Upon the Shock Response of Tantalum: Cold Work and Dilute Alloying, JEREMY MILLETT, AWE — The response of the body centred cubic metal tantalum to shock loading has been studied for several decades, due to its use by the military in explosively formed projectiles. It can also be considered as an ideal body centred cubic metal, thus rendering it ideal for studies of fundamental mechanical and microstructural behaviour. Previous studies on well controlled, annealed specimens has shown that deformation is controlled by the motion of rather than the generation of $a/2\langle 111 \rangle\{110\}$ screw dislocations in straight segments, which result in little if any post shock hardening. In situ-shear strength measurements have also shown a significant strength reduction behind the shock front, suggesting that the motion of these dislocations acts as a stress relief mechanism. Similar effects have also been noted in tungsten and its alloys, but very recently, measurements in niobium and molybdenum show shear strength to be near constant behind the shock front. Other factors, such as variation of Peierls stress effecting ease of dislocation generation and the propensity to twin also have a strong effect upon the shock response. In this presentation, we return to tantalum, investigating the differences in shock response between a low dislocation density (annealed) and high dislocation density (cold rolled) material. We also examine the effects of dilute alloying through the addition of 2.5wt% tungsten to tantalum. Results are discussed in terms of the shear strength and its variation with time behind the shock front.

10:00AM H25.00009 High Strain Rate Behavior of Nanoporous Tantalum¹, CARLOS J. RUESTES, Instituto de Ciencias Basicas, Univ. Nac. Cuyo., EDUARDO M. BRINGA, CONICET - Instituto de Ciencias Basicas, Univ. Nac. Cuyo., ALEXANDER STUKOWSKI, Lawrence Livermore National Laboratory, JOAQUIN F. RODRIGUEZ NIEVA, Massachusetts Institute of Technology, GRACIELA BERTOLINO, CONICET - Centro Atomico Bariloche, YIZHE TANG, MARC A. MEYERS, University of California, San Diego — Nano-scale failure under extreme conditions is not well understood. In addition to porosity arising from mechanical failure at high strain rates, porous structures also develop due to radiation damage. Therefore, understanding the role of porosity on mechanical behavior is important for the assessment and development of materials like metallic foams, and materials for new fission and fusion reactors, with improved mechanical properties. We carry out molecular dynamics (MD) simulations of a Tantalum (a model body-centered cubic metal) crystal with a collection of nanovoids under compression. The effects of high strain rate, ranging from $10^7 s^{-1}$ to $10^{10} s^{-1}$, on the stress strain curve and on dislocation activity are examined. We find massive total dislocation densities, and estimate a much lower density of mobile dislocations, due to the formation of junctions. Despite the large stress and strain rate, we do not observe twin formation, since nanopores are effective dislocation production sources. A significant fraction of dislocations survive unloading, unlike what happens in fcc metals, and future experiments might be able to study similar recovered samples and find clues to their plastic behavior during loading.

¹Research funded by PICT2008-1325, PICT2009-0092 and SeCTyP.

10:12AM H25.00010 High-Pressure Strength Determination via Quasi-Elastic Optimization Analysis, JUSTIN BROWN, TRACY VOGLER, JIM ASAY, Sandia National Laboratories — The analysis of unloading profiles from ramp wave experiments on Sandia's Z machine for the purposes of extracting strength information can be greatly influenced by the presence of a window. An impedance mismatch between the sample and the window generates a reflected ramp wave which perturbs the incoming wave, particularly at later times when, during unloading, the material strength becomes evident. In an effort to analyze the waveforms for an accurate estimate of the strength, the experimental data is coupled with optimized numerical simulations. Simulations were performed with LASLO, a one-dimensional magneto-hydrodynamics code. The deviatoric response was calculated using a modified rate-independent Steinberg - Guinan model in which a quasi-elastic response was implemented during unloading by linearly varying the shear modulus. A best fit of relevant parameters in this strength model along with the magnetic field at the drive surface were estimated over the course of thousands of simulations using the Dakota optimization package. These results may then be used to estimate the in situ wave profiles from which the strength can be extracted. Initial results will be presented for ramp wave compression of tantalum with a lithium fluoride window to peak stresses of ~ 120 GPa. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

10:24AM H25.00011 Calculation of diffusivity and viscosity of Al-Cu molten mixtures using molecular dynamics¹, ROBERT RUDD, WILLIAM CABOT, KYLE CASPERSEN, JEFF GREENOUGH, TOMORR HAXHIMALI, PAUL MILLER, DAVID RICHARDS, FREDRICK STREITZ, Lawrence Livermore National Lab — We use equilibrium classical molecular dynamics and Green-Kubo techniques to calculate the diffusivity and viscosity of Al-Cu molten mixtures. We calculate both the self-diffusivities and the Maxwell-Stefan diffusivities, and evaluate the validity of the Darken relation for this system. We compare the results with those from experiments reported in the literature. We have constructed an analytic model that is fit to the MD results. This transport model has been implemented in a continuum hydrodynamics code. Both the continuum code and extremely large-scale molecular dynamics have been used to simulate the development of vortices due to the Kelvin-Helmholtz instability in a shear layer, and we discuss the results of that comparison.

¹This work was performed under the auspices of the US Dept. of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344.

10:36AM H25.00012 Mechanical Behaviour of Light Metal Alloys at High Strain Rates. Computer Simulation on Mesoscale Levels, VLADIMIR SKRIPNYAK, EVGENIYA SKRIPNYAK, Tomsk State University, LOTHAR W. MEYER, NORMAN HERZIG, Nordmetall GmbH, NATALIYA SKRIPNYAK, Tomsk State University, TOMSK STATE UNIVERSITY TEAM, NORDMETALL GMBH TEAM — Researches of the last years have allowed to establish that the laws of deformation and fracture of bulk ultrafine-grained and coarse-grained materials are various both in static and in dynamic loading conditions. Development of adequate constitutive equations for the description of mechanical behavior of bulk ultrafine-grained materials at intensive dynamic influences is complicated in consequence of insufficient knowledge about general rules of inelastic deformation and nucleation and growth of cracks. Multi-scale computational model was used for the investigation of deformation and fracture of bulk structured aluminum and magnesium alloys under stress pulse loadings on mesoscale level. The increment of plastic deformation is defined by the sum of the increments caused by a nucleation and gliding of dislocations, the twinning, meso-blocks movement, and grain boundary sliding. The model takes into account the influence on mechanical properties of alloys an average grains size, grain sizes distribution of and concentration of precipitates. It was obtained the nucleation and gliding of dislocations caused the high attenuation rate of the elastic precursor of ultrafine-grained alloys than in coarse grained counterparts.

10:48AM H25.00013 Estimation of spectral characteristics of particles ejected from free surfaces of metals and liquids under shock wave effect, ALLA GEORGIEVSKAYA, VICTOR RAEVSKY, RFNC-VNIIEF — The authors present approximated relations for estimations of the basic characteristics of flow of particles ejected from free surface of substance after shock wave arrival (shock-wave ejecta). The problem is considered as a particular case of the Richtmayer-Meshkov instability. Periodic perturbations on free surface, which are sinusoidal and having triangular shape, are considered as the initial perturbations causing formation of jets and particles. The medium is assumed to be liquid with surface tension. The role of viscosity is estimated. In the work, the authors obtained equations for estimations of the following characteristics of the particle flow: - dependence of integral mass of ejected substance on time; - space-time distribution of density of ejected substance; - space-time distribution of velocity of ejected substance; - distribution of particles in sizes; - correlation of sizes and velocities of particles. Estimations are presented concerning influence of shear strength and plasticity on substance ejecta. Analytical relations are compared with results of numerical calculations and experiments."

Tuesday, February 28, 2012 8:00AM - 11:00AM —
Session H26 DCOMP GSNP: Focus Session: Friction, Fracture and Deformation Across Length Scales - Friction Across Length Scales 257B

8:00AM H26.00001 Rock Friction from the Nanoscale to the San Andreas Fault, DAVID L. GOLDSBY, Brown University — Nucleation of earthquakes (EQs) and the resistance of faults to shearing during EQs are determined by nano-to-micro- scale frictional processes that occur on tectonic-scale faults. A first-order observation from rock-friction studies is that of ageing, i.e., the linear increase in friction with the log of the time of stationary contact, manifest as a positive or negative dependence of friction on sliding rate. A necessary condition for EQ nucleation is a negative rate dependence of friction. In spite of the success of friction 'laws' which encapsulate the rate and time dependences of friction in fitting experimental data and reproducing natural phenomena in EQ models, these laws lack a physical basis. Atomic force microscope (AFM) experiments on silica-silica contacts explore the physics of ageing, more specifically increases in adhesion of nanometers-sized contacts with time (Li et al., *Nature*, 2011). The experiments reveal prominent ageing which increases with humidity, as in rock friction tests, without increases in contact area due to creep (the canonical explanation for ageing in rock-friction tests). Ageing in the AFM tests is in fact much larger than in rock-friction tests, a discrepancy explained with a simple multi-asperity contact model. At EQ slip rates (≥ 1 m/s) a variety of dynamic fault-weakening mechanisms may decrease the shear resistance of faults, which would have important consequences for the magnitudes of EQ stress drops, strong ground motions and accelerations, for the EQ energy budget, and for the state of stress on faults. Experiments on rocks found in the Earth's crust for slip rates up to ~ 0.4 m/s over ~ 40 mm of slip, reveal a dramatic $1/V$ decrease in frictional strength above a characteristic weakening velocity V_w of ~ 0.1 m/s (Goldsby and Tullis, *Science*, 2011). Friction is also revealed to be a nearly pure function of slip rate, i.e., it adjusts to the ambient slip rate over only microns of slip. The observations are explained by 'flash heating', whereby microscopic asperity contacts become intensely frictionally heated and weakened above V_w . Dramatically lower friction due to flash heating may explain why heat flow along active faults like the San Andreas Fault is much lower than expected. Strong velocity-weakening friction and the rapid strength recovery with decreasing slip rate from flash heating may explain why EQ ruptures propagate as slip pulses rather than as cracks.

8:36AM H26.00002 Avalanche Distributions and the Effect of Inertia in Strained Amorphous Solids¹, K. MICHAEL SALERNO, MARK O. ROBBINS, Johns Hopkins University, CRAIG MALONEY, Carnegie Mellon University — We present results from two and three-dimensional simulations of a disordered, binary Lennard-Jones solid under quasi-static, steady-state shear. The solid responds to the applied shear strain with bursts of particle movement and plasticity. The energy E of these avalanches spans a wide range and follows a power-law distribution $N(E) \propto E^{-\tau}$ with three distinct exponents, depending on the importance of inertia. In the limit of overdamped dynamics, or no inertia, we find $\tau \approx 0.8$, consistent with previous energy minimization simulations. As inertia becomes more important, the system approaches an unstable critical point where $\tau = 1$. In the underdamped limit, where inertia plays a large role, the distribution of avalanches follows a power-law with exponent $\tau = 1.4$ with an excess of system-spanning events. The three regimes have distinct finite-size-scaling exponents. The fact that consistent exponents are found in two and three dimensions indicates that both may be in the mean-field limit. Spatial correlations in avalanches under different damping regimes will be contrasted.

¹Supported by NSF DMR-1006805

8:48AM H26.00003 Dynamic Phase Diagram and Jamming for Driven Dislocation Assemblies, CHARLES REICHHARDT, CYNTHIA REICHHARDT, CAIZHI ZHOU, IRENE BEYERLEIN, Los Alamos National Laboratory — By using large scale numerical simulations for driven dislocations in 2D, we show that the resulting dynamic phase diagram has the same features found for driven vortex matter and charge density waves in the presence of random disorder. For low loads the system is pinned or jammed. Just above the onset of motion we observe strong velocity fluctuations with $1/f$ noise properties and bimodal velocity distributions associated with rapidly fluctuating dislocation structures. At higher loads there is a dynamic reordering into a state of partially ordered domain walls with a pronounced drop in the velocity fluctuations as well as a reduction in the noise power. These features have all the hallmarks observed for dynamic phases such as the pinned, fluctuating, and dynamical reordering transitions found in driven vortex matter. We discuss the implications of work in terms of dynamic phase transitions at the onset of motion and the onset of the dynamical ordering.

9:00AM H26.00004 Scale invariant avalanches: a critical confusion, OSVANNY RAMOS, Laboratoire PMCN, University Lyon 1, 43 bd. du 11 novembre 1918, 69622 Villeurbanne, France — In the last decades considerable efforts have been devoted to understanding single events related to friction, fracture and unjamming transition, commonly denominated avalanches. However, in many different natural scenarios -from subcritical fracture to earthquake dynamics- these events are of all scales; a situation that has often been interpreted within the formalism of critical phenomena, and having as a relevant consequence the inherently unpredictability of scale-invariant avalanches. A revision of this interpretation which departs from standard ideas is presented here, resulting in [1]: (i) critical systems are not necessarily unpredictable; (ii) slowly driven systems evolving through power-law distributed avalanches are not necessarily critical; and (iii) scale-invariant avalanches are not necessarily unpredictable. Simple simulations and granular experiments [2] confirm the findings.

[1] O. Ramos, Scale invariant avalanches: a critical confusion; in B. Veress and J. Szigethy (eds.) Horizons in Earth Science Research. Vol. 3 (Nova Science Publishers) pp 157-188 (2011) arXiv:1104.4991v1.

[2] O. Ramos, E. Altshuler, and K. J. Måløy, Avalanche prediction in a self-organized pile of beads, Phys. Rev. Lett. 102, 078701 (2009).

9:12AM H26.00005 Unjamming of amorphous films probed with a transverse shear ultrasonic oscillator, JULIEN LEOPOLDES, GUILLAUME CONRAD, XIAOPING JIA, Université Paris Est, France, LPMDI TEAM — Friction between solids depends essentially on the response of the interfacial amorphous layer to shear and compressive stresses. Hence, the transition from static to dynamic friction corresponds to the unjamming transition of confined amorphous materials [1]. With a shear ultrasonic oscillator, we study the boundary lubrication due to molecular films confined between a plane and a sphere [2]. We observe a linear viscoelastic behaviour at low oscillation amplitude and a nonlinear frictional microslip regime at high amplitude. In a new set of experiments, the system is brought near the unjamming transition by applying a static force. The interfacial layer softens before unjamming, as indicated by the linear response of the oscillator. We suggest an interpretation based on a stress-induced decrease of the free volume, and propose a corresponding heuristic model. Last, we show how ultrasonic in-plane oscillations of ~ 10 nm amplitude can trigger unjamming, and we discuss the possible related mechanisms.

[1] P. Thomson and G. Grest and M.O. Robbins, Phys. Rev. Lett **68**, 3448 (1992)

[2] J. Léopoldès and X. Jia, Phys. Rev. Lett **105**, 266101 (2010)

9:24AM H26.00006 Universality of Deformation Down to the Nanoscale, NIR FRIEDMAN, Department of Physics, University of Illinois at Urbana-Champaign, ANDREW T. JENNINGS, Division of Engineering and Applied Sciences, Caltech, GEORGIOS TSEKENIS, Department of Physics, University of Illinois at Urbana-Champaign, JU-YOUNG KIM, Division of Engineering and Applied Sciences, Caltech, MOLEI TAO, Department of Computing and Mathematical Sciences, Caltech, JONATHAN T. UHL, None, JULIA R. GREER, Division of Engineering and Applied Sciences, Caltech, KARIN A. DAHMEN, Department of Physics, University of Illinois at Urbana-Champaign — Deformation on macroscopic scales is often modeled as a continuous process, which in reality occurs via a sequence of nanometer-sized discrete slips. We report statistical analyses of slip size distributions obtained by uniaxial compression experiments on nano-crystals of different crystal structures and sizes down to 75 nm. We show that a simple mean field theory (MFT) correctly predicts the statistical behavior by collapsing data using the MFT exponents and scaling function. This study demonstrates that a simple model captures the statistics and universality class of discrete deformation events in a variety of metallic nano-crystals down to the smallest experimentally accessed length scales.

9:36AM H26.00007 Boundary lubrication under pressure: could the friction jump down, instead of up? , ANDREA VANOSI, SISSA & CNR-IOM DEMOCRITOS, Trieste, Italy, ANDREA BENASSI, CNR-IENI, Milano, Italy, NICOLA VARINI, ICHEC, Dublin, Ireland, ERO TOSATTI, SISSA & CNR-IOM DEMOCRITOS, ICTP, Trieste, Italy — The sliding friction during pressure squeezeout of a boundary lubricated contact has been shown [1,2] to undergo upward jumps every time a lubricant atomic layer is expelled. Here we ask the question whether the jump could not be downward. Whereas most studies focus on the layered structure which the confined lubricant takes in the normal direction, the element we wish to consider is a possible change of parallel periodicity occurring at the squeezeout transition. Such changes have been reported in simulations [3], but their effect has not been discussed so far. One possible effect could be a transition of the slider-lubricant interface commensurability, producing a switch of the frictional mechanism, from lubricant melting-freezing in a commensurate state, to superlubric in an incommensurate one – in this case with a drop of friction for increasing load. We exemplify this effect by MD simulations, where we replace for convenience the open squeezeout system with a closed system, where the lubricant is sealed between the sliders. As the number of layers drops under pressure, the planar lubricant structural lattice parameter also drops. This change reflects in a sliding friction jump, which is easily observed to be downwards. The potential observability of load-induced friction drops will be discussed.

[1] J.N. Israelachvili et al., Science 240, 189 (1988).

[2] J. Gao et al., J. Phys. Chem. B 102, 5033 (1998).

[3] U. Tartaglino et al., J. Chem. Phys. 125, 014704 (2006).

9:48AM H26.00008 Plasticity as a Depinning Phase Transition , GEORGIOS TSEKENIS, University of Illinois at Urbana-Champaign, PAK YUEN CHAN, None, THOMAS FEHM, Ludwig-Maximilians-Universität Muenchen, JONATHAN T. UHL, None, JONATHAN DANTZIG, NIGEL GOLDENFELD, KARIN DAHMEN, University of Illinois at Urbana-Champaign — Crystalline materials deform in an intermittent way via slip-avalanches, which exhibit a variety of scale-invariant behaviors that have been interpreted as a pinning-depinning transition. We use discrete dislocation dynamics at zero temperature to resolve the temporal profiles of slip-avalanches and extract the finite-size scaling properties of the dislocation system, thus going beyond gross aggregate statistics. We provide a comprehensive set of scaling exponents, which establishes that the dynamics of plasticity, in the absence of hardening, is consistent with the mean field interface depinning universality class, even though there is no quenched disorder. Finally, we show how Phase Field Crystal simulations shed light on the effect of temperature on intermittent dislocation dynamics and its critical scaling behavior.

10:00AM H26.00009 Tribo-induced melting and temperature gradients at sliding asperity contacts , J. KRIM, L. PAN, D.J. LICHTENWALNER, North Carolina State University, A.I. KINGON, Brown University — Tribo-induced nanoscale surface melting mechanisms have been investigated by means of a combined QCM-STM technique [1] for a range of Au and Au-Ni alloys with varying compositional percentages and phases. The QCM-STM setup allows studies to be performed at sliding speeds of up to m/s, and also reveals valuable information concerning tip-substrate temperature gradients.[3] A transition from solid-solid to solid-“liquid like” contact was observed for each sample at sufficiently high asperity sliding speeds. Pure gold, solid-solution and two-phase Au-Ni (20 at.% Ni) alloys were compared, which are materials of great relevance to MEMS RF switch technology.[2] The transition points agree favorably with theoretical predictions for their surface melting characteristics. We acknowledge NSF and AFOSR support for this research.

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[2] Zhenyin Yang; Lichtenwalner, D.J.; Morris, A.S.; Krim, J.; Kingon, A.I, Journal of Microelectromechanical Systems, April 2009, Volume: 18 Issue:2, 287-295

[3] C.G. Dunkle, I.B. Altfeder, A.A. Voevodin, J. Jones, J. Krim and P.Taborek, J. Appl. Phys., 107, art#114903, (2010)

10:12AM H26.00010 Formation of Stable Metallic Nanocontacts by mechanical annealing¹ , CARLOS SABATER, Dep. of Applied Physics University of Alicante, Spain, CARLOS UNTIEDT, Dep. App. Phys. Univ. Alicante, SP, JUAN JOSE PALACIOS, Dep. of Condensed Matter Physics, Univ. Autonoma de Madrid, MARIA JOSE CATURLA, Dep. App. Phys. Univ. Alicante, SP — Metallic nanocontacts (NC) can be fabricated using STM or related techniques. In these experiments the size of the NC can be followed, down to the atomic contact, by measuring its electrical conductance. Such evolution will normally differ for each experimental realization and therefore conductance histograms are used to identify preferential configurations. It can be shown that occasionally there are some atomic configurations that can be repeated during consecutive cycles of mechanical deformation of the contacts. Here we report experiments for gold NC where the same trace of conductance can be obtained for hundreds of cycles of formation and rupture. We have studied the process leading to such repetitiveness of the traces and found that this is obtained when limiting the indentation depth between the two surfaces to a conductance value of approximately 5-6 G_0 . Using molecular dynamics simulations we have obtained the same behaviour and observed how, after repeated indentations, the two metallic contacts are shaped into a stable configuration by mechanical annealing. This confirms and explains the fact that repeated indentation of a tip into a metallic substrate can be used as a method to sharpen or clean STM tips, but only when such indentation does not exceed a limit.

¹Acknowledgment: Spanish Government through Consolider CSD2007-0010 and FIS 2010-21883-C02-01

10:24AM H26.00011 Scaling in earthquake models with inhomogeneous damage¹ , RACHELE DOMINGUEZ, Randolph-Macon College, KRISTY TIAMPO, University of Western Ontario, C.A. SERINO, W. KLEIN, Boston University — We study the scaling of earthquake models that are variations of Olami-Feder-Christensen and Burridge-Knopoff models, in order to explore the effect of spatial inhomogeneities on earthquake-like systems when interaction ranges are long, but not necessarily longer than the distances associated with the inhomogeneities of the system. For long ranges and without inhomogeneities, such models have been found to produce scaling similar to GR scaling found in real earthquake systems. In the earthquake models discussed here, damage is distributed inhomogeneously throughout and the interaction ranges, while long, are not longer than all of the damage length scales. We find that the scaling depends not only on the amount of damage, but also on the spatial distribution of that damage.

¹This work was funded by the DOE through grant DE-FG02-95ER14498 and the NSERC and Aon Benfield/ICLR Industrial Research Chair in Earthquake Hazard Assessment.

10:36AM H26.00012 Stress Corrosion Fracture of Silicate Glasses: How Far Can Water Penetrate? , ELISABETH BOUCHAUD, CEA-Saclay ESPCI ParisTech, CINDY ROUNTREE, FABRICE COUSIN, CEA-Saclay, FREDERIC LECHENAULT, ENS Paris, STEPHANE CHAPULIOT, AREVA, LAURENT PONSON, I D Alembert Paris, JEAN-PHILIPPE BOUCHAUD, CFM Paris — Although glass can be considered as homogeneous at scales as small as a few tens of nanometers, since it exhibits no density fluctuations beyond, its amorphous structure makes it a disordered material with respect to fracture properties. Fluctuations of the orientations of Si-O bonds with respect to the external stress make it unlikely that bonds closest to the crack tip break first, despite the high stress concentration. As a consequence, glass behaves in a quasi-brittle manner rather than in a purely elastic way. *In situ* Atomic Force Microscopy experiments tracking the slow progression of a stress corrosion crack seemed to show indeed the opening and growth of nano size flaws ahead of the tip. However, these results are controversial, because of artifacts which may seriously affect the observations. Furthermore, the low diffusion coefficient of water in silica should forbid hydrolysis at a distance from the crack tip, except at the free surface. Nevertheless, our recent neutron reflectivity experiments show that water actually penetrates into the material during stress corrosion fracture. Comparing two experiments performed for different crack velocities shows that the diffusion coefficient is hugely increased under stress, allowing for bond breakings at ~ten nanometers ahead of the main crack tip.

10:48AM H26.00013 Magnetic friction: From Stokes to Coulomb behavior¹, MARTIN MAGIERA, SEBASTIAN ANGST, ALFRED HUCHT, DIETRICH E. WOLF, Faculty of Physics and CeNIDE, University of Duisburg-Essen, D-47048 Duisburg, Germany — We demonstrate that in a ferromagnetic substrate, which is continuously driven out of equilibrium by a field moving with constant velocity v , at least two types of friction may occur when v goes to zero: The substrate may feel a friction force proportional to v (Stokes friction), if the field changes on a time scale which is longer than the intrinsic relaxation time. On the other hand, the friction force may become independent of v in the opposite case (Coulomb friction). These observations are analogous to e.g. solid friction. The effect is demonstrated in both, the Ising (one spin dimension) and the Heisenberg model (three spin dimensions), irrespective which kind of dynamics (Metropolis spin-flip dynamics or Landau-Lifshitz-Gilbert precessional dynamics) is used. For both models the limiting case of Coulomb friction can be treated analytically. Furthermore we present an empiric expression reflecting the correct Stokes behavior and therefore yielding the correct cross-over velocity and dissipation. arXiv:1111.2494

¹Financial support by the German Research Foundation (DFG, via SFB616) and the German Academic Exchange Service (DAAD, PROBRAL programme) is acknowledged.

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H27 GMAG DMP FIAP: Invited Session: McGroddy Prize, Adler Lectureship, and Pake Prize: Superconductivity and Spin Transport 258AB

8:00AM H27.00001 Assembling, understanding, auguring phase diagrams for Fe-based superconductivity¹, PAUL CANFIELD, Ames Laboratory and Department of Physics, Iowa State University — The quest for improved examples of novel, potentially useful, superconductors reached another milestone in 2008 with the discovery of Fe-based superconductivity in wide range of structurally related arsenide and selenide compounds. In particular, the AFe_2As_2 ($\text{A} = \text{Ba}, \text{Sr}, \text{Ca}$) compounds proved to have the highly desirable combination of intriguing properties that imply intimate coupling between electronic, magnetic and structural degrees of freedom, exceptionally high and relatively isotropic upper critical field curves and readily grown, homogeneous single crystals. Over the past three years the CMP community has been able to develop a broad and deep empirical understanding of substitutional and pressure based phase diagrams of these materials that is leading to theoretical as well as synthetic insights. In this talk I will broadly review some of our key findings and speculate about future directions for research in this field.

¹Work at the Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

8:36AM H27.00002 James C. McGroddy Prize for New Materials Lecture: New Superconductors and other Research in New Materials¹, ROBERT CAVA, Department of Chemistry, Princeton University — Superconductors and other electronic materials can often display subtle relationships between their structural characteristics and their electronic properties. Though the primary interest in these relationships is within the condensed matter physics community, often at their foundation are the concepts of bonding and structure familiar to inorganic and solid state chemists. Thus a hybridized view, combining physics and chemistry, is one way of approaching the discovery and characterization of new materials. In this talk I will describe some of our research in this context and comment on some broader aspects of interdisciplinary research in new materials.

¹The authors work on superconductivity and new materials has been supported by DOE, NSF, and AFOSR.

9:12AM H27.00003 David Adler Lectureship Award in the Field of Materials Physics: Racetrack Memory - a high-performance, storage class memory using magnetic domain-walls manipulated by current, STUART PARKIN, IBM Almaden Research Center, San Jose, California — Racetrack Memory is a novel high-performance, non-volatile storage-class memory in which magnetic domains are used to store information in a “magnetic racetrack” [1]. The magnetic racetrack promises a solid state memory with storage capacities and cost rivaling that of magnetic disk drives but with much improved performance and reliability: a “hard disk on a chip”. The magnetic racetrack is comprised of a magnetic nanowire in which a series of magnetic domain walls are shifted to and fro along the wire using nanosecond-long pulses of spin polarized current [2]. We have demonstrated the underlying physics that makes Racetrack Memory possible [3,4] and all the basic functions - creation, and manipulation of a train of domain walls and their detection. The physics underlying the current induced dynamics of domain walls will also be discussed. In particular, we show that the domain walls respond as if they have mass, leading to significant inertial driven motion of the domain walls over long times after the current pulses are switched off [3]. We also demonstrate that in perpendicularly magnetized nanowires there are two independent current driving mechanisms: one derived from bulk spin-dependent scattering that drives the domain walls in the direction of electron flow, and a second interfacial mechanism that can drive the domain walls either along or against the electron flow, depending on subtle changes in the nanowire structure. Finally, we demonstrate thermally induced spin currents are large enough that they can be used to manipulate domain walls.

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[3] L. Thomas, R. Moriya, C. Rettner and S.S.P. Parkin, Science 330, 1810 (2010).

[4] X. Jiang et al. Nat. Comm. 1:25 (2010) and Nano Lett. 11, 96 (2011).

9:48AM H27.00004 George E. Pake Prize Lecture: Pulsed Laser Deposition and the Oxide Electronics Revolution, T. VENKATESAN, NUSNNI-NanoCore, National University of Singapore — The discovery of the Pulsed Laser Deposition (PLD) Process at Bellcore was followed by a stream of advances in the epitaxial growth of oxides and a variety of heterostructures and interfaces. Today Oxide Electronics is a fascinating field with a great deal of new Science and potential for applications. Following a discussion of these events, my talk will focus on the adventure involved in creating a new company, Neocera, and, at the same time, pushing ahead in the evolving field of oxide electronics. There, electron spin, pairing, and alignment to create superconductivity and magnetism have opened up new frontiers for research and materials development.

10:24AM H27.00005 A New Avenue towards Colossal Magnetoresistance in Organic Tunneling Junctions, JIAN SHEN, Department of Physics, Fudan University, Shanghai, China and Department of Physics and Astronomy, The University of Tennessee — A major challenge for the field of organic spintronics is how to achieve large magnetoresistance (MR) in a reliable manner. We have developed a new approach that dramatically improves MR of organic spin valves. Our approach involves using buffer layer assisted growth to prepare magnetic nanodot layers on top of the organic spacer layer. Interdiffusion between magnetic electrode and organic spacer layer has been largely suppressed in devices prepared by this method. Consequently, devices become highly reliable and large magnetoresistance up to a few hundred percent has been obtained. Moreover, we have attempted to insert a single magnetic nanodot layer inside the organic spacer layer. In such a tunneling junction device, even when the electrodes are nonmagnetic, a colossal MR up to 100000% has been achieved at relatively high temperatures. The underlying mechanism has been discussed based on temperature-dependent I-V curves and resistivity measurements.

Tuesday, February 28, 2012 8:00AM - 11:00AM – Session H28 DMP: Focus Session: Dopants and Defects in Semiconductors - Si 258C

8:00AM H28.00001 Reliability of III-V electronic devices – the defects that cause the trouble¹

, SOKRATES T. PANTELIDES, Department of Physics and Astronomy and Department of Electrical Engineering and Computer Science, Vanderbilt University, Nashville, TN — Degradation of electronic devices by hot electrons is universally attributed to the generation of defects, but the mechanisms for defect generation and the specific nature of the pertinent defects are not known for most systems. Here we describe three recent case studies [1] in III-V high-electron-mobility transistors that illustrate the power of combining density functional calculations and experimental data to identify the pertinent defects and associated degradation mechanisms. In all cases, benign pre-existing defects are either depassivated (irreversible degradation) or transformed to a metastable state (reversible degradation). This work was done in collaboration with R.D. Schrimpf, D.M. Fleetwood, Y. Puzyrev, X. Shen, T. Roy, S. DasGupta, and B.R. Tuttle. Devices were provided by D.F. Brown, J. Speck and U. Mishra, and by J. Bergman and B. Brar.

[1] Y. S. Puzyrev et al., Appl. Phys. Lett. **96**, 053505 (2010); T. Roy et al., Appl. Phys. Lett. **96**, 133503 (2010); X. Shen et al., J. Appl. Phys. **108**, 114505 (2010).

¹Work supported in part by ONR MURI grant N-00014-08-100655. The author is also affiliated with Oak Ridge National Laboratory, Oak Ridge, TN

8:36AM H28.00002 Near-Interface Defects in SiO₂/SiC MOS Devices¹, A.F. BASILE, P.M. MOONEY, Simon

Fraser University — The implementation of SiO₂/SiC MOSFETS for high power applications has been hindered by the high density of near-interface states. We have developed a method to distinguish both the energy and spatial distribution of defect states near insulator-semiconductor interfaces through a comparison of the thermal emission energy extracted from constant capacitance transient spectroscopy (CCDLTS) measurements and the interface Fermi energy (F_P). The dependence of F_P on trap filling voltage at the CCDLTS peak temperature is determined from temperature-dependent 1MHz C-V curves. Capture by tunneling into oxide traps is detected in 4H- and 6H-SiC capacitors fabricated by oxidation followed by NO-annealing, with the difference in thermal emission energies consistent with the conduction band offsets of the two polytypes at the SiO₂/SiC interface. Comparison with results from first principles calculations suggests that the observed oxide traps are $C_O=C_O$ and interstitial Si [1]. SiC defects having energies close to the SiC conduction band are suggested to be carbon di-interstitial defects, $(C_2)_i$, introduced during standard oxidation [1]. Well-known traps introduced in SiC by ion-implantation are observed in 4H-SiC MOS capacitors fabricated by N-implantation followed by standard oxidation, thus validating this new method [2].

1. A.F. Basile, *et al.*, J. Appl. Phys. **109**, 064514 (2011)

2. A.F. Basile, *et al.*, J. Appl. Phys. **109**, 114505 (2011).

¹Natural Sciences and Engineering Council, Canada

8:48AM H28.00003 Doping in Si/SiO₂ Structures: A first-principles metadynamics study ,

NICHOLAS LANZILLO, Rensselaer Polytechnic Institute, PHILIP SHEMELLA, IBM Research - Zurich, SAROJ NAYAK, Rensselaer Polytechnic Institute, WANDA ANDREONI, ALESSANDRO CURIONI, IBM Research - Zurich, RENSSELEAR POLYTECHNIC INSTITUTE COLLABORATION, IBM RESEARCH - ZURICH COLLABORATION — Dopant diffusion in semiconductor devices is a field of study with tremendous technological importance. We have performed first-principles metadynamics simulations of the diffusion of n-type dopants at the Si/SiO₂ interface using the ab-initio MD method. After the generation of a vacancy in the Si region, arsenic, phosphorus and silicon atoms show varying mechanisms of diffusion, including both substitutional and interstitial. Although at the near-interface silicon region arsenic is the first to diffuse interstitially, its interstitial position is more stable and thus less likely to diffuse across the interface relative to phosphorus and silicon. As arsenic crosses the interface, however, its relative stability decreases with respect to phosphorus and silicon and diffusion into the oxide becomes unfavorable. This is in agreement with experimentally observed arsenic pile-up at the Si/SiO₂ interface. We quantify the diffusion mechanisms by comparing free energy barriers in the silicon region as well as at the interface. We find the largest barriers exist for silicon, while the smallest barriers exist for arsenic.

9:00AM H28.00004 The lifetime recovery puzzle in intermediate band materials: A new experimental approach ,

MARK WINKLER, Massachusetts Institute of Technology, DANIEL RECHT, JACOB KRICH, MICHAEL AZIZ, Harvard University, TONIO BUONASSISI, Massachusetts Institute of Technology — We have recently observed that deep-level impurities in silicon – such as the chalcogens S and Se – can drive an insulator-to-metal transition. The existence of this transition has potential ramifications for the development of intermediate band (IB) solar cells, and significant progress has recently been made toward explaining the origin of this transition. Recently, however, theoretical disagreement has arisen regarding whether impurity concentrations beyond the insulator-to-metal transition should result in increased non-radiative recombination rates or instead yield “lifetime recovery.” Very few measurements of carrier lifetime in IB-candidates have been reported that could help clarify this issue, which has important impacts on the selection of IB-materials and the design of IB solar cells. We have developed a technique based on transient optical absorption to measure the trapping rate of the intermediate states and will discuss the results of these measurements in the hyperdoped silicon system (Si doped with chalcogens to concentration $>10^{20}\text{cm}^{-3}$). We will also discuss the impact of these measurements on the current theoretical disagreement.

9:12AM H28.00005 Single-Electron Capacitance Spectroscopy of Individual Dopants in Silicon ,

MATTHEW DENINNO, MOREWELL GASSELLER, JAMES HARRISON, STUART TESSMER, Michigan State University, SVEN ROGGE, Centre for Quantum Computation and Communication Technology, School of Physics, The University of New South Wales, ROGER LOO, MATTY CAYMAX, IMEC, Belgium — Motivated by recent transport experiments and proposed atomic-scale semiconductor devices, we present measurements that extend the reach of scanned-probe methods to discern the properties of individual dopants tens of nanometers below the surface of a silicon sample. Using a capacitance-based approach, we have both spatially resolved individual subsurface boron acceptors and spectroscopically detected single holes entering and leaving these minute systems of atoms. A resonance identified as the B^+ state is shown to shift in energy from acceptor to acceptor. The resonance is absent in a control sample that does not contain the boron acceptors. By directly measuring the quantum levels and testing the effect of dopant-dopant interactions, this method represents a valuable tool for the development of future atomic-scale semiconductor devices.

9:24AM H28.00006 Charge States of Individual Group V Donors on n-doped Si(111)-(2x1)

Surface¹, VERONIKA BRAZDOVA, PHILIPP STUDER, CYRUS F. HIRJIBEHDIN, STEVEN SCHOFIELD, NEIL J. CURSON, DAVID R. BOWLER, University College London — Functionality of semiconductor devices now relies upon only a few atoms and study of individual dopants in silicon has thus been rapidly growing in importance. Group V donors are especially interesting due to their potential applications in quantum computing and spintronics. The charge state of the dopants is of fundamental importance for conventional semiconductor devices as well as in concept QIP and spintronic devices. We combine density functional theory simulations and ion implantation and cross-sectional scanning tunneling microscopy (XSTM) to study individual Group V donors in cleaved n-doped Si(111)-(2x1) surface. We present a detailed analysis of the dopant-induced charging effects and discuss the surface charge dependence on the local reconstruction induced by the individual dopants.

¹Supported by the EPSRC grant COMPASSS

9:36AM H28.00007 First-principles calculations for Er impurities in Si

LARS BJAALIE, LARS ISMER, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — Erbium-doped Si is a promising material for the development of silicon-based light sources that can interface with CMOS technology, optical fiber, and spin centers for quantum computing. Using density functional theory with a screened hybrid functional we examine the structural and electronic properties of Er(III) impurities in Si, focusing on the site preference and the Er effects on the electrical properties of the Si host. We find that Er is stable either at the tetrahedral interstitial site or at the substitutional site, depending on the Fermi-level position; Er sitting at the hexagonal interstitial site is higher in energy at all Fermi levels, in agreement with experimental observations. In p-type Si, i.e., for Fermi levels near the valence band, Er prefers the tetrahedral interstitial site and acts as a donor. In n-type Si, i.e., for Fermi levels near the conduction band, Er prefers the substitutional site and acts as an acceptor. We will also discuss the impurity-to-band optical transitions determined from calculated configuration coordinate diagrams.

9:48AM H28.00008 Deactivation of deep level impurities in hyperdoped silicon

CHRISTIE SIMMONS, MARK WINKLER, JOSEPH SULLIVAN, Massachusetts Institute of Technology, DANIEL RECHT, MICHAEL AZIZ, Harvard School of Engineering and Applied Sciences, TONIO BUONASSISI, Massachusetts Institute of Technology — Extremely high concentrations of deep level impurities in silicon have exhibited unique properties of interest for optoelectronic and photovoltaic applications. For example, silicon hyperdoped with chalcogens demonstrates significant infrared absorption at wavelengths longer than the band edge of silicon. Hyperdoped silicon is fabricated by high-dose ion implantation followed by pulsed laser melting and rapid re-solidification. The result is a metastable supersaturated solid solution with doping concentrations orders of magnitude above the room temperature solubility limit. Thermal annealing results in a deactivation of the sub-gap absorption in this material, suggesting that the precise chemical state of the deep level impurities is a critical component of the enhanced absorption. To gain further insight to the absorption mechanism and the stability this material, we present a detailed investigation of the deactivation induced by rapid thermal annealing of silicon hyperdoped with sulfur.

10:00AM H28.00009 Single crystal silicon hyperdoped with transition metals

DANIEL RECHT, Harvard University, MATTHEW SMITH, JOSEPH SULLIVAN, Massachusetts Institute of Technology, SUPAKIT CHARNVANICHBORIKARN, Australian National University, MARK WINKLER, Massachusetts Institute of Technology, JAMES WILLIAMS, Australian National University, TONIO BUONASSISI, SILVIJA GRADEČAK, Massachusetts Institute of Technology, MICHAEL AZIZ, Harvard University — Silicon hyperdoped with sulfur and selenium by ion implantation and pulsed laser melting has recently been shown to undergo an insulator to metal transition. While experimental and theoretical investigations have begun to unravel the nature of this transition, little has been done to generalize this work to other dopants. This talk will discuss recent progress in hyperdoping silicon with transition metal dopants focusing on challenges not present in the silicon-chalcogen system. In particular, experimental results (e.g., SIMS, RBS, TEM) on the role of dopant selection and resolidification velocity in preventing segregation and cellular breakdown of the solidification front will be addressed in detail. In addition, measurements of the optoelectronic properties of silicon hyperdoped with transition metal dopants will be reported.

10:12AM H28.00010 Theoretical and Experimental Framework of an Insulator-to-Metal Transition in Selenium-Hyperdoped Silicon

ELIF ERTEKIN, University of Illinois, MARK WINKLER, Massachusetts Institute of Technology, DANIEL RECHT, AURORA SAID, MICHAEL AZIZ, Harvard University, TONIO BUONASSISI, JEFFREY GROSSMAN, Massachusetts Institute of Technology — Following the discovery of black silicon in 1998, hyperdoping - doping to concentrations orders of magnitude larger than the solubility limit - has emerged as a promising method for designing semiconductors with unique optical and electronic properties. Black silicon (silicon hyperdoped with chalcogens), synthesized by pulsed laser techniques, has recently received substantial interest owing to its broad, sub-band gap absorption down to photon energies as low as 0.5 eV, suggesting applications towards infrared detection and intermediate band photovoltaics. Until now, there has not been a clear explanation of these properties. In this presentation, we combine computational and experimental evidence to probe the origin of sub-band gap optical absorption and metallicity in black silicon. Temperature-dependent conductivity measurements show that black silicon undergoes an insulator-to-metal transition at a critical dopant concentration. Our computational analysis based on density functional theory and quantum Monte Carlo methods suggest that the enhanced optical properties result from this insulator-to-metal transition that appears to be a classic impurity-driven Mott transition, driven largely by many-body effects.

10:24AM H28.00011 Optical Absorption Mechanisms in Sulfur Hyper-doped Silicon

JOSEPH SULLIVAN, Department of Mechanical Engineering, Massachusetts Institute of Technology, DANIEL RECHT, Harvard School of Engineering and Applied Sciences, CHRISTIE SIMMONS, Department of Mechanical Engineering, Massachusetts Institute of Technology, MICHAEL AZIZ, Harvard School of Engineering and Applied Sciences, TONIO BUONASSISI, Department of Mechanical Engineering, Massachusetts Institute of Technology — Silicon that is doped with sulfur, a deep-level donor, to concentrations approaching 1% at. demonstrates sub-band gap optical absorption, and has potential applications as an intermediate band solar cell material and a short-wavelength infrared (SWIR) photodetector. Understanding the nature of the absorption mechanism will aid in creating future devices with this exciting material. To elucidate the absorption mechanism, the reflectivity and absorption coefficient have been measured to photon energies down to 75 meV. We report on these new measurements as well as data fitting that give insight into absorption mechanism within these materials.

10:36AM H28.00012 Atomistic study of heavy doping in Si nanowires¹

MAHESH NEUPANE, University of California, Riverside, CA 92506, RAJIB RAHMAN, Sandia National Laboratories, Albuquerque, NM 87185, USA, ROGER LAKE, University of California, Riverside, CA 92506 — Dopant atoms are becoming increasingly important in the nanoscaled field-effect transistors (FET) because of their tendency to influence device parameters such as sub-threshold current-voltage characteristics and gate-to-channel electrostatic coupling. Achieving high doping concentrations is essential for the realization of Si nanowire FET where low resistance contacts or tunnel junctions and narrow depletion widths are needed. In an effort to understand the dopants effect on these devices as a function of scaling parameters, we use self-consistent field (SCF) tight-binding (TB) method as implemented in NEMO3D to obtain an accurate quantitative description of the band structure, confinement geometries and valley-orbit interaction from a full band-structure technique as a function of dopant location, concentration and applied electrical field. Our method solves the Poisson equation iteratively coupled with the atomistic TB Hamiltonian for charge self-consistency to provide an accurate description of the electrostatics. Our simulations show how the band structure of the nanowire is affected by the presence of few impurities.

¹This work was supported by the Microelectronics Advanced Research Corporation Focus Center on Nano Materials (FENA). Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy

10:48AM H28.00013 Femtosecond-laser hyperdoping: controlling sulfur concentrations in silicon for band gap engineering, MENG-JU SHER, MARK WINKLER, YU-TING LIN, BENJAMIN FRANTA, ERIC MAZUR, Harvard University — Doping silicon to concentrations above the metal-insulator transition threshold yields a novel material that has potential for photovoltaic applications. By focusing femtosecond laser pulses on the surface of a silicon wafer in a sulfur hexafluoride (SF₆) environment, silicon is doped with 1% atomic sulfur. This material exhibits near-unity, broadband absorption from the visible to the near infrared (< 0.5 eV, deep below the silicon band gap), and metallic-like conduction. These unusual optical and electronic properties suggest the formation of an intermediate band. We report on the femtosecond laser doping techniques we employ and the resulting material properties. By changing the laser parameters and ambient environment we can control the dopant profiles, crystallinity, and surface morphology. We perform optical absorption and temperature-dependent Hall measurements to investigate electron transport and to identify the energy states of the sulfur donors.

Tuesday, February 28, 2012 8:00AM - 11:00AM —

Session H29 GQI: Focus Session: Superconducting Qubits: Amplifiers and Read-out 259A

8:00AM H29.00001 Frequency tunable non-degenerate Josephson amplifier for qubit readout¹, FLAVIUS SCHACKERT, MICHAEL HATRIDGE, KATRINA SLIWA, BALEEGH ABDO, LUIGI FRUNZIO, MICHEL DEVORET, Yale University, Dept. of Applied Physics — We have developed a new ultra low noise microwave amplifier based on the Josephson parametric converter (JPC), which overcomes a practical weakness of devices of previous generations: having sufficient frequency tunability to easily match the qubit readout frequency. The JPC consists of two superconducting microwave resonators that are coupled to each other through a ring of four Josephson junctions, threaded by a magnetic flux and providing the non-linearity for the amplification process. The non-linearity is of the trilinear form involving the minimal number of modes, and allows ideal non-degenerate parametric amplification at the quantum limit of noise. In our new tunable version, the junctions responsible for amplification are shunted by a cross of four larger junctions, which for our purpose can be regarded as linear inductors, as in the work of Roch et al.[1]. The JPC has now a unique bias point at any applied flux and is tunable over more than half a gigahertz. We are currently using this amplifier in conjunction with a quantum non-demolition measurement of a transmon qubit and have observed quantum jumps with fidelity larger than 90%. [1] N. Roch, E. Flurin, F. Nguyen, P. Morfin, P. Campagne-Ibarcq, M. H. Devoret, and B. Huard, in preparation.

¹Work supported by IARPA, ARO, and NSF.

8:12AM H29.00002 Microstrip SQUID amplifiers for quantum information science, M.P. DEFEO, B.L.T. PLOURDE, Syracuse University — Recent progress in SQUID amplifiers suggests that these devices might approach quantum-limited sensitivity in the microwave range, thus making them a viable option for measurement of superconducting quantum systems. In the microstrip SQUID amplifier configuration, gains of around 20dB are possible at frequencies of several hundred MHz, and the gain is limited by the maximum voltage modulation available from the SQUID. One route for increasing the voltage modulation involves using larger resistive shunts, however maintaining non-hysteretic device operation requires smaller junction capacitances than is possible with conventional photolithographically patterned junctions. Operating at higher frequencies requires a shorter input coil which reduces mutual inductance between the coil and washer and therefore gain. We have fabricated microstrip SQUID amplifiers using submicron Al-AIO_x-Al junctions and large shunts. The input coil and SQUID washer are optimized for producing high gain at frequencies in the gigahertz range. Recent measurements of gain and noise temperature will be discussed as well as demonstrations of these devices as a first stage of amplification for a superconducting system.

8:24AM H29.00003 Measurement of the phase non-reciprocity of the Josephson parametric converter¹, BALEEGH ABDO, KATRINA SLIWA, ARCHANA KAMAL, FLAVIUS SCHACKERT, MICHAEL HATRIDGE, LUIGI FRUNZIO, MICHEL DEVORET, Applied Physics - Yale University — Non-reciprocal devices such as circulators and isolators play a pivotal role in many microwave experiments on quantum superconducting circuits. However, non-reciprocity in these devices is achieved using ferrites and permanent magnets which are not suitable for on chip integration. We have built a symmetric two port device by pairing two Josephson parametric converters (JPCs) working in pure conversion mode, each of which is driven with an independent pump tone. We observed a non-reciprocal phase shift between the two ports, which depends on the phase difference between the two pumps. The present noiseless system constitutes an important step towards the implementation of a noiseless gyrator, the main building block of an on-chip circulator for back-action free quantum measurement.

¹Work supported by IARPA, ARO and NSF

8:36AM H29.00004 Performance of the doubly pumped four-wave Josephson parametric amplifier¹, KATRINA SLIWA, ANIRUDH NARLA, MICHAEL HATRIDGE, FLAVIUS SCHACKERT, SHYAM SHANKAR, ARCHANA KAMAL, BALEEGH ABDO, LUIGI FRUNZIO, MICHEL DEVORET, Applied Physics Dept., Yale University — The degenerate Josephson Parametric Amplifier (JPA) is a promising quantum-limited amplifier for the measurement of mesoscopic systems. In the single pump scheme, the amplification process utilizes two photons at the drive frequency to produce a signal and an idler photon. However the large reflected pump tone at the drive frequency strongly acts back on the measured system. Several circulators prevent this back action, but come at a non-negligible cost in system noise temperature. Two drive tones symmetrically detuned from the original drive frequency provide the necessary pump energy but with the reflected tones now far removed from the signal frequency. We have investigated the performance of the doubly pumped JPA with pump detunings from 50 to 1000 MHz. The expected gain profile has been measured with at least 20 dB of gain and no loss of bandwidth. A gigahertz range of tunability, no degradation in noise temperature, and improvements in dynamic range are also expected.

¹Work Supported by IARPA, ARO, and NSF

8:48AM H29.00005 Analytical Calculation of Gain and Noise of DC SQUID Microwave Amplifier, ARCHANA KAMAL, MICHEL DEVORET, Departments of Physics and Applied Physics, Yale University, JOHN CLARKE, Department of Physics, University of California, Berkeley — The dc SQUID microwave amplifier, based on Josephson junctions, is employed in a wide spectrum of applications ranging from dark matter detection to the readout of superconducting qubits. A crucial advantage offered by this device is the separation of input and output channels, unlike conventional Josephson parametric amplifiers, so that it does not require a nonreciprocal device such as a circulator for its operation. The mechanism underlying the directional gain in the SQUID microwave amplifier, however, has so far remained elusive. We present a first principles, analytical calculation, based on scattering theory, of a practical SQUID amplifier which elucidates the underlying nonlinear mode mixing responsible for the directional operation of the device. The gain and quantum noise characteristics of a SQUID operated as a microwave voltage amplifier are discussed. Work supported by IARPA and ARO (AK, MHD and JC) and NSF (AK and MHD).

9:00AM H29.00006 Observing quantum jumps of a transmon qubit with a Josephson parametric converter¹, S. SHANKAR, M. HATRIDGE, F. SCHACKERT, K. GEERLINGS, T. BRECHT, K. SLIWA, B. ABDO, L. FRUNZIO, R.J. SCHOELKOPF, M.H. DEVORET, Applied Physics Dept., Yale University — A high fidelity linear quantum non-demolition (QND) readout of a superconducting qubit opens up the possibility of observing quantum jumps and is a prerequisite for quantum feedback and error correction. This readout is challenging since the qubit, the readout resonator and the following amplifier chain have to be simultaneously optimized to achieve the desired performance. We fabricated a superconducting transmon qubit at 5.7 GHz coupled to a compact resonator at 7.5 GHz, designed to produce a dispersive shift (χ) of 6 MHz of the resonator frequency when the qubit is excited. The resonator linewidth matches χ to produce maximum readout contrast in a transmission measurement, while maintaining a Purcell limited T_1 of about 3 μ s. Using a Josephson parametric converter that is tuned to match the resonator frequency, we achieved a system noise temperature of the following amplifier chain of about 0.5 K, roughly thrice the standard quantum limit. Using these optimized parameters, we measured the qubit state with about 5 photons in the readout resonator and observed quantum jumps with fidelity above 90 %. Further, by looking at the statistics of the jumps and the evolution of the qubit population in single shot traces, we find that the average qubit T_1 during the readout matches the Purcell limited T_1 , as expected for a QND measurement.

¹Work supported by IARPA, ARO and NSF.

9:12AM H29.00007 Quantum measurement in action with the transmon qubit¹, M. HATRIDGE, S. SHANKAR, F. SCHACKERT, K. GEERLINGS, T. BRECHT, K. SLIWA, B. ABDO, L. FRUNZIO, R.J. SCHOELKOPF, M.H. DEVORET, Applied Physics Dept., Yale University — High fidelity, rapid quantum non-demolition readout of superconducting qubits greatly facilitates tests of single qubit measurement theory. We have realized such readout in an experiment comprised of a transmon coupled to a compact resonator, which is in turn connected via an isolator and circulator to a tunable Josephson parametric converter (JPC) operated as a phase-preserving parametric amplifier. When the qubit state is measured with an rf tone corresponding to an average cavity circulating power of 5 photons, fidelity exceeds 90% for a measurement duration of 240 ns ($\sim 0.1 T_1$). This performance allows the observation of quantum trajectories of the qubit, showing discrete jumps and a bimodal distribution of measurement results, despite the linear character of the amplifier. This provides further support for the quantum nature of superconducting artificial atoms. We have conducted Stern-Gerlach type experiments, in which the qubit is repeatedly measured along different axes. Results are in good agreement with theoretical predictions of the effect of partial measurement on qubit state evolution.

¹Work supported by IARPA, ARO, and NSF.

9:24AM H29.00008 Monitoring the state of a superconducting quantum bit using weak measurements¹, CHRIS MACKLIN, R. VIJAY, D.H. SLICHTER, STEVEN WEBER, KATER MURCH, R. NAIK, UC Berkeley, QNL, ALEXANDER N. KOROTKOV, Department of Electrical Engineering, University of California, Riverside, CA 92521, USA, I. SIDDIQI, UC Berkeley, QNL — We demonstrate continuous weak measurement of the state of a superconducting transmon qubit in the circuit QED architecture using a Josephson parametric amplifier. The near quantum-limited noise performance of the amplifier enables us to obtain a high-fidelity measurement record which can be used to reconstruct the qubit state evolution during measurement by employing the quantum Bayesian formalism. While simultaneously driving the qubit at its Larmor frequency and measuring it weakly, we are able to resolve the spectral signature of Rabi oscillations present in the measurement record with a high signal-to-noise ratio (SNR). We discuss current limitations in this measurement scheme and suggest ways to further optimize the SNR. Our results suggest a route to implement quantum feedback to steer the state of a superconducting qubit.

¹This research is supported by the ARO QCT program.

9:36AM H29.00009 Stabilizing Rabi oscillations in a superconducting qubit using quantum feedback¹, R. VIJAY, CHRIS MACKLIN, D.H. SLICHTER, STEVEN WEBER, KATER MURCH, R. NAIK, UC Berkeley, QNL, ALEXANDER N. KOROTKOV, Department of Electrical Engineering, University of California, Riverside, CA 92521, USA, I. SIDDIQI, UC Berkeley, QNL — Recent progress in the development of quantum-noise-limited superconducting parametric amplifiers has enabled high-fidelity, continuous measurements of superconducting quantum bits (qubits). We exploit this functionality while leveraging improved coherence times in transmon qubits to show that it is now possible to obtain a faithful record of real-time qubit dynamics during measurement. We weakly measure the qubit while it is continuously driven at the Larmor frequency. The phase of the resulting Rabi oscillations diffuses slowly, primarily due to the measurement. We monitor this phase diffusion and correct for it by feeding back on the qubit drive amplitude. This locks the Rabi oscillations to a classical reference signal and the oscillations persist indefinitely with a reduced visibility set by the feedback efficiency. We perform tomography on the feedback stabilized state and suggest routes to further optimize the feedback efficiency. Such capabilities suggest a measurement based route for implementing continuous quantum error correction.

¹This research is supported by the ARO QCT program

9:48AM H29.00010 High fidelity readout of a superconducting qubit using heralded state preparation¹, J.E. JOHNSON, UC Berkeley, C. MACKLIN, D.H. SLICHTER, R. VIJAY, UC Berkeley, QNL, E. WEINGARTEN, JOHN CLARKE, UC Berkeley, I. SIDDIQI, UC Berkeley, QNL — We report measurements of a superconducting flux qubit, coupled via a shared inductance, to a quasi-lumped element 5.78-GHz readout resonator formed by the parallel combination of an interdigitated capacitor and a meander line inductor. A Josephson parametric amplifier with near-quantum-limited noise performance is used to increase the measurement sensitivity. We demonstrate a continuous, high-fidelity readout with sufficient bandwidth and signal-to-noise ratio to resolve quantum jumps in the flux qubit. We achieve a readout fidelity of 91%, limited primarily by T_1 decay between state preparation and measurement. The fast, high-visibility, QND character of the readout allows for many successive readouts within a time T_1 . We exploit this capability to herald pure ground and excited state ensemble populations by post-selecting only for certain states after an initial readout. This method enables us to eliminate errors due to imperfect state preparation, increasing the fidelity to 94%. We also present a precise budget of fidelity loss and an analysis of the readout backaction.

¹This work was funded in part by the U.S. Government and by BBN Technologies.

10:00AM H29.00011 Experimental approaches to improve the single shot measurement fidelity of a superconducting charge qubit, YANBING LIU, SRIKANTH SRINIVASAN, ANTHONY HOFFMAN, ANDREW HOUCK, Princeton University — We discuss various experimental approaches to improve the single shot measurement fidelity of a superconducting charge qubit. Dispersive readout is optimized on a transmon coupled to a superconducting coplanar waveguide resonator. Measurement parameters, such as microwave power and frequency are varied. Also control theory is adapted to construct a genetic algorithm which optimizes the shape of the drive pulse. Additionally, we attempt to reduce noise and increase SNR by employing a SLUG amplifier. Using these techniques, we discuss the feasibility of reaching the measurement fidelity needed for scalable quantum computation with superconducting circuits.

10:12AM H29.00012 Multiplexed dispersive readout for the superconducting phase qubit, DANIEL SANK, R. BARENDs, J. BOCHMANN, B. CHIARO, Y. CHEN, J. KELLY, M. LENANDER, E. LUCERO, M. MARIANTONI, A. MEGRANT, C. NEILL, P. O'MALLEY, P. ROUSHAN, A. VAINSENCHEr, J. WENNER, T. WHITE, Y. YIN, ANDREW CLELAND, JOHN M. MARTINIS, UC Santa Barbara — Scaling to multiple qubit circuits requires state readout with maximum reliability and the minimum number of readout lines. Here, we introduce a multiplexed readout scheme for superconducting phase qubits. We replace our standard readout SQUIDs with inductively coupled resonators so that the measured state of the qubit (left or right side of the potential well) is read out as a shift of the resonator frequency. We connected several readout resonators to a single feedline and use a multi-tone microwave reflection measurement to simultaneously read out the states of multiple qubits using a single cable. Together with the compact lumped LC resonator design, the efficiency of chip space usage is greatly improved.

10:24AM H29.00013 Ground State Misidentification in Superconducting Qubits, JAMES WENNER, Y. CHEN, J. KELLY, H. WANG, E. LUCERO, B. CHIARO, R. BARENDs, M. LENANDER, M. MARIANTONI, A. MEGRANT, C. NEILL, P. O'MALLEY, P. ROUSHAN, D. SANK, A. VAINSENCHEr, T. WHITE, Y. YIN, J. ZHAO, A.N. CLELAND, JOHN M. MARTINIS, UC Santa Barbara — To achieve fault tolerant quantum computation, it is necessary to maximize measurement fidelity and minimize readout-induced measurement errors. A new protocol was developed to measure $P_1(|g\rangle)$, the probability of measuring the excited state without exciting the qubit, while not including stray tunneling present in superconducting phase qubits. We have confirmed the expected trend in $P_1(|g\rangle)$ with device temperature. We then compared $P_1(|g\rangle)$ for phase qubits with different readout mechanisms and found that it is $\sim 3\%$ for our dispersive readout scheme and $\sim 1.5\%$ for our prior SQUID-based readout scheme. We have further applied microwave power to the flux bias and microwave drive lines to understand the source of this difference.

10:36AM H29.00014 Autoresonant readout of a high Q resonator coupled to a superconducting quantum bit¹, KATER MURCH, STEVEN WEBER, R. VIJAY, UC Berkeley, QNL, ERAN GINOSSAR, Physics Department, University of Surrey, STEVEN M. GIRVIN, Physics Department, Yale University, I. SIDDIQI, UC Berkeley, QNL — The frequency of a nonlinear oscillator changes with oscillation amplitude. When a high-Q, nonlinear oscillator is excited with a frequency chirped drive, the system can respond at either low or high oscillation amplitude depending on whether the drive excitation is below or above a critical value, respectively – a phenomenon known as autoresonance. We exploit this nonlinear phenomenon to read out the state of a superconducting transmon qubit coupled to a high-Q nonlinear resonator. Because the excitation is non-equilibrium, the resonator can be read out faster than its energy decay time. The fidelity for mapping the qubit state onto the oscillator can be as high as 80% and is limited by the T_1 lifetime of the qubit, and readily achievable pulse parameters.

¹This research was supported by the IARPA CSQ program.

10:48AM H29.00015 Qubit Measurement with a Nonlinear Cavity Detector Beyond Linear Response, CATHERINE LAFLAMME, AASHISH CLERK, McGill University — We consider theoretically the use of a driven, nonlinear superconducting microwave cavity to measure a coupled superconducting qubit. This is similar to setups studied in recent experiments.^{1,2} In a previous work, we demonstrated that for weak coupling (where linear response theory holds) one misses the quantum limit on QND detection in this system by a large factor proportional to the parametric gain.³ Here we calculate measurement backaction beyond linear response by using an approximate mapping to a detuned degenerate parametric amplifier having both linear and dispersive couplings to the qubit. We find surprisingly that the backaction dephasing rate is far more sensitive to corrections beyond linear response than the detector response. Thus, increasing the coupling strength can significantly increase the efficiency of the measurement. We interpret this behavior in terms of the non-Gaussian photon number fluctuations of the nonlinear cavity. Our results have applications to quantum information processing and quantum amplification with superconducting microwave circuits.

¹M. Hatridge *et al.* Phys.Rev.B, 83,134501 (2011)

²F.R. Ong *et al.* PRL 106,167002 (2011)

³C. Laflamme and A.A. Clerk, Phys. Rev. A 83, 033803 (2011)

Tuesday, February 28, 2012 8:00AM - 11:00AM – Session H30 GQL: Semiconductor Qubits - Device Development 259B

8:00AM H30.00001 Screening of charged impurities with multi-electron singlet-triplet spin qubits in quantum dots¹, JASON KESTNER, EDWIN BARNES, NGA NGUYEN, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland - College Park — Charged impurities in semiconductor quantum dots comprise one of the main obstacles to achieving scalable fabrication and manipulation of singlet-triplet spin qubits. We theoretically show that using dots that contain several electrons each can help to overcome this problem through the screening of the rough and noisy impurity potential by the excess electrons [1]. We demonstrate how the desired screening properties turn on as the number of electrons is increased, and we characterize the properties of a double quantum dot singlet-triplet qubit for small odd numbers of electrons per dot. We show that the sensitivity of the multi-electron qubit to charge noise may be an order of magnitude smaller than that of the two-electron qubit.

[1] E. Barnes, J.P. Kestner, N.T.T. Nguyen, and S. Das Sarma, arXiv:1108.1399.

¹This work supported by LPS-NSA, IARPA, and CNAM.

8:12AM H30.00002 Measurements of undoped accumulation-mode SiGe quantum dot devices, KEVIN ENG, MATHEW BORSELLI, KEVIN HOLABIRD, IVAN MILOSAVLJEVIC, ADELE SCHMITZ, PETER DEELMAN, BIQIN HUANG, MARKO SOKOLICH, LESLIE WARREN, THOMAS HAZARD, ANDREY KISELEV, RICHARD ROSS, MARK GYURE, ANDREW HUNTER, HRL Laboratories, LLC — We report transport measurements of undoped single-well accumulation-mode SiGe quantum dot devices with an integrated dot charge sensor. The device is designed so that individual forward-biased circular gates have dominant control of dot charge occupancy, and separate intervening gates have dominant control of tunnel rates and exchange coupling. We have demonstrated controlled loading of the first electron in single and double quantum dots. We used magneto-spectroscopy to measure singlet-triplet splittings in our quantum dots: values are typically ~ 0.1 meV. Tunnel rates of single electrons to the baths can be controlled from less than 1 Hz to greater than 10 MHz. We are able to control the (0,2) to (1,1) coupling in a double quantum dot from under-coupled ($t_c < kT \sim 5\mu\text{eV}$) to over-coupled ($t_c \sim 0.1$ meV) with a bias control of one exchange gate. Sponsored by the United States Department of Defense. Approved for Public Release, Distribution Unlimited. The views expressed are those of the author and do not reflect the official policy or position of the Department of Defense or the U.S. Government.

8:24AM H30.00003 Fabrication of dual-gated devices on undoped Si/SiGe heterostructures¹

Y. DOVZHENKO, K. WANG, C. PAYETTE, Department of Physics, Princeton University, Princeton, New Jersey 08544, C.-H. LEE, C. W. LIU, Department of Electrical Engineering, National Taiwan University, Taipei, Taiwan, ROC, J. R. PETTA, Department of Physics, Princeton University, Princeton, New Jersey 08544 — Undoped accumulation mode Si/SiGe heterostructures have recently emerged as a promising platform for the fabrication of few-electron silicon spin qubits. Spin blockade has been observed in an accumulation mode double dot [1] and a record mobility of $1.6 \text{ million cm}^2/(\text{Vs})$ has been achieved in undoped wafers grown at National Taiwan University [2]. We develop a fabrication process for dual-gated accumulation mode structures and form a stable two-dimensional electron gas by applying positive bias to a global top gate. The resulting 2DEG has charge densities of $2 - 5 \times 10^{11}/\text{cm}^2$ and mobilities up to $200,000 \text{ cm}^2/(\text{Vs})$. We present preliminary data from quantum point contacts fabricated in this geometry.

References:

[1] M. G. Borselli *et al.*, Appl. Phys. Lett. **99**, 063109 (2011).

[2] T. M. Lu *et al.*, Appl. Phys. Lett. **94**, 182102 (2009).

¹Funded by the Sloan and Packard Foundations, NSF, and DARPA through HRL Laboratories

8:36AM H30.00004 Optimization of realistic silicon double quantum dots through simulation

, ERIK NIELSEN, SUZEY GAO, RALPH YOUNG, RICHARD MULLER, Sandia National Laboratories — We present results obtained using a newly developed semiclassical and Poisson-Schrodinger simulation tool which is able to simultaneously optimize many solution parameters. We discuss the benefit this capability has on realistic device design, and report general trends seen when targeting few-electron quantum dots in silicon and silicon-germanium structures. This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

8:48AM H30.00005 Anatomy of the exchange gate action in undoped accumulation-mode SiGe quantum dot devices

, A.A. KISELEV, R.S. ROSS, M.G. BORSELLI, K. ENG, K.S. HOLABIRD, T.M. HAZARD, M.F. GYURE, HRL Laboratories LLC, 3011 Malibu Canyon Road, Malibu CA 90265 — We discuss simulations of an undoped accumulation-mode SiGe device containing an electrostatically formed double quantum dot in its active area. We validate our virtual model by extensive device characterization (in terms of gate actions, dot addition energies, etc.) and quantitative comparisons to concurrent experimental data. Next, we trace and map in detail the turn-on of the inter-dot exchange interaction by the exchange gate located between the dot gates. Of primary interest is the ability to control (i.e., both to completely shut off and to gradually modulate in the neV to μeV range) the exchange energy between the two separated electrons. We identify a potential obstacle to proper device operation, the formation of additional dot states under the progressively more forward-biased exchange gate. This effect is limited, however, to the case of large dot gate diameter and/or large dot-dot separation. Lastly we quantify and analyze the consequences of cross-capacitance between adjacent exchange and dot gates. Sponsored by the United States Department of Defense. Approved for public release, distribution unlimited.

9:00AM H30.00006 Effect of fixed charge gate oxide defects on the exchange energy of a multi-valley silicon double quantum dot¹

, RAJIB RAHMAN, ERIK NIELSEN, RICK MULLER, MALCOLM CARROLL, Sandia National Laboratories — Exchange interaction at the MOS interface has been proposed as a qubit coupling approach for both MOS quantum dots and donor qubits. An intrinsic source of disorder in the MOS system is the charge defects in silicon dioxide, nanometers away from the interface and qubit electrons. The presence of a charge defect so near the qubit can significantly perturb the confinement potential and alter the intended coupling. Using a large-scale atomistic tight-binding method coupled to a full configuration interaction technique, we investigate the role of these defects on the two-electron coupling of a double quantum dot (DQD) as a function of detuning bias. We show how the multi-valley character of silicon is manifested in the two-electron spectrum, and hence in the exchange energies of excited triplet states corresponding to different valley configurations. Our results show that defects near the tunnel barrier can adversely affect the tunability of the DQD, while defects distributed asymmetrically relative to the two dots can act as an additional detuning source.

¹Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

9:12AM H30.00007 Modeling split gate tunnel barriers in lateral double top gated Si-MOS nanostructures

, AMIR SHIRKHORSHIDIAN, University of New Mexico, NATHANIEL BISHOP, RALPH YOUNG, JOEL WENDT, MICHAEL LILLY, MALCOLM CARROLL, Sandia National Labs — Reliable interpretation of quantum dot and donor transport experiments depends critically on understanding the tunnel barriers separating the localized electron state from the 2DEG regions which serve as source and drain. We analyze transport measurements through split gate point contacts, defined in a double gate enhancement mode Si-MOS device structure. We use a square barrier WKB model which accounts for barrier height dependence on applied voltage. This constant interaction model is found to produce a self-consistent characterization of barrier height and width over a wide range of applied source-drain and gate bias. The model produces similar results for many different split gate structures. We discuss this models potential for mapping between experiment and barrier simulations. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility. The work was supported by the Sandia National Laboratories Directed Research and Development Program. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:24AM H30.00008 Enhancement-mode buried strained-silicon channel double quantum dot

, T.M. LU, N.C. BISHOP, T. PLUYM, J. MEANS, P.G. KOTULA, J. CEDERBERG, L.A. TRACY, J. DOMINGUEZ, M.P. LILLY, M.S. CARROLL, Sandia National Laboratories — We demonstrate a relaxed-SiGe/strained-Si enhancement-mode gate stack for quantum dots. The devices were fabricated within a 150 mm Si foundry setting that uses implanted ohmics and chemical-vapor-deposited dielectrics. Thermal budget was minimized to prevent Ge/Si interdiffusion and strain relaxation. A mobility of $1.6 \times 10^5 \text{ cm}^2/\text{Vs}$ at $5.8 \times 10^{11}/\text{cm}^2$ is measured in Hall bars that witness the same device process flow as the quantum dot. Periodic Coulomb blockade measured in a double-top-gated lateral quantum dot nanostructure terminates with open diamonds up to $\pm 10 \text{ mV}$ of dc voltage across the device. Charge sensing indicates a lithographically defined double quantum dot with tunable coupling. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility. The work was supported by the Sandia National Laboratories Directed Research and Development Program. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:36AM H30.00009 Hybrid Donor-Dot Devices made using Top-down Ion Implantation for Quantum Computing, EDWARD BIELEJEC, NATHAN BISHOP, MALCOLM CARROLL, Sandia National Laboratories — We present progress towards fabricating hybrid donor – quantum dots (QD) for quantum computing. These devices will exploit the long coherence time of the donor system and the surface state manipulation associated with a QD. Fabrication requires detection of single ions implanted with 10's of nanometer precision. We show in this talk, 100% detection efficiency for single ions using a single ion Geiger mode avalanche (SIGMA) detector integrated into a Si MOS QD process flow. The Nanoimplanter (nl) a focused ion beam system is used for precision top-down placement of the implanted ion. This machine has a 10 nm resolution combined with a mass velocity filter, allowing for the use of multi-species liquid metal ion sources (LMIS) to implant P and Sb ions, and a fast blanking and chopping system for single ion implants. The combination of the nl and integration of the SIGMA with the MOS QD process flow establishes a path to fabricate hybrid single donor-dot devices. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:48AM H30.00010 Computer assisted design of poly-silicon gated enhancement-mode, lateral double quantum dot devices for quantum computing, NATHANIEL BISHOP, RALPH YOUNG, Sandia National Labs, CARLOS BORRAS PINILLA, HAROLD STALFORD, University of Oklahoma, Norman, ERIK NIELSEN, RICHARD MULLER, RAJIB RAHMAN, LISA TRACY, JOEL WENDT, MICHAEL LILLY, MALCOLM CARROLL, Sandia National Labs — We discuss trade-offs of different double quantum dot and charge sensor lay-outs using computer assisted design (CAD). We use primarily a semi-classical model, augmented with a self-consistent configuration interaction method. Although CAD for quantum dots is difficult due to uncontrolled factors (e.g., disorder), different ideal designs can still be compared. Comparisons of simulation and measured dot characteristics, such as capacitance, show that CAD can agree well with experiment for relevant cases. CAD results comparing several different designs will be discussed including a comparison to measurement results from the same designs. Trade-offs between poly-silicon and metal gate lay-outs will also be discussed. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility. The work was supported by the Sandia National Laboratories Directed Research and Development Program. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

10:00AM H30.00011 Correlation functions of the electric and magnetic fields in the vicinity of a metal surface¹, LUKE LANGSJOEN, ROBERT JOYNT, MAXIM VAVILOV, AMRIT POUDEL, University of Wisconsin - Madison — The Johnson noise-induced relaxation rate of a charge or spin qubit for a transition at a particular frequency in the vicinity of a metal boundary is proportional to the temporal Fourier component at that frequency of the electric or magnetic correlation function evaluated at the position of the qubit. These correlation functions are shown to be greatly enhanced compared to the blackbody result in the near vicinity of the metal due to the contribution of evanescent waves. As such, we expect a measurable enhancement of qubit decoherence due to the contribution of evanescent waves. We use a Green's dyadic approach to calculate the correlation functions of the fluctuating electric and magnetic fields in the vicinity of a conducting surface. In a local treatment of the dielectric properties of the metal this enhancement diverges as the inverse cube of the distance from the boundary, and for distances less than the order of the Fermi wavelength of the metal a nonlocal treatment is necessary to obtain an accurate result. We present a calculation of the correlation function for the full range of distances.

¹DOD, ARMY W911NF-11-1-0030

10:12AM H30.00012 Fabrication and measurement of quantum dots in double gated, dopantless Si/SiGe heterostructures, DANIEL WARD, ROBERT MOHR, JONATHAN PRANCE, JOHN GAMBLE, DON SAVAGE, MAX LAGALLY, SUSAN COPPERSMITH, MARK ERIKSSON, University of Wisconsin-Madison — Significant progress has been made towards quantum dot spin qubits in Si/SiGe single and double quantum dots. In the past, these structures have been created by depleting a modulation-doped 2DEG that forms at the Si/SiGe interface. The modulation doping in such devices is believed to be a source of charge noise. Recently, undoped structures have been explored for the formation of both 2DEGs and quantum dots in Si/SiGe. Here we discuss measurements on double gated, dopantless quantum dots in Si/SiGe heterostructures. The devices are based on a new "island mesa" design incorporating micro-ohmic contacts. We present transport measurements on a double quantum dot showing a smooth transition from single dot to double dot behavior.

10:24AM H30.00013 Unintentional Quantum Dots in Silicon: Deducing the Location and Cause, TED THORBECK, NIST and University of Maryland: JQI, CNAM, NEIL M. ZIMMERMAN, NIST — When attempting to use local gates to electrostatically define quantum dots in silicon, additional unintentional quantum dots (U-QDs) that are not defined by the gates are often observed. U-QDs are typically blamed on random charged defects such as dopants or interface traps. We use measured gate capacitances and a capacitance simulator to determine the location of the U-QDs with a precision of a few nanometers. Since we have observed U-QDs in similar locations in multiple devices, we suggest that some U-QDs are not caused by random charged defects instead are a systematic but unanticipated consequence of the fabrication. We will discuss strain as a potential cause of the U-QDs. This allows us to suggest methods to reduce the frequency of U-QDs in future devices. Given the variety of groups suffering from U-QDs and the simplicity of this technique, we think that many groups might benefit from our methods.

10:36AM H30.00014 The divacancy in SiC: A new solid-state qubit, LUKE GORDON, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — The nitrogen-vacancy center in diamond has attracted interest due to promising applications as a room-temperature solid-state qubit (the basic unit of a quantum computer). It is, however, desirable to identify defects that possess similar properties, but in alternative semiconductors that are either cheaper or more technologically mature. One notable defect system is the divacancy in 4H-SiC, which has recently been the subject of extensive experimental investigation. In this work, we employ advanced computational methods, particularly density functional theory using a hybrid functional, to investigate the stability and excitation energies of multiple forms of the divacancy in the various polytypes of silicon carbide. The hybrid functional gives band gaps and lattice parameters that are in excellent agreement with experiments. This allows for quantitative predictions of defect levels and zero-phonon line energies for excitation and emission processes, aiding in experimental identification of these defects.

10:48AM H30.00015 Large Stark effect for Li donor spins in Si, LUKE PENDO, ERIN HANDBERG, South Dakota School of Mines, VADIM SMELYANSKIY, NASA Ames Research Center, ANDRE PETUKHOV, South Dakota School of Mines — We study the effect of a static electric field on lithium donor spins in silicon. The anisotropy of the effective mass leads to the anisotropy of the quadratic Stark susceptibility, which we determined using the Dalgarno-Lewis exact summation method [1]. The theory is asymptotically exact in the field domain below Li-donor ionization threshold, relevant to the Stark-tuning Electron Spin Resonance (ESR) experiments [2]. With the calculated Stark susceptibilities at hand, we were able to predict and analyze several important physical effects. In particular, we demonstrate that the Stark effect anisotropy, combined with unique valley-orbit splitting of a Li donor in Si, spin-orbit interaction and specially tuned external stress, may lead to a very strong modulation of the donor spin g-factor by the electric field. Also we investigate the influence of random strains on the g-factor shifts and quantify the random strain limits and requirements to Si material purity necessary to observe the ESR-Stark shifts experimentally. Finally, we discuss possible applications of our results to quantum information processing with Li spin qubits in Si.

[1] A. Dalgarno and J. T. Lewis, Proc. Roy. Soc. 233, 70 (1955).

[2] F. R. Bradbury et al. Phys. Rev. Lett. 97, 176404 (2006).

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H31 DMP: Focus Session: Topological Insulators: Synthesis and Characterization:
Bulk Crystals 260

8:00AM H31.00001 Low carrier concentration crystals of the topological insulator $\text{Bi}_2\text{Te}_2\text{Se}$, SHUANG JIA, HUIWEN JI, E. CLIMENT-PASCUAL, M.K. FUCCILLO, M.E. CHARLES, Department of Chemistry, Princeton University, JUN XIONG, N.P. ONG, Department of Physics, Princeton University, R.J. CAVA, Department of Chemistry, Princeton University — We report the characterization of $\text{Bi}_2\text{Te}_2\text{Se}$ crystals obtained by the modified Bridgman and Bridgman-Stockbarger crystal growth techniques. X-ray diffraction study confirms an ordered Se-Te distribution in the inner and outer chalcogen layers, respectively, with a small amount of mixing. The crystals displaying high resistivity ($> 1 \Omega\text{cm}$) and low carrier concentration ($\sim 5 \times 10^{16}/\text{cm}^3$) at 4 K were found in the central region of the long Bridgman-Stockbarger crystal, which we attribute to very small differences in defect density along the length of the crystal rod. Analysis of the temperature dependent resistivities and Hall coefficients reveals the possible underlying origins of the donors and acceptors in this phase.

8:12AM H31.00002 Structural study of topological insulator $\text{Bi}_2(\text{Se}_{3-x}\text{Te}_x)$, KEESEONG PARK, University of Virginia, Charlottesville, Virginia 22904, USA., DESPINA LOUCA, University of Virginia, Charlottesville, Virginia 22904, USA, ANNA LLOBET, Lujan Neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — With neutron diffraction, we systematically investigated the local and average structures of topological insulator $\text{Bi}_2(\text{Se}_{3-x}\text{Te}_x)$ ($x=0, 1, 1.5, 2$, and 3) from 5 to 500 K. The average crystal structure of Bi_2Se_3 is rhombohedral R-3m symmetry with 2 unique chalcogen sites. This gives rise to 2 types of Bi-(Se/Te) bonds in quintuple layer composed of Se1-Bi-Se2 –Bi-Se1 layers, covalent Se1-Bi bond with the bonding length of 2.85 Å and ionic Se2-Bi bond with the bonding length of 3.07 Å at 5 K. The Se1-Se1 bonds between quintuple layers are governed by Van der Waals of the length of 3.47 Å at 5 K. With increasing temperature, it is observed that the quintuple layer unit contracts from the anti-parallel motion of the Bi-(Se1)₃ tetrahedra toward the Se2-center layer. Also such a contraction implies the Van der Waals bonding between quintuple layers weakens with temperature. A similar temperature dependence of atomic structure is observed on Bi_2Se_3 .

8:24AM H31.00003 Hole doping of p-type thin topological insulators, INNA KORZHOVSKA, LUKAS ZHAO, ZHIYI CHEN, HAIMING DENG, LIMIN HUANG, City College of New York - CUNY, SIMONE RAOUX, JEAN JORDAN-SWEET, IBM Research - Yorktown, MYRIAM SARACHIK, STEPHEN O'BRIEN, LIA KRUSIN, City College of New York - CUNY — Recent studies of intrinsically n-type topological insulator (TI) Bi_2Se_3 demonstrated that doping with Cu introduces electrons into this system, and that in the narrow range of doping $\text{Cu}_x\text{Bi}_2\text{Se}_3$ becomes a superconductor below Tc 5 K. It is presumed that Cu intercalates into Van der Waals gaps in the tetradymite structure of layered Bi_2Se_3 , although this remains to be confirmed. We report on hole doping experiments on the naturally p-type Te-based TIs: thin films of Bi_2Te_3 and nanocrystalline plates of Sb_2Te_3 . The samples were iodine doped either during the growth or by the exposure to iodine vapor. Transport measurements on films indicate a very unusual T³ temperature dependence of longitudinal resistivity. It drops significantly below 30 K with decreasing temperature, although the drop appears arrested by a metal-insulator transition in the 300 mK range. Magnetization measurements on nanoplates indicate the development of large diamagnetic signal. These results will be discussed in comparison with the superconductivity obtained by Cu doping in Bi_2Se_3 . * Supported in part by NSF-DMR-1122594.

8:36AM H31.00004 Synthesis and Characterization of New Topological Insulators¹, KOUJI SEGAWA, Institute of Scientific and Industrial Research, Osaka University — In this talk, I will show detailed information on synthesizing process and characterization results of new topological insulator (TI) materials with interesting properties. Among the synthesized materials, TlBiSe_2 was the first ternary TI and has the largest bulk band gap [1], $\text{TlBi}(\text{S}_{1-x}\text{Se}_x)_2$ presents a topological phase transition with unexpected Dirac mass [2], BiTe_2Se presents a large bulk resistivity [3], and $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ has finally achieved the surface-dominated transport in bulk single crystals [4]. It is essentially easy to grow single crystals of all the chalcogenides above, because those compounds melt congruently at relatively low temperatures. Therefore, the melt-growth method is applicable if the raw materials are in a sealed condition, e.g., in a quartz tube. However, crucial techniques for obtaining high-quality samples vary between the systems. Besides the growth method, characterizations of the transport properties, ARPES, the X-ray diffraction, and quantitative chemical analysis will also be presented.

This work is in collaboration with A. A. Taskin, S. Sasaki, Zhi Ren, K. Eto, T. Minami, and Y. Ando (Osaka Univ.), and T. Sato, S. Souma, H. Guo, K. Sugawara, K. Kosaka and K. Nakayama, and T. Takahashi (Tohoku Univ.).

[1] T. Sato, Kouji Segawa, T. Takahashi, Y. Ando *et al.*, Phys. Rev. Lett. **105**, 136802 (2010).

[2] T. Sato, Kouji Segawa, Y. Ando, T. Takahashi *et al.*, Nature Physics, **7**, 840 (2011).

[3] Zhi Ren, Kouji Segawa, Y. Ando *et al.*, Phys. Rev. B (Rapid Comm.) **82**, 241306(R) (2010).

[4] A. A. Taskin, Kouji Segawa, and Y. Ando *et al.*, Phys. Rev. Lett. **107**, 016801 (2011).

¹This work was supported by JSPS(KAKENHI 19674002 and 20371297, and Next-Generation World-Leading Researchers Program), MEXT (Innovative Area “Topological Quantum Phenomena” KAKENHI 22103004), and AFOSR (AOARD 10-4103).

9:12AM H31.00005 Transport properties of new Pb-based Topological Insulators¹, KAZUMA ETO, SATOSHI SASAKI, KOUJI SEGAWA, YOICHI ANDO, Institute of Scientific and Industrial Research, Osaka University — A topological insulator (TI) has a gapped insulating bulk and a gapless metallic surface. So far, such materials as $\text{Bi}_{1-x}\text{Sb}_x$, Bi_2Se_3 , and TlBiSe_2 are known to be TIs. Recently, several theoretical predictions have been made for new TI materials. In this work, we focus on the Pb-based ternary chalcogenides as new candidate TIs. We have grown a number of single crystals in the systems of Pb-Bi-Se, Pb-Bi-Te, Pb-Sb-Te and Pb-(Sb,Bi)-Te. After selecting single-phase samples, we measured the transport properties to check for their bulk-insulating nature. It was found that $\text{Pb}(\text{Sb}_x\text{Bi}_{1-x})_2\text{Te}_4$ shows a change in the carrier type at around $x=0.55$ as inferred both by the thermopower and by the Hall effect, but the temperature dependences of the resistivity remained metallic in all the samples studied. We discuss the prospect of making a bulk-insulating material in the Pb-based TIs.

¹This work was supported by JSPS (KAKENHI 23-4376 and NEXT Program), MEXT (Innovative Area “Topological Quantum Phenomena”) and AFOSR-AOARD. KE expresses his special thanks for the Research Fellowship for Young Scientists by JSPS.

9:24AM H31.00006 Millikelvin transport of high quality Bi_2Se_3 crystals at high pressure, KEVIN KIRSCHENBAUM, Center for Nanophysics and Advanced Materials, Physics Dept., University of Maryland, JASON JEFFRIES, NICHOLAS BUTCH, Lawrence Livermore National Laboratory, PAUL SYERS, Center for Nanophysics and Advanced Materials, Physics Dept., University of Maryland, JAMES HAMLIN, BRIAN MAPLE, University of California at San Diego, JOHNPIERRE PAGLIONE, Center for Nanophysics and Advanced Materials, Physics Dept., University of Maryland — In this study we present electronic transport in Bi_2Se_3 single crystals in a diamond anvil pressure cell. Reaching temperatures down to 20 mK and pressures exceeding 30 GPa we measure changes in electrical resistivity, magnetoresistance, and the Hall effect and discuss the results as they pertain to topologically interesting behavior.

9:36AM H31.00007 Entropy transport in Bi_2Se_3 , BENOÎT FAUQUÉ, AURELIE COLLAUDIN, KAMRAN BEHNIA, LPEM (UPMC-CNRS), ESPCI, 75005 Paris, France, NICK BUTCH, JOHNPIERRE PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park, Maryland 20742, USA, STEFFEN WIEDMANN, High Field Magnet Laboratory, Institute for Molecules and Materials, Radboud University Nijmegen, 6525 ED Nijmegen, The Netherlands — Bi_2Se_3 and Bi_2Te_3 are well known compounds in the thermoelectricity community as they present a high figure of merit [1]. Although the thermoelectric power of Bi_2Se_3 has been extensively studied at high temperature, little is known about its behaviour at the low temperature limit. In this presentation, we will report the results of our entropy measurement of Bi_2Se_3 at low temperature and high magnetic field for a bulk carrier concentration from 10^{17}cm^{-3} to 10^{19}cm^{-3} . In all compounds we show significant quantum oscillations in the Seebeck and Nernst responses. Based on the bulk Fermi surface, we propose a simple description of the entropy transport measurement in Bi_2Se_3 (in the range of concentrations studied). Indeed, Bi_2Se_3 (non compensated system) appears as a complementary system of bismuth [2] and graphite [3] (compensated systems) to understand the entropy transport in the low carrier concentration limit.

[1] G.S. Nolas et al, Thermoelectrics Basic Principles and New Materials Developments, Springer.

[2] K.Behnia et al, PRL, 98, 166602 (2007)

[3] Z.Zhu et al, Nature Physics, 6, 26 (2009)

9:48AM H31.00008 Search and Design of Topological Insulators by High-throughput Method, KESONG YANG, WAHYU SETYAWAN, SHIDONG WANG, Department of Mechanical Engineering and Materials Science, Duke University, JEFF MULLLEN, MARCO BUONGIORNO-NARDELLI, Department of Physics, North Carolina State University, STEFANO CURTAROLO, Department of Mechanical Engineering and Materials Science, Duke University, DUKE TEAM, NCSU TEAM — Topological insulators (TIs) have attracted enormous interest because of their novel surface conduction effects which are protected by time-reversal symmetry. A high-purity TI with a highly insulating bulk is necessary to realize the potential practical applications of this class of materials. Therefore, numerous attempts are being made to search for TIs with desired properties (e.g., a large band gap and amenability to high-quality crystal growth). In this presentation, we will introduce an effective high-throughput approach to search and design TIs from a vast electronic structure database such as Inorganic Crystal Structure Database (ICSD) and Heusler alloys.

10:00AM H31.00009 Effects of Intrinsic Defects on Topological Insulator Behavior: Theory and Experiments on Ternary Tetradymite Compounds¹, DUANE D. JOHNSON, LIN-LIN WANG, AFTAB ALAM, MIANLIANG HUANG, SRINIVASA THIMMAIAH, TOM LOGRASSO, ADAM KAMINSKI, None, PAUL C. CANFIELD, Division of Materials Science and Engineering, Ames Laboratory and Iowa State University — Ternary tetradymites $\text{Bi}_2\text{Te}_{3-x}\text{Se}_x$ are predicted to be topological insulators via density functional theory (DFT) surface band structure calculations. Experimentally, we find that Bi_2Se_3 and Bi_2Te_3 form a continuous solid solution at the two non-equivalent group VI sites with different site preferences for Se and Te. The DFT formation energies for ordered and partially ordered compounds agree well with experimental data. Importantly, we calculated the intrinsic defect formation energies of binary and ternary tetradymites, and find they correlate well with the bulk conductivity measurement. Angle resolved photoemission spectroscopy confirms the existence of the Dirac cone in the surface band of $\text{Bi}_2\text{Te}_2\text{Se}$.

¹Supported by DE-AC02-07CH11358 at the Ames Laboratory operated by Iowa State University

10:12AM H31.00010 Transport properties of chalcogenide and related topological insulator bulk crystals, R.B. LILLIANFELD, HELIN CAO, TAI-LUNG WU, IREK MIOTKOWSKI, YONG P. CHEN, Purdue University — Three-dimensional (3D) topological insulators (TIs) have attracted strong theoretical and experimental interest in the condensed matter community. We have used the Bridgman method to synthesize various chalcogenide and related 3D TI crystals. We present an experimental survey of a group of binary, tertiary, and quaternary bulk crystals of various compositions of Bi, Sb, Ge, Se, Te, and S. Our survey includes systems without intentional doping, as well as systems doped with magnetic and non-magnetic impurities. We present magnetotransport data over a range of temperatures. We also measure thin films exfoliated from these bulk crystals to examine efficacy of carrier modulation through an applied gate voltage. We discuss the results of these measurements in the context of TI properties, with the ultimate goal of identifying systems that display electronic transport properties consistent with an insulating bulk and spin-helical Dirac fermion surface states.

10:24AM H31.00011 Bulk Excitations in single crystal Bi_2Se_3 : Electron Energy Loss Spectroscopy Study, SZ-CHIAN LIQU, F.T. HUANG, R. SANKAR, M.-W. CHU, F.C. CHOU, C.H. CHEN, Center for Condensed Matter Sciences, National Taiwan University, CENTER FOR CONDENSED MATTER SCIENCES, NATIONAL TAIWAN UNIVERSITY COLLABORATION — Bi_2Se_3 with larger figure of merit has been used in room-temperature thermoelectric applications. Furthermore, it is also one of a handful known topological insulators. Most of recent studies were focused on the topological surface states of Bi_2Se_3 while few of them studied the electronic excitations of bulk Bi_2Se_3 . Here, we report studies of electronic excitations of single-crystal Bi_2Se_3 by electron energy-loss spectroscopy (EELS). EELS spectrum in bulk Bi_2Se_3 reveals several spectral features at ~ 7 , ~ 16.8 , ~ 26.4 and ~ 28.4 eV. The peaks at ~ 26.4 and ~ 28.4 eV are due to excitations from Bi 5d electrons. The ~ 7 and ~ 16.8 eV peaks are easily identified as bulk-plasmon excitations according to the frequency-dependent complex dielectric function derived from experimental spectrum with Kramers-Krönig analysis. Furthermore, momentum (q)-dependent EELS spectra along [110], [300] and [001] directions were also performed in this study. When momentum transfer q is parallel [110] and [300] directions, the 16.8 eV-peak (bulk plasmon) significantly shift to higher energy (up to 23 eV) with increasing q values, while this peak shifts less than 1 eV when momentum transfer q is parallel to [001] direction, revealing the distinct anisotropy of bulk plasmon dispersions. Detailed characteristics of this anisotropic behavior will also be discussed.

10:36AM H31.00012 Insights on the electronic and vibrational properties of Bi(111) from first principles¹, MARISOL ALCANTARA ORTIGOZA, ROLF HEID, KLAUS-PETER BOHNEN, Karlsruhe Institute for Technology, IRINA SKLYADNEVA, Donostia International Physics Center, NEHA NAYYAR, TALAT S. RAHMAN, University of Central Florida, EUGENE CHULKOV, Donostia International Physics Center — Bi(111) is known to have surface electron carriers close to Γ as well as hole carriers at Γ and along the ΓM directions. The lattice dynamics of Bi(111) is however largely unknown. We investigate both the electronic structure and lattice dynamics of Bi(111) films via density-functional-theory and density-functional-perturbation-theory calculations taking into account the spin-orbit coupling (SOC). While the splitting of the branches is dominated by the SOC almost everywhere along the ΓM direction, around the zone boundary (M), the delocalized character of this state plays an important role. Reducing the thickness of a film decreases the band gap progressively. At ~ 3 -nm thickness, the highest valence band re-crosses the Fermi level and creates extra electron pockets. We find, however, that the lattice dynamics of Bi(111) is robust with respect to film thickness. Bi(111) has a number of “high-lying” surface modes in the optical band almost everywhere along the ΓKM and ΓM directions, most notably, a vertical mode slightly above the bulk band. Surface acoustic modes are also present as well as some “low frequency” optical modes in small regions of the zone. A comparison with recent measurements will be presented, as well as the possible implications on the electron-phonon coupling.

¹Work supported in part by DOE-BES grant DE-FG02-07ER46354

10:48AM H31.00013 Electron beam irradiation effect on Bi_2Se_3 topological insulator nanodevices¹, ZHIYONG WANG, PENG WEI, XINFEI LIU, JING SHI, Department of Physics and Astronomy, University of California Riverside — Nanofabrication is found to introduce excess charge carriers and results in a strong metallic state in Bi_2Se_3 . The uncontrolled carrier density causes the Fermi level to rise to the conduction band. To verify the effect of the electron beam lithography (EBL), we have measured the carrier density of Bi_2Se_3 nanodevices before and after EBL with a range of electron beam energies and doses and find that the Fermi level rises in both n- and p-type devices. To effectively control the position of the Fermi level, we have developed a nanofabrication-free technique for Bi_2Se_3 nanodevices, with which the initial state of the bulk materials can be well preserved. We deliberately choose p-type Ca-doped Bi_2Se_3 devices and systematically introduce more electrons using successive EBL. Resistivity temperature dependence shows that the Fermi level position is gradually tuned from the valence band into the band gap. Further fine tuning of the Fermi level is accomplished by applying a gate voltage to the devices. An increase of a factor of 10 in mobility has been observed in the device as the Fermi level is brought into the band gap, which is consistent with the suppressed backscattering of the surface states in topological insulators.

¹This work was supported in part by DOE and NSF.

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H32 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides - Conducting Domain Walls and Conduction Mechanisms 261

8:00AM H32.00001 Conduction of topologically-protected charged ferroelectric domain walls¹, WEIDA WU, YOICHI HORIBE, NARA LEE, S-W. CHEONG, Department of Physics and Astronomy and Rutgers Center for emergent materials, Rutgers University, Piscataway, NJ 08854 USA, JEFFERY GUEST, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, Illinois 60439 USA — We report on the observation of nanoscale conduction at ferroelectric domain walls in hexagonal HoMnO_3 protected by the topology of multiferroic vortices using *in situ* conductive atomic force microscopy, piezo-response force microscopy, and kelvin-probe force microscopy at low temperatures. Conductance spectra reveal that only negatively charged tail-to-tail walls, in contrast to positively charged head-to-head walls, exhibit ohmic-like conduction in addition to Schottky-like rectification. Our results pave the way for understanding the semiconducting properties of the domains and domain walls in small-gap ferroelectrics.

¹NSF-DMR-0844807, NSF-DMR-1104484 and DE-AC02-06CH11357

8:12AM H32.00002 Electrical dressing of domain walls in hexagonal ErMnO_3 , DENNIS MEIER, JAN SEIDEL, UC Berkeley, ANDRES CANO, European Synchrotron Radiation Facility, KRIS DELANEY, UC Santa Barbara, YU KUMAGAI, ETH Zuerich, MAXIM MOSTOVOY, University of Groningen, NICOLA A. SPALDIN, MANFRED FIEBIG, ETH Zuerich, RAMAMOORTHY RAMESH, UC Berkeley — Domain walls are natural mobile nanoscale objects that can exhibit structural, physical, and chemical properties which drastically differ from the surrounding bulk material. This applies to a large variety of phenomena including chemical/electrical transport, multiferroicity, or superconductivity. Unfortunately, in contrast to bulk materials, very little is known about involved length scales and control parameters when it comes to domain walls and experimental evidence is highly desirable. Here, we report on electrical dressing of trimerization-polarization walls in ErMnO_3 . Using piezoforce-response microscopy and conductive atomic force microscopy we reveal that two characteristic length scales are to be distinguished: A first one corresponding to the structural / ferroelectric changes occurring at the wall and a second one referring to the associated electric properties. Furthermore, we demonstrate the response of the electrically dressed walls to external electric fields and develop a model that explains this response. Our results are expected to generally apply to domain walls in ferroelectric semiconductors and provide new insight into the interplay of charge and lattice degrees of freedom at domain walls.

8:24AM H32.00003 Anisotropic conductance at improper ferroelectric domain walls, JAN SEIDEL, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, DENNIS MEIER, Department of Physics, University of California, Berkeley, CA 94720, USA, ANDRES CANO, European Synchrotron Radiation Facility, 6 Rue Jules Horowitz, 38043 Grenoble, France, KRIS DELANEY, Materials Research Laboratory, University of California, Santa Barbara, CA 93106, USA, YU KUMAGAI, Department of Materials, ETH Zurich, Wolfgang-Pauli-Strasse, 8093 Zurich, Switzerland, MAXIM MOSTOVOY, Zernike Institute for Advanced Materials, University of Groningen, 9747 AG Groningen, The Netherlands, NICOLA SPALDIN, MANFRED FIEBIG, Department of Materials, ETH Zurich, Wolfgang-Pauli-Strasse, 8093 Zurich, Switzerland, RAMAMOORTHY RAMESH, Department of Materials Science and Engineering, University of California, Berkeley, CA 94720, USA — Domain walls in ferroelectric oxides hold great potential for the development of new device paradigms in oxide nanoelectronics due to their field-tunable functionality. They are also of fundamental interest for studies of ferroic and low-dimensional systems physics. We investigate the electronic conductance of ferroelectric domain walls in the improper ferroelectric ErMnO_3 . We show that the conductance is a continuously tunable function of the domain wall orientation, with a range of an order of magnitude. We explain the observed behavior using first-principles density functional and phenomenological theories, and relate it to the extraordinary stability of the inherent head-to-head and tail-to-tail domain walls in hexagonal manganites, which is a direct consequence of the improper ferroelectric character of these materials.

8:36AM H32.00004 Conduction at domain walls in insulating $\text{Pb}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{O}_3$ thin films, JILL GUYONNET, IAROSLAV GAPONENKO, STEFANO GARIGLIO, PATRYCJA PARUCH, DPMC, University of Geneva — Ferroic domain walls are intrinsically nanoscale and often present functional properties beyond those of their parent material. One of the most striking examples is the recent discovery of electrical conduction¹ at domain walls in multiferroic BiFeO_3 . Different scenarios have been proposed to explain the observed conduction, generally relating it to the complex nature of domain walls specific to BiFeO_3 .² Here, we report on scanning probe microscopy studies of domain-wall-specific conduction in thin films of tetragonal ferroelectric (PZT). Our measurements show nonlinear asymmetric current-voltage characteristics with strong thermal activation at $T > 150$ K. Moreover, the average current signals remain stable over the duration of measurement (up to four days). In light of recent transmission electron microscopy measurements at 180° domain walls in PZT,³ we discuss the possible conduction mechanisms, highlighting the role of electrode asymmetry and microscopic domain wall structure promoting local defect segregation.

¹Seidel et al., Nat. Mat. **8**, 229 (2009)

²Lubk et al., PRB **80**, 104110 (2009); Chiu et al., Adv. Mat. **23**, 1530 (2011); Farokhipoor et al., PRL **107**, 127601 (2011)

³Jia et al., Sci. **331**, 1420 (2011)

8:48AM H32.00005 Interplay between polarization and conductivity in BiFeO_3 thin films, SAEEDH FAROKHIPOOR, BEATRIZ NOHEDA PINUAGA, Zernike Institute for Advanced Materials, Netherlands — BiFeO_3 (BFO) is a rhombohedrally distorted, ferroelectric, antiferromagnetic perovskite and one of the few room temperature multiferroics. We've previously reported on conduction at 71° domain walls in BFO thin films grown on SrRuO_3 -buffered SrTiO_3 substrates. For clarifying the origin of conductivity in domain/domain walls, the conduction mechanisms have been extensively studied. The large current regime is determined by Schottky emission from the tip. The migration of oxygen vacancies to the domain walls lowers the Schottky barrier heights at the interface with the metallic tip compared to that in the domains, which results in the observed difference of conductivity in domains and domain walls. In this work we investigate the tunability of the conductivity upon changes in the electrode's work function, as well as the interplay between polarization and conductivity in BFO thin films.

9:00AM H32.00006 Tunable Metallic Conductivity in Ferroelectric Nanodomains, P. MAKSYM-MOVYCH, Oak Ridge National Laboratory, Oak Ridge, TN, A.N. MOROZOVSKA, Institute for Semiconductor Physics, National Academy of Science of Ukraine, P. YU, Department of Materials Science and Engineering, University of California, Berkeley, CA, E.A. ELISEEV, Institute for Problems of Materials Science, National Academy of Science of Ukraine, Y.-H. CHU, Department of Materials Science and Engineering, National Chiao Tung University, R. RAMESH, Department of Materials Science and Engineering, University of California, Berkeley, CA, A.P. BADDORF, S.V. KALININ, Oak Ridge National Laboratory, Oak Ridge, TN — Domain wall conductivity in ferroelectric and multiferroic oxides is an essential example of new electronic properties created by topological defects. So far electron transport through domain walls in canonical BiFeO₃ and PbZr_{0.2}Ti_{0.8}O₃ (PZT) ferroelectrics has been dominated by thermally activated hopping, concealing the enabling physics and limiting potential applications. We will present a pioneering observation of metallic conductivity in nanoscale ferroelectric domains in PZT, that unambiguously identifies a new conduction channel created through the bulk of the oxide film [1]. From a corollary theoretical analysis, we conclude that metallic conductance is enabled by the interplay of charging and flexoelectric effects at tilted and curved walls of the nanodomain. Furthermore, both type and density of carriers can be tuned by manipulation of the order parameter. Thus, a new family of electronic properties may be found in multiferroic and topologically nanostructured complex oxides. [1] Maksymovych et al, *Nano Lett.* in review (2011). Research conducted at the Center for Nanophase Materials Sciences, sponsored by BES, U. S. DOE.

9:12AM H32.00007 Ultrafast p-d charge-transfer carrier dynamics of multiferroic BiFeO₃, Y.M. SHEU, S.A. TRUGMAN, Y.-S. PARK, Center for Integrated Nanotechnologies, LANL, Los Alamos, NM 87545, S.-W. CHEONG, Department of Physics and Astronomy, Rutgers University, NJ 08854, Q. JIA, A.J. TAYLOR, R.P. PRASANKUMAR, Center for Integrated Nanotechnologies, LANL, Los Alamos, NM 87545 — We report first comprehensive understanding of ultrafast carrier dynamics in bulk single crystal BiFeO₃. From a wavelength dependent optical pump-probe measurement, we find that the photoexcited carriers relax to the bottom of band through electron-phonon coupling with a ~ 1 ps time constant that does not significantly change across the antiferromagnetic transition. Following relaxation, carriers leave the conduction band or original excited electronic configuration and decay via radiative recombination, which is supported by our photoluminescence spectroscopy, reported for the first time.

9:24AM H32.00008 Photocurrent effect of epitaxial tetragonal-like BiFeO₃ thin film, KANGHYUN CHU, CHANG-SU WOO, SEUNG JIN KIM, Department of Physics, KAIST, JI HO SUNG, WONMO LEE, MOON-HO JO, Department of Materials Science and Engineering, POSTECH, CHAN-HO YANG, Department of Physics, KAIST — Photovoltaic effect in ferroelectrics has recently received many attentions due to potential applications related to optoelectronic devices and solar cells. Here we report photocurrent effect of highly elongated “tetragonal-like” BiFeO₃ thin films grown on LaAlO₃ (001) substrates using pulsed laser deposition technique. Spatially resolved photocurrent measurements are performed with varying photon wavelength and polarization. Being combined with local ferroelectric domain structure by piezoresponse force microscopy, the spatially resolved techniques make a pathway to explore inter-relation between electric polarization and photon polarization. This study might deepen our understating of light induced conduction phenomena in ferroelectrics.

9:36AM H32.00009 Intrinsic defects in BiFeO₃: Energetics and implication for magnetism, TULA R. PAUDEL, SITARAM S. JASWAL, EVGENY Y. TSYMBAL, University of Nebraska, Lincoln — We investigate energetics of the intrinsic defects in bulk multiferroic BiFeO₃ and explore their implication for magnetization in this compound using a first-principles approach based on density functional theory. We find that dominant defects in oxidizing conditions are Bi and Fe vacancies and in reducing conditions are O and Bi vacancies. When enforcing charge neutrality, the calculated carrier concentration shows that the BiFeO₃ grown in oxidizing conditions has p-type conductivity. The conductivity decreases with oxygen partial pressure and the material becomes insulating with tendency for n-type conductivity. We find that the Bi and Fe vacancies produce a magnetic moment of $\sim 1 \mu_B$ and $\sim 5 \mu_B$ per vacancy, respectively, for p-type BiFeO₃ and none for insulating BiFeO₃. O vacancies do not introduce any moment for both p-type and insulating BiFeO₃. Calculated magnetic moments due to intrinsic defects are consistent with those reported experimentally for the bulk BiFeO₃, however do not explain the large magnetization observed in some experiments on thin-film BiFeO₃.

9:48AM H32.00010 Dielectric screening enhanced Hall mobility in doped ferroelectrics, WOLTER SIEMONS, MICHAEL A. MCGUIRE, VALENTINO R. COOPER, MICHAEL D. BIEGALSKI, ILIA N. IVANOV, GERALD E. JELLISON, LYNN A. BOATNER, BRIAN C. SALES, HANS M. CHRISTEN, Oak Ridge National Laboratory — A low electron mobility is the key limitation that prevents widespread device applications of complex oxide materials. However, in some perovskites, for example SrTiO₃ and KTaO₃, high mobilities in excess of $10,000 \text{ cm}^2 \text{ s}^{-1} \text{ V}^{-1}$ are measured. Together with this dramatic increase in mobility as temperature is lowered, their dielectric constants also increase from a few hundred at room temperature to near 20,000 at low temperatures, suggesting a correlation between the dielectric constant and the mobility. By using electron-doped ferroelectric crystals of composition KTa_{1-x}Nb_xO₃, where the ferroelectric transition temperature can be tuned by changing the Ta:Nb ratio, we demonstrate an enhancement of the Hall mobility by a factor of 2-3 at the Curie temperature up to room temperature. We conclude that the mobility in these doped ferroelectrics peaks at the Curie temperature due to the increased dielectric constant, which reduces charge carrier scattering by impurities. Enhanced mobility could result in faster oxide transistors, boost the performance of thermoelectric devices, and enable more efficient photovoltaic materials. Supported by ORNL's LDRD program (W.S., H.M.C., V.C., G.E.J.), U.S. DOE, BES, MSED (M.A.M., B.C.S.) and SUFD (M.D.B., I.N.I.).

10:00AM H32.00011 The persistence of ferroelectric distortions in electron-doped BaTiO₃: microscopic origins and critical behavior, YONG WANG, JOHN BURTON, SITARAM JASWAL, EVGENY TSYMBAL, University of Nebraska - Lincoln — To explore possible novel applications of the prototypical ferroelectric oxides we perform theoretical studies of electron-doping in BaTiO₃. The presence of conduction electrons in a ferroelectric opens the possibility of bi-stable behavior directly in a conducting material which may lead to new functionalities. It is known, however, that conduction electrons screen the long range Coulomb interactions responsible for polar instabilities. Interestingly though, our first-principle density functional calculations reveal that ferroelectric distortions can persist in electron-doped BaTiO₃ up to 0.01 e/unit cell, consistent with experimental results [1], suggesting that ferroelectricity and conductivity can coexist. To elucidate the competition between the long range Coulomb interactions and the short range bonding effects we have developed an adequate electrostatic model. Using this model, we reproduce the polarization vs. doping behavior obtained from first-principles and derive an analytical expression for the critical doping above which ferroelectric distortions disappear. [1] T. Kolodiazhnyi et al, Phys. Rev. Lett. 104, 147602 (2010).

10:12AM H32.00012 Multiphysics model of semiconducting ferroelectrics and its application to memory devices, NATHANIEL NG, KAUSHIK BHATTACHARYA, California Institute of Technology — Ferroelectrics are used in many electronic devices, in particular as transistors for ferroelectric memory devices. The behavior of these materials are often described via the classic time-dependent Ginzburg Landau model, where they are treated as insulators. However, it is well known that ferroelectrics are in fact wide band-gap semiconductors. It then follows that capturing the key aspects of semiconductor physics—band bending at the interface, Fermi levels, depletion layers, require ferroelectrics to be treated as semiconductors. In this work, we introduce a model that addresses these difficulties, yet at the same time is consistent with both the time-dependent Ginzburg Landau model and the classic drift-diffusion model in semiconductors. Unlike other models, our model makes no a priori assumptions on the space charge and polarization distributions and is not restricted to equilibrium profiles. We first demonstrate that charge carriers migrate to neutralize electric fields across 90° domain walls. Finally, we attempt a full simulation of a ferroelectric transistor and model current flow, electric field and polarization distributions.

10:24AM H32.00013 Conduction mechanism in $\text{BiFeO}_3\text{-CoFe}_2\text{O}_4$ columnar nanostructure, YI-CHUN CHEN, Department of Physics, National Cheng Kung University, YING-HUI HEISH, CHEN-WEI LIANG, Department of Materials Science and Engineering, National Chiao Tung University, JIA-MING LIOU, Department of Physics, National Cheng Kung University, YA-PING CHIU, Department of Physics, National Sun Yat-Sen University, QING HE, Advanced Light Source, Lawrence Berkeley National Laboratory, QIAN ZHAN, Department of Materials Physics and Chemistry, University of Science and Technology Beijing, YING-HAO CHU, Department of Materials Science and Engineering, National Chiao Tung University — Multiferroic materials, which possess interaction between more than one ferroic ordering parameters, had attracted great scientific and technological interests. Among the bi-phase magneto-electric nanostructures, $\text{BiFeO}_3\text{-CoFe}_2\text{O}_4$ (BFO-CFO) is a model system with ferroelectricity and ferrimagnetism coupling to each other through stress mediation. In this study, we investigated the electron transport behavior and the leakage-current mechanism in high quality nano-composite BFO-CFO thin films. The CFO nanopillars were heteroepitaxially embedded in a BFO matrix grown on SrTiO_3 substrates. Macroscopic vertical transport result showed the interface limit model was the dominant mechanism of the large leakage. Local conduction in epitaxial BFO-CFO nanostructures was studied by conducting atomic force microscope (C-AFM) while the nature of band structure variation was demonstrated by scanning tunneling microscope (STM). This study provides a basic explanation of leakage mechanism in self-assembled composite material system.

10:36AM H32.00014 Current-Controlled Negative Differential Resistance Due to Joule Heating In TiO_2 , A.M. BRATKOVSKY, Hewlett-Packard Laboratories, Palo Alto, A.S. ALEXANDROV, S.E. SAVEL'EV, Loughborough Inst. Technology, UK, D.B. STRUKOV, UC Santa Barbara, Santa Barbara, R.S. WILLIAMS, Hewlett-Packard Laboratories, Palo Alto — We show that Joule heating causes current-controlled negative differential resistance (CC-NDR) in TiO_2 memristive systems by constructing an analytical model of the current-voltage characteristics based on polaronic transport for Ohm's law and Newton's law of cooling and fitting this model to experimental data. This threshold switching is the "soft breakdown" observed during electroforming in TiO_2 and other transition-metal oxide based memristors, as well as a precursor to "ON" or "SET" switching of unipolar memristors from their high to their low resistance states. The shape of the V-I curves is a sensitive indicator of the nature of the polaronic conduction, which apparently follows an adiabatic regime [1].

[1] A.S. Alexandrov, A.M. Bratkovsky, B. Bridle, S.E. Savel'ev, D. Strukov, and R.S. Williams, Appl. Phys. Lett. 99, xxx (2011).

10:48AM H32.00015 Physical and Electrical Characterization of HfO_2 , HfSiO_4 , and ZrSiO_4 Memristors Based on Sol-Gel Synthesis, J.L. TEDESCO, WALTER ZHENG, S. POOKPANRATANA, A.A. HERZING, P.P. KAVURI, O.A. KIRILLOV, N.V. NGUYEN, C.A. RICHTER, National Institute of Standards and Technology — To date, most memristive devices have been fabricated by using TiO_2 or TaO_x dielectric films. In order to explore the possible advantages of other high- κ dielectrics in memristive devices, memristors were fabricated with HfO_2 , HfSiO_4 , and ZrSiO_4 layers synthesized from sol-gels. X-ray photoelectron spectroscopy measurements are consistent with reported spectra of HfO_2 , HfSiO_4 , and ZrSiO_4 films, but contain significant amounts of carbon. The films also have low densities and are flat, as measured by vacuum ultraviolet spectroscopic ellipsometry and optical profilometry measurements, respectively. This flat morphology is different from previous solution-processed dielectric films that exhibited rough surfaces [1]. Transmission electron microscopy measurements were also used to characterize these dielectric films. Current-voltage measurements indicate that, despite the contamination, the memristors exhibit nonvolatile bipolar resistive switching. The retention times measured for these memristors are $\sim 10^6$ s. Capacitance and conductance measurements of these memristors indicate differences between the ON and OFF states, which will be discussed further. [1] J.L. Tedesco, et al., ECS Trans. 35, 111 (2011).

Tuesday, February 28, 2012 8:00AM - 11:00AM – Session H33 GERA FIAP: Focus Session: Scaleable Technologies for Photovoltaics 106

8:00AM H33.00001 Solar Glitter – Microsystems Enabled Photovoltaics, GREGORY N. NIELSON, Sandia National Laboratories — Many products have significantly benefitted from, or been enabled by, the ability to manufacture structures at an ever decreasing length scale. Obvious examples of this include integrated circuits, flat panel displays, micro-scale sensors, and LED lighting. These industries have benefited from length scale effects in terms of improved performance, reduced cost, or new functionality (or a combination of these). In a similar manner, we are working to take advantage of length scale effects that exist within solar photovoltaic (PV) systems. While this is a significant step away from traditional approaches to solar power systems, the benefits in terms of new functionality, improved performance, and reduced cost for solar power are compelling. We are exploring scale effects that result from the size of the solar cells within the system. We have developed unique cells of both crystalline silicon and III-V materials that are very thin (5-20 microns thick) and have very small lateral dimensions (on the order of hundreds of microns across). These cells minimize the amount of expensive semiconductor material required for the system, allow improved cell performance, and provide an expanded design space for both module and system concepts allowing optimized power output and reduced module and balance of system costs. Furthermore, the small size of the cells allows for unique high-efficiency, high-flexibility PV panels and new building-integrated PV options that are currently unavailable. These benefits provide a pathway for PV power to become cost competitive with grid power and allow unique power solutions independent of grid power.

8:36AM H33.00002 Perspective on the Practical Limits and Roadmap for Nanostructured Photovoltaics, RICHARD R. LUNT, Michigan State University, VLADIMIR BULOVIC, Massachusetts Institute of Technology — The practical efficiency limits for nanostructured photovoltaics including organic small molecule, dye-sensitized, polymer, and colloidal-quantum-dot architectures are assessed *a posteriori*. Five decades since Shockley and Queisser derived the theoretical power conversion efficiency limit of single-junction photovoltaic cells, researchers have still not demonstrated such high performance for any photovoltaic device system. Hence, in evaluating the achievable performance of a comparatively new photovoltaic technologies, such as nanostructured PVs, it is prudent to estimate the upper limit of achievable efficiencies based on trends of the best technical demonstrations across the nanostructured platforms. This analysis is utilized to give a clear perspective on the potential market viability of these technologies in the near future and outline the challenges necessary to overcome this threshold. These technologies are compared and contrasted to provide an overview for the potential of each for reducing thermal losses with "Third Generation" concepts accessible to nanostructured PVs that can subsequently impact cost structures.

8:48AM H33.00003 Role of radiative recombination in 1 eV GaInNAs solar cells, IAN R. SELLERS, University of Oklahoma, WEI-SIN TAN, KATHERINE SMITH, STEPHEN DAY, STEWART HOOPER, MATTHIAS KAUER, Sharp Laboratories of Europe — High quality GaInNAs p-i-n solar cells with depletion widths in excess of $1\mu\text{m}$ for material absorbing in the practically important 1eV band gap regime are presented [1]. This is achieved through optimization of post-growth rapid thermal annealing at a temperature of $\sim 910^\circ\text{C}$. Despite the improvements in material quality evidenced by a low background impurity concentration and improved minority carrier collection, the external quantum efficiency remains limited to $\sim 50\%$. This is attributed to losses due to efficient radiative recombination in the bulk GaInNAs intrinsic region enhanced via localization of carriers in alloy fluctuations.

[1] Sellers *et al.* Applied Physics Letters 99, 151111 (2011)

9:00AM H33.00004 Device architectures for efficient photovoltaics from hard-to-dope semiconductors, STEVEN BYRNES, WILLIAM REGAN, WILL GANNETT, ALEX ZETTL, FENG WANG, Department of Physics, University of California at Berkeley, Berkeley, CA, and Materials Sciences Division, Lawrence Berkeley National Laboratory — In the search for cheap and efficient next-generation solar cells, much attention and effort has focused on semiconductor absorber materials which are difficult to dope both p and n, because of self-compensation, trap creation, or other effects. Such materials include oxides, sulfides, nanoparticles, organics, and so on. Even when the material itself has desirable electrical and optical properties for photovoltaic performance, the lack of a p-n homojunction architecture hampers device efficiency. Heterojunctions are a frequent solution, but compatible semiconductors are often unavailable or suboptimal. Therefore, we have explored new, cost-effective device architectures that promise performance comparable to a p-n homojunction, but which require neither bipolar doping nor compatible materials for heterojunctions. These architectures have the potential to bring emerging hard-to-dope semiconductors into technological and commercial relevance.

9:12AM H33.00005 Efficiency Analysis and Demonstration of Split-Junction Photovoltaic Solar Cells, HAN CHEN, EMIR MAGDEN, CHANDLER DOWNS, THOMAS VANDERVELDE, Tufts University — Recently, it has been proposed that separating solar radiation with a split-junction solar cell can result in higher overall conversion efficiencies, than are possible for monolithic designs. This hypothesis is investigated by simulating and analyzing 2+1 split junction cells for efficiency comparisons with theoretical and actual multi-junction cells. Ideal band-gaps for simultaneously operating photovoltaic and thermophotovoltaic cells have been determined. With the new configuration, it is shown that the efficiency achievements previously set by Ge/InGaAs/InGaP cells can be surpassed. A total increase in power output is observed during field tests using a Cassegrain split-junction concentrator with a dichroic lens (1.1 micron cutoff wavelength). Proposed benefits such as reduced heat load on the solar cell and ease of lattice constant matching in cell design are also validated. Additionally, with the flexibility of the concentrator assembly, it is shown that similar split-junction configurations with matching dichroic lenses allow for significant improvements in high efficiency solar cell technology.

9:24AM H33.00006 Electronic structure and optical spectra of Bulk and Nanocrystalline CuInS_2 ¹, MICHAEL MEHL, ALEXANDER EFROS, Naval Research Laboratory, Washington DC, ANDREW SHABAEV, George Mason University, Fairfax VA — Chalcopyrite CuInS_2 is a promising candidate for semiconductor photovoltaic devices. Here we study the behavior of the electronic structure and optical spectra of nanocrystalline CuInS_2 . We determine the bulk band structure using the HSE06 Hybrid Density Functional as implemented in the Vienna Ab-initio Simulation Package (VASP). We find an equilibrium structure in good agreement with experiment, and a direct band gap of 1.2 eV, as compared to the experimental value of 1.5 eV. The band gap is extremely sensitive to the position of the sulfur atoms, which suggests that it can be controlled in part by the doping of the In site with Ga. CuInS_2 is nearly cubic, so we fit the first-principles band structure to a k.p Hamiltonian with invariants consistent with the departure for cubic symmetry. This Hamiltonian is then used to describe the hole spectra in a CuInS_2 nanocrystal. We show the symmetry breaking inherent in the chalcopyrite structure can activate the optically passive ground hole state in the nanocrystal, and discuss the resulting optical behavior of the nanocrystal.

¹Work supported by the US Office of Naval Research

9:36AM H33.00007 Impact of a high resistivity transparent (HRT) layer on ultra-thin CdTe devices¹, HASITHA MAHABADUGE, KRISTOPHER WIELAND, The University of Toledo, ALVIN COMPAAN, The University of Toledo; Xunlight 26 Solar, LLC — Pushing the limits of the absorber layer thickness to submicron levels without compromising the efficiency in CdTe devices is important for several reasons. Reducing the thickness of the CdTe layer can increase the manufacturing speed and lower the material usage, production time, cost and energy needed for production. Thickness fluctuations in these submicron devices can lead to shunting when these fluctuations are comparable to the absorber layer thickness. Introducing a high resistivity transparent (HRT) layer in the device structure can reduce such shunting. We find that the impact of the HRT layer is higher for ultra-thin absorber layers. In this study, the effect of using sputtered ZnO as the HRT layer was investigated for devices with a 0.2 μm CdTe layer. Our results show a 40% increase in efficiency in the CdTe devices with the HRT layer compared to the devices without the HRT layer. The increase in efficiency is primarily from improved fill factor due to an increase in shunt resistance from 0.15 kohm-cm² to 0.32 kohm-cm². As a result of increased shunt resistance there is an increase in the efficiency as well as a substantial increase in the yield for small dot cells.

¹Work supported by Xunlight 26 Solar and the Ohio Third Frontier Advanced Energy Program.

9:48AM H33.00008 Solution-based synthesis of crystalline silicon thin films from liquid silane inks, GANJIGUNTE R.S. IYER, GURUVENKET S., JUSTIN M. HOEY, KENNETH J. ANDERSON, DOUGLAS L. SCHULZ, ORVEN F. SWENSON, S. ELANGO VAN, P. BOUDJOUK, ERIK K. HOBBIE, North Dakota State University — Silicon (Si) dominates the photovoltaics industry and there is a need for new approaches that can significantly reduce fabrication cost. In this context, we report a non-vacuum, solution-based process for the synthesis of crystalline silicon (c-Si) thin films from liquid cyclohexasilane (CHS) in a platform that is readily applicable to large-area flexible devices. UV-polymerization during spin coating leads to the formation of thin films, which were crystallized via thermal and laser annealing. Structural changes in the films were examined using SEM, AFM and Raman spectroscopy. Subsequent chemical annealing through atmospheric-pressure hydrogen plasma treatment led to a four-decade enhancement in film conductivity, which we attribute to a disorder-order transition in a bonded Si network.

10:00AM H33.00009 Device modeling for organic solar cells¹, LUNMEI HUANG, ROBERT KRASNY, Department of Mathematics, University of Michigan, KYLE RENSHAW, Department of Physics, University of Michigan, STEPHEN FORREST, Department of Physics, Department of Electrical Engineering and Computer Science, and Materials Science and Engineering, University of Michigan — Organic solar cells (OSCs) are expected to play an important role in addressing our future energy needs due to their low cost and low processing requirements compared to inorganic solar cells (ISCs). However the efficiency of OSCs is still too low in comparison with ISCs for widespread applications. The biggest loss of quantum efficiency (QE) in OSCs is due to the limited free carrier generation occurring at the donor-acceptor (D-A) interface. Excitons (bound electron-hole pairs) are generated in the bulk by photo-absorption, but only a portion of them reach the D-A interface where they can dissociate into free charge carriers. Therefore, better understanding and control of exciton diffusion, free carrier generation and recombination are critical in order to improve QE for OSCs. To elucidate the physics of OSCs and aid in experimental studies, we developed a drift-diffusion model to describe the dynamics of excitons and free charge carriers. Our model predicts the performance of OSC devices by calculating their QE and current-voltage curves (I-V), as well as many other important physical quantities, such as the internal electric field, and the concentration and flux of excitons and free carriers. The effect of exciton and free carrier mobility, device temperature, and layer thickness, will be discussed. Furthermore, the exciton dissociation mechanism widely described by Onsager's model, will be investigated in detail.

¹The authors thank NSF(CHE-0934098) for financial support of this work.

10:12AM H33.00010 Combined Photo and Thermionic Energy Conversion with Doped Diamond Electron Emitters, TIANYIN SUN, FRANZ KOECK, ROBERT NEMANICH, Arizona State University — Conversion of heat into electrical energy has been demonstrated using low effective work function diamond films achieved with n-type doping and surface hydrogen termination. Recently, visible light photo-electron emission has been demonstrated from the same diamond, and this work suggests that this effect could be utilized for a new approach to solar energy conversion namely combined photo and thermionic energy conversion. This work presents a spectroscopic study of photo- and thermionic electron emission from nitrogen doped diamond films on silicon substrates. In this experiment the diamond samples are heated from 100 °C to 500 °C, while being illuminated with light from 240 to 600 nm. The emission spectra show a significant increase of photo-emission intensity with elevated temperature and a lowering of the effective work function. The results are discussed in terms of the photo and thermal excitation, the carrier transport and the electron statistics. The results indicate the potential of diamond films in a combined photo and thermionic energy conversion solar cell. This research is supported through the Office of Naval Research.

10:24AM H33.00011 Metal nanoparticle-graphene superstructures as electrodes for solar cells¹, ANNA ZANIEWSKI, MARIA SCHRIVER, GLORIA LEE, A. ZETTL, Dept. of Physics, UC Berkeley — We present metal nanoparticle and graphene superstructures as a potential electrode for solar cells. We show the effect of various metallic nanoparticles on the work function, sheet resistance, and optical properties of graphene layers. The geometries studied include nanoparticles on single layer graphene, and embedded in a graphene sandwich. We discuss the application of these electrodes to organic and silicon solar cells.

¹Director, Office of Energy Research, Materials Sciences and Engineering Division, of the US Department of Energy under Contract No. DE-AC02-05CH11231

10:36AM H33.00012 Study of the crystalline phases in paste coating deposition of CIGS, IVAN DAVOLI, IVAN COLANTONI, Università di Roma Tor Vergata, Dipartimento di Fisica, SURFACE ANALYSES LABORATORY COLLABORATION — One or two microns of CIGS can absorb most of the incident solar radiation because $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ have a direct band gap with a high absorption coefficient. The theoretical predictions explain that the optimum photovoltaic performance should be provided by a high gallium concentration, but experimentally is observed that above 30% of Ga the efficiency is reduced. This contradictory behaviour is not completely understood. Using paste coating technique for CIGS deposition, we have recently shown a strong correlation among Ga concentration, structural properties and compound stoichiometry. The desired stoichiometric compound will be obtained varying the concentration of the basic elements in the paste. Our diffraction data show that the maximum of the crystalline phase is reached when CIGS have a Ga concentration higher. Furthermore the SEM EDX quantitative analysis performed on the same samples have shown the presence of different phases. Such a phases separation find a theoretical explanation as ODC (Ordered Defect Compound) in Cu-poor system. X-ray absorption spectroscopy reveals the structure around a specific atomic species and allow us to understand the type of phases in chalcopyrite structure.

10:48AM H33.00013 A large-area, LED-based spectral response measurement system for solar PV device characterization, BEHRANG HAMADANI, JOHN ROLLER, HOWARD YOON, BRIAN DOUGHERTY, National Institute of Standards and Technology — Accurate and reliable measurement of the spectral responsivity (SR) of a solar cell is an important step in evaluating the electrical performance of competing photovoltaic (PV) technologies. We have investigated ways to measure the spectral responsivity, and hence the external quantum efficiency, of solar cells using measurement techniques that employ light emitting diodes (LEDs). Our setup includes one or more plates of compactly-installed, high-powered LEDs each containing up to 32 different LEDs that span the wavelength range of 375 nm to 1200 nm. Each LED plate is placed at the entrance of a tapered, highly reflective light guide for light mixing and large-area projection. Two unique measurement techniques have been investigated at NIST. The first technique consists of an LED sweep algorithm where a pulsed signal is applied to a given LED and the photogenerated current from the device under test is recorded using a lock-in technique. In the second SR technique, 32 variable-frequency, pulsed signals are applied to all LEDs at the same time, while recording the photogenerated current by a spectrum analyzer in the frequency domain. We will describe the uniqueness and advantages offered by each technique in detail and compare the accuracy of the two methods. A scheme for providing light bias and its impact on the SR measurements will be reported.

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H34 DCP: Focus Session: Nano II: Nanoscale Materials and Properties I 107A

8:00AM H34.00001 Nanoelectronics Meets Biology, CHARLES LIEBER, Harvard University, Dept. of Chemistry and Chemical Biology — Nanoscale materials enable unique opportunities at the interface between the physical and life sciences, and the interface between nanoelectronic devices and biological systems makes possible communication between these two diverse systems at the length scale relevant to biological function. In this presentation, the development of nanowire nanoelectronic devices and their application as powerful tools for the life sciences will be discussed. First, a brief introduction to nanowire nanoelectronic devices as well as comparisons to other electrophysiological tools will be presented to illuminate the unique strengths and opportunities enabled at the nanoscale. Second, illustration of detection capabilities including signal-to-noise and applications for real-time label-free detection of biochemical markers down to the level of single molecules will be described. Third, the use of nanowire nanoelectronics for building interfaces to cells and tissue will be reviewed. Multiplexed measurements made from nanowire devices fabricated on flexible and transparent substrates recording signal propagation across cultured cells, acute tissue slices and intact organs will be illustrated, including quantitative analysis of the high simultaneous spatial and temporal resolution achieved with these nanodevices. Specific examples of subcellular and near point detection of extracellular potential will be used to illustrate the unique capabilities, such as recording localized potential changes due to neuronal activities simultaneously across many length scales, which provide key information for functional neural circuit studies. Last, emerging opportunities for the creation of powerful new probes based on controlled synthesis and/or bottom-up assembly of nanomaterials will be described with an emphasis on nanowire probes demonstrating the first intracellular transistor recordings, and the development of “cyborg” tissue. The prospects for blurring the distinction between nanoelectronic and living systems in the future will be highlighted.

8:36AM H34.00002 Charge Retention by Monodisperse Gold Clusters on Surfaces Prepared Using Soft Landing of Mass Selected Ions, GRANT JOHNSON, Pacific Northwest National Laboratory, THOMAS PRIEST, University of Louisville, JULIA LASKIN, Pacific Northwest National Laboratory — Monodisperse gold clusters have been prepared on surfaces in different charge states through soft landing of mass-selected ions. Gold clusters were synthesized in methanol solution by reduction of a gold precursor with a weak reducing agent in the presence of a diphosphine capping ligand. Electrospray ionization was used to introduce the clusters into the gas-phase and mass-selection was employed to isolate a single ionic cluster species which was delivered to surfaces at well controlled kinetic energies. Using in-situ time of flight secondary ion mass spectrometry (SIMS) it is demonstrated that the cluster retains its 3+ charge state when soft landed onto the surface of a fluorinated self assembled monolayer on gold. In contrast, when deposited onto carboxylic acid terminated and conventional alkyl thiol surfaces on gold the clusters exhibit larger relative abundances of the 2+ and 1+ charge states, respectively. The kinetics of charge reduction on the surface have been investigated using in-situ Fourier Transform Ion Cyclotron Resonance SIMS. It is shown that an extremely slow interfacial charge reduction occurs on the fluorinated monolayer surface while an almost instantaneous neutralization takes place on the surface of the alkyl thiol monolayer. Our results demonstrate that the size and charge state of small gold clusters on surfaces, both of which exert a dramatic influence on their chemical and physical properties, may be tuned through soft landing of mass-selected ions onto selected substrates.

8:48AM H34.00003 Transitioning the Superfluid Helium Droplet Assembly into a Technology: Synthesis of Nanometer Scale Energetic Films using SHeDA, S.B. EMERY, K.B. RIDER, B.K. LITTLE, R. CLEAVER, C.M. LINDSAY, Air Force Research Laboratory Energetic Materials Branch — Since the pioneering work of the Toennies, Scoles, and Northby groups in the early 1990's, dozen of instruments around the world have been constructed to produce and study beams of superfluid helium nanodroplets. The technique has been exploited to shed light on a wide range of topics in chemical physics such as atomic scale manifestations of superfluidity, chemistry at ultra-low temperatures, and the assembly of exotic Van der Waals complexes to name a few. The helium droplet method has been considered for more applied use as a tool for isotope enrichment, low-fragmentation ionization mass spectrometry, and synthesizing/depositing core-shell spintronic nanoparticles. Indeed, the helium droplet methodology is in the midst of transitioning from a novel cryogenic nano-scale matrix in which to perform fundamental research into a technology for synthesizing, characterizing, and manipulating material. This talk describes our efforts to engineer a robust, user-friendly, broadly-tunable helium droplet apparatus capable of synthesizing composite nanoparticles and depositing them into films. This device is now being used to assemble and deposit metallic nanoparticles, and the efficiency of the process is being investigated. The physical details of the design, performance of the instrument, and our progress at understanding the deposition process will be presented. Distro 96ABW-2011-0266.

9:00AM H34.00004 Screened Charge Model in the Treatment of Electrostatic Interactions¹, BO WANG, HANNAH LEVERENTZ, Department of Chemistry, University of Minnesota, DONALD TRUHLAR, Department of Chemistry and Supercomputing Institute, University of Minnesota — Partial atomic charges play an important role in molecular simulations of complex systems, and they are widely used to compute the electrostatic interactions in various methods. We propose a screened charge model to include charge penetration and screening effects in electrostatic modeling. In the screened charge model, the atomic charge density of an atom in a molecule is represented by a spherical smeared charge plus a point charge at the nucleus. The new model is illustrated for the electronically embedded combined quantum mechanical and molecular mechanical (QM/MM) calculations and for the electrostatically embedded many-body (EE-MB) method. For a test set of 40 complexes, the mean unsigned error of QM/MM electrostatic interactions between QM and MM regions is reduced from 8.1 to 2.8 kcal/mol and that for QM/MM induction interactions from 1.9 to 1.4 kcal/mol. In a test of five water hexamers, the mean unsigned error of the EE-MB binding energies of the clusters is decreased by a factor of 2 at both the pairwise additive (PA) and three-body (3B) levels. Moreover, we have found that the charges derived by fitting electrostatic potentials with the screened charge method are less sensitive to the positions of the fitting points, and the quality of the fit to the electrostatics is improved.

¹This work is supported by NSF and AFOSR.

9:12AM H34.00005 Magnetic Superatom Assemblies and their Transport Properties¹, LIN ZHU, J. ULISES REVELES, V. MENDEL, A. REBER, SHIV KHANNA, Department of Physics, Virginia Commonwealth University — We had recently shown that magnetic superatoms can be formed by embedding 3d transition metal atoms in metallic clusters of otherwise non-magnetic elements. The hybridization between the localized exchange split atomic orbitals in 3d elements with superatomic orbitals can help stabilize the magnetic state. Through first principles studies on the electronic structure and magnetic moment of $Mg_n TM$ ($TM = Sc, Ti, V, Cr, Mn, Fe, Co, \text{ and } Ni$) clusters, we had identified $Mg_8 Fe$ to be a stable magnetic superatom. In this work, we will present our investigations on the magnetic properties of the assemblies of such superatoms and the nature of electronic transport through such assemblies with various electrodes. The effects of the contact geometry and gate voltage on the conductance are also studied.

¹We gratefully acknowledge support from U. S. Department of Energy (DOE) through grant DE-FG02-11ER16213.

9:24AM H34.00006 Fabrication and Characterization of Electrodeposited Nanoporous Alloys¹, KYLA KOBOSKI, NATHAN GRABER, EVAN NELSEN², JENNIFER HAMPTON, Hope College — Nanoporous Ni and NiFe thin films were created by electrodeposition of NiCu and NiFeCu followed by electrochemical dealloying to remove the Cu component. The structure and composition of the resulting materials, before and after the dealloying step, was characterized using scanning electron microscopy and energy dispersive spectroscopy. The electrochemical double-layer capacitance was measured to estimate the active surface area. The catalytic behavior of these complex nanoporous materials was investigated using hydrogen evolution as a model reaction.

¹This material is based upon work supported by the National Science Foundation under NSF-RUI Grant No. DMR-1104725, NSF-REU Grant No. PHY/DMR-1104811, and NSF-MRI Grant No. CHE-0959282.

²Rhodes College

9:36AM H34.00007 Strongly Size-Dependent High-Temperature Behavior of Bismuth Oxide Nanoparticles, GERRIT GUENTHER, Technische Universität Darmstadt, Materials Science, Petersenstr. 23, 64287 Darmstadt, Germany, RALF THEISSMANN, EINAR KRUIS, Nanostructures and Technology, University Duisburg-Essen, Bismarckstr. 81, 47057 Duisburg, Germany, OLIVIER GUILLON, Institute for Materials Science, Friedrich-Schiller-Universität Jena, Löbdergraben 32, 07743 Jena, Germany — Oxide nanostructures show very strong size-dependent changes in their thermal and chemical stability and reactivity. The degree of these changes depends on the type and strength of bonds at the surface: The higher the surface energy the stronger the size-dependence. Inorganic compounds are governed by strong and long ranging bonds which result e.g. in generally high melting points and surface energies. So the properties of such nanostructures could shed more light on the role that the material's surface plays. This is demonstrated here by experiments with size-selected bismuth oxide nanoparticles between 5 and 60 nm ($\pm 5\%$). Characterization of the particles revealed a metastable $\beta - Bi_2O_3$ structure. That testifies a size-driven crossover in phase stability below a critical particle size. Heating experiments up to the evaporation point were performed inside the synthesis-chamber as well as with in-situ TEM, in-situ XRD and a high-temperature nanocalorimeter. Different atmospheres were used. For the first time a melting point reduction in oxide nanoparticles was directly shown: For example 10 nm particles melted max. 40% and evaporated 12% below the bulk values which is a considerably stronger size-effect than for metals ($\leq 5\%$).

9:48AM H34.00008 Borane derivatives: A New Class of Superhalogens, DEVLEENA SAMANTA, Virginia Commonwealth University, BISWARUP PATHAK, RAJEEV AHUJA, Uppsala University, PURUSOTTAM JENA, Virginia Commonwealth University — Halogens have the largest electron affinities of all elements in the periodic table, that of Cl being the highest, namely 3.6 eV. Superhalogens have electron affinities that far exceed that of halogens. Based on density functional theory calculations, we show that the Wade-Mingo's rule, well known for describing the stability of closo-boranes ($B_n H_n^{2-}$), can be used to design a new class of superhalogens by tailoring the size and composition of borane derivatives. These superhalogens do not have to have either a metal or a halogen atom unlike conventional superhalogens. We show this by taking $B_{12}H_{13}$ and $CB_{11}H_{12}$ as examples. Also, these superhalogens can be used as building blocks of hyperhalogens of the form $M(B_{12}H_{13})_2$ and $M(CB_{11}H_{12})_2$ ($M=Li, Na, K, Rb, Cs$). This finding opens the door to an untapped source of superhalogens and weakly coordinating anions with potential applications.

10:00AM H34.00009 Configurational thermodynamics of alloyed nanoparticles: a first-principles cluster expansion study¹, LIN-LIN WANG, Division of Materials Science and Engineering, Ames Laboratory, DUANE D. JOHNSON, Division of Materials Science and Engineering, Ames Laboratory and Iowa State University — Transition-metal, alloyed core-shell nanoparticles (NPs) continue to be studied as heterogeneous catalysts because they are found to improve catalytic activity and selectivity for many energy-conversion processes. However, thermodynamic investigations have been limited mostly to NP core-shell preference, rather than both geometric structure and its chemical decoration. Here, by extending cluster expansion methods to treat alloyed nanoparticles, we study the configurational thermodynamics of bimetallic NPs, using databases from density functional theory calculations. We find that the interplay between the ordering tendency and the core-shell segregation tendency can induce site-specific preferences around the NP, as we exemplify, e.g., in AgAu. Such simulations will provide information needed for further understanding of the structure-function relationships in NP catalysis.

¹Supported by the DOE/BES under DE-FG02-03ER15476 (Catalysis) and DE-AC02-07CH11358 at the Ames Laboratory operated by Iowa State University

10:12AM H34.00010 Sintering of multi-metallic nanoparticles, VINEETHA MUKUNDAN, Purdue University, BIRGID WANJALA, RAMESHWORI LOUKRAKAM, JIN LUO, JUN YIN, CHUAN-JIAN ZHONG, Binghamton University, OANA MALIS, Purdue University — During the thermal treatment employed to activate the Pt-based nano catalysts used in fuel cell applications, the particles undergo structural transformations that affects their chemical performance. The mechanisms of coalescence and grain growth in bimetallic/trimetallic nanoparticles supported on planar silica on silicon are investigated using in-situ synchrotron based X-ray diffraction in the temperature regime 400-900C. The sintering process was found to be accompanied by lattice contraction and L10 chemical ordering. The mass transport involved in sintering is attributed to grain boundary diffusion and its corresponding activation energy is estimated from data analysis.

10:24AM H34.00011 Temperature dependence of Raman spectroscopy of molecular iodine trapped in zeolite crystals, WENHAO GUO, DINGDI WANG, JUANMEI HU, ZIKANG TANG, SHENGWANG DU, Physics Department, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong — Molecular iodine has been pursued for many practical applications, such as molecular clock, molecule-based quantum information processing, due to its narrow-linewidth hyperfine optical transitions. But because of its low vapor pressure, the experimental setup employing a free-space-based iodine vapor cell is very space-consuming. Recently, it is reported that the iodine molecule can be loaded into the channels of zeolite crystals, the density there could be orders improved and its space orientation can be precisely controlled. It may drastically reduce the size of molecular iodine experiment setup, and have many potential applications in microchip technology. We have studied the Raman spectroscopy of iodine molecule confined in zeolite crystals, AlPO₄-5 (AFI) and AlPO₄-11 (AEL), under different temperatures. The results show that in AEL, where the molecules are intensely confined, the ground vibrational states are close to that of an ideal 1D harmonic oscillator, while in AFI, where the molecules have a bit more freedom, they vibrate like in the free space, but with a loosened spring. And we come up a reasonable theoretical model to explain the Raman width dependence on temperature for these systems

10:36AM H34.00012 Single molecule thermodynamics and nanopore-based thermometry, JOSEPH E. REINER, Physics Department, Virginia Commonwealth University, JOSEPH W.F. ROBERTSON, Physical Measurement Laboratory, NIST, LISA K. BURDEN, Biology Department, Wheaton College, DANIEL L. BURDEN, Chemistry Department, Wheaton College, JOHN J. KASIANOWICZ, Physical Measurement Laboratory, NIST — The nanopore-based resistive pulse method measures the reduction in ionic current caused by the interaction of single molecules with the pore. It has great promise in addressing problems across a range of fields that include biomedicine and genomics. The technique requires the residence time of the molecules in the pore to exceed the inverse bandwidth of the detection system ($\sim 10 \mu s$). Efforts are underway to improve this by molecular modification of the pore wall, but little effort has focused on modifying the solution conditions in and around the pore. We address this issue by precisely controlling the solution temperature around a protein ion channel (alpha hemolysin) via laser-induced heating of gold nanoparticles. In this technique, the nanopore serves dual roles as both a highly local thermometer and single molecule sensor. Preliminary data suggests that the solution temperature can be controlled over a wide range, the nanopore conductance can be used to directly measure rapid changes in temperature, and the temperature change can dramatically alter the interaction kinetics of single molecules with the nanopore. The method will improve the development of biochip sensors and lead to a new platform for single molecule thermodynamic studies.

10:48AM H34.00013 On the Stability and Dynamics of Atmospheric Pre-Nucleation Clusters, VILLE LOUKONEN, University of Helsinki, Department of Physics, Helsinki, FI-00014 University of Helsinki, Finland, I-FENG W. KUO, Lawrence Livermore National Laboratory, Chemical Sciences Division, Livermore, CA 94550 USA, MATTHEW J. MCGRATH, Department of Biophysics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan, HANNA VEHKAMAKI, University of Helsinki, Department of Physics, Helsinki, FI-00014 University of Helsinki, Finland — Atmospheric new-particle formation is a complex physical phenomenon with far-reaching consequences: currently, the role of aerosols is one of the main uncertainties in predicting the climate change. However, the molecular-level particle formation mechanisms are poorly understood. It is believed that sulfuric acid is the key player with possible contributions from various base molecules, ions or organics. Here we present results from first-principles molecular dynamics simulations of molecular clusters of sulfuric acid and two atmospherically relevant bases, ammonia and dimethylamine. The dynamics and stability of the studied clusters (sulfuric acid)_n•(ammonia)_{n-1} and (sulfuric acid)_n•(dimethylamine)_n where $n = 2, 3, 4$ were probed for 45 ps at T=300K at BPE/TZV2P level of theory. The stability of the clusters is largely dependent on the H-bonding patterns and in most cases the equilibrium patterns emerged within the first 10 ps. Curiously, even after the equilibrium was reached the clusters showed pronounced bond rearrangement: the number of bonds remained the same, but the individual atoms forming the bonds changed. Regardless of this behavior, the clusters remained bound together.

Tuesday, February 28, 2012 8:00AM - 11:00AM —
Session H35 DCP: Focus Session: DFT III: Weak Bonding and Liquid Phase Systems 107B

8:00AM H35.00001 Weakly Interacting Subsystems in DFT, TROY VAN VOORHIS, MIT Department of Chemistry — In chemistry, one is frequently interested in systems that are composed of weakly interacting fragments: a solute dissolved in a solvent phase, the base pairs in DNA, molecules in a crystal. In all these cases, our physical picture is that electronic states of the assembly emerge from small perturbations of states localized on the fragments. In frustrating fashion, standard functionals completely fail to reproduce this qualitative picture: the excited states of molecular assemblies are dominated not by local, valence excitations, but by spurious charge transfer states; weak van der Waals forces that hold molecules together are typically absent; excess spin and charge tend to be strongly delocalized even when the physical coupling between centers is extremely weak. In this talk we will discuss how truly nonlocal density functionals can mollify these trends. In particular, we will highlight the recent derivation and implementation of nonlocal van der Waals density functionals that account for long-range correlation in terms of two-point density interactions.

8:36AM H35.00002 Towards Efficient and General Method for Many-Body van-der-Waals Interactions, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG, Berlin — Van der Waals interactions are intrinsically many-body phenomena, arising from collective electron fluctuations in a given material. Adiabatic connection fluctuation-dissipation theorem (ACFDT) allows to compute the many-body vdW interactions accurately. However, the ACFDT computational cost is prohibitive for real materials, even when the random-phase approximation is employed for the response function. We show how the problem of computing the long-range many-body vdW energy for real systems can be solved efficiently by mapping the system (molecule or condensed matter) onto a collection of quantum harmonic oscillators. Currently, our method, which couples density-functional theory with the many-body dispersion energy (DFT+MBD), is developed for non-metallic system [A. Tkatchenko, R. A. DiStasio Jr., R. Car, M. Scheffler, submitted]. The DFT+MBD method includes the hybridization effects by using the Tkatchenko-Scheffler approach [PRL 102, 073005 (2009)], the long-range Coulomb screening through classical electrodynamics [B. U. Felderhof, Physica 29, 1569 (1974)], and the many-body vdW energy from the coupled-fluctuating dipole model [M. W. Cole et al., Mol. Simul. 35, 849 (2009)]. The successes of the DFT+MBD approach and the many challenges that lie ahead will be discussed.

8:48AM H35.00003 Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals, LEEOR KRONIK, Weizmann Institute of Science, Israel, NOA MAROM, University of Texas at Austin, Austin, TX, ALEXANDRE TKATCHENKO, MARIANA ROSSI, VIVEKANAND V. GOBRE, Fritz-Haber-Institut, Germany, ODED HOD, Tel Aviv University, Israel, MATTHIAS SCHEFFLER, Fritz-Haber-Institut, Germany — We present a comparative assessment of the accuracy of two approaches for evaluating dispersion interactions: inter-atomic pair-wise corrections and semi-empirical meta-generalized-gradient-approximation (meta-GGA) based functionals. This is achieved by employing conventional (semi-)local and (screened-)hybrid functionals, as well as semi-empirical hybrid and non-hybrid meta-GGA functionals of the M06 family, with and without pair-wise Tkatchenko-Scheffler corrections. All those are tested against the benchmark S22 set of weakly bound systems, a representative larger molecular complex, and a representative dispersively bound solid. We also compare our results with those obtained from Grimme's pair-wise correction (DFT-D3) and Langreth-Lundqvist functionals (vdW-DF1/2). We find that the semi-empirical kinetic-energy-density dependence of the M06 functionals mimics some of the non-local correlation needed to describe dispersion. However, long-range contributions are still missing. Pair-wise corrections provide for a satisfactory level of accuracy irrespectively of the underlying functional.

9:00AM H35.00004 *Ab-initio* liquid water with hybrid functionals and dispersion interactions¹, ZHAOFENG LI, Princeton University, XIFAN WU, Temple University, ROBERT DISTASIO JR., ROBERTO CAR, Princeton University — We report *ab-initio* molecular dynamics simulations of liquid water using the hybrid PBE0 functional plus self-consistent dispersion forces based on the scheme of Ref.² Simulations were performed at T=300K and at T=330K to approximately account for nuclear quantum effect on the oxygen-oxygen(O-O) RDF, as suggested by previous path integral simulations. Focusing on O-O RDF, we find that the combined effect of the hybrid functional and of the dispersion interactions significantly improves the agreement of the simulated structure with experiment.

¹This work is supported by NSF CHE-0956500 and DOE-DE-SC0005180.

²A. Tkatchenko and M. Scheffler, Phys. Rev. Lett. **102**, 073005 (2009).

9:12AM H35.00005 Understanding the role of London dispersion forces in molecular surface processes, VALENTINO R. COOPER, Oak Ridge National Laboratory — The interactions and dynamics of molecules at surfaces and within pores are essential to many chemical processes, ranging from molecular storage to catalysis and self-assembly. A molecular level understanding of molecule-surface interactions is crucial for tuning surface/pore selectivity and reactivity. While it is clear that strong chemisorption bonds facilitate these interactions, the role of weaker van der Waals (vdW) forces, which include London dispersion and π - π stacking interactions, are often unknown or overlooked. Recent advances in density functional theory (DFT) have now made it possible to reliably account for London dispersion interactions. In this paper, I will discuss the use of one such technique, the Rutgers-Chalmers vdW non-local correlation functional,^{1,2} to demonstrate how the inclusion of London dispersion forces is critical for a truly first principles understanding of processes sensitive to molecule-surface interactions, such as the loading of H₂ within porous materials and the chemisorption of organic molecules at surfaces. These works highlight the fundamental importance of London dispersion interactions in the broader context of chemical physics. This work was supported by the Department of Energy, BES, Materials Sciences and Engineering Division.³

¹M. Dion, H. Rydberg, E. Schröder, B. I. Lundqvist and D. C. Langreth, Phys. Rev. Lett., **92**, 246401 (2004)

²T. Thonhauser, V. R. Cooper, S. Li, A. Puzder, P. Hyldgaard, and David C. Langreth, Phys. Rev. B, **76**, 125112 (2007)

³Collaborators: Guo Li, Isaac Tambllyn, Yungok Ihm, Jun-Hyung Cho, Shixuan Du, Jeffrey B. Neaton, Hong-Jun Gao, Zhenyu Zhang, James R. Morris

9:48AM H35.00006 First principles Monte Carlo simulations of vapor-liquid equilibria: Density functionals, basis sets, and dispersion corrections¹, J. ILJA SIEPMANN, University of Minnesota, MATTHEW J. MCGRATH, Kyoto University, I-F. WILLIAM KUO, Lawrence Livermore National Laboratory, CHRISTOPHER J. MUNDY, Pacific Northwest National Laboratory — Gibbs ensemble Monte Carlo simulations are used to compute the vapor-liquid equilibria for water, methanol, and methane using Kohn-Sham density functional theory. Results for BLYP and PBE functionals, BLYP with Grimme D2 and D3 dispersion corrections, and various basis sets are compared. Although none of the combinations of functional, dispersive correction, and basis set is found to yield highly accurate predictions for liquid densities, vapor pressures, and heats of vaporization for all three compounds, the results for dispersion corrected BLYP with large basis set are promising.

¹Research support from the National Science Foundation is gratefully acknowledged.

10:00AM H35.00007 Incorporation of an Improved Radial Distribution Function into Classical DFT, JOOST DE GUSSEM, ERIN MCGARRITY, Delft Technical University — An expression for the radial distribution function $g(\vec{r})$ for a fluid can be found using classical density functional theory. We use this expression in place of the mean-field value (*e.g.*, $g = 1$ for Lennard Jones fluids) in the excess Helmholtz free energy functional for the pair interactions to achieve self-consistent density profiles. We will discuss the differences found with this improved choice for $g(\vec{r})$ compared to other, simpler approximations. We will show results for liquid-vapor systems containing hard-sphere fluids with Lennard-Jones and dipolar interactions.

10:12AM H35.00008 Solvation of the chloride anion in water: ab initio simulations, CUI ZHANG, Department of Chemistry, University of California, Davis, DAVIDE DONADIO, Department of Chemistry, University of California, Davis and Max Planck Institute for Polymer Research, 55128 Mainz, Germany, FRANCOIS GYGI, Department of Computer Science, University of California, Davis, GIULIA GALLI, Department of Chemistry, University of California, Davis and Department of Physics, University of California, Davis — We studied the structural, vibrational and electronic properties of the chloride anion in water using ab initio molecular dynamics. Our investigation has three main objectives: understand the range of perturbation exerted by the anion on the water hydrogen bonded network; identify signatures of the anion perturbation in infrared spectra of the solution and study the extent of charge localization on the anion, as predicted by semi-local (PBE) and hybrid functionals (PBE0). In agreement with recent experiments, we find that the presence of the anion substantially affects only the hydrogen bonding in the first solvation shell, due to a decrease of the dipole moment of the first shell water molecules and thus a weakening of the hydrogen bonds. Such a weakening leads to a slightly blue shifted band in the computed IR spectra. While structural and vibrational properties of the solution are similar within PBE and PBE0, the electronic properties exhibit marked differences.

10:24AM H35.00009 Entropy of Liquid Water from Ab Initio Molecular Dynamics, LEONARDO SPANU, CUI ZHANG, Chemistry Department University of California Davis, GIULIA GALLI, Chemistry Department and Physics Department University of California Davis — The debate on the structural properties of water has been mostly based on the calculation of pair correlation functions. However, the simulation of thermodynamic and spectroscopic quantities may be of great relevance for the characterization of liquid water properties. We have computed the entropy of liquid water using a two-phase thermodynamic model and trajectories generated by ab initio molecular dynamics simulations [1]. In an attempt to better understand the performance of several density functionals in simulating liquid water, we have performed ab initio molecular dynamics using semilocal, hybrid [2] and van der Waals density functionals [3]. We show that in all cases, at the experimental equilibrium density and at temperatures in the vicinity of 300 K, the computed entropies are underestimated, with respect to experiment, and the liquid exhibits a degree of tetrahedral order higher than in experiments. We also discuss computational strategies to simulate spectroscopic properties of water, including infrared and Raman spectra.

[1] C.Zhang, L.Spanu and G.Galli, *J.Phys.Chem. B* 2011 (in press)

[2] C.Zhang, D.Donadio, F.Gygi and G.Galli, *J. Chem. Theory Comput.* 7, 1443 (2011)

[3] C.Zhang, J.Wu, G.Galli and F.Gygi, *J. Chem. Theory Comput.* 7, 3061 (2011)

10:36AM H35.00010 Mean-field Density Functional Theory of Triple Junction¹, CHANG-YOU LIN, MICHAEL WIDOM, ROBERT F. SEKERKA, Department of Physics, Carnegie Mellon University, Pittsburgh, PA 15232, USA — A triple junction in a three-phase fluid system is modeled by a mean-field density functional theory. We use a variational approach to find the Euler-Lagrange equations. Analytic solutions are obtained in the two-phase regions at large distances from the triple junction. We employ a triangular grid and use a successive over-relaxation method to find numerical solutions in the entire domain for the special case of equal interfacial tensions for the two-phase interfaces. We use the Kerins-Boiteux formula to obtain a line tension associated with the triple junction. This line tension turns out to be negative. We associate line adsorption with the change of line tension as the governing potentials change.

¹We appreciate the support of Department of Physics, Carnegie Mellon University for this work.

10:48AM H35.00011 Structural and vibrational properties of sulphate-water clusters from ab-initio calculations, QUAN WAN, LEONARDO SPANU, Department of Chemistry, University of California, Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis — Hydrated clusters of sulfuric acid derivatives play an important role in many processes of interest, e.g. environmental sciences and electrochemistry. Determining their structural and electronic properties is a challenging task: they exhibit a complex free energy landscape and there is no direct experimental measurement of their geometry, which is usually inferred from spectral signatures obtained, e.g. by infrared (IR) measurements [1]. We have used *ab initio* molecular dynamics simulations to investigate the stability, electronic properties and IR of sulphate-water clusters containing 12 and 13 water molecules. We discuss how the entire hydrogen bonded network of the cluster may be affected by the presence of a single, additional water molecule, leading to geometrical arrangements not yet identified in experiments. We also show that clusters with different structures may have similar IR spectra, thus making it difficult to use spectral signatures to unequivocally determine the cluster geometry. Finally we discuss the electronic properties of the clusters and in particular differences obtained in the computed ionization potentials when using semi-local and hybrid functionals.

[1] Zhou *et al.* *J. Chem. Phys.* 11, 111102 (2006)).

Tuesday, February 28, 2012 8:00AM - 11:00AM – Session H36 DCP: Focus Session: Environment II: Green Processes 107C

8:00AM H36.00001 Using Molecular Simulation to Develop New Materials for Energy and Environmental Applications¹, EDWARD MAGINN, University of Notre Dame — We face two enormous challenges in the coming decades. First, we must find ways to provide clean, affordable energy to an ever-growing population. Second, as underdeveloped countries advance, we must find ways to provide access to advanced technologies that enhance human wellbeing. What makes these two challenges even more daunting is that they both must be met using sustainable technologies; simply relying on old dirty technologies is not an option. In this talk, I will show how approaches rooted in chemical physics are being used to develop new materials that can be used to meet these challenges. In particular, I will give examples where molecular-based simulations are being used in three areas: 1) the discovery of new ionic liquid solvents for capturing CO₂ produced from fossil fuel combustion; 2) the development of new refrigerants that have better performance and significantly lower global warming potentials than existing refrigerants; and 3) fundamental investigations of actinide ions in solution, with the objective of developing new separation processes for nuclear waste remediation and fuel reprocessing technologies.

¹Support provided by the U.S. Department of Energy

8:36AM H36.00002 Highly Selective CO₂/CH₄ Gas Uptake by a Halogen-Decorated Borazine-Linked Polymer, THOMAS REICH, SWAYAMPRAKASH BEHERA, KARL JACKSON, PURU JENA, HANI EL-KADERI, Virginia Commonwealth University — We report herein a synergistic approach that combines synthesis and characterization of a new borazine-linked polymer, BLP-10(Cl), and theoretical calculations based on density functional theory to investigate its performance in small gas storage and separation. We focus on the binding of H₂, CO₂, and CH₄. The choice of these gases is motivated by their impact on energy and the environment. Given the relatively small and similar kinetic diameter of the CH₄ and CO₂ molecules, their efficient separation remains a nontrivial task. In the case of a dihydrogen molecule interacting with the chlorinated borazine, we find the H₂ to be bound molecularly with a bond length of 0.75 Å and at a distance of 2.76 Å from the boron site. CO₂ and CH₄, on the other hand, interact with the central ring system of borazine at a distance of 3.12 Å and 3.33 Å respectively. The bond length between the carbon and oxygen atoms of CO₂ is 1.16 Å while the distance between the carbon and hydrogen of CH₄ is 1.10 Å. The binding affinities of all gases with the chlorinated borazine rings obtained from using the M06 exchange-correlation potential agree very well with experimental data collected from pure gas component isotherms. Theoretical investigations also indicate that all of the gas molecules preferentially interact with the borazine ring rather than the phenyl substituent of the nitrogen atoms which highlight the significance of including polarizable building blocks in adsorbent materials.

8:48AM H36.00003 Carbon dioxide intercalation in Na-fluorohectorite clay at near-ambient conditions¹, JON OTTO FOSSUM², Department of Physics, Norwegian University of Science and Technology, HENRIK HEMMEN, ERLEND G. ROLSETH, DAVI FONSECA, ELISABETH LINDBO HANSEN, Department of Physics, Norwegian University of Science and Technology - NTNU, TOMAS PLIVELIC, MAX IV Laboratory, Lund University, Sweden — A molecular dynamics study by Cygan et al.[1] shows the possibility of intercalation and retention of CO₂ in smectite clays at 37 °C and 200 bar, which suggests that clay minerals may prove suitable for carbon capture and carbon dioxide sequestration. In this work we show from x-ray diffraction measurements that gaseous CO₂ intercalates into the interlayer space of the synthetic smectite clay Na-fluorohectorite. The mean interlayer distance of the clay when CO₂ is intercalated is 12.5 Å at 20 °C and 15 bar. The magnitude of the expansion of the interlayer upon intercalation is indistinguishable from that of the dehydrated-monohydrated intercalation of H₂O, but this possibility is ruled out by careful repeating the measurements exposing the clay to nitrogen gas. The dynamics of the CO₂ intercalation process displays a higher intercalation rate at increased pressure, and the rate is several orders of magnitude slower than that of water or vapor at ambient pressure and temperature.

[1] Cygan, R. T.; Romanov, V. N.; Myshakin, E. M. *Natural materials for carbon capture*; Technical report SAND2010-7217; Sandia National Laboratories: Albuquerque, New Mexico, November, 2010.

¹Supported by the Research Council of Norway CLIMIT Program

²Present address: Centre for Advanced Study - CAS, Oslo, Norway

9:00AM H36.00004 Monoethanolamine adsorption on TiO₂ (110) for solid supported CO₂ capture¹, DEYU LU, KATHRIN MULLER, Center for Functional Nanomaterials, Brookhaven National Laboratory, SANJAYA SENANAYAKE, Chemistry Department, Brookhaven National Laboratory, DAVID STARR, Center for Functional Nanomaterials, Brookhaven National Laboratory — Solid supported CO₂ capture materials are drawing substantial attention as a promising, cost-effective and environmentally friendly alternative to aqueous amine based CO₂ capture. Recently CO₂ capture was observed from monoethanolamine (MEA) adsorbed TiO₂ powders. In order to facilitate the rational design of future solid CO₂ capture materials, it is very important to understand the interaction between MEA and the TiO₂ surface at the atomic level and how it affects the CO₂ capture capabilities. In this work, we report a combined experimental and theoretical study of MEA adsorption on rutile TiO₂ (110). We found that 1 ML of MEAs can form a stable and ordered pattern on TiO₂ (110). However, the amine group in MEA (the CO₂ capture site) binds preferably to the TiO₂ surface in the gauche mode. The binding energy of the gauche mode is about 0.8 eV larger than the trans mode, where the amine group is free, causing the present MEA/TiO₂ system unable to capture CO₂. We found that this large binding energy difference is originated from a combination of surface donor-acceptor bonds, H-bonds, and dipole-induced dipole interaction. Our study suggests that these effects are key factors to design future amine-based solid supported CO₂ capture materials.

¹Work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886

9:12AM H36.00005 Investigation of nanoparticle transformations to guide the design of greener products and processes¹, JAMES HUTCHISON, University of Oregon — Nanoscale particles and products containing nanoparticles hold promise as higher performance materials; however, there are concerns that the production and use of nanoparticles might negatively impact human health or the environment. Within the context of greener nanoscience we aim to maximize the benefits, while minimizing hazards, of nanoscale products. A significant gap in the knowledge needed to develop greener products and processes is our understanding of the formation and transformation of nanoparticles. Such studies of nanoparticle dynamics are technically challenging and few studies have been reported. In this presentation, I will describe convenient methods to monitor nanoparticle dynamics and show how knowledge of nanoparticle transformations can guide the design of greener products and processes. In one example, chemically-modified transmission electron microscopy (TEM) grids are used to directly visualize silver nanoparticle transformations on surfaces. By indexing the TEM grids, it was possible to examine the same nanoparticles repeatedly throughout exposure to different environments. These studies show that larger particles can act as a source of smaller nanoparticles and that much larger particles also produce nanoparticles. With this knowledge, an improved design of nanoparticle coatings for antimicrobial fabrics was developed. A second example involves the use of small angle x-ray scattering (SAXS) to monitor nanoparticle formation reactions in solution in real-time. A combination of beam-line and lab-scale SAXS measurements, combined with simultaneous optical studies, showed that particle growth and coalescence compete under typical synthesis conditions, leading to loss of structural definition of the product. This mechanistic insight, in turn, guided the design of efficient and greener syntheses of well-defined nanoparticles.

¹This work was supported through the Safer Nanomaterials and Nanomanufacturing Initiative and funded by the Air Force Research Laboratory (under Agreement No. FA8650-05-1-5041) and the W. M. Keck Foundation

9:48AM H36.00006 Ceria Nanoparticles: Environmental Impacts on Particle Structure and Chemistry¹, DONALD BAER, PRABHAKARAN MUNUSAMY, AJAY KARAKOTI, SUNTHARAMPILLAI THEVUTHASAN, EMSL Pacific Northwest National Laboratory, SATYA KUCHIBHATLA, Battelle Science and Technology India, SUDIPTA SEAL, University of Central Florida — Ceria nanoparticles are widely studied for catalytic, energy, environmental and bio-medical applications. The performance of ceria often depends on the ability of Cr to switch between +3 and +4 oxidation states. This paper summarizes observations of the impact that synthesis route, processing conditions, storage and environmental conditions have on the chemical and physical properties of ceria nanoparticles. Particles less than 10 nm in diameter are highly dynamic and change their oxidation state not just as a function of size, but also as a function of aging (time) and environmental conditions. During particle nucleation and growth, both particle size and oxidation state change with time. These observations suggest that interpretations of experimental results based primarily on particle size may be misleading. Raman and microXRD studies indicate that these changes can be more complex than anticipated. Because synthesis, analysis and relevant operational conditions often place particles in different environments, understanding how particles change with time in operational conditions is essential to predicting their properties. Time and environmentally induced changes may also play a significant role in the discrepancies reported in various studies.

¹Supported by US DOE and NIH some work conducted in EMSL

10:00AM H36.00007 Solubility and transport of cationic and anionic patterned nanoparticles, JIAYE SU, HONGXIA GUO, Beijing National Laboratory for Molecular Sciences, Joint Laboratory of Polymer Sciences and Materials, MONICA OLVERA DE LA CRUZ, Department of Materials Science, Northwestern University — Diffusion and transport of nanoparticles (NPs) through nanochannels is important for desalination, drug delivery, and biomedicine. Their surface composition dictates their efficiency separating them by reverse osmosis, delivering into cells, as well as their toxicity. We analyze bulk diffusion and transport through nanochannels of NPs with different hydrophobic-hydrophilic patterns achieved by coating a fraction of the NP sites with positive or negative charges via explicit solvent molecular dynamics simulations. The cationic NPs are more affected by the patterns, less water soluble, and have higher diffusion constants and fluxes than their anionic NPs counterparts. The NP-water interaction dependence on surface pattern and field strength explains these observations. For equivalent patterns, anionic NPs solubilize more than cationic NPs since the Coulomb interaction of free anionic NPs, which are much stronger than hydrophobic NP-water interactions, are about twice that of cationic NPs.

10:12AM H36.00008 Hydrogen bond density and strength analysis on hydrated Rutile (110) and Cassiterite (110) surfaces, NITIN KUMAR, Department of Physics, Penn State University, PAUL KENT, Center for Nanophase Materials Sciences and Chemical Sciences Division, Oak Ridge National Laboratory, ANDREI BANDURA, St. Petersburg State University, DAVID WESOLOWSKI, Chemical Sciences Division, Oak Ridge National Laboratory, JAMES KUBICKI, Department of Geosciences, Penn State University, JORGE SOFO, Department of Physics, Penn State University — We study the dynamics of water on the surface of cassiterite (110) and rutile (110) using ab-initio molecular dynamics simulation. Water adsorbs and dissociates on these surfaces. This dynamic equilibrium is dominated by the hydrogen bond (h-bond) network at the surface. The h-bond density analysis shows that adsorbed water molecules form higher average number of h-bonds on rutile (~2.3) as compared to the cassiterite surface (~2.1). On the other hand, bridging oxygen atoms form higher average number of h-bonds on cassiterite (~1.4) than rutile surface (~1.2). Dissociated species are found to have same average number of hydrogen bonds on both surfaces. As a consequence, the rutile surface has higher density of h-bonds at the surface than cassiterite, however, their strength is lower [N. Kumar et al., J. Chem. Phys. 134, 044706 (2011)]. This delicate balance is responsible for the different dynamical properties of both surfaces.

10:24AM H36.00009 Microfluidics and Stimulus-Responsive Materials – The Key to Next Generation Chemical Sensors for Widely Distributed Environmental Monitoring¹, DERMOT DIAMOND, Dublin City University — The fields of chemical sensing and microfluidics have promised much, but in terms of functional devices, have delivered relatively little. Issues like biofouling and surface degradation mean that sensor characteristics change rapidly in real samples. Consequently, chemical sensors must be regularly recalibrated to ensure the information they send is reliable. This results in complex and very costly devices that must integrate fluidics, standards, and waste storage, as well as sampling and analytical procedures. The fundamental challenge for realizing sensors for widely distributed environmental monitoring is this - how can we produce low cost sensing platforms that can function reliably in an autonomous manner for periods up to years? The key to progress lies in new, and more sophisticated materials that can respond to external stimuli, and communicate with the external world. For example, materials that can be activated from a passive state, reversibly bind and release targeted guest molecules, and return to a passive form. Activation and deactivation happen as part of an external control system, which can be local (chemical in nature) or external (e.g. photonic), and the material reports its status (passive, activated-free, activated-occupied) optically materials can be incorporated into more sophisticated platforms, such as micelles, beads, or complete fluidic systems that are much more biomimetic in nature than current platforms. They include polymer actuators that expand and contract dramatically under an external stimulus (e.g. light), enabling valve and pumping functions to be fully integrated into the microfluidic device. This lecture, I will present some of the exciting possibilities for chemical sensing that are now beginning to emerge through breakthroughs in fundamental materials science.

¹Science Foundation Ireland - 07/CE/I1147 - “CLARITY: Centre for Sensor Web Technologies.”

Tuesday, February 28, 2012 8:00AM - 11:00AM – Session H37 SPS: SPS Undergraduate Research III 108

8:00AM H37.00001 Fabrication of Micromirror Templates Using a Focused CO₂ Laser¹, SONIA PEREZ, Henderson State University, BEN PETRAK, KUMARASIRI KONTASINGHE, ANDREAS MULLER, University of South Florida — Micromirrors are an important component in quantum optics, for example in Fabry-Perot microcavities, where light can be recirculated within small volumes. Recently, a CO₂ laser method has been demonstrated as a way to fabricate micromirror templates with an exceptionally high surface quality. However, these templates typically vary in size significantly, which is undesirable in many applications, for example when arrays are needed. Here we address this problem by implementing a feedback method, which uses the light emitted by the sample during the ablation process. By measuring the intensity of the light emitted and correcting, in real time, the laser intensity, we can control the feature size to be less than 5 percent.

¹This work was supported by NSF REU program (award No DMR-1004873).

8:12AM H37.00002 High-power, narrow-bandwidth laser based on a tapered amplifier¹, MICHAEL YANAKAS, ANTHONY VIVONA, MICHAEL LIM, Dept. of Physics and Astronomy, Rowan University — We have constructed a high-power, tunable, narrow-bandwidth, cw laser based on a semiconductor tapered amplifier at a wavelength of 780 nm. Bandwidth narrowing to less than 1 MHz is accomplished with an intra-cavity interference filter, while 10 GHz of continuous tuning is possible with a cavity mirror mounted on a PZT stack. The laser output has a slope efficiency of 0.5 W/A, optical output power of 0.7 W, and will be used for laser cooling of atomic rubidium.

¹Supported in part by NSF PHY0613659.

8:24AM H37.00003 Depth of focus in digital holography using spatial partially coherent light¹, KRISTEN BINZ, Wake Forest University, XIAO YU, DAVID CLARK, MYUNG K. KIM, University of South Florida — Digital holography is a powerful, but young, imaging technology that has a vast array of applications; its strength lies in the ability to numerically focus on any plane within a sample from a single hologram and to use both amplitude and phase information from the intensity field to reconstruct the sample's 3D characteristics on a computer. The quality of many holograms, however, is compromised by speckle and other interference noise associated with the high-coherence lasers often used to illuminate the sample. Speckle noise may be diminished by lowering the coherence length of the source. In our experiments, partially coherent light was created by directing a laser beam through a rotating ground glass. We aimed to discern whether the coherence of the source could be systematically altered by changing the position of the ground glass within the focused laser beam. We anticipated that altering the coherence length would also systematically change the depth of focus. Initial results support our hypotheses.

¹This work was supported by NSF REU program (award No DMR-1004873)

8:36AM H37.00004 Photocatalytic properties of nanostructured TiO₂ surfaces¹, LAUREN MOORE, Northeastern University, TIMOTHY LUTTRELL, MATTHIAS BATZILL, University of South Florida — Photocatalytic chemical reactions are actively explored for direct production of chemical fuels from sun light through electrolysis or for the clean-up of organic pollutants through photocatalysis. Titanium dioxide is a prototypical photocatalyst which has been studied extensively. However, there are still unanswered questions regarding the relationship between surface morphology and photocatalytic properties. In this study, we used ion beam assisted surface nanopatterning and UV-catalysis to investigate the dependence of photoreactivity on surface nanostructures. Energetic argon gas ions were used to induce self-formation of nanopatterns on TiO₂ surfaces and the structure formation was characterized by atomic force microscopy. The influence of the surface structure on the photochemical properties was assessed through photocatalytic degradation of methyl orange in aqueous solution with a flat sample and a nanopatterned sample of TiO₂, respectively. The resulting absorbance spectrums were then compared.

¹This work was supported by NSF REU program (award No DMR-1004873).

8:48AM H37.00005 Pushing the Limits of Nanoscale Imaging in Atomic Force Microscopy , JACOB CVETICH, VASUDEVA RAO ARAVIND, BENJAMIN LEGUM, Clarion University, CLARION UNIVERSITY TEAM — The invention of scanning probe microscopy has revolutionized the field of nanotechnology. Atomic force microscopy is a branch of scanning probe microscopy in which an extremely sharp tip (~ 50 nm diameter) is held in contact with a sample surface. By maintaining constant force between the tip and the sample, the topography of a sample surface can be measured with high precision. The lateral resolution in this technique is however limited by the size of the tip. In this presentation, we present a method to deconvolve the effect of tip size and obtain higher resolution than presented by the experimentally obtained topographic image.

9:00AM H37.00006 Scanning Tunneling Microscopy of Fe Doped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$, BRIAN KOOPMAN, Clark University, W.D. WISE, KAMALESH CHATTERJEE, MIT, GENDA GU, Brookhaven National Laboratory, E.W. HUDSON, Penn State University, M.C. BOYER, Clark University — We will present a low temperature scanning tunneling microscopy (STM) study of the high-temperature superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ (Bi-2212) which has been intentionally doped with magnetic (Fe) impurities in order to locally disrupt superconductivity around the impurities. We examine spatial variations in the density of states in the vicinity of Fe impurities, and compare our results with previous STM studies of Ni doped Bi-2212. Notable differences between Fe and Ni impurities include differences in the number and energy locations of the impurity peaks. Our analysis shows that Fe is a weaker magnetic impurity than Ni and that the particle-hole symmetry present in the spectra of Ni impurities is not as obvious in Fe impurities. By studying how these impurities interact with superconductivity in Bi-2212 we hope to understand more about the superconducting mechanism in high-temperature superconductors.

9:12AM H37.00007 Theoretical & Experimental Design & Optimization of Multilayer Mirrors for Soft X-Ray Reflection , BAKARI HASSAN, FRANCK DELMOTTE, EVGUENI MELTCHAKOV, None — The reflection of soft X-rays is relevant for the development of ultra fast attosecond cameras, X-ray lithography, and the study of solar storms. Soft X-rays are typically absorbed, as opposed to reflected, due to all materials' absorptive nature. Co/C-am multilayers composed of 40 layers were deposited on Si & SiO_2 substrates by Magnetron Sputtering technique and were characterized by grazing-incidence diffraction. Theoretical interfacial roughness and layer thicknesses were simulated using the commercial software IMD, while experimental values were estimated by fitting the reflectivity data. Low reflectivity values were observed at the locations of Bragg peaks. However, through deposition optimization, reflectivity values could potentially reach values above 60%.

9:24AM H37.00008 Domain Coarsening Within the Ising Model on the Hyperbolic Plane¹ , JAMES MOLCHANOFF, Math, West Virginia Wesleyan University, HOWARD L. RICHARDS, Physics, Marshall University — In spite of its simplicity, both the dynamics and equilibrium statistics of the Ising model are nontrivial. Previous studies in this REU have shown that the dynamics of metastable decay is very different in the hyperbolic plane than in the Euclidean plane. Here we perform Monte Carlo simulations of domain coarsening in the hyperbolic plane. We find that domain coarsening occurs more slowly than in the Euclidean plane.

¹Research performed at Marshall University's REU in scientific computing, supported by National Science Foundation grant OCI-1005117.

9:36AM H37.00009 Quantum chaos: an introduction via chains of interacting spins-1/2 , AVIVA GUBIN, LEA SANTOS, Yeshiva University — We discuss aspects of quantum chaos by focusing on spectral statistical properties and structures of eigenstates of quantum many-body systems. Quantum systems whose classical counterparts are chaotic have properties that differ from those of quantum systems whose classical counterparts are regular. One of the main signatures of what became known as quantum chaos is a spectrum showing repulsion of the energy levels. We show how level repulsion may develop in one-dimensional systems of interacting spins-1/2 which are devoid of random elements and involve only two-body interactions. We present a simple recipe to unfold the spectrum and emphasize the importance of taking into account the symmetries of the system. In addition to the statistics of eigenvalues, we analyze also how the structure of the eigenstates may indicate chaos. This is done by computing quantities that measure the level of delocalization of the eigenstates.

9:48AM H37.00010 Solving the Feynman–Gell-Mann Equation for the Electron , GRAHAM MILLER, DANIEL FINKENSTADT, U.S. Naval Academy, Physics Department — There are very few cases for which the Dirac equation can be solved exactly. Moreover, the techniques familiar from undergraduate quantum mechanics provide little help in solving its linear differential equations. Working instead with a two-component formalism, the transformed Dirac equation can be solved for cases of constant electric and magnetic fields for an electron. This approach was recommended in the famous 1958 paper by Feynman and Gell-Mann and has the form: $(i\hbar \frac{\partial}{\partial t} - V)^2 = -\hbar^2 c^2 |\nabla - i\frac{e}{\hbar} \vec{A}|^2 - e\hbar c \vec{\sigma} \cdot (\vec{B}c + i\vec{E}) + (mc^2)^2$, when acting on a two component spinor φ . We will show the solution of this equation for the cases of parallel E & B fields, perpendicular fields, perhaps oblique fields and finish with a discussion of the Hydrogen atom. Through taking the nonrelativistic limits, these solutions can be verified for well-known conditions.

10:00AM H37.00011 Second harmonic generation and non-linear corrections to the high frequency susceptibility of a multiferroic material , PHILIP JAVERNICK, TRINANJAN DATTA, Augusta State University — We consider the effects of non-linear (second order) corrections to the high-frequency susceptibilities of a material that is simultaneously ferroelectric and a canted antiferromagnet (multiferroic). The non-linear corrections introduce a second harmonic term in the magnetic, electric, and multiferroic susceptibilities. Using the Landau-Lifshitz equation of motion for the magnetic components and the Landau-Khalatnikov relaxation equation for the electric polarization we theoretically compute the non-linear corrections to the susceptibilities for the optic antiferromagnetic mode, the acoustic mode, and the electric susceptibilities up to second order. Using realistic material parameters we find that the corrections have either a noticeable or negligible effect on the first order susceptibility values.

10:12AM H37.00012 Aluminum Nitride Nanofibers fabricated using Electrospinning and Nitridation¹ , XENIA BARBOSA, University of Puerto Rico at Humacao, EVA CAMPO, JORGE SANTIAGO, University of Pennsylvania, IDALIA RAMOS, University of Puerto Rico at Humacao, UPPEN-UPR PREM COLLABORATION² — Aluminum Nitride (AlN) and other nitride semiconductors are important materials in the fields of optoelectronics and electronics. AlN nanofibers were synthesized using electrospinning and subsequent heating under N_2 and NH_3 atmospheres. The precursor solution for electrospinning contains aluminium nitrate and cellulose acetate. The electrospun nanofibers were heated in N_2 to eliminate the polymer and produce Al_2O_3 , and then nitridized at a temperature of 1200°C under NH_3 flow. Scanning Electron Microscopy (SEM) observations demonstrate the production of fibers with diameters ranging from a few nanometers to several micrometers. X-Ray Diffraction and UV-VIs analyses show the production of AlN nanofibers with hexagonal wurzite structure and a band gap of approximately approximately 6 eV. Current-Voltage measurements on a single AlN fiber with gold electrodes suggest the formation of a Schottky contact The fabrication method and results from the fibers characterization will be presented.

¹This work was funded by NSF-DMR-0934195

²This work was funded by PENN-UPR No. NSF-DMR-0934195

10:24AM H37.00013 Formation of Nanostructures at Gold Surfaces Exposed to Femtosecond Laser Pulses, KELSIE NIFFENEGGER, Auburn University, BRIAN DEMASKE, VASILY ZHAKHOVSKY, IVAN OLEYNIK, University of South Florida — The evolution of free-standing gold film irradiated by ultrashort laser pulses was simulated using molecular dynamics. The spatially non-uniform deposition of laser energy was modeled by a two-dimensional temperature profile applied during time of electron-ion energy exchange. Our simulations show that the ultrafast two-dimensional heating results in the melting and pressurization of a thin surface layer. Due to a non-uniform stress distribution, this molten layer expands to form a jet-like protrusion at the laser pulse's focal point. Above some critical stress, many voids start to nucleate forming a foam-like material covered by a thin liquid shell/cupola. The still expanding cupola may rupture forming a rim around the newly-developed crater. All these processes lead to complicated surface morphology, which becomes frozen at the nanosecond time scale. Geometrical characteristics of simulated surface profiles, including crater depth and size of frozen bubbles, agree well with experiment. Our simulations help to provide better insight into the atomistic mechanisms of nanostructure formation.

10:36AM H37.00014 Gold coated nanoparticles on silicon substrate, SIRAK MELAKU, None — The study of Gold nanoparticles is very captivating because of their significance and applications as catalysts in restructuring technologies that are used for manufacturing medicine, energy production, transportation, computation, communication, and environmental changes. In this experiment, I have analyzed the morphology of gold nanoparticles using different techniques. A sputter coating technique was used to deposit gold on silicon substrate. During the process, depositions were performed using varying plasma coating times and voltages. The Gold nanoparticles were then analyzed using the Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM). The AFM and SEM data revealed that the coating surface morphology was dependent upon deposition conditions.

10:48AM H37.00015 Simulations of surface plasmons launched on gold nanogratings, IAN WHITE, JENNIFER STEELE, Department of Physics and Astronomy, Trinity University — A gold nanograting with a dielectric coating containing fluorescent molecules can enhance the intensity of fluorescence at certain frequencies due to the excitation of surface plasmons. Fluorescence is enhanced by two mechanisms: (1) an enhanced electromagnetic field at the excitation frequency of the fluorophores and (2) surface plasmon modes providing extra decay channels for fluorophores. Previous studies on corrugated film gratings show that coupling to higher diffraction order plasmons occur with lower efficiency. We find that for wire gratings, fluorophores couple to higher order plasmon modes on both sides of the gold wires with uniform efficiency. We also measure directional enhanced fluorescence on both the active (reflection) and substrate (transmission) side of the gratings. In this work, gold nanogratings with a dielectric coating were modeled using COMSOL Multiphysics software, which solves Maxwell's equations in the region of the grating. As the thickness of the dielectric layer containing the fluorophores is increased, the plasmon modes shift. The behavior of the gratings was simulated as a function of height of the gold wires and thickness of the dielectric coating. These simulations will inform future experiments.

Tuesday, February 28, 2012 8:00AM - 11:00AM – Session H39 Electronic Structure: Calculations II 109B

8:00AM H39.00001 Variational investigations of the electronic structure and energy of finite hydrogen systems with the Gutzwiller wave function within local correlation matrix renormalization approximation¹, YONGXIN YAO, JUN LIU, CAI-ZHUANG WANG, KAI-MING HO, Iowa State University and Ames Laboratory-U.S. DOE — We introduce the correlation matrix renormalization Hartree-Fock (CMR-HF) method in which the many-body Hamiltonian of a multi-electronic system is solved using a variational Gutzwiller-type wave-function. The Gutzwiller approximation is generalized to renormalize the one-electron density matrix and two-electron correlation matrix of the system. To achieve a clear presentation of the concept and methodology, we describe the detailed formalisms for a finite hydrogen system with minimal basis set. The resulting expectation value of the Hamiltonian have clear parallels to terms in the standard uncorrelated Hartree-Fock method, allowing an iterative self-consistent field solution of the many-electron problem analogous to the Hartree-Fock solution. We have applied the method to a series of hydrogen clusters to compare with the results of several other quantum chemical calculation methods.

¹Work at Ames Laboratory was supported by the US Department of Energy, Basic Energy Sciences, Division of Materials Science and Engineering.

8:12AM H39.00002 Real-time time-correlation approach for x-ray absorption and emission spectra¹, F.D. VILA, A.J. LEE, J.J. REHR, Dept. of Physics, U. of Washington, Seattle, WA 98195 — We present a real-time approach for calculations of X-ray absorption (XAS) and emission spectra (XES) from deep core-levels, based on time-correlation functions. XAS and XES have traditionally been calculated using Fermi's golden rule in frequency space, and alternatively, using real-space Green's function (RSGF) methods. Recently, however, with the advent of very high brightness pulsed x-ray sources, calculations of time-dependent response have become a focus of attention. Here we obtain the time-correlation functions by propagating the initial, dipole-excited wavefunction with a Crank-Nicolson time-evolution operator.² The initial state is obtained using projector augmented wave (PAW) transition matrix elements and, for XAS, the propagation is carried out in the presence of a core hole. The approach is implemented using an extension of SIESTA and can be applied both to molecular and extended systems. Illustrative examples are presented for several systems, and yield results in good agreement with RSGF and Fermi golden rule approaches using FEFF and StoBe respectively. Finally, we discuss improvements in order to include dynamic many-body effects.

¹Supported by NSF Grant PHY-0835543 (AL, FDV) and DOE BES Grant DE-FG03-97ER45623 (JJR), and facilitated by the DOE CMCSN Grant DE-FG02-08ER46540L.

²Y. Takimoto *et al.*, J. Chem. Phys. **127**, 154114 (2007).

8:24AM H39.00003 Calculation of Phonon Satellites in Electron Spectral Functions¹, SPENCER WILLIAMS, J.J. KAS, J.J. REHR, University of Washington, M. VERSTRAETE, Universite de Liege — We describe a first principles approach for calculations of phonon satellites in the electron self-energy and spectral function. The method is based on cumulant expansion techniques [1] applied to the self-energy model of Eiguen and Ambrosch-Draxl [2] with the dynamical matrix and electron-phonon couplings obtained from ABINIT [3]. In particular, the electron-phonon couplings are calculated from the Eliashberg functions as in [4], and the phonon DOS is obtained from a many-pole/Lanczos representation of the phonon Green's function [5]. The method is illustrated with results for a number of systems.

[1] F. Aryasetiawan *et al.*, Phys. Rev. Lett. **77**, 2268 (1996).

[2] A. Eiguen and C. Ambrosch-Draxl, Phys. Rev. Lett. **101**, 036402 (2008).

[3] X. Gonze *et al.*, Comput. Materials Science **25**, 478 (2002).

[4] S. Y. Savrasov and D. Y. Savrasov Phys. Rev. B **54**, 16487 (1996).

[5] F. Vila *et al.*, Phys. Rev. B **76**, 014301 (2007).

¹Supported by NSF Grant PHY-0835543.

8:36AM H39.00004 Atomic Multiplets in X-ray spectroscopies revisited¹, BERNARD DELLEY, Paul Scherrer Institut, CMT, WHGA123, CH-5232, Villigen PSI, FRANÇOIS VERNAY, University of Perpignan, France, ANNE-CHRISTINE ULDREY, Paul Scherrer Institut, CMT, WHGA123, CH-5232, Villigen PSI — Atomic multiplets are known since a long time to produce specific, crystal field dependent, fingerprints of open d- and f- shells in X-ray spectroscopies. Older computer programs originating from gas-phase optical spectroscopy of atoms tend to be difficult to apply to crystal field environments with lower symmetries. In order to study changes of X-ray absorption near edge spectra and resonant inelastic X-ray scattering (RIXS) across symmetry lowering phase transitions, a new multiplet program was developed. Starting from a Dirac-Slater spherical atom calculation we evaluate electron-electron interaction and crystal field in the Hilbert space spanned by the open shells by diagonalization. The crystal field can be simply defined by nominal charges and cartesian atomic positions relative to the core-hole atom. To overcome limitations of the model and for fitting known spectra, spin-orbit splitting, el-el interaction and crystal-field can be scaled independently. The nominal charges may be taken as further crystal field parameters. Various XAS and RIXS examples will be discussed, in particular in view of the polarisation dependence and symmetry of the crystal.

¹Supported by grant SNF 200021-129970.

8:48AM H39.00005 Simulation of electron-energy-loss spectra including both diffraction and solid-state effects¹, MICAH PRANGE, MARK OXLEY, Vanderbilt University and ORNL, MARIA VARELA, ORNL, STEPHEN PENNYCOOK, ORNL and Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University and ORNL — Aberration-corrected scanning transmission electron microscopes yield probe-position-dependent electron-energy-loss spectra (EELS) that can potentially provide spatial mapping of the underlying electronic states. EELS calculations, however, typically describe excitations by a plane wave travelling in vacuum, neglecting diffraction and interference effects. Here we report the development and initial application of a methodology that combines a full electronic-structure calculation with beam propagation in a thin film. The simulations are based on PAW plane-wave calculations of the excitation spectrum of the material and Bloch wave simulations of the probe propagation.

¹This work was supported in part by DOE grant no. DE-FG02-09R46554 (MPP, MPO, STP), by the DOE Basic Energy Sciences (SJP,MV,STP) and by the McMinn Endowment at Vanderbilt University (STP).

9:00AM H39.00006 Precise all-electron response functions from a combined spectral sum and Sternheimer approach: application to EXX-OEP, MARKUS BETZINGER, CHRISTOPH FRIEDRICH, STEFAN BLÜGEL, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — The optimized-effective-potential (OEP) method is used to construct local potentials from non-local, orbital-dependent functionals, e.g., exact exchange (EXX). The method involves two response functions, which have to be converged to very high precision to obtain smooth and stable local potentials. Usually, this requires an exceptionally large orbital basis, leading to very costly calculations, especially for all-electron methods such as FLAPW [1]. In this work, we propose a scheme that combines the usual spectral sum from standard perturbation theory with a radial Sternheimer approach. It also comprises a, albeit small, Pulay-type correction, which refines the results especially for small basis sets. We demonstrate that with this new approach already the conventional minimal LAPW basis set is sufficient to yield precise response functions. Furthermore, very few unoccupied states are required, which reduces the computational cost considerably. The numerically important Sternheimer contribution arises from the potential dependence of the LAPW basis functions and is constructed by solving inexpensive radial differential equations. We show results for complex transition-metal oxides.
[1] M. Betzinger *et al.*, Phys. Rev. B **83**, 045105 (2011)

9:12AM H39.00007 Electronic band structure of lanthanum bromide and strontium iodide from many-body perturbation theory calculations¹, DANIEL ABERG, Lawrence Livermore National Laboratory, PAUL EHART, Chalmers University of Technology, BABAK SADIGH, Lawrence Livermore National Laboratory — Rare-earth based scintillators represent a challenging class of scintillator materials due to pronounced spin-orbit coupling and subtle interactions between d and f states that cannot be reproduced by standard electronic structure methods such as density functional theory. In this contribution we present a detailed investigation of the electronic band structure of LaBr₃ using the quasi-particle self-consistent GW (QPscGW) method. This parameter-free approach is shown to yield an excellent description of the electronic structure of LaBr₃. Specifically we reproduce the correct level ordering and spacing of the 4f and 5d states, which are inverted with respect to the free La atom, the band gap as well as the spin-orbit splitting of La-derived states. We furthermore present electronic structure calculations using G₀W₀ for the important scintillator material SrI₂. We explicitly take into account spin-orbit coupling at all levels of the theory. Our results demonstrate the applicability and reliability of the GW approach for rare-earth halides and complex halides. They furthermore provide an excellent starting point for investigating the electronic structure of rare-earth dopants such as Ce and Er.

¹Prepared by LLNL under Contract DE-AC52-07NA27344. The authors acknowledge support from the National Nuclear Security Administration (NNSA) Office of Nonproliferation Research and Development (NA-22).

9:24AM H39.00008 First-principles studies of Ce and Eu doped inorganic materials as candidates for scintillator gamma ray detectors¹, ANDREW CANNING, Lawrence Berkeley National Laboratory, UC Davis, SLIM CHOUROU, STEPHEN DERENZO, Lawrence Berkeley National Laboratory — We have performed high-throughput DFT based (GGA+U) band structure calculations for new Ce and Eu doped wide band gap inorganic materials to determine their potential as candidates for gamma ray scintillator detectors. These calculations are based on determining the 4f ground state level of the Ce and Eu relative to the valence band of the host as well as the position of the Ce and Eu 5d excited state relative to the conduction band of the host. We find many classes of candidate materials where the 5d is in the conduction band preventing scintillation. Even when the Eu and Ce 4f and 5d levels are placed well in the gap of the host, traps on the host can also prevent the energy of the gamma ray transferring to the Eu or Ce. We therefore also performed calculations for host hole traps and electron traps to compare their energies to the Ce and Eu 4f and 5d levels.

¹The work was supported by the US Department of Homeland Security and was carried out at the Lawrence Berkeley National Laboratory under US Department of Energy Contract No. DE-AC02-05CH11231.

9:36AM H39.00009 Test of Variational Methods for Molecular and Solid State Properties by Application to Hyperfine Interaction in Phosphorous Atom, T.P. DAS, R.H. PINK, S.R. BADU, Department of Physics, University at Albany, SUNY, ARCHANA DUBEY, Department of Physics, University of Central Florida, R.H. SCHEICHER, Department of Physics, Uppsala University, LEE CHOW, Department of Physics, University of Central Florida — As part of our program for testing the accuracy of variational methods for studying energy and wave-function dependent molecular and solid state properties, namely the Variational Hartree-Fock Many Body Perturbation Theory (VHFMBPT) and Variational Density Functional Theory (VDFT), we have studied the magnetic hyperfine interaction for ^{31}P nucleus in the ground state. Our investigations provide hyperfine constants of +35.2MHz by the VHFMBPT and -11.2 MHz by VDFT procedures as compared to +55.055 MHz from experiment [1]. The VHFMBPT procedure provides the same signs for one-electron and many-body contributions as obtained earlier [2] by the HFMBPT procedure which uses the needed one-electron atomic wave-functions for the occupied and unoccupied states obtained by solving the Hartree-Fock equations through numerical integration, and not variationally as in the VHFMBPT procedure. Possible avenues for improved agreement by both variational procedures will be suggested. [1] N.C. Dutta, C. Matsubara, R.T. Pu and T.P. Das, Phys. Rev. Lett. 21, 1139 (1963) and references therein, [2] T.P. Das Hyperfine Interactions 34, 149 (1987) and reference therein to the experimental result for phosphorous atom. [3] Alfred Owusu, R.W. Dougherty, G. Gowri, J. Andriessen, T.P. Das, Phys. Rev. A 56, 305 (1997) and references therein.

9:48AM H39.00010 Sharp transition for single polarons in one-dimensional models with non-diagonal Su-Schrieffer-Heeger coupling, DOMINIC J.J. MARCHAND, PHILIP C.E. STAMP, University of British Columbia, NIKOLAY V. PROKOF'EV, University of Massachusetts, MONA BERCIU, University of British Columbia — Ever since Landau pointed out the possibility of an electron becoming self-trapped in its own lattice distortion, people have looked for sharp transitions in polaronic states. Gerlach and Löwen [1] proved the absence of such a transition in the case of a gapped (i.e. optical) phonon branch and an electron-phonon coupling $g(q)$ depending only on the phonon momentum q . Whether a sharp transition could be found in other models remained an open question for the last twenty years. By presenting both unbiased Diagrammatic Monte Carlo results for the single polaron with Su-Schrieffer-Heeger (SSH) coupling to optical phonons, and supporting results from no less than three other numerical and analytical approximations, we believe our previous work and that of our collaborators [2] to be the first unequivocal demonstration of a sharp transition in a polaronic system. Here we expand this work to more general models that include either an additional diagonal Holstein coupling to optical phonons, or a SSH coupling to acoustic phonons. The survival of the sharp transition in these models is investigated using the Bold Diagrammatic Monte Carlo method and the Momentum Average approximation. References: [1] Rev. Mod. Phys. 63, 63 (1991) [2] Phys. Rev. Lett. 105, 266605 (2010)

10:00AM H39.00011 Many-Pole Model Calculations of Inelastic Losses in XPS¹, J.J. KAS, J.J. REHR, University of Washington, M. GUZZO, L. REINING, Ecole Polytechnique — Inelastic losses such as satellites in x-ray photo-emission spectra (XPS) are difficult to treat theoretically due to the importance of many-body effects beyond the quasi-particle approximation. Here we present an approach based on an exponential (i.e., cumulant) representation² of the one-particle Green's function, together with³ a many-pole model of the dielectric function, which incorporates dynamic effects beyond the GW approximation. In this method the photo-electron is treated as in inverted LEED state which couples to the system via neutral, quasi-boson excitations. The approach yields an approximation to the XPS in terms of a convolution of a quasi-particle calculation and a spectral function that includes contributions from both intrinsic and extrinsic excitations,⁴ as well as interference between them. The method is illustrated with recent experimental results.⁵

¹Supported by DOE BES grant DE-FG03-97ER45623.

²M. Guzzo et al., Phys. Rev. Lett. **107**, 166401 (2011)

³J. Kas et al., Phys. Rev. B **76**, 195116 (2007)

⁴L. Hedin et al., Phys. Rev. B **58**, 15565 (1998)

⁵Guzzo, op. cit.

10:12AM H39.00012 Low Energy Positron Interactions with Biological Molecules, INDIKA WAN- NIARACHCHI, CAROLINE MORGAN, Physics Department, Wayne State University, BERNHARD SCHLEGEL, Chemistry Department, Wayne State University, GARY KEDZIORA, AFRL/DSRC, Wright-Patterson AFB, LARRY BURGGRAB, Engineering Physics, Air Force Institute of Technology, MICHAEL PAK, SHARON HAMMES-SCHIFFER, Chemistry Department, Penn State University — There is some experimental evidence that positrons can produce distinctive molecular fragmentation patterns. It is known that tuning the incident positron energy to near resonance with molecule vibrations can strongly enhance the positron annihilation probability for a molecule.¹ This suggests that fragmentation induced by slow positrons may provide valuable complementary information to existing techniques for identification and study of proteins. In order to study this concept, we are developing a general quantum method for reliably calculating the density distribution for positrons bound to large biological molecules using NEO/GAMESS. We developed transferrable atom-centered positron basis sets for first-principles calculations for molecules containing O, N, C, and H. The positron density in the bound state is concentrated near the most electronegative atomic sites so that e^-e^+ annihilation will be most likely to occur in these regions for low incident positron energies leading to positron trapping in the bound state. Using the basis sets and approximations we have tested to predict where annihilation occurs can ultimately help us understand the resulting fragmentation patterns of larger biological molecules.

¹Gribakin, Young, and Surko, Rev. Mod. Phys. 82 (2010) 2577

10:24AM H39.00013 Atomic Probing Structures of Electrolytes at Graphene Surface: Insights from X-ray Scattering and Molecular Dynamics, HUA ZHOU, PAUL FENTER, Argonne National Laboratory, PANCHAPAKESAN GANESH, PAUL KENT, DEEN JIANG, ARIEL CHIALVO, PASQUALE FULVIO, SHENG DAI, Oak Ridge National Laboratory, GUANG FENG, MICHAEL ROUHA, PETER CUMMINGS, Vanderbilt University, VOLKER PRESSER, JAKE MCDONOUGH, YURI GOGOTSI, MATTHEW WANDER, KEVIN SHUFORD, Drexel University — The interactions of electrolyte fluids with carbon-based electrodes control many complex interfacial processes encountered in electrochemical energy storage systems. However, our knowledge of the atomic/nanoscale reactivity at interfaces of electrolytes with electrodes remain scares due to the incomplete understanding of interfacial structures and processes in-situ and real-time encountered in real operation conditions. In this talk, we will present our efforts to obtain a molecular-scale perspective of the interactions of electrolytes with carbon surfaces near “real world” conditions. Structures of various electrolytes including slat aqueous and ionic liquids on atomically flat graphene (epitaxially grown on a SiC substrate), an ideal model fluid-solid interface system, were investigated by coupling high-resolution interface X-ray scattering techniques with molecular modeling-simulation approaches. These results provide a base-line for understanding relevant electrolyte/carbon interactions and will lead to fundamentally new insights and provide unique tests of atomistic fluid-solid interface models for energy storage systems.

10:36AM H39.00014 Charge Transfer Resistance of a Pristine Graphitic Carbon Interface, BRAD CORSO, ISRAEL PEREZ, PHILIP COLLINS, University of California, Irvine — Electron transfer to and from graphitic carbons is highly sensitive to the chemistry of the graphitic carbon surface. It is known that pristine graphitic carbon has a much higher interfacial resistance than defective carbon; however, a quantitative measure of the difference is limited by the difficulty of preparing truly pristine, defect-free surfaces. Here, we use an individual single-walled carbon nanotube (SWNT) and its single defect sensitivity to ensure that the graphitic carbon surface is pristine. The interfacial charge transfer resistance is measured in the context of a MnO₂-coated SWNT, a pseudocapacitor device whose charge cycling performance is found to be limited by the chemistry of the carbon interface. In our devices, the SWNT is uniformly coated with 250-350 nm of MnO₂ and cyclic voltammetry is analyzed using an equivalent circuit model to determine the charge transfer resistance. We prove that the defect-free carbon interface is less active than disordered interfaces of carbon or of metallic electrodes. This research is supported by the NEES Energy Frontier Research Center of the U.S. DOE Office of Basic Energy Sciences (#DESC0001160).

10:48AM H39.00015 Applications of Light Element X-ray Raman Spectroscopy and Hard X-ray Emission Spectroscopy to the Electronic Structure of Energy Storage Materials: Prospects and Initial Results from the Spectroscopy Program at SSRL, DENNIS NORDLUND, WENG TSU-CHIEN, DIMOSTHENIS SOKARAS, SLAC National Accelerator Laboratory, STANFORD SYNCHROTRON RADIATION LABORATORY TEAM — We present the applicability of x-ray raman spectroscopy of light elements and hard x-ray emission to probe the electronic structure of energy storage materials under in-situ conditions. In particular, recent advances in resolution and throughput of x-ray raman spectroscopy (XRS) offer the capability to measure 1s x-ray absorption profiles of light elements such as lithium, boron, carbon, nitrogen and oxygen with less than 0.3eV resolution in the order of 10s of minutes. Initial results from the Spectroscopy program at SSRL and collaborations with groups in various energy storage fields will be presented, with an emphasis on Lithium Batteries and Hydrogen Storage applications.

Tuesday, February 28, 2012 8:00AM - 11:00AM —
Session H40 DBIO DPOLY: Focus Session: Protein Association II: Aggregation and Fibril Formation 156A

8:00AM H40.00001 The Physics of Amyloid Aggregation and Templating in Prions¹, DANIEL COX, Dept. of Physics, UC Davis — The problem of self-assembled amyloid aggregation of proteins in structures with beta-strands perpendicular to a one dimensional grown axis is interesting at a fundamental level (is this the most generic end state of proteins?), from a biological level (if the self-assembly can be regulated it is of use in contexts like spider silk and bacterial colony formation), for human public health (aggregation unregulated induces diseases like mad cow and Alzheimer's), and for possible materials applications (e.g., in tissue scaffolding). In this presentation, I will review the work of my group in examining the possibility that the left-handed beta helix (LHBH) structure can be the building block of the aggregates of mammalian prion and yeast prion proteins. I will also discuss our efforts to assess the possibility of a novel pH driven structural switch between LHBH and alpha-helical forms in the ordered half of the mammalian prion protein, and now the possibly pH stabilized LHBH structure can template aggregate growth of the disordered half of the protein, identified in numerous experimental studies as most relevant to disease.

¹Support from US NSF I2CAM International Materials Institute Award, Grant DMR-0844115 is gratefully acknowledged

8:36AM H40.00002 Early-Aggregation Studies of Polyglutamine in Solution, AARON FLUITT, JUAN DE PABLO, University of Wisconsin-Madison — Several neurodegenerative diseases, notably Huntington's disease, are associated with certain proteins containing extended polyglutamine tracts. In all polyglutamine diseases, the age of onset is inversely correlated with the length of the polyglutamine domain beyond some pathological threshold. Diseased cells are characterized by intranuclear inclusions rich in aggregated polyglutamine. Experimental evidence suggests that oligomeric aggregate species, not mature amyloid fibrils, are the species most toxic to the cell. Little is known about the structures and aggregation dynamics of polyglutamine oligomers due to their short lifetimes. A better understanding of the pathway through which polyglutamine peptides form oligomeric aggregates will aid the design of therapies to inhibit their toxic activity. In this work, we report structural characterization of polyglutamine monomers and dimers from atomistic molecular dynamics simulations in explicit water. Umbrella sampling simulations reveal that the stability of the dimer species with respect to the disassociated monomers is an increasing function of the chain length.

8:48AM H40.00003 Search for Length Dependent Stable Structures of Polyglutamine Proteins with Replica Exchange Molecular Dynamic¹, ALEXANDER KLUBER, ROBERT HAYRE, DANIEL COX, University of California Davis — Motivated by the need to find beta-structure aggregation nuclei for the polyQ diseases such as Huntington's, we have undertaken a search for length dependent structure in model polyglutamine proteins. We use the Onufriev-Bashford-Case (OBC) generalized Born implicit solvent GPU based AMBER11 molecular dynamics with the parm96 force field coupled with a replica exchange method to characterize monomeric strands of polyglutamine as a function of chain length and temperature. This force field and solvation method has been shown among other methods to accurately reproduce folded metastability in certain small peptides, and to yield accurately de novo folded structures in a millisecond time-scale protein. Using GPU molecular dynamics we can sample out into the microsecond range. Additionally, explicit solvent runs will be used to verify results from the implicit solvent runs. We will assess order using measures of secondary structure and hydrogen bond content.

¹Research supported by NSF grant DMR-0844115

9:00AM H40.00004 Lysozyme Aggregation and Fibrillation Monitored by Dynamic Light Scattering, LOUIS NEMZER, BRET FLANDERS, JEREMY SCHMIT, CHRISTOPHER SORENSEN, Department of Physics - Kansas State University — The aggregation of amyloidogenic proteins provides a rich phase space with significant biomedical implications, including a link with several age-related diseases. We employed dynamic light scattering to monitor the aggregation of lysozyme, a model protein, from a monomeric state until the formation of micron-sized fibrils. For an aqueous lysozyme solution buffered at pH 2, the auto-correlation function of the scattered light intensity was found to be well-fit by a single exponential function with decay time $\tau = 1/(2Dq^2) = 0.25$ ms, which corresponds to a mean hydrodynamic radius (R_H) of 2.2 nm, very likely generated by monomers. Ethanol (4% v/v final concentration) induced a partial unfolding, to $R_H = 4.6$ nm. The subsequent addition of 70 mM KCl was found to shrink the size back to $R_H = 2.5$ nm, as expected when a denatured protein refolds due to partial screening of the intramolecular repulsion. However, further aggregation was not observed. At pH 4, using a low-salt acetate buffer, more ethanol (10% v/v) was required to initiate unfolding, but once it occurred, larger aggregates formed. These results are consistent with the model that partial unfolding, which exposes beta-motif secondary structure, is a prerequisite for aggregation and fibrillation, but the aggregation fate depends on the protein charge state (pH) and screening (salt concentration).

9:12AM H40.00005 Primary nucleation and linear aggregation: novel methods take us further

, GONZALO GARCIA, Department of Chemistry, University of Cambridge — Understanding linear aggregation has long been of interest in the study of proteins, as it is relevant in several human diseases such as Alzheimer's Disease. While much work has been carried out experimentally and numerically, relatively little has been done to develop an analytical model for the time evolution and scaling behaviour of such systems. Here, we present a novel mathematical framework, guided by physical insight, for approaching these problems. We then apply this to derive an exact expression for the evolution of the polymer length distribution of an amyloid system, driven by primary nucleation, taking into account both elongation and depolymerisation. This is presented in terms of a perturbative expansion, and is valid for negligible monomer depletion. We then apply a similar framework to solve a similar system that also includes an arbitrary number of conformational intermediates before reaching the final conformation - we uncover the time evolution of the total mass of polymers in the final conformational state, and demonstrate various properties about its time-scaling behaviour. We then apply self-consistent iterative schemes, starting from these solutions, to derive a series of approximate analytical models for these systems, taking monomer depletion into account.

9:24AM H40.00006 The Mechanisms of Aberrant Protein Aggregation

, SAMUEL COHEN, Harvard University, University of Cambridge, MICHELE VENDRUSCOLO, CHRIS DOBSON, TUOMAS KNOWLES, University of Cambridge — We discuss the development of a kinetic theory for understanding the aberrant loss of solubility of proteins. The failure to maintain protein solubility results often in the assembly of organized linear structures, commonly known as amyloid fibrils, the formation of which is associated with over 50 clinical disorders including Alzheimer's and Parkinson's diseases. A true microscopic understanding of the mechanisms that drive these aggregation processes has proved difficult to achieve. To address this challenge, we apply the methodologies of chemical kinetics to the biomolecular self-assembly pathways related to protein aggregation. We discuss the relevant master equation and analytical approaches to studying it. In particular, we derive the underlying rate laws in closed-form using a self-consistent solution scheme; the solutions that we obtain reveal scaling behaviors that are very generally present in systems of growing linear aggregates, and, moreover, provide a general route through which to relate experimental measurements to mechanistic information. We conclude by outlining a study of the aggregation of the Alzheimer's amyloid-beta peptide. The study identifies the dominant microscopic mechanism of aggregation and reveals previously unidentified therapeutic strategies.

9:36AM H40.00007 Amyloid growth: combining experiment and kinetic theory

, TUOMAS KNOWLES, SAMUEL COHEN, MICHELE VENDRUSCOLO, CHRISTOPHER DOBSON, University of Cambridge — The conversion of proteins from their soluble forms into fibrillar amyloid nanostructures is a general type of behaviour encountered for many different proteins in the context of disease as well as for the generation of a select class of functional materials in nature. This talk focuses on the problem of defining the rates of the individual molecular level processes involved in the overall conversion reaction. A master equation approach is discussed^{1 2} and used in combination with kinetic measurements to yield mechanistic insights into the amyloid growth phenomenon.

¹Cohen et al, J Chem Phys 2011, 135, 065106

²Knowles et al, Science, 2009, 326, 1533-1537

9:48AM H40.00008 Scaling exponents report on changes in the mechanism of filamentous

growth, LUKE RAJAH, SAMUEL COHEN, Department of Chemistry, University of Cambridge, SARA LINSE, ERIK HELLSTRAND, Chemistry Department and Molecular Protein Science, Lund University, CHRIS DOBSON, TUOMAS KNOWLES, Department of Chemistry, University of Cambridge — We analyse the scaling behaviour in the proliferation and growth of protein nanostructures. We show that changes in scaling exponents that govern the lag time of the reaction within a given system can be identified with mechanistic changes that affect a molecular step in the assembly pathway. In this study, we focused on fibril growth from a representative protein, insulin, and an unstructured peptide, A β 42. Our results reveal that the scaling exponent contains contributions not only from the dominant secondary nucleation mechanism in the systems studied, but also from the primary nucleation step even in cases where the generation of nuclei from the primary pathway is significantly smaller than from the secondary pathway. These results shed light on the origin of the scaling behaviour of filamentous growth.

10:00AM H40.00009 Control the kinetics and pathway of insulin fibril formation

, ZHONGLI ZHENG, BENXIN JING, Y. ELAINE ZHU, University of Notre Dame — Protein fibrils have been proposed as possible toxic agents for many amyloid related diseases, such as Alzheimer's disease, however the reaction pathway toward the amyloid fibrillation remain inadequately understood. In this work, we examine the conformational transition of human insulin as the model amyloid protein by single-molecule fluorescence spectroscopy and imaging. By controlling the pH cycling, insulin monomer and oligomers are indentified at given pH variation condition. Furthermore, low frequency ac-electric fields are employed to control the insulin aggregation from its monomers in a microchannel. It is observed that lag time to induce insulin fibrillation can be significantly shortened, in compasson to the commonly used cooling and seeding methods, and exhibits a strong dependence on applied ac-field strength. Additionally, the structure of insulin aggregates under ac-electric fields is observed to be drastically different from that under the temperature control.

10:12AM H40.00010 Time-Dependent and Low Temperature Studies of Amyloidogenic and Non-amyloidogenic Proteins by Dielectric Relaxation Spectroscopy

, DONALD BARRY, SHAUN MARSHALL, SHELBY HUNT, Worcester Polytechnic Institiute, FLORIN DESPA, University of California, Davis, IZABELA STROE, Worcester Polytechnic Institiute — We present dielectric relaxation spectroscopy measurements of amyloidogenic Abeta (1-42) and non-amyloidogenic Abeta (42-1) proteins over a frequency range of 10 mHz to 10 MHz. Measurements were performed as a function of time from 0 to 24 h and temperature range of 193K-283K. Two relaxation peaks, alpha and beta, were observed at temperatures above 193 K. These peaks are attributed to the bulk and bound water. As a function of time, the dielectric signal of the Abeta (1-42) shifts towards the dielectric signal of the solvent while for the Abeta (42-1) the dielectric signal does not change. The activation energies of Abeta (1-42) and Abeta (42-1) were calculated and significant differences were found. We attribute these variations to structural changes that affect the hydration map of Abeta (1-42) aggregates. Our results are in agreement with theoretical predictions.

10:24AM H40.00011 Applying microfluidic techniques in quantitative studies of protein aggregation

, THERESE HERLING, University of Cambridge — Protein aggregation and fibrillation is involved in a number of devastating diseases, of which we have a limited understanding at present. Microfluidic techniques can be used in developing quantitative assays to study individual aspects of protein aggregation. Under certain conditions bovine insulin aggregates to give spherulites; spherical structures with fibrils growing and branching out from a central core. Drawing a parallel to actin polymerisation of the cell's cytoskeleton, fibril growth generates force. The force generated by polymerisation at fibril ends during spherulite growth can be measured in a microfluidic environment (TPJ Knowles et al, PNAS, 2009). By measuring the bending of four polydimethylsiloxane walls by a growing spherulite positioned in the centre, the force generated by polymerisation at fibril termini can be calculated. By growing the spherulites with a constant flow of monomer, the maximum force able to be generated by fibril growth, the stall force, can be calculated. This gives insight into the energy landscape of protein aggregation.

10:36AM H40.00012 Anomalous Formation of Multilayer Protein Aggregates on the Surface of Nanotubular TiO_2 ¹, JACOB FORSTATER, ALFRED KLEINHAMMES, YUE WU, Department of Physics and Astronomy, University of North Carolina at Chapel Hill — Significant evidence links protein aggregation to the pathology and progression of most protein misfolding diseases. Protein aggregation also poses a significant problem for the safe and cost-effective production of therapeutic proteins. A comprehensive understanding of these problems requires both a detailed understanding native protein-protein interactions as well as an understanding of how protein-material interactions may alter protein aggregation phenomenon. Here we report on the anomalous formation of multilayered protein aggregates of globular proteins on the surface of TiO_2 nanotubes. Our findings suggest that minor alterations of the surface hydration properties of the nanotubes may drastically alter protein aggregation phenomenon. We further highlight the role of electrostatic and Van der Waals forces in this aggregation process.

¹ Authors acknowledge support by NSF DMR-0906547

10:48AM H40.00013 Effect of Lipid Bilayer on Human Islet Amyloid Polypeptide Self Assembly, CHI-CHENG CHIU, SADANAND SINGH, JUAN J. DE PABLO, University of Wisconsin-Madison — Aggregates of human islet amyloid polypeptides (hIAPP, also known as human amylin) are commonly found in the pancreatic β -cells of type II diabetes patients. Experimental studies have shown that small aggregates of hIAPP, that arise during the assembly process, lead to membrane leakage and are highly cytotoxic. Due to the fast assembly kinetics, it is difficult to study the early aggregation of hIAPP experimentally. In this work, we use molecular simulation with a coarse grained (CG) model to investigate the oligomerization of hIAPP with and without the presence of lipid bilayers. We develop a CG protein model that reproduces the three thermodynamically stable structures of hIAPP, namely α -helix, β -hairpin, and unstructured coil, and the corresponding free energy differences calculated by atomistic molecular simulations. The aggregated structure of hIAPP also agrees with that proposed by NMR experiments. We further investigate the assembly of hIAPP in the presence of a lipid bilayer and its effect on the membrane leakage. Comparing our results with the mechanism proposed based on experimental data provides a better understanding of the origins of hIAPP self assembly and its toxicity.

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H43 DBIO: Invited Session: Physics of Systems Biology 157AB

8:00AM H43.00001 Robustness of Biological Circuits, MARC KIRSCHNER, Department of Systems Biology, Harvard Medical School, Boston MA, USA — In responding to inputs biological systems do many types of calculations, some of which serve to maximize the signal and suppress noise. Physiology faces similar requirements and to fulfill these many sensory systems such as vision and hearing are designed to respond logarithmically to the fold change over initial conditions, a property known as “Weber’s Law.” Mathematical modeling of the ancient Wnt signaling circuit suggested that a key design feature of that pathway was to provide a robust logarithmic output and as a consequence it does not respond robustly in a linear or hyperbolic way. We confirmed this behavior in *Xenopus* embryos and in human colorectal cells in culture. However, to read a robust logarithmic output from the Wnt pathway in the form of fold change in the levels of beta catenin, the responding transcriptional circuit must be able to compare initial and final levels of beta catenin accurately. This is exactly what we found in *Xenopus* embryos. What kind of transcriptional pathway has this property? Examination of the detailed promoter of a classic wnt responsive gene showed that two domains contribute to the calculation: the well known TCF/LEF sites that bind beta catenin near the coding sequence and a functional DNA feature upstream, which is unresponsive to beta catenin. The TCF/LEF sites on their own respond in a linear mode to the beta catenin concentration. The upstream functional feature confers the logarithmic response. Knowledge of the pathway structure should allow us to define a “Weber’s Law” circuit that allows transcriptional systems to suppress noise by responding to fold change rather than to simple saturation.

8:36AM H43.00002 Epigenetic switches and network transitions, MASAKI SASAI, Nagoya University — We investigate dynamics of gene networks which are regulated by both the fast binding/unbinding of transcription factors to/from DNA and the slow processes of chromatin structural change or histone modification. This heterogeneous dynamics consisting of different time scales is analyzed by the mean-field approximation and the stochastic simulation to show that the network exhibits multiple metastable states and is characterized by transitions among them. We discuss distribution and fluctuation of states of the core gene network of embryonic stem cells as an example of such heterogeneous dynamics and the simulated transitions are compared with the experimental data on the distribution of stem cell states.

9:12AM H43.00003 Specificity and Self Recognition in Immunity, ARUP K. CHAKRABORTY, Massachusetts Institute of Technology — No abstract available.

9:48AM H43.00004 Landscape and Flux Framework for Non-Equilibrium Networks: Kinetic Paths and Rate Dynamics, JIN WANG, Stony Brook University — We developed a general framework to quantify three key ingredients for dynamics of nonequilibrium systems through path integrals in length space. First, we identify dominant kinetic paths as the ones with optimal weights, leading to effective reduction of dimensionality or degrees of freedom from exponential to polynomial so large systems can be treated. Second, we uncover the underlying nonequilibrium potential landscapes from the explorations of the state space through kinetic paths. We apply our framework to a specific example of nonequilibrium network system: lambda phage genetic switch. Two distinct basins of attractions emerge. The dominant kinetic paths from one basin to another are irreversible and do not follow the usual steepest descent or gradient path along the landscape. It reflects the fact that the dynamics of nonequilibrium systems is not just determined by potential gradient but also the residual curl flux force, suggesting experiments to test theoretical predictions. Third, we have calculated dynamic transition time scales from one basin to another critical for stability of the system through instantons. Theoretical predictions are in good agreements with wild type and mutant experiments. We further uncover the correlations between the kinetic transition time scales and the underlying landscape topography: the barrier heights along the dominant paths. We found that both the dominant paths and the landscape are relatively robust against the influences of external environmental perturbations and the system tends to dissipate less with less fluctuations. Our theoretical framework is general and can be applied to other nonequilibrium systems.

10:24AM H43.00005 Experimental evolution in budding yeast, ANDREW MURRAY, Harvard University — I will discuss our progress in analyzing evolution in the budding yeast, *Saccharomyces cerevisiae*. We take two basic approaches. The first is to try and examine quantitative aspects of evolution, for example by determining how the rate of evolution depends on the mutation rate and the population size or asking whether the rate of mutation is uniform throughout the genome. The second is to try to evolve qualitatively novel, cell biologically interesting phenotypes and track the mutations that are responsible for the phenotype. Our efforts include trying to alter cell morphology, evolve multicellularity, and produce a biological oscillator.

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H44 DPOLY: Focus Session: Nano to Mesoscale Structure in Ordered Systems: Liquid Crystal Topology and Defects 157C

8:00AM H44.00001 Polymer Physics Prize Break —

8:36AM H44.00002 Chiral Self-Assembly¹, ROBERT MEYER², Physics Department, Brandeis University, Waltham, MA 02454 — Chirality, the lack of reflection symmetry, at the molecular level has a profound influence on the ordering of molecular assemblages at the macroscopic scale. The example discussed here is the self-assembly of monolayers of rod-like fd virus particles, with the virus particles oriented on the average perpendicular to the plane of the layer, like a single layer of a smectic-A liquid crystal. Because these virus particles are chiral, they would prefer a twisted packing, which is incompatible with the layer structure. The twisted packing can only appear locally, at layer edges or in isolated defects in the interior of the layer. As chirality increases, the twisted regions achieve lower energy, until they can drive remarkable transformations to structures with longer edges and/or a greater number of defects.

¹Supported by the MRSEC at Brandeis University, NSF-MRSEC-0820492

²Director, MRSEC at Brandeis University

9:12AM H44.00003 Pillar-Assisted Epitaxial Assembly of Focal Conic Domain Arrays in Smectic-A Liquid Crystals, DANIEL BELLER, APIRADEE HONGLAWAN, MARCELLO CAVALLARO, RANDALL KAMIEN, KATHLEEN STEBE, SHU YANG, University of Pennsylvania — We demonstrate a versatile approach to tailor the spacing and symmetry of periodic arrays of toric focal conic domains (TFCDs) over a large area via confinement of smectic-A liquid crystals (SMA LCs) in patterned substrates. Arrays of pillars with variable dimensions are employed to direct the assembly of TFCDs, determining both the domain positions and the size of the defects. Highly ordered square and hexagonal arrays of TFCDs result from topographical confinement of the LC in square and hexagonal arrays of pillars. Focal conic domains are shown to form only when the confined geometry provides sufficient area so that substrate-induced planar alignment of LC molecules is energetically favorable. Since the spacing and symmetry of the TFCD array can be readily pre-determined by the arrangement of the directing pillars, this pillar-assisted assembly technique serves as a model study for directed assembly of liquid crystals in three dimensions and offers improvements to the capability of LC-based templates for device fabrication and lithography.

9:24AM H44.00004 Shape and chirality transitions in twisted nematic elastomer ribbons: Finite element simulation studies, VIANNEY GIMENEZ-PINTO, Liquid Crystal Institute, Kent State University, FANGFU YE, University of Illinois, Urbana, BADEL MBANGA, University of Massachusetts, Amherst, JONATHAN SELINGER, ROBIN SELINGER, Liquid Crystal Institute, Kent State University — We use finite element simulation studies to explore transitions of shape and chirality in nematic elastomer ribbons with a twisted director configuration. Recent experimental and theoretical studies demonstrated that these fascinating materials show reversal of macroscopic chiral sense under a change of temperature, and explored shape selection as a function of the sample's aspect ratio. We explore these phenomena via three dimensional finite element simulation studies. For ribbons with width/thickness ratio above a threshold value, we find that on heating the sample undergoes a sequence of shape transitions from right handed helix – right handed twisted ribbon – flat ribbon – left handed twisted ribbon – left handed helix. Ribbons with width/thickness ratio below the threshold show fewer shape transitions, from right handed twisted ribbon – flat ribbon – left handed twisted ribbon. These results are in qualitative agreement with theoretical predictions, provide insight into experimental observations, and demonstrate the value of finite element methods for future engineering design of nematic elastomer devices.

9:36AM H44.00005 Frustrated orientational order on extrinsic geometries¹, BADEL L. MBANGA, GREGORY M. GRASON, Department of Polymer Science and Engineering, University of Massachusetts, Amherst, CHRISTIAN D. SANTANGELO, Department of Physics, University of Massachusetts, Amherst — The ground state of an anisotropic liquid on a curved surface has topological defects due to the surface's Gaussian curvature. The extrinsic geometry of the surface, however, frustrates the ground state arising from Gaussian curvature alone, changing the defect configurations in the ground state or expelling them from the surface altogether. We study nematic order on unduloids - a family of undulated cylinders with constant mean curvature spanning from the cylinder to a chain of spherical droplets - arising in systems ranging from liquid bridges to fluid membranes. We identify structural transitions in which pairs of disclinations of opposite signs are nucleated as the unduloid progresses from cylinder to spheres, explicitly separating the role of intrinsic geometry, which nucleates disclinations to screen Gaussian curvature, and extrinsic geometry, which expels defects from the neck. We describe some implications for the pinching off of a cylinder.

¹This work is supported as part of Polymer-Based Materials for Harvesting Solar Energy, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001087.

9:48AM H44.00006 Topology of knots and links in chiral nematic colloids, SLOBODAN ZUMER, University of Ljubljana and Jozef Stefan Institute, SIMON COPAR, University of Ljubljana, IGOR MUSEVIC, University of Ljubljana and Jozef Stefan Institute, MIHA RAVNIK, University of Oxford, UROS TKALEC, Jozef Stefan Institute — Nematic braids formed by disclinations entangling colloidal particles in chiral and achiral nematic liquid crystals are geometrically stabilized and restricted by topology. We report how self-linking number enables a classification of entangled defect lines [1, 2] and how a simple rewiring scheme for the orthogonal crossing of two half integer disclinations, based on a tetrahedral rotation of two relevant disclination segments allows us to predict nematic braids and their self-linking numbers. We further describe how using of laser micromanipulation enable the knotting of defect lines in chiral nematic colloids into knots and links of arbitrary complexity [3]. Colloids stabilized by nematic braids based on all knots and links with up to six crossings, including Hopf link, Star of David, Borromean rings are realized. We demonstrate how topology leads to the engineering of complex soft materials.

[1] S. Copar and S. Zumer, Nematic Braids: Topological Invariants and Rewiring of Disclinations, Phys. Rev. Lett. 106, 177801 (2011).

[2] S. Copar, T. Porenta and S. Zumer, Nematic Disclinations as Twisted Ribbons, Phys. Rev. E 84, 051702 (2011).

[3] U. Tkalec, M. Ravnik, S. Copar, S. Zumer and I. Musevic, Reconfigurable Knots and Links in Chiral Nematic Colloids, Science 333, 62 (2011).

10:00AM H44.00007 Modeling texture transitions in cholesteric liquid crystal droplets¹, ROBIN SELINGER, VIANNEY GIMENEZ-PINTO, SHIN-YING LU², JONATHAN SELINGER, ANDREW KONYA, Kent State University — Cholesteric liquid crystals can be switched reversibly between planar and focal-conic textures, a property enabling their application in bistable displays, liquid crystal writing tablets, e-books, and color switching “e-skins.” To explore voltage-pulse induced switching in cholesteric droplets, we perform simulation studies of director dynamics in three dimensions. Electrostatics calculations are solved at each time step using an iterative relaxation method. We demonstrate that as expected, a low amplitude pulse drives the transition from planar to focal conic, while a high amplitude pulse drives the transition from focal conic back to the planar state. We use the model to explore the effects of droplet shape, aspect ratio, and anchoring conditions, with the goal of minimizing both response time and energy consumption.

¹Supported by Ohio Board of Regents

²now at Micron Technology, Inc.

10:12AM H44.00008 Necklaces of Liquid Crystal Beads: Nematic Drops Constrained on Thin Cellulosic Fibers, PEDRO ALMEIDA, YONG GENG, FCT/UNL, EUGENE TERENTJEV, University of Cambridge, MARIA HELENA GODINHO, FCT/UNL, CENIMAT COLLABORATION, CAVENDISH LABORATORY COLLABORATION — Liquid crystal droplets dispersed in a continuous matrix have important applications in electro-optical devices. They also produce intriguing topological defect structures due to the confinement of the liquid crystal by closed boundaries that impose alignment at the interface. In this work we use a simple method to generate stable liquid crystal droplets topologically equivalent to a toroid by depositing tiny volumes of a nematic liquid on cellulosic micro-fibers (1 μm diameter) suspended in air. This system can exhibit non-trivial point topological defects which can be energetically unstable against expanding into ring defects, depending on the fibers constraining geometries. By changing temperature, the system remains stable and allows the study of the defects evolution near the nematic-isotropic transition showing qualitatively different behavior on cooling and heating processes. The necklaces of such liquid crystal drops constitute excellent systems for fundamental studies and open new perspectives for applications. This work was sponsored by Air Force Office of Scientific Research, Air Force Material Command, USAF, under grant number FA8655-10-1-3020. The US Government is authorized to reproduce and distribute reprints for Governmental purpose notwithstanding any copyright notation thereon. Other support includes the Portuguese Science and Technology Foundation grant SFRH/BD/63574/2009 and projects PEst-C/CTM/LA0025/2011 (Strategic Project - LA 25 - 2011-2012, PTDC/CTM/099595/2008, PTDC/FIS/110132/2009 and Windsor Treaty grant 2009-10 UR55.

10:24AM H44.00009 Controlling the location of defects in nematic shells, ALBERTO FERNANDEZ-NIEVES, Georgia Tech, TERESA LOPEZ-LEON, MAURIZIO NOBILI, CHRISTOPHE BLANC, University of Montpellier 2 — We study nematic shells with four $s=+1/2$ defects and vary the elastic constant anisotropy of the liquid crystal by approaching the nematic-to-smectic phase transition temperature. We find the defects ultimately arrange themselves along a great circle, consistent with recent expectations. Changing the elastic constant anisotropy provides an alternative route to changing the shell thickness inhomogeneity for controlling the defects location.

10:36AM H44.00010 Structures in liquid crystalline shells at a nematic-smectic transition¹, JAN LAGERWALL, Seoul National University, Grad. School of Convergence Science & Technology, Korea, HSIN-LING LIANG, Inst. of Organic Chemistry, Johannes Gutenberg University Mainz, Mainz, Germany, PER RUDQUIST, Chalmers University of Technology, Dept. for Microtechnology & Nanoscience, Goteborg, Sweden — Liquid crystalline shells display phenomena that are fascinating from a fundamental physics point of view and they also hold promise for innovative applications e.g. for advanced colloids. The key feature of these shells is the unavoidable presence of topological defects, the types and numbers of which depend on the phase as well as the geometrical features of the shell. Here we present our investigation of the complex internal reordering phenomena occurring in a liquid crystalline shell undergoing a transition between the nematic and smectic phases. In the smectic phase, the topological and geometrical constraints of a spherical shell with symmetric boundary conditions imposed on the developing 1D quasi-long-range order create a conflict that triggers a series of buckling instabilities, resulting in two different characteristic defect patterns. We will also show very recent results on shells with asymmetric boundary conditions, giving rise to beautiful complex patterns, some transitory, some stable. The phase transition between nematic and smectic order yields varying textures depending on the shell size and thickness, and on the specific alignment types at the shell in- and outside, respectively.

¹Supported by grants 2011-0012184 (NRF, Korea) and 490-20100024 (AICT, SNU, Korea)

10:48AM H44.00011 Visualizing, manipulating, and imprinting π -wall defects in self-assembled colloidal membranes, MARK ZAKHARY, THOMAS GIBAUD, C. NADIR KAPLAN, EDWARD BARRY, Brandeis University, RUDOLF OLDENBOURG, Marine Biology Laboratory, ROBERT B. MEYER, ZVONIMIR DOGIC, Brandeis University — Geometric frustration and the resulting topological defects play an important role in determining the structural, mechanical and optical properties of materials. Here we describe the behavior of a new type of defect, called a π -wall, in a model system of colloidal membranes composed of chiral rod-like *fd* viruses. We use complimentary optical microscopy techniques to study the structure and energetics of π -walls, and develop a model based on the analogy between liquid-crystals and superconductors to determine the structure and energetics of π -walls. We then focus on π -wall formation, showing that π -walls naturally assemble through a unique coalescence process in which chiral frustration plays an essential role. π -walls can also be artificially created and engineered using externally applied optical forces.

Tuesday, February 28, 2012 8:00AM - 11:00AM —

Session H45 DPOLY: Focus Session: Thin Film Block Copolymers - Phase Behavior 159

8:00AM H45.00001 Polymer Physics Prize Break —

8:36AM H45.00002 Controlling the Orientation of Block Copolymer Thin Films with Selective and Neutral Nanoparticles, MISANG YOO, SEYONG KIM, Korea University, BUMJOON J. KIM, Korea Advanced Institute of Science and Technology, JOONA BANG, Korea University — The bottom up approach using self-assembly of block copolymers (BCP) have been considered as a powerful technique which can resolve the limitations of conventional nanolithograph. For practical applications, the perpendicular orientation of microdomains with respect to the substrate is a prerequisite. However in most cases, one of the domains has a preferential interaction with the substrate and this interaction induces parallel orientation of the microdomains. To overcome the preferential interaction and to obtain vertically orientated BCP microdomains, diverse approaches have been developed. Previously, we synthesized thermally stable core-shell gold nanoparticles using UV cross-linkable BCP and also precisely tuned the surface property of nanoparticles which are selective and neutral to PS and PMMA by adjusting the composition of polymeric ligand. Moreover, we demonstrated the effect of selective and neutral gold nanoparticles on the orientation of PS-PMMA thin films. Herein, we further investigated the effect of selective and neutral gold nanoparticles on the orientation of BCP thin films of lamellar and cylindrical BCP according to the film thickness. The thin film morphologies were characterized with AFM and SEM.

8:48AM H45.00003 Assembly and Photo-Induced Disorder in Block Copolymer-Additive Systems¹, LI YAO, JAMES WATKINS, University of Massachusetts Amherst — Additives that hydrogen bond selectively to one block of a weakly ordered or disordered block copolymer can drive phase segregation to yield well ordered materials. Here we show that the addition of D- or L-tartaric acid to low molecular weight, weakly segregated poly(ethylene oxide-block-tert-butyl acrylate), PEO-b-PtBA, induces strong segregation and well ordered morphologies as evidenced by Small Angle X-ray Scattering. This strong interaction between enantiopure tartaric acid and the PEO block also suppresses PEO crystallinity at room temperature. While the addition of racemic tartaric acid does not strengthen segregation nor does it suppress PEO crystallization. The UV-exposure of well ordered films of PEO-b-PtBA/tartaric acid blends containing a photo acid generator followed by a post-exposure bake results in the deprotection of the tert-butyl acrylate block to yield poly(acrylic acid) (PAA). Since PAA and PEO are miscible and tartaric acid can interact strongly with either block, the system becomes disorder, resulting in a photo-induced disordering transition which can be exploited to pattern the surfaces. The kinetic behavior of the disordering transition upon deprotection of PtBA to PAA was studied using Grazing-Incidence Small-Angle X-ray Scattering.

¹Funding from Center for Hierarchical Manufacturing (CHM); Facility support from Materials Research Science and Engineering Center at University of Massachusetts Amherst (MRSEC UMASS) and Cornell High Energy Synchrotron Source (CHESS)

9:00AM H45.00004 Diblock copolymer morphologies in ultra thin films under shear, MARCO PINNA, ANDREI ZVELINDOVSKY, University of Central Lancashire, XIAOHU GUO, Daresbury Laboratory, CHRISTINE STOKES, University of Central Lancashire — We demonstrate that the shear alignment and the shear-induced transitions in sphere-forming diblock copolymer single layer and bilayer films observed experimentally can be explained by cell dynamics simulation, a simple model with a Ginzburg-Landau Hamiltonian. In two layer films the spheres align in various arrangements, like (100) or (110) bcc plains, or transform to cylinders depending on the shear rate and the temperature. We present a nontrivial alignment mechanism of a single layer of spherical domains in shear via slug-like movement of transient cylindrical micelles. In addition, we clarify the formation of the perpendicular cylinders, found in the recent particle based simulation. We also present results on lamellae shearing in ultra-thin films.

9:12AM H45.00005 Structure and dynamics of random block copolymers in the bulk and thin films, MARCUS MÜLLER, BIRGER STEINMÜLLER, Georg-August University, Göttingen, Germany, KEITH H. HAMBRECHT, GRANT D. SMITH, DMITRY BEDROV, University of Utah, Salt Lake City — Using a soft, coarse-grained model and a Lennard-Jones bead-spring model, we study the morphology of random block copolymers in the bulk and in contact with a hard wall that preferentially attracts one component. We show that both coarse-grained models yield similar equilibrium morphologies at intermediate and long length scales, and identify a mapping between the parameters of the two models. For most parameters we observe a disordered, microemulsion-like morphology. We study the single-chain dynamics in the bulk and in contact with a preferential surface. The relaxation times of the soft, coarse-grained model is about two orders of magnitude faster than the Lennard-Jones bead-spring model. In both models the relaxation time increases with segregation but the Lennard-Jones bead-spring model is additionally slowed down by the densification of the local packing at low temperatures. We employ the soft, coarse-grained model to generate starting configurations for the bead-spring model. Then, the bead-spring model is quenched below its glass transition temperature, and we investigate the local mechanical properties of the disordered, yet structured morphology.

9:24AM H45.00006 Macrophase Separation of Block Copolymer Blends in Thin Films, LANCE WILLIAMSON, PAUL NEALEY, University of Wisconsin — The behavior of macrophase-separating blends of symmetric polystyrene-*b*-poly(methyl methacrylate) block copolymers in thin films on non-preferential surfaces was characterized with respect to the blends' molecular weights and composition. When the molecular weight ratio of block copolymers is at least five, the blends segregate into a domain of nearly pure small block copolymer with a small lamellar period and a domain of about equal volume fraction of each block copolymer with a larger lamellar period. The composition and structure of these blends was determined by analyzing the period and area fraction of each phase from plan-view scanning electron micrographs. The lamellae propagate through the thickness of the film. The use of block copolymer blends has potential in block copolymer lithography as a strategy to pattern different period structures in the same film.

9:36AM H45.00007 Phase segregation at the sub-5-nm scale using high χ Poly(ethylene oxide-*b*-dimethylsiloxane) copolymers, DAMIEN MONTARNAL, GLENN FREDRICKSON, EDWARD KRAMER, CRAIG HAWKER, Materials Research Laboratory, UCSB — Silicon containing block copolymers, such as Poly(styrene-*b*-dimethylsiloxane) (PS-PDMS), have recently received significant attention for nanolithographic applications [Jung et al., Nano Letters 2010, 10, 1000]. PDMS provides indeed a robust and highly selective mask to oxygen reactive ion etching. In addition, the high Flory-Huggins $\chi_{PS-PDMS}$ parameter (about 0.3 at room temperature) favors the segregation of low molecular weight (16 kg/mol) block copolymers (BCPs) into well-organized structures with pitch as small as 17 nm. In an effort to downscale further the size of structures formed by BCP, we decided to turn to copolymers with even higher χ parameters. Copolymers of Poly(ethylene oxide) (PEO) and PDMS are known to have extremely high χ parameters (0.4 -1.1) [Galin et al., Macromolecules, 1981, 14, 677], but their bulk and thin film properties have not been investigated in detail. PEO-PDMS BCPs were synthesized by chain coupling via a versatile copper-activated azide-alkyne click reaction. The unusually high χ parameter between EO and DMS allowed strong phase segregation to occur in copolymers with molecular weight as low as 5kg/mol. The full pitch were found to be less than 10 nm and we report on their bulk and thin film characteristics.

9:48AM H45.00008 Decoupling Bulk Thermodynamics and Wetting Characteristics of Block Copolymer Thin Films¹, SANGWON KIM, University of Minnesota, Twin Cities, PAUL NEALEY, University of Wisconsin, Madison, FRANK BATES², University of Minnesota, Twin Cities — The incorporation of a random copolymer molecular architecture has been known to induce notable changes in the physical properties, often with commercial implications. In this presentation, the consequences of controlled degrees of epoxidation on both bulk and thin-film properties of poly(isoprene) blocks in poly(styrene-*b*-isoprene) (PS-PI) diblock copolymers and poly(isoprene) (hPI) homopolymers have been studied, where the products after epoxidation are denoted as hPI_{xn} and PS-PI_{xn}. Small angle X-ray scattering and dynamic mechanical spectroscopy were conducted on PS-PI_{xn} to calculate the effective interaction parameters χ_{eff} between the PS and PI_{xn} blocks in bulk (3-D) while the surface energy of thin-film PI_{xn} (2-D) was estimated based on contact angle measurements on hPI_{xn} and lamellar orientations of thin-film PS-PI_{xn}. A non-linear change with a minimum at the intermediate degrees of modification is observed for χ_{eff} in bulk whereas thin-film experiments suggest that the surface energy of PI_{xn} increases linearly with epoxidation. This decoupling of bulk and thin-film thermodynamic behaviors is attributed to the different roles that a random copolymer architecture plays in establishing 3-D order versus wetting at a 2-D surface.

¹Financial support for this work was provided by the Nanoscale Science and Engineering Center (NSEC).

²Corresponding Author

10:00AM H45.00009 Continuity and connectivity of lamellar-forming block copolymers in thin films, IAN CAMPBELL, MARK STOYKOVICH, University of Colorado, Boulder — Thin films of block copolymers are emerging as a low-cost lithographic material. In order to effectively utilize this class of materials, the structure of the self-assembled morphologies in thin films must be well understood. In this work, the network structure formed by a lamellar diblock copolymer of polystyrene (PS) and poly(methyl methacrylate) (PMMA) was explored as the compositional symmetry was varied through homopolymer addition. The volume fraction of PMMA was varied from 0.45 to 0.55. The long-range connectivity of the PS and PMMA domains, as well as the branch and endpoint density, was characterized. Increasing the compositional asymmetry of the copolymer system leads to interconnected networks that span arbitrarily large areas, increased branch density, and decreased endpoint density. The network structure for each copolymer system also depends on annealing time, annealing temperature, and surface chemistry of the substrate. Improved understanding of the variability in lamellar morphologies will enable the selection of copolymers, annealing conditions, and surface chemistries to fabricate lithographic masks by self-assembly.

10:12AM H45.00010 Theoretical and Experimental Investigations of Contact Hole Shrink using PS-PMMA Block Copolymers, VALERIY GINZBURG, PHILLIP HUSTAD, JEFFREY WEINHOLD, RAHUL SHARMA, VIVIAN CHUANG, PETER TREFONAS, The Dow Chemical Company — One possible application of block copolymer directed self-assembly (DSA) involves rectification or "shrink" of contact holes in a polarity switched photoresist (see, e.g., J. Cheng et al., ACS Nano 8, 4815 [2010]). The block copolymer (e.g., PS-PMMA) undergoes ordering inside the cylindrical hole; the central (PMMA) domain is then etched out so that the hole diameter is effectively reduced. We utilize strong segregation theory (SST) and numerical self-consistent field theory (SCFT) to calculate the phase behavior of the block copolymers as function of their molecular weight and composition, as well as the contact hole diameter and the surface chemistry of the walls. The model predictions were compared with experimental data, and a good agreement was found. The results illustrate how modeling can serve to guide block copolymer selection for DSA contact hole rectification application.

10:24AM H45.00011 Tailoring block copolymer morphology via control of topographical surface: A self consistent field theoretic study, XIANGGUI YE, BRIAN J. EDWARDS, BAMIN KHOMAMI, Materials Research and Innovative Laboratory, Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, TN 37996 — It is well known that chemically patterned or topologically complex substrates can direct self-assembly of adsorbed layers or thin films of block copolymers. In this study we have examined the self-assembly of a lamella-forming diblock copolymer guided by topological complexity, namely, substrates composed of trenches with different heights and widths. In general, when the substrate is neutral to both blocks of the copolymer, the perpendicular lamella morphology is obtained. However, when the substrate has a preferred affinity to one of the blocks, a host of novel morphologies including different bi-continuous network structures can be created by judiciously manipulating the trench height and width. Overall, this study clearly demonstrates the impact of this class of simulations in rational design of morphologies in thin multi-component polymeric films with application to technologies such as filtration, and high-surface area membranes.

10:36AM H45.00012 Silicon patterning using self-assembled PS-b-PAA diblock copolymer masks for anti-reflective black silicon fabrication via plasma etching, XIN ZHANG, CHRISTOPHER J. METTING, SEAN FACKLER, ROBERT M. BRIBER, Department of Materials and Engineering, University of Maryland, College Park, MD 20742, USA, ANDREI B. SUSHKOV, H. DENNIS DREW, Department of Physics, University of Maryland, College Park, MD 20742, USA — The diblock copolymer of poly(styrene-b-acrylic acid) is a novel self-assembling mask material for pattern transfer applications. This material system has high dry etch selectivity and can produce a variety of feature types and size scales. Different vertical profiles were produced by altering the etch recipes and diblock copolymer or SiO₂ mask processing. This patterning technique is used to fabricate antireflective silicon metamaterials that show broadband anti-reflection properties in the visible and infrared wavelength range (<5% total reflection). These materials are potentially useful for solar cell and light sensing applications. Similar surface roughening by chemical etch, porous silicon, nanowires and other methods have been used previously to reduce reflectance from material interfaces for photovoltaics and antireflection applications. Unlike these methods, the BCP self-assembled pattern transfer via RIE produces robust patterns that are tunable in both the horizontal and vertical directions without harsh chemicals or expensive catalysts. This simple and rapid process can also be applied to semiconductors other than silicon.

10:48AM H45.00013 Assembly of block copolymer films between chemically patterned and chemically homogeneous surface, JEONG IN LEE, HUIMAN KANG, HYO SEON SUH, CHRISTOPHER THODE, University of Wisconsin, LEI WAN, HGST, ABELRADO HERNANDEZ, University of Wisconsin, YASUHIKO TADA, HIROSHI YOSHIDA, Hitachi Ltd., JUAN DE PABLO, PAUL NEALEY, University of Wisconsin — Many technologically useful block copolymer systems other than poly(styrene-block-methylmethacrylate) are currently not amenable for directed assembly because one of the blocks has a lower surface energy, segregates to the free surface of the film, and disrupts directed assembly of the film (at least with respect to realizing perpendicularly oriented through-film domains) on the underlying chemical pattern. Cross-linkable random copolymer mats were developed as well as methods to deposit them on the surfaces of block copolymer films. The chemistry of these “top coats” can be tuned to impart preferential and non-preferential wetting properties towards the blocks of the block copolymer films. The three-dimensional morphology of block copolymers assembled between lithographically-defined chemically patterned surfaces and top coats of varying wetting properties were characterized using specialized sample preparation techniques and cross-sectional scanning electron microscopy. The resulting structures compare favorably with molecular simulations. A primary technological objective of the top coat strategy is to direct the assembly of block copolymer systems that allow for sub-10 nm patterning and perpendicularly oriented domains.

Tuesday, February 28, 2012 8:00AM - 11:00AM — Session H46 DPOLY: Invited Session: Polymer Physics Prize 160ABC

8:00AM H46.00001 Polymer Physics Prize Lecture: Polyelectrolyte complexes: New routes to useful soft materials, MATTHEW TIRRELL, University of Chicago — Mixtures of oppositely charged polyelectrolytes may form precipitates (phase-separated solids) or coacervates (phase-separated fluids). Coacervates have been known for a long time to have interesting properties such as very low interfacial tension with water and a resultant ability to coat surfaces, engulf particles and invade porous media. Most prior work on coacervate complexes has been done with structurally complex (e.g., gum Arabic), biologically derived macromolecules (e.g., gelatin). Our work is focusing on phase behavior and self-assembly in classes of structurally simpler polymers. Polypeptides are one such class, where we can produce anionic, cationic and neutral, water-soluble polymers all with the same backbone and varying in small side-group structures. We are able to demonstrate very general patterns in phase behavior over different members of this class of polymers. Coacervate formation is the rule rather than the exception in these materials, with such formation quite strongly peaked at balanced stoichiometry of the polyelectrolyte components. One molar salt is usually sufficient to dissolve the coacervate phases that form. Block copolymer mixtures containing oppositely charged blocks can form self-assembled structures: micelles with diblocks and hydrogels with triblocks. The structure and properties of these assemblies can be tuned based on knowledge of the bulk phase behavior response to molecular weight, stoichiometry and salt concentration. Examples of phase behavior and structure-property relationship will be discussed.

8:36AM H46.00002 Physical and Biological Properties of Engineered Protein Hydrogels, DAVID TIRRELL, California Institute of Technology — Injectable hydrogels show substantial promise for use in minimally invasive tissue engineering and drug delivery procedures. A new injectable hydrogel material, developed from recombinant telechelic proteins expressed in *E. coli*, demonstrates shear thinning by three orders of magnitude at large strains. Large amplitude oscillatory shear illustrates that shear thinning is due to yielding within the bulk of the gel, and the rheological response and flow profiles are consistent with a shear-banding mechanism for yielding. The sharp yielding transition and large magnitude of the apparent shear thinning allow gels to be injected through narrow gauge needles with only gentle hand pressure. After injection the gels reset to full elastic strength in seconds due to rapid reformation of the physical network junctions, allowing self-supporting structures to be formed. The shear thinning behavior is largely independent of the midblock length, enabling genetic engineering to be used to control the equilibrium modulus of the gel without loss of the characteristic yielding behavior. The shear-banding mechanism localizes shear stresses during flow into narrow regions of the gel, allowing more than 95% of seeded cells to survive the injection process.

9:12AM H46.00003 Enhancing Biopolymer Dynamics through Destruction, JENNIFER ROSS, University of Massachusetts Amherst — Microtubules are cytoskeletal filaments that organize intracellular space structurally and through active transport along their lengths. They need to be organized and remodeled quickly during development of differentiated cells or in mitosis. Much work has focused on remodeling from the ends because these long polymers can stochastically disassemble through dynamic instability or be actively disassembled. Microtubule-severing enzymes are a novel class of microtubule regulators that create new ends by cutting the filament. Thus, these proteins add a new dimension to microtubule regulation by their ability to create new microtubule ends. Interestingly, despite their destructive capabilities, severing has the ability to create new microtubule networks in cells. We are interested in the inherent biophysical activities of these proteins and their ability to remodel cellular microtubule networks. Interestingly, despite their destructive capabilities, severing has the ability to create new microtubule networks in cells. We use two-color single molecule total internal reflection fluorescence imaging to visualize purified severing enzymes and microtubules *in vitro*. We have examined two families of severing enzymes to find that their biophysical activities are distinct giving them different network-regulating abilities.

9:48AM H46.00004 Cellular Reconstitution: Building Biomolecular Systems from the Bottom Up, DANIEL FLETCHER, University of California, Berkeley — No abstract available.

Tuesday, February 28, 2012 8:00AM - 11:00AM — Session H48 DPOLY: Polymer Gels and Solutions 161

8:00AM H48.00001 Polymer Physics Prize Break —

8:36AM H48.00002 Phase Segregation and Dynamics in Strongly Interacting Small Molecule Additive - Block Copolymer Surfactant Complexes , ROHIT KOTHARI, Polymer Science and Engineering, University of Massachusetts Amherst (UMASS Amherst), AHMED KHALIL, H. HENNING WINTER, Chemical Engineering, UMASS Amherst, JAMES J. WATKINS, Polymer Science and Engineering, UMASS Amherst — Rheology and Small Angle X-Ray Scattering (SAXS) were used to investigate order to disorder transitions (ODTs) and disorder to order transitions (DOTs) of poly(ethyleneoxide-*b*-propyleneoxide-*b*-ethyleneoxide) block copolymer surfactants mixed with hydrogen-bond-donating small molecule additives. A series of additives having a core benzene ring and systematic variation in the number of carboxylic or hydroxyl groups attached to the ring were of particular interest. Ordered cylindrical morphologies, confirmed using SAXS, were obtained only in a certain additive concentration region. ODTs were characterized by sudden changes in the linear viscoelastic properties in low frequency region upon increasing temperature. The locations of ODTs varied widely with hydrogen-bond-donating ability of the functional group and were found to be strongly dependent on the number of functional groups attached to the ring. For a given additive, the temperature at which ODT occur was strong function of the additive loading, whereas the linear viscoelastic properties of the ordered state were little changed upon varying additive concentration in ordered region. The location and dynamics of DOTs upon cooling were comparable to the ODTs upon heating. Studies using these model systems provide insight into the design of well-ordered hybrid materials.

8:48AM H48.00003 Using Mesoscopic Models to Design Strong and Tough Biomimetic Polymer , ISAAC G. SALIB, University of Pittsburgh, Pittsburgh, PA 15261, USA , GERMAN V. KOLMAKOV, New York City College of Technology, CUNY, New York, NY 11201, USA, BENJAMIN J. BUCIOR, University of Pittsburgh, Pittsburgh, PA 15261, USA, ORIT PELEG, MARTIN KROGER, THIERRY SAVIN, VIOLA VOGEL, ETH Zurich, CH-8093 Zurich, Switzerland, KRZYSZTOF MATYJASZEWSKI, Carnegie Mellon University, Pittsburgh, PA 15213, USA, ANNA C. BALAZS , University of Pittsburgh, Pittsburgh, PA 15261, USA — Using computational modeling, we investigate the mechanical properties of polymeric materials composed of coiled chains, or globules, which encompass a folded secondary structure and are crosslinked by labile bonds to form a network. In the presence of an applied force, the globules can unfold into linear. Our goal is to determine how to tailor the labile intra- and inter-molecular bonds within the network to produce material exhibiting both toughness and strength. We use the lattice spring model (LSM) to simulate the globules and the crosslinked network. We utilize our modified Hierarchical Bell model (MHBM) to simulate the rupture and reforming of N parallel bonds. We demonstrate that the mechanical properties of the system are sensitive to the values of N_{in} and N_{out} , the respective values of N for the intra- and inter-molecular bonds. We find that the strength of the material is mainly controlled by the value of N_{out} , with the higher value of N_{out} providing a stronger material. We also find that if N_{in} is smaller than N_{out} , the globules can unfold under the tensile load before the sample fractures and thus, can increase the ductility of the sample.

9:00AM H48.00004 Synthesis and Characterization of Poly(hydroxyethyl methacrylate) Hydrogels Bearing Reversibly Associating Side Groups¹ , CHRISTOPHER LEWIS, JIAHUI LI, MITCHELL ANTHAMATTEN, University of Rochester — Poly(hydroxyethyl methacrylate) (poly(HEMA)) is a technologically important hydrogel that can be processed into different shapes and is best known for its role in contact lenses. However, applications of water swollen polyHEMA are limited by its poor mechanical properties. We are studying the influence of reversibly associating side groups on the behavior of poly(HEMA) hydrogels. In non-polar media, it is well known that ureidopyrimidinone (UPy) groups self-associate to form hydrogen bonded dimers (DDAA); however their behavior in water-swollen hydrogels is unclear. A series of poly(HEMA) linear polymers of controlled molecular weight with varying UPy content have been prepared using a reversible addition-fragmentation chain transfer (RAFT) polymerization technique. UPy content significantly reduces water swelling and improves mechanical properties. The degree of hydrogen bonding within water swollen hydrogels is studied, and properties of functional hydrogel polymers and networks are compared to an unswollen hydrophobic analog.

¹The authors acknowledge funding provided by the National Science Foundation under Grant DMR-0906627

9:12AM H48.00005 Thermoreversible Supramolecular Ion Gels via Hydrogen Bonding , YU LEI, TIMOTHY LODGE, Department of Chemistry, University of Minnesota — Ion gels are a novel class of functional materials of broad interest for advanced applications. We have developed a thermoreversible supramolecular ion gel system consisting of a poly(2-vinylpyridine-*b*-ethylene oxide-*b*-2-vinylpyridine) (P2VP-PEO-P2VP) triblock copolymer, a poly(4-vinylphenol) (PVPh) linear homopolymer, and an ionic liquid, 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide ([EMI][TfSA]), where a highly inter-connected transient polymer network is formed by hydrogen bonding between the P2VP endblocks and PVPh cross-linkers. This system exhibits novel physical properties, such as interesting dynamics and homopolymer clustering in the cross-links. The applicability of time-temperature superposition to this system is striking, resulting in a master curve that extends over 20 orders of magnitude in reduced frequency. The hydrogen-bonded phase can arrange into a hexagonally packed cylindrical morphology with long-range ordering, which reveals very slow kinetics and is thermodynamically stable only within a narrow temperature window. The highly tunable relaxation dynamics as well as shear modulus might enable materials design for specific applications.

9:24AM H48.00006 Hydrogen Bonding Based Layer-by-Layer Assembly of Poly(vinyl alcohol) with Weak Polyacids , HYOMIN LEE, REMY MENSIRE, ROBERT COHEN, MICHAEL RUBNER, Massachusetts Institute of Technology — Multilayer thin films that consist of poly(vinyl alcohol) (PVA) and weak polyacids such as poly(acrylic acid) (PAA) and poly(methacrylic acid) (PMAA) were prepared by hydrogen bonding interactions. Both the degree of hydrolysis and molecular weight of PVA were investigated in terms of their influence on growth behavior and pH stability. Multilayer films containing PVA and PAA could be assembled successfully only by using partially hydrolyzed PVA and low pH solutions. By comparing films containing PAA with those containing a more strongly interacting partner, PMAA, it was shown that the extent of PVA hydrolysis becomes significant only when weak hydrogen bonding pairs such as PVA and PAA were used. pH-triggered dissolution experiments demonstrated that the degree of hydrolysis can be used as an additional parameter by which to tune the pH stability of the film. Also, the presence of an abundance of free hydroxyl and carboxylic acid groups in the multilayer allowed enhanced pH stability to be obtained by thermal and chemical methods as well as numerous opportunities for post-assembly functionalization.

9:36AM H48.00007 Gelation in a model 1-component system with adhesive hard-sphere interactions, JUNG MIN KIM, University of Delaware, AARON EBERLE, National Institute of Standards and Technology, JUN FANG, Arkema Inc., NORMAN WAGNER, University of Delaware — Colloidal dispersions can undergo a dynamical arrest of the disperse phase leading to a system with solid-like properties when either the volume fraction or the interparticle potential is varied. Systems that contain low to moderate particulate concentrations form gels whereas higher concentrations lead to glassy states in which caging by nearest neighbors can be a significant contributor to the arrested long-time dynamics. Colloid polymer mixtures have been the prevalent model system for studying the effect of attraction, where attractions are entropically driven by depletion effects, in which gelation has been shown to be a result of phase separation [1]. Using the model 1-component octadecyl coated silica nanoparticle system, Eberle et al. [2] found the gel-line to intersect the spinodal to the left of the critical point, and at higher concentrations extended toward the mode coupling theory attractive driven glass line. We continue this study by varying the particle diameter and find quantitative differences which we explain by gravity.

1. Lu, P.J., et al., Nature, 2008. 453(7194): p. 499-504.
2. Eberle, A.P.R., N.J. Wagner, and R. Castaneda-Priego, Physical Review Letters, 2011. 106(10).

9:48AM H48.00008 Concentration Fluctuations in Polymer Solutions under Extensional Flow, MICHAEL VILLET, MICHAEL CROMER, GLENN FREDRICKSON, GARY LEAL, University of California, Santa Barbara, ROMAN STEPANYAN, MARKUS BULTERS, DSM Ahead, Geleen, Netherlands — Polymer solutions under flow are known to exhibit stress-concentration coupling that can anisotropically amplify concentration fluctuations. This phenomenon has been extensively studied for shear flow, but is less well understood for extensional flows. Using a two-fluid model, we study concentration fluctuation amplification in polymer solutions under a variety of extensional flows, including mixed shear and extension.

10:00AM H48.00009 Crossover length scale for viscosity experienced by Gold nanoparticles in semi dilute polymer solution, INDERMEET KOHLI, RAMI OMARI, ASHIS MUKHOPADHYAY, Wayne State University — Gold nanoparticles (Au NPs) were used as a probe to characterize the crossover length scale for viscosity in semi dilute poly (ethylene glycol) (PEG)-water solutions. Fluctuation correlation spectroscopy (FCS) was used to measure the diffusion of these NPs as a function of their size (5-20 nm), PEG concentration (0 to 40%w/w) and PEG molecular weight (5 kDa to 35 kDa). Our results indicate that for particles with radius $R > R_g$, usual hydrodynamic conditions can be applied, but for particles with radius $R \leq R_g$, the diffusion is approximately an order of magnitude faster than that predicted by Stokes Einstein (SE) relation. The results imply that radius of gyration R_g of the polymer gives the crossover length scale from nanoviscosity to macroviscosity. The relative viscosity experienced by the particles was scaled as $\eta/\eta_0 = \exp(b(R_g/\xi)^a)$, where η_0 is the water viscosity, ξ is the correlation length, $a = 0.70 \pm 0.03$ and $b = 1.59 \pm 0.07$.

10:12AM H48.00010 Kinetics of Narrowly dispersed Latex Formation in a Surfactant-free Emulsion Polymerization of Styrene in Acetone-Water Mixture¹, HE CHENG, ZHIYONG LI, CHARLES HAN, Intitue of Chemistry Chinese Academy of Sciences — The kinetics of narrowly dispersed latex formation in a surfactant-free emulsion polymerization of styrene in acetone-water was studied by a combination of transmission electron microscopy and light scattering. The critical nuclei were experimentally observed and the formation of narrowly dispersed PS latex is proved to be originated from competitive growth kinetics. Spherical nuclei were regenerated via a microphase inversion of PS oligomer in 50% volume fraction acetone-water mixture at 70°C. They follow a polydispersed log-normal distribution and the smallest nucleus with $R_s 1.1\text{nm}$ is similar to critical nuclei. Note the spherical nuclei are not necessarily narrowly dispersed. Competitive growth kinetics makes smaller nuclei grow much faster than large nuclei in the subsequent polymerization process, resulting in narrowly dispersed PS latex. Two kinds of PS seed particles were added, separately, into two parallel surfactant-free emulsion polymerization batches of styrene in acetone-water mixture at 70°C. It was found that the size of seed particles almost does not change, but the small size PS latex grows rapidly. Our fitting results proves competitive growth kinetics proposed by Vanderhoff and coworkers.

¹The authors appreciate the financial support of the National Basic Research Program of China (973 Program, 2012CB821500), and National Natural Scientific Foundation of China (Young Scientists Fund) (20804052)

10:24AM H48.00011 Cluster Growth in Aqueous Sugars Observed by Dynamic Light Scattering¹, TRI TRAN², DAVID SIDEBOTTOM, Creighton University — Dynamic light scattering of aqueous sugar solutions as a function of sugar concentration and temperature reveal the development of sugar clusters occurring in two stages. At low volume fractions of sugar, a so-called cluster phase consisting of nearly monodisperse clusters forms with a mean cluster mass that increases in proportion to the volume fraction. At a critical volume fraction, near where the clusters begin to overlap, a second stage ensues wherein cluster-cluster aggregation forces a more rapid, power law growth in advance of a percolation threshold observed near 83 wt% sugar.

¹This research supported by funding from NIH grant number 1R01EB009644-01

²first year graduate student will present

10:36AM H48.00012 Boson peak in L-cysteine: a Raman scattering study, THAMIRES LIMA, HERCULANO MARTINHO, Universidade Federal do ABC — The Boson peak is a distinctive feature of many glassy and disordered crystalline solids. Recently it has been suggested that similar feature may be correlated to anharmonic transitions observed in macromolecules like DNA and proteins. In the present work we studied the low frequency ($15 - 600 \text{ cm}^{-1}$) Raman scattering response of L-cysteine and L-Cysteine hydrochloride with different hydration levels in the $15 - 270 \text{ K}$ temperature range. Our analyzes will be concerned to understand the water rule in the Boson peak inelastic light signal, its correlation to the dynamic transitions at $T^* \sim 80 \text{ K}$ and $T_D \sim 280 \text{ K}$, and its microscopic origin as well.

10:48AM H48.00013 Low temperature dynamic transitions of L-cysteine and L-proline amino acids: a specific heat study, MARIANA ISHIKAWA, THAMIRES LIMA, HERCULANO MARTINHO, Universidade Federal do ABC — Studies have shown that several macromolecules present two dynamic transitions at $T^* \sim 80 \text{ K}$ and $T_D \sim 280 \text{ K}$ which have intrinsic correlation to their biological activity. The present work concerns the detailed analysis of the low temperature transition at T^* by specific heat. This transition is usually described as originated on the CH₂SH dynamics. We compared the experimental results with simulations based on rigid rotor specific heat model by Caride and Tsallis [J. Stat. Phys. **35**, 187 (1984)] and we found an excellent agreement.

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H49 DPOLY: Focus Session: Fluctuation-Induced Forces in Soft Matter & Polymeric Systems - Casimir and Interfacial Forces 162A

8:00AM H49.00001 Polymer Physics Prize Break –

8:36AM H49.00002 Casimir Interaction at Soft Interfaces , EHSAN NORUZIFAR, JEF WAGNER, University of California, Riverside, HSIANG-KU LIN, University of California, Riverside / MIT, UMAR MOHIDEEN, ROYA ZANDI, University of California, Riverside — We study Casimir interaction due to the thermal fluctuations between colloidal particles on the membranes and fluid interfaces. To calculate the Casimir energy we employ the scattering formalism. In this technique the shape and material properties of the colloids are encoded in their scattering matrices. The energy is calculated by combining the scattering matrices with the universal translation matrices, which convert between the bases used to compute scattering for each colloid, but otherwise are independent of the physical and chemical properties of the colloids and the interface. We show that in the scattering formalism one can easily implement various geometries and material properties and more importantly calculate the energy for all separation regimes.

8:48AM H49.00003 Critical Casimir Interactions: New fluctuation forces in colloidal science , PETER SCHALL, Institute of Physics, University of Amsterdam — Casimir forces arise from the confinement of fluctuations between two walls. Critical Casimir forces provide thermodynamic analogues of quantum-mechanical Casimir forces and arise from the confinement of concentration fluctuations of a critical solvent. These forces act also between colloidal particles that are suspended in this solvent, giving rise to temperature-dependent attractive interactions between the particles. We use these temperature-dependent forces to control colloidal phase transitions. In this talk, I will present a new index and density-matched model system that allows direct observation of these phase transitions with confocal microscopy. In three dimensions and real time, we follow how a colloidal gas freezes into a colloidal liquid, and the colloidal liquid freezes into a solid, all driven by critical Casimir forces. We measure the critical Casimir particle pair potential directly from the pair correlation function, and use Monte Carlo simulations to map the complete gas-liquid-solid phase diagram. Excellent agreement with the experimental observations is obtained. Our measurements include microgravity experiments on board the International Space Station (ISS) to elucidate non-equilibrium assembly of the particles achieved by controlled temperature quench.

9:00AM H49.00004 Thermodynamic Casimir effect in the large- n limit: Exact results for slabs with free surfaces , F.M. SCHMIDT, Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany, M. HASENBUSCH, Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany, A. HUCHT, S. RUTKEVICH, D. GRÜNEBERG, H.W. DIEHL, Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany — The $O(n)$ ϕ^4 -model for a three-dimensional slab of thickness L and infinite lateral extension is investigated in the large- n limit. The effective (Casimir-like) forces that are induced between the two confining boundary planes by thermodynamic fluctuations in such systems at and near bulk criticality are studied. While systems with periodic or antiperiodic boundary conditions perpendicular to the planes are translationally invariant and thus can be treated analytically, the physical relevant case of free boundary conditions leads to a breaking of translational invariance perpendicular to the boundary planes. In the large- n limit one arrives at a spherical model with separate constraints for each layer parallel to the confining surfaces. The resulting self-consistent Schrödinger-type equation is solved numerically at and near the bulk critical temperature to obtain the large- n limit of the scaling functions of the Casimir force and the excess free energy. The Casimir amplitude is calculated with high accuracy to take the value $\Delta_C = -0.01077340685025(10)$. The Casimir force scaling function shows a minimum below the bulk critical temperature similar to the $n = 2$ result.

9:12AM H49.00005 Fluctuation-induced forces in a fluid membrane under tension , ROYA ZANDI, University of California, Riverside — We develop an exact method to calculate thermal Casimir forces between inclusions of arbitrary shapes and separation, embedded in a fluid membrane whose fluctuations are governed by the combined action of surface tension, bending modulus, and Gaussian rigidity. Each object's shape and mechanical properties enter only through a characteristic matrix, a static analog of the scattering matrix. We calculate the Casimir interaction between two elastic disks embedded in a membrane. In particular, we find that at short separations the interaction is strong and independent of surface tension.

9:48AM H49.00006 The Casimir forces between inclusions in a fluid membrane , HSIANG-KU LIN, ROYA ZANDI, UMAR MOHIDEEN, LEONID PRYADKO, University of California at Riverside — We discuss the fluctuation-induced force, a finite-temperature analogue of the Casimir force, between two foreign inclusions embedded in a stretchable fluid membrane. Specifically, we suggest a Green's-function-based method to calculate the Casimir interaction in cases where the fluctuations of a planar membrane are governed by Helfrich Hamiltonian, including the surface tension σ and both bending κ and Gaussian $\bar{\kappa}$ rigidities. For two circular inclusions in a fluid membrane, the Casimir energy scales as the inverse power law of the separation and is greatly reduced beyond the characteristic length $\ell_0 = \sqrt{\kappa_0/\sigma_0}$. The impact of line tension is also discussed.

10:00AM H49.00007 Aspect-ratio dependence of thermodynamic Casimir forces , ALFRED HUCHT, DANIEL GRUENEBERG, FELIX M. SCHMIDT, Fakultät für Physik, Universität Duisburg-Essen, 47058 Duisburg, Germany — We consider the three-dimensional Ising model in a $L_\perp \times L_\parallel \times L_\parallel$ cuboid geometry with finite aspect ratio $\rho = L_\perp/L_\parallel$ and periodic boundary conditions along all directions. For this model the finite-size scaling functions of the excess free energy and thermodynamic Casimir force are evaluated numerically by means of Monte Carlo simulations [1]. The Monte Carlo results compare well with recent field theoretical results for the Ising universality class at temperatures above and slightly below the bulk critical temperature T_c . Furthermore, the excess free energy and Casimir force scaling functions of the two-dimensional Ising model are calculated exactly for arbitrary ρ and compared to the three-dimensional case. We give a general argument that the Casimir force vanishes at the critical point for $\rho = 1$ and becomes repulsive in periodic systems for $\rho > 1$.

[1] Alfred Hucht, Daniel Grüneberg, and Felix M. Schmidt, Phys. Rev. E 83, 051101 (2011)

10:12AM H49.00008 Field-Theoretic Simulations of Bicontinuous Microemulsions in Polymer Blends , KRIS DELANEY, GLENN FREDRICKSON, UC Santa Barbara — Long diblock copolymers introduced into a blend of thermodynamically incompatible homopolymers can act as a surfactant to suppress macroscopic phase separation of the blend. As the fraction of diblock copolymer is varied, an isotropic Lifshitz tricritical point is observed in the mean-field equations, demarking the crossover from macrophase to microphase separation. Close to the Lifshitz point, fluctuations are strong enough to suppress the low-temperature formation of a well-ordered microphase leading to the appearance of a long-lived bicontinuous microemulsion characterized by micron-scale continuous domains. In this work, we discuss computational strategies for simulating the equilibrium formation of the microemulsion using field-theoretic methods. We address the challenges involved with accurately localizing the order-disorder transition in a fluctuating theory, and the handling of strong fluctuations close to the Lifshitz point.

10:24AM H49.00009 Looking Down at Adsorption Dynamics: Filament Height Measurements with TIRFM , DAVID WELCH, ZVONIMIR DOGIC, Brandeis University — Polymer adsorption is important in several contexts such as chromatography, colloid stabilization, and bio-fouling. Despite a cross-disciplinary interest in the subject, there are not many techniques to observe single-molecule adsorption events in real time. We use TIRF microscopy to accomplish this using the biological polymer f-actin adsorbed to a microscope slide via the well-known depletion interaction. We find TIRFM is able to quantitatively measure filament height, and we compare our results to theoretical predictions and previous results obtained from other systems.

10:36AM H49.00010 Partial osmotic compressibility of binary mixtures of colloidal nanoparticles and PEG, JINXIN FU, MELISSA GOLEB, H. DANIEL OU-YANG, Lehigh University — Proposed originally by Oosawa and Asakura, polymer crowding-induced attractive force between colloidal particles is being used in a variety of applications ranging from protein crystallization to nanoparticle sorting. While the force has been well studied for a pair of micro particles in the presence of polymers, direct measurement of such force between nanoparticles is very difficult. To investigate effects of crowding polymers, we propose an approach to measure the colloidal osmotic compressibility and virial coefficients in the presence of polymers and compare experimental results with theoretical models. The materials we investigated are binary mixtures of fluorescent polystyrene nanospheres (100 – 210 nm in diameter) and polyethylene glycol (PEG). Using fluorescence microscopy to examine the change of the particle concentration in an optical trap, which exerts no force upon PEG, allows us to measure the partial osmotic compressibility of the particles. The measured partial compressibility and its virial expansion are compared with theoretical calculations to elucidate the competing effects of polymer crowding and adsorption.

10:48AM H49.00011 ABSTRACT WITHDRAWN —

Tuesday, February 28, 2012 8:00AM - 11:00AM —
Session H50 DPOLY: Polymer Melts 162B

8:00AM H50.00001 Polymer Physics Prize Break —

8:36AM H50.00002 Coil-Globule Transition of Polymer – Tricriticality of Theta, ASHOK DASMAHA-PATRA, Department of Chemical Engineering, Indian Institute of Technology Guwahati, Guwahati-781039, Assam — We demonstrate the tricriticality of the theta point in the coil-to-globule transition of a single flexible polymer chain by dynamic Monte Carlo (DMC) simulation. For homopolymer, at the tricritical point, the second order theta transition line approaches the first order collapse transition line as the chain length approaches the thermodynamic limit. Theta point of homopolymer has been estimated by following the ideal behavior of chain at the theta point. Temperature at which the constant volume specific heat (C_v) shows a peak is considered as the collapse temperature and the transition is of first order. In T-N plane, collapse temperature approaches towards the theta temperature as the chain length approaches to the thermodynamic limit. For copolymer (with periodic distribution of comonomer along the chain), the collapse temperature increases with increasing the stickiness parameter (viz., higher solvophobicity of the comonomers relative to monomers) and approaching towards the theta as the value of the stickiness parameter increases. Theta points of copolymers have been estimated from the theta point of homopolymer under the condition of the ideality of the theta point. The collapse temperatures for copolymer have been in a manner similar to homopolymers. Theta temperature vs. stickiness parameter represents a second order line whereas collapse temperature vs. stickiness parameter represents a first order line. We demonstrate that as the stickiness parameter increases, these two lines meet each other, close to the “tricritical” theta temperature.

8:48AM H50.00003 Microscopic Theory of Nanoparticle Diffusivity in Entangled and Unentangled Polymer Melts, UMI YAMAMOTO, KENNETH SCHWEIZER, University of Illinois, Urbana-Champaign — We present a statistical dynamical theory at the level of forces for the violation of the Stokes-Einstein (SE) diffusion law of a spherical nanoparticle in entangled and unentangled polymer melts. Based on a combination of mode-coupling and polymer physics ideas, the non-hydrodynamic friction coefficient is related to microscopic structure and the length-scale-dependent polymer melt collective density fluctuation dynamics. When local packing correlations are neglected, analytic expressions are derived for the non-hydrodynamic diffusivity as a function of particle size, polymer radius-of-gyration, tube diameter, degree of entanglement and temperature; local packing effects are numerically investigated under athermal and attractive conditions. The conditions for the recovery of the SE law are qualitatively distinct for unentangled and entangled melts, and entanglement effects are the origin of large SE violations consistent with recent experiments. The influences of melt packing fraction and interfacial attraction strength are also qualitatively different depending on whether the polymers are entangled or not. The anomalous time-dependence of the nanoparticle mean square displacement is studied using a self-consistent Generalized Langevin Equation approach.

9:00AM H50.00004 Effect of Secondary Structure on the Persistence Length of a Poly N-substituted Glycine, HANNAH K. MURNEN, ADRIANNE M. ROSALES, University of California Berkeley, STEVEN R. KLINE, National Institute of Standards and Technology, RONALD N. ZUCKERMANN, Lawrence Berkeley National Laboratory, RACHEL A. SEGALMAN, University of California Berkeley — A polymer containing helical secondary structure is shown to be nearly as flexible as a chemically analogous polymer containing no structure. Polypeptides or poly N-substituted glycines are a class of sequence specific polymers in which chain shape can be controlled via monomer choice involving both sterics and chirality. In this study, a polypeptoid containing aromatic chiral sidechains was synthesized. Classical measurements such as circular dichroism and NMR have shown previously that the bulky chiral side chains cause the polypeptoid to adopt a helical conformation. However, small angle neutron scattering demonstrated that in acetonitrile, the persistence length of the helical polypeptoid was approximately 1 nm, only about 15% of the fully extended helical length. This small persistence length indicates that the chain likely adopts several conformations in solution and is not rigidly locked into its helical shape throughout the entire length of the polymer

9:12AM H50.00005 Gibbs Ensemble Calculations of Phase Coexistence in Supramolecular Assembly of Block Copolymers, ZOLTAN MESTER, NATHANIEL LYND, GLENN FREDRICKSON, University of California Santa Barbara — We propose a new self-consistent field theory method for calculating phase behavior in reversibly bonded supramolecular polymer melts. Previous studies formulated models for supramolecular assembly in the grand canonical ensemble to make use of the constraints imposed on the chemical potentials of the products from chemical equilibrium. Instead, we formulate the model in the canonical ensemble by including a term in the Hamiltonian that accounts for the reaction favorability/penalty. The chemical equilibrium statement is obtained by optimizing the Hamiltonian with the amount of reacted polymer. The canonical partition function can be easily adapted to the Gibbs ensemble whereby phase boundaries between coexisting phases can be conveniently simulated. As an illustration of our method, we examine a blend of AB diblock and B homopolymer with the ability to reversibly bond to form ABB diblock. In the limits of infinite reaction favorability and penalty, the system approaches cases of an ABB diblock-B homopolymer blend when the AB diblock is the limiting reactant and an AB diblock-B homopolymer blend, respectively. The interplay between reactant ratios (stoichiometry) and reaction favorability/penalty is explored for intermediate values of reactivity.

9:24AM H50.00006 Pressure-induced structural transition in an one-component polymer poly(4-methyl-1-pentene) in its melted state, AYANO CHIBA, Keio University, Japan, NOBUMASA FUNAMORI, KAZUYA NAKAYAMA, University of Tokyo, Japan, YASUO OHISHI, Japan Synchrotron Radiation Research Institute (Spring-8), Japan, STEPHEN M. BENNINGTON, Rutherford Appleton Laboratory, UK, SANJAY RASTOGI, Loughborough University, UK, ANUJ SHUKLA, European Synchrotron Radiation Facility, France, KAZUHIKO TSUJI, Keio University, Japan, MIKIHITO TAKENAKA, Kyoto University, Japan — Liquid-liquid transitions or amorphous-amorphous transitions are well-known in systems with small molecular or structural units, such as those seen in water, phosphorus, and silica glass. We studied pressure-induced structural change for isotactic poly(4-methyl-1-pentene) in its melted state, and found a structural transition for this one-component polymer melt. High-pressure in-situ x-ray diffraction and specific-volume measurements on the polymer melt have uncovered discontinuities in the pressure dependences of microscopic structure as well as those of macroscopic density. The results suggest the occurrence of a liquid-liquid phase transition.

9:36AM H50.00007 Anomalous diffusion of a polymer chain in an unentangled melt, JEAN FARAGO, Universite de Strasbourg, HENDRIK MEYER, ALEXANDER SEMENOV, CNRS — Contrary to common belief, the hydrodynamic interactions (HI) in polymer melts are not screened beyond the monomer length and are important in transient regimes. We show that the viscoelastic HI effects (VHI) lead to anomalous dynamics of a tagged chain in an unentangled melt at $t < t_N$ (t_N , the Rouse time). The chain centre-of-mass (CM) mean-square displacement is enhanced (as compared to the Rouse diffusion) by a large factor increasing with chain length. We develop an analytical theory of VHI-controlled chain dynamics yielding negative CM velocity autocorrelation function which quantitatively agrees with our MD simulations without any fitting parameter. It is also shown that the Langevin friction force, when added in the model, strongly affects the short- t CM dynamics which, however, can remain strongly enhanced. The transient VHI effects thus provide the dominant contribution to the subdiffusive CM motion universally observed in simulations and experiments on polymer melts.

9:48AM H50.00008 Representation of Polymer melts as soft liquids with effective pair interactions, ANTHONY CLARK, MARINA GUENZA, University of Oregon — Descriptions at various levels of coarse-graining are of great interest in understanding the complex structure and dynamics of polymer liquids, as relevant processes take place at a wide variety of length and time scales. In this talk we present and analytically characterize effective interaction potentials to map a polymer melt onto a liquid of soft spheres or soft-colloid chains, with each soft colloid representing the center of mass of a chain or large subsection of a chain. The thermodynamics of the coarse-grained system using the effective potentials can be shown to agree with the thermodynamics of monomer-level descriptions across a range of thermodynamic states. The scaling of the effective pair potentials beyond the physical extent of the polymer with increasing chain interpenetration is shown to be essential to capturing the contribution to the thermodynamics of the melt due to many-polymer interactions in the soft coarse-grained description, despite its vanishingly small effect on structural correlations. Further development of the theory will consider its extension from soft-colloid chains to lower level bead and spring level descriptions with the aim of gaining insight into the thermodynamic properties of these widely used models.

10:00AM H50.00009 Entropy of Mixing: Rigid vs. Flexible Molecules: Effect of Varying Solvent on Dissolution Temperature, ERIC B. SIROTA, ExxonMobil Research and Engineering Company, HASNAIN RANGWALLA, ExxonMobil Chemical Company, PAWEL PECZAK, ExxonMobil Research and Engineering Company — We report a study of the dissolution temperature of n-hexacontane, as a function of concentration, with 52 different solvents, aimed at understanding the effect of molecular flexibility on the entropy-of-mixing. The entropy-of-mixing of rigid molecules is commonly expected to go as $\ln(\text{mole fraction})$, while for flexible polymers it is expected to follow Flory-Huggins $\ln(\text{volume fraction})$. By isolating the entropy-of-mixing, we have experimentally found that rigidity, through ring structures, causes deviations from the Flory-Huggins behavior; and we have proposed and derived a cross-over form for the entropy-of-mixing which varies between $\ln(\text{volume fraction})$ and $\ln(\text{mole fraction})$ according to molecular rigidity.

10:12AM H50.00010 Polymeric Fluid Flow Over Superhydrophobic Surfaces, LUCAS LANDHERR, STEVEN HUDSON, KALMAN MIGLER, National Institute of Standards and Technology — Superhydrophobic (SHP) surfaces are characterized by their exceptionally low surface energies and distinct surface roughnesses that create a vapor layer between the fluid and the surface. The reduced contact area at the interface can create a dewetted state resulting in slip, drag reduction, and improved flow of fluids. Most previous superhydrophobic studies have utilized simple liquids (e.g. water) in focusing on characterization of the quiescent interface and on drag reduction or slip modifications of fluid flow. As polymeric fluid flows have exhibited similar slip and drag reduction phenomena, this study attempts to utilize SHP surfaces to improve the flow behavior of more complex multi-component fluids, such as polymer solutions. By merging the research fields of SHP surfaces and polymer fluids, we investigate the potential to enhance slip and drag reduction effects as a result of surface interactions. Microfluidic channels, interfacial rheometry and goniometry are used to evaluate slip length and fluid flow.

10:24AM H50.00011 Reconstructing Polymer Melt Dynamics Sped up due to Large-Scale Coarse-Graining, IVAN LYUBIMOV, MARINA GUENZA, University of Oregon — A theoretical approach to rescale the artificially fast dynamics of highly coarse-grained polymer melts is extended to chains represented as soft particles. The effective pair potential derived from first-principles to represent polymer chains with soft interactions is used to perform mesoscale molecular dynamics simulations of coarse-grained melts. This potential ensures the reproduction of the correct global structure and thermodynamics, but entropic and frictional corrections are necessary to reconstruct realistic dynamics. The behavior of the system is described by generalized Langevin equations derived for different levels of coarse-graining. The explicit analytical dependence on the thermodynamic and molecular parameters enhances the predictive power of the reconstruction method. The dynamics, reconstructed from mesoscale simulation, is in quantitative agreement with experiments and atomistic simulations.

10:36AM H50.00012 Steric Constraints in Fractal-Regime Star Polymers, GREGORY BEAUCAGE, DURGESH RAI, RAMANTH RAMACHANDRAN, University of Cincinnati, KEDAR RATKANTHAR, NIKOS HADJICHRISTIDIS, University of Athens, HONG KUNLUN, DAVID UHRIG, Oak Ridge National Laboratory — Star polymers at high functionality, f , and high arm length, z_{arm} , display a collapsed core structure described by Daoud and Cotton in a colloidal regime (CR). At lower functionality ($f < \sim 8$) and relatively low arm length, stars display a polymeric structure in a fractal regime (FR). For FR stars in good solvents the arms display steric interactions analogous to polymer chains tethered to a surface. We have used small-angle neutron scattering to quantify, for the first time, this steric interaction so as to understand the approach to the CR as a function of z_{arm} and f as well as temperature and solvent type. Experimental data from model star polymers and literature data from polyurethane stars are considered as examples.

10:48AM H50.00013 Capillary break-up, gelation and extensional rheology of hydrophobically modified cellulose ethers, VIVEK SHARMA, SIMON HAWARD, Massachusetts Institute of Technology, OLIVIA PESSINET, Ecole des Mines, ASA SODERLUND, PHIL THRELFALL-HOLMES, AkzoNobel, GARETH MCKINLEY, Massachusetts Institute of Technology — Cellulose derivatives containing associating hydrophobic groups along their hydrophilic polysaccharide backbone are used extensively in the formulations for inks, water-borne paints, food, nasal sprays, cosmetics, insecticides, fertilizers and bio-assays to control the rheology and processing behavior of multi-component dispersions. These complex dispersions are processed and used over a broad range of shear and extensional rates. The presence of hydrophobic stickers influences the linear and nonlinear rheology of cellulose ether solutions. In this talk, we systematically contrast the difference in the shear and extensional rheology of a cellulose ether: ethylhydroxyethyl-cellulose (EHEC) and its hydrophobically-modified analog (HMEHEC) using microfluidic shear rheometry at deformation rates up to 10^6 inverse seconds, cross-slot flow extensional rheometry and capillary break-up during jetting as a rheometric technique. Additionally, we provide a constitutive model based on fractional calculus to describe the physical gelation in HMEHEC solutions.

Tuesday, February 28, 2012 8:00AM - 11:00AM –

Session H51 DCMP DFD: Colloids II: Crystals and Phase Transitions Boston Convention Center 154

8:00AM H51.00001 Effects of vacancies and interstitials on the phonon modes in a 2D colloidal crystal¹, LICHAO YU, SUNGCHEOL KIM, Brown University, DI YIN, Wuhan University and Brown University, ALEXANDROS PERTSINIDIS, Sloan-Kettering Institute, New York, XINSHENG LING, Brown University — We report a study of the effects of vacancies and interstitials on the phonon modes in a 2D colloidal crystal. By applying the equi-partition theorem, we extract the dispersion relation of the lattice vibrations in a two-dimensional colloidal crystal using real-time video microscopy. We find that both longitudinal and transverse modes in the spectrum are softened by the existence of vacancies and interstitials.

¹This work was supported by a grant from NSF-DMR.

8:12AM H51.00002 Normal modes of various colloidal crystals¹, FENG WANG, YI PENG, ZIREN WANG, YILONG HAN, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China, SOFT MATTER AND VIDEO MICROSCOPY LAB TEAM — We measured the vibrational normal modes from particle displacements in various microgel colloidal crystals including monolayers, multi-layer thin films, three-dimensional normal and superheated crystals by video microscopy. Their density of states all agree with the Debye's theory in the low-frequency regime, but the fluctuation of the frequency is similar to that of the eigenvalues of random matrices: the distributions of the frequency spacings between successive normal modes are the Wigner surmise, the spectral rigidities are logarithmic, and the distributions of vibrational amplitudes in the majority of modes are Gaussian. In addition, the first a few low-frequency modes are plane waves and dominate the thermal vibration, and the majority of modes are delocalized.

¹This work was supported by Hong Kong GRF Grants No. 601208 and No. 601911.

8:24AM H51.00003 Microscopic observation of dynamics and structure in microgel suspensions¹, MELAKU MULUNEH, Harvard University, JORIS SPRAKEL, Wageningen University, The Netherlands, HANS WYSS, Eindhoven University of Technology, The Netherlands, JOHAN MATTSSON, University of Leeds, UK, DAVID WEITZ, Harvard University — We use 3D confocal microscopy to understand the packing dynamics and structure of fluorescently labeled p(NIPAm-co-AAc) microgel colloidal particles. Such systems respond to changes in temperature, pH, and polymer content by changing size, morphology, and interaction behavior. We conduct experiments to understand this behavior in detail: our results show that the dynamics are dominated by attraction driven crystallization and concentration at low pH and concentration only at high pH. Crystal nucleation occurs homogeneously in the suspensions and does not appear to be restricted to geometric boundaries. The growth of crystals is nucleation-limited and can complete on the order of hours. Structural analysis of the crystals formed indicates that the stacking style is insensitive to charge, concentration, size, and stiffness of the particles and remains FCC.

¹This work is supported by the Harvard MRSEC (DMR-0820484), and the NSF (DMR-1006546)

8:36AM H51.00004 Homogeneous Melting of 3D Superheated Colloidal Crystals¹, ZIREN WANG, FENG WANG, YI PENG, YILONG HAN, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, SOFT MATTER & VIDEO MICROSCOPY LAB TEAM — We locally superheated the interior of thermal-sensitive microgel colloidal crystals and measured the homogenous melting by video microscopy. The nucleation was typically started from a local strong-vibrating region instead of precursor defects. We found that the nucleation time $t \sim (\phi - \phi_m)^{-2}$ and critical nucleus size $r^* \sim (\phi - \phi_m)^{-1}$ as predicted by the classical nucleation theory, while the observed non-spherical critical nuclei and the merging of subcritical nuclei are beyond the classical nucleation theory. At the superheated limit where the incubation time vanishes, the Lindemann parameter approaches 0.18 which just equals to that at the liquid-solid interface. Beyond the superheated limit, the melting becomes like a spinodal decomposition rather than a nucleation process.

¹This work was supported by Hong Kong SAR GRF Grants No. 601208 & 601911.

8:48AM H51.00005 Polyhedral assembled colloids (PACs); a new family of colloids with facets, NOBUHIRO YANAI, JING YAN, QIAN CHEN, STEVE GRANICK, University of Illinois at Urbana Champaign — We introduce a new class of colloids with polyhedral morphology that self-assemble into well-defined clusters and crystals by means of directional attraction between facets. These micron-sized particles are prepared by controlled crystallization of metal ions and organic bridging ligands in solution. They are characterized by distinct polyhedral morphology, rhombic dodecahedra in this work. Unlike spheres that isotropically interact along a curved surface, rhombic dodecahedra particles in suspension associate in a directional facet-to-facet fashion, forming clusters whose elemental units are orderly not only in interparticle distance but also mutual orientation. Furthermore, by changing the particle concentration during the self-assembly, we observe two types of hexagonal arrangement of these rhombic dodecahedra.

9:00AM H51.00006 Measuring every particle's size in a confocal microscopy experiment, ERIC WEEKS, Physics Dept., Emory University, REI KURITA, Institute of Industrial Science, University of Tokyo — We have developed a technique to estimate the radius of every particle observed in a confocal microscopy experiment. From simulations, we verify that the particle radii are estimated to high accuracy in a variety of samples: dense colloidal suspensions, colloidal gels, and binary samples. This method allows us to determine *in situ* the particle size distribution. Furthermore, this method lets us find relationships between individual particle size and dynamical behaviors. First, crystal nucleation occurs in regions that are locally more monodisperse. Second, in dense samples, particle mobility is well correlated with the local volume fraction, defined as the true particle volume divided by the particle's Voronoi volume.

9:12AM H51.00007 Vibrational Phonon Modes of Two-Dimensional Soft-Particle Colloidal Crystals with Hard-Particle Dopants¹, MATTHEW GRATALE, PETER YUNKER, KE CHEN, Department of Physics and Astronomy, University of Pennsylvania, KEVIN APTOWICZ, Department of Physics, West Chester University, ARJUN YODH, Department of Physics and Astronomy, University of Pennsylvania — We study the phonon modes of two-dimensional colloidal crystals consisting of random distributions of "soft" NIPA microgel particles and "hard" polystyrene particle dopants. Thus, the effective springs connecting nearest-neighbors are very stiff, very soft, or of intermediate stiffness, corresponding to three possible inter-particle potentials present in the crystals. We employ video microscopy to derive the phonon modes of corresponding "shadow" crystals with the same geometric configuration and interactions as the experimental colloidal system, but absent damping [1,2,3]. Long wavelength, Debye-like behavior is found at low frequencies, regardless of the number of hard polystyrene particles present in the crystal. Hard particles are primary participants at high frequencies, while soft spheres are primary participants at intermediate frequencies. [1] Chen *et al.*, PRL **105**, 025501 (2010). [2] Kaya *et al.*, Science **329**, 656 (2010). [3] Ghosh *et al.* PRL **104**, 248305 (2010).

¹This work is supported by NSF grant DMR-0804881, Penn MRSEC grant DMR11-20901, and NASA grant NNX08AO0G

9:24AM H51.00008 Direct observation of the nucleation in colloidal solid-solid transitions¹ , YI PENG, FENG WANG, ZIREN WANG, YILONG HAN, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China — We studied the solid-solid transitions between square and triangular lattices in thermal sensitive microgel colloidal thin films by video microscopy. A novel two-step nucleation process was observed in a locally heated single crystalline domain: typically a ~60-particle liquid nucleus was first from the square lattice and then rapidly transformed to a solid nucleus with triangular lattice. Such a post-critical triangular-lattice nucleus grew linearly and induced grain boundaries around it. Nuclei were triggered by the merging of stronger vibrating areas instead of precursor defects. The critical nucleus size was measured from the mean first passage time of the nucleus size.

¹This work was supported by GRF grants 601208 and 601911.

9:36AM H51.00009 Colloidal gas-liquid transition: tuning nucleation and growth by Critical Casimir forces , DUC NGUYEN, PhD, PETER SCHALL, Dr — The nucleation and growth of the liquid phase has been well studied in simulations, but direct experimental observations remain challenging. Here we present a detailed study of the colloidal gas-liquid transition induced by Critical Casimir forces that allow direct control over particle interactions via temperature-dependent solvent fluctuations. We show that with the direct control over particle interactions we can “freeze” a dilute colloidal gas into a dense colloidal liquid. By using dynamic light scattering to follow the evolution of liquid aggregates we observe three clearly distinct regimes: nucleation, interface limited- and diffusion limited growth. We elucidate these regimes directly in real space by using confocal microscopy. In the nucleation regime, we determine the Gibbs free energy, interfacial tension and chemical potential of the liquid aggregates directly from their size distribution. In the growth regime, we can directly follow the attachment of particles, and the collapse of liquid aggregates to large drops. Our critical Casimir colloidal system allows us to control all stages of nucleation and growth with temperature, thereby providing unprecedented insight into this gas-liquid transition.

9:48AM H51.00010 Temperature control of colloidal phases by Critical Casimir forces – a simulation study , MINH TRIET DANG, VAN DUC NGUYEN, Van der Waals-Zeeman Institute, University of Amsterdam, Netherlands, ANA VILA VERDE, PETER BOLHUIS, Van't Hoff Institute for Molecular Science, University of Amsterdam, Netherlands, PETER SCHALL, Van der Waals-Zeeman Institute, University of Amsterdam, Netherlands, VAN DER WAALS-ZEEMAN INSTITUTE, UNIVERSITY OF AMSTERDAM, NETHERLANDS COLLABORATION, VAN'T HOFF INSTITUTE FOR MOLECULAR SCIENCE, UNIVERSITY OF AMSTERDAM, NETHERLANDS COLLABORATION — Critical Casimir forces arising from the confinement of critical solvent fluctuations between the surfaces of colloidal particles have recently been shown a promising route to control colloidal assembly. Such forces are strongly temperature dependent, and thus allow for direct temperature control of colloidal interactions. However, colloidal phase transitions controlled by this highly temperature-dependent potential are still poorly understood. Here, we report Monte Carlo simulations of critical Casimir-driven colloidal phase behavior using input potentials directly measured in experiments. We map the gas-liquid coexistence region using Gibbs ensemble simulations and the solid-fluid coexistence boundaries using Gibbs-Duhem integration, and determine the gas-liquid critical point by applying scaling theory. The constructed gas-liquid-solid phase diagram agrees quantitatively with that observed in experiments. Remarkably, the simulated gas-liquid coexistence curve exhibits 3D Ising scaling despite the strong temperature dependence of the pair potentials.

10:00AM H51.00011 Colloidal aggregation in microgravity by critical Casimir forces¹ , SANDRA VEEN, PETER SCHALL, OLEG ANTONIUK, Van der Waals Zeeman Institute - University of Amsterdam, MARCO POTENZA, MATTEO ALAIMO, University of Milan, STEFANO MAZZONI, European Space Agency, GERARD WEGDAM, Van der Waals Zeeman Institute - University of Amsterdam, VAN DER WAALS ZEEMAN INSTITUTE - UNIVERSITY OF AMSTERDAM COLLABORATION, OPTICS AND MICROGRAVITY RESEARCH LABORATORY - UNIVERSITY OF MILAN COLLABORATION, PHYSICAL SCIENCE UNIT HUMAN SPACEFLIGHT AND OPERATIONS - EUROPEAN SPACE AGENCY COLLABORATION — We study aggregation and crystal growth of spherical Teflon colloids in binary liquid mixtures in microgravity by the critical Casimir effect. The critical Casimir effect induces interactions between colloids due to the confinement of bulk fluctuations (density or concentration) near the critical point of liquids. The strength and range of the interaction depends on the length scale of these fluctuations which increase as one approaches the critical point. The interaction potential can thus be tuned with temperature. We follow the growth of structures in real time with Near Field Scattering. Measurements are performed in microgravity in order to study pure diffusion limited aggregation, without disturbance by sedimentation or flow.

¹NWO/NSO/ESA

10:12AM H51.00012 Light transport through soft colloidal glasses , SOFIA MAGKIRIADOU, Harvard Physics Department, Cambridge, MA, USA, JIN-GYU PARK, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA, YOUNG-SEOK KIM, Korea Electronics Technology Institute, S.Korea, GI-RA YI, Department of Engineering Chemistry, Chungbuk National University, S. Korea, VINOTHAN N. MANOHARAN, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA — We have developed a novel colloidal system for the fundamental study of light propagation through disordered media. Our colloids contain core-shell particles with scattering cores and transparent shells which are self-assembled into amorphous, glassy configurations. The core-shell structure of the particles allows us to independently control two key parameters for light propagation: their scattering cross-section, which is determined by the cores, and their spacing, which is determined by the shells. Thus, our system is ideally suited for the study and manipulation of the optical properties of disordered materials. In particular, we aim to investigate how photonic stop bands arise in disordered media and how near-field coupling between scatterers affects light transport. We intend to use this knowledge to make amorphous colloids with various angularly-independent structural colors.

10:24AM H51.00013 3D Dynamic Light Scattering of Microgel Suspensions , JOHN HYATT¹, ALBERTO FERNANDEZ-NIEVES², Georgia Institute of Technology, GEORGIA TECH TEAM — We use 3D cross-correlated dynamic light scattering to investigate suspensions of microgels. We will discuss some of the theory behind this technique and present results from size- and pH-tunable pNIPAM microgels cross-linked with PEG and copolymerized with acrylic acid.

¹Graduate student in Georgia Tech Soft Condensed Matter Laboratory.

²PI of Georgia Tech Soft Condensed Matter Laboratory.

10:36AM H51.00014 Using colloidal packings as templates for structuring drugs , JAMES WILKING, Harvard University, ANDRÉ STUDART, ETH, SEBASTIAN KOLTZENBURG, BASF, RODRIGO GUERRA, ESTHER AMSTAD, Harvard University, JENS RIEGER, BASF, DAVID WEITZ, Harvard University — Many pharmaceutical compounds are poorly soluble in water; this is problematic because most pharmaceuticals are delivered orally and must dissolve in the gastrointestinal fluid in order to be taken up by the body. We introduce a simple method for increasing the dissolution rates of poorly water-soluble organic actives. We demonstrate that by structuring the compounds within the interconnected, nanoscale pore space of a colloidal packing we create composites which rapidly disintegrate in water, exposing the nanostructured organic active and leading to improved dissolution rates.

10:48AM H51.00015 Spin coating of superparamagnetic colloids with applied magnetic fields¹

, WENCESLAO GONZÁLEZ-VIÑAS, MOORTHY PICHUMANI, University of Navarra — We report experimental results on the behavior of dilute superparamagnetic colloids under shear stresses (using a commercial spin-coater and varying its rate of rotation) with applied magnetic fields. For the case of zero field, we compare the results obtained for different kind of particles (non-magnetic [1] vs PS based [2] vs silica based [3]) and solvents by analyzing the dried deposits obtained from the spin coating. All the data collapse in a single curve, when the appropriate scaling for the film thickness is performed. This agreement allows us to define a reference to measure the relative change in viscosity, when a magnetic field is applied during the spin coating. Thus, we show the magnetorheological properties of colloidal dispersions. These results shed light into the aggregation and clustering dynamics for colloids under external fields with shear and provide a new method to study the rheological properties of colloids.

[1] M. Giuliani et al. "Dynamics of crystal structure formation in spin-coated colloidal films" J. Phys. Chem. Lett. 1(9), 1481 (2010)

[2] M. Pichumani et al. "Spin-coating of dilute magnetic colloids in a magnetic field" Magnetohydrodynamics, 47(2), 191 (2011)

[3] M. Pichumani et al. In preparation

¹This work is partly supported by the Spanish Government Contract No. FIS2008-01126. M.P. acknowledges the financial support from the "Asociación de Amigos de la Universidad de Navarra"

Tuesday, February 28, 2012 8:00AM - 11:00AM — Session H52 GSNP DFD: Focus Session: Extreme Mechanics - Rods 153C

8:00AM H52.00001 Dynamic curling of a naturally curved Elastica¹, BASILE AUDOLY, Institut Jean le Rond d'Alembert, University Paris 6 and CNRS — We consider the motion of a naturally curved Elastica that has been flattened onto a hard surface. When it is released from one end, the Elastica lifts off the surface and curls dynamically into a moving spiral. The motion is governed by inertia, bending and geometric nonlinearity. At long times, the dynamics follows a self-similar regime: the size of the spiral grows like the cubic root of time, while the velocity of the front reaches a constant value. The asymptotic velocity is derived analytically, and compared to numerical simulations and to experiments.

¹Joint work with Andrew Callan-Jones and Pierre-Thomas Brun

8:36AM H52.00002 The Mechanics of Curly Hair, JAMES MILLER, Massachusetts Institute of Technology, ARNAUD LAZARUS, BREANNA BERRY, MIT, BASILE AUDOLY, Institut d'Alembert (University Paris 6), PEDRO REIS, MIT — We explore the oft-neglected role of intrinsic natural curvature on the mechanics of elastic rods. Our testbed, a hanging hair, is a deceptively simple system that exhibits complex mechanics and geometrically nonlinear behavior. Through a combination of precision desktop-scale experiments, numerical simulations, and theoretical analysis, we seek physical insight into the nontrivial configurations adopted by a naturally curved elastic rod that is suspended under its own weight. In particular, we aim to gain predictive understanding of the transition from planar to non-planar solutions as well as the localization of torsion in the non-planar configurations. The experimentally observed behavior of our custom-fabricated naturally curved rods is captured well by simulations and is rationalized through scaling arguments.

8:48AM H52.00003 The Shape of a Ponytail and the Statistical Physics of Hair Fiber Bundles, RAYMOND E. GOLDSTEIN, University of Cambridge, PATRICK B. WARREN, Unilever R&D Port Sunlight, ROBIN C. BALL, University of Warwick — From Leonardo to the Brothers Grimm our fascination with hair has endured in art and science. Yet, a quantitative understanding of the shapes of a hair bundles has been lacking. Here we combine experiment and theory to propose an answer to the most basic question: What is the shape of a ponytail? A model for the shape of hair bundles is developed from the perspective of statistical physics, treating individual fibers as elastic filaments with random intrinsic curvatures. The combined effects of bending elasticity, gravity, and bundle compressibility are recast as a differential equation for the envelope of a bundle, in which the compressibility enters through an "equation of state." From this, we identify the balance of forces in various regions of the ponytail, extract the equation of state from analysis of ponytail shapes, and relate the observed pressure to the measured random curvatures of individual hairs.

9:00AM H52.00004 Following the equilibria of slender elastic rods, ARNAUD LAZARUS, JAMES MILLER, PEDRO REIS, Massachusetts Institute of Technology — We present a novel continuation method to characterize and quantify the equilibria of elastic rods under large geometrically nonlinear displacements and rotations. To describe the kinematics we exploit the synthetic power and computational efficiency of quaternions. The energetics of bending, stretching and torsion are all taken into account to derive the equilibrium equations which we solve using an asymptotic numerical continuation method. This provides access to the full set of analytical equilibrium branches (stable and unstable), a.k.a bifurcation diagrams. This is in contrast with the individual solution points attained by classic energy minimization or predictor-corrector techniques. We challenge our numerics for the specific problem of an extremely twisted naturally curved rod and perform a detailed comparison against a precision desktop-scale experiments. The quantification of the underlying 3D buckling instabilities and the characterization of the resulting complex configurations are in excellent agreement between numerics and experiments.

9:12AM H52.00005 The elasticity of magnetic chains: From self-buckling to self-assembly, DOMINIC VELLA, EMMANUEL DU PONTAVICE, CAMERON HALL, ALAIN GORIELY, OCCAM, University of Oxford — Spherical neodymium magnets have become a popular toy in recent years. In this talk, we present the results of some experimental and theoretical investigations into the peculiar elastic-like behaviour exhibited by chains of these magnetic spheres. We show how the dipole-dipole interactions between spheres penalise deformation, and we find that the form of this penalty is different for a long chain compared to a short chain. Finally, we investigate the dynamic self-assembly of these chains into cylindrical structures.

9:24AM H52.00006 Spontaneous and Deterministic Three-dimensional Curling of Pre-strained Elastomeric Strips: From Hemi-helix to Helix, JIANGSHUI HUANG, JIA LIU, BENEDIKT KROLL, KATIA BERTOLDI, ZHIGANG SUO, DAVID CLARKE, Harvard University — A variety of three dimensional curls are produced by a simple generic process consisting of pre-straining one elastomeric strip, joining it to another and then releasing the bi-strip. The hemi-helix, one kind of three dimensional curls, consists of multiple, alternating helical sections of half wavelength in opposite chiralities and separated by perversions. The hemi-helix wavelength and the number of perversions are determined by the strip cross-section, the constitutive behavior of the elastomer and the value of the pre-strain. Topologically, the perversions also separate regions of the helix deforming principally by bending from those where twisting dominates. Changing the prestrain and the ratio between the thickness and the width induce a phase separation of hemi-helical structure, helical structure and hybrid structure which have similarities to coiled polymer molecules and plant tendrils.

9:36AM H52.00007 Snakes Out of the Plane¹, ANDREW MCCORMICK, BRUCE A. YOUNG, L. MAHADEVAN, Harvard University — We develop a new computational model of elastic rods, taking into account shear and full rotational dynamics, as well as friction, adhesion, and collision. This model is used to study the movement of snakes in different environments. By applying different muscular activation patterns to the snake, we observe many different patterns of motion, from planar undulation to sudden strikes. Many of the most interesting behaviors involve the snake rising out of the horizontal plane in the vertical direction. Such behaviors include a sand snake sidewinding over the hot desert sand and a cobra rearing up into a defensive striking position. Experimental videos of live snakes are analyzed and compared with computational results. We identify and explain a new form of movement previously unobserved: “collateral locomotion.”

¹A.M. acknowledges support from the NDSEG program.

9:48AM H52.00008 Analysis of the fluid mechanical sewing machine, PIERRE-THOMAS BRUN, Institut Jean le Rond d'Alembert/Lab. FAST, UPMC, Univ Paris-Sud, CNRS, BASILE AUDOLY, Institut Jean le Rond d'Alembert, UPMC, CNRS, NEIL RIBE, Lab FAST, UPMC, Univ Paris-Sud, CNRS — A thin thread of viscous fluid falling onto a moving belt generates a surprising variety of patterns, similar to the stitch patterns produced by a traditional sewing machine. By simulating the dynamics of the viscous thread numerically, we can reproduce these patterns and their bifurcations. The results lead us to propose a new classification of the stitch patterns within a unified framework, based on the Fourier spectra of the motion of the point of contact of the thread with the belt. The frequencies of the longitudinal and transverse components of the contact point motion are locked in most cases to simple ratios of the frequency Ω_c of steady coiling on a surface at rest (i.e., the limit of zero belt speed). In particular, the “alternating loops” pattern involves the first five multiples of $\Omega_c/3$. The dynamics of the patterns can be described by matching the upper (linear) and the lower (non-linear) portions of the thread. Following this path we propose a toy model that successfully reproduces the observed transitions from the steady dragged configuration to sinusoidal meanders, alternating loops, and the translated coiling pattern as the belt speed is varied.

10:00AM H52.00009 Microfabrication of a spider-silk analogue through the liquid rope coiling instability¹, FREDERICK P. GOSSELIN, DANIEL THERIAULT, MARTIN LEVESQUE, Ecole Polytechnique de Montreal — Spider capture silk outperforms most synthetic materials in terms of specific toughness. We developed a technique to fabricate tough microstructured fibers inspired by the molecular structure of the spider silk protein. To fabricate microfibers (with diameter $\sim 30\mu m$) with various mechanical properties, we yield the control of their exact geometry to the liquid rope coiling instability. This instability causes a thread of honey to wiggle as it buckles when hitting a surface. Similarly, we flow a filament of viscous polymer solution towards a substrate moving perpendicularly at a slower velocity than the filament flows. The filament buckles repetitively giving rise to periodic meanders and stitch patterns. As the solvent evaporates, the filament solidifies into a fiber with a geometry bestowed by the instability. Microtraction tests performed on fibers show interesting links between the mechanical properties and the instability patterns. Some coiling patterns give rise to high toughness due to the sacrificial bonds created when the viscous filament loops over itself and fuse. The sacrificial bonds in the microstructured fiber play an analogous role to that of the hydrogen bonds present in the molecular structure of the silk protein which give its toughness to spider silk.

¹We acknowledge the funding from FQRNT, NSERC and CFI.

10:12AM H52.00010 Buckling Instability and Stress Propagation in Rods with Elastic Support, ZI CHEN, Biomedical Engineering, Washington Univ. in St. Louis, WANLIANG SHAN, Mechanical & Aerospace Engineering, Princeton Univ., ANKITA GUMASTE, Neuroscience & Behavioral Biology, Emory Univ., WINSTON SOBOYEJO, Mechanical & Aerospace Engineering, Princeton Univ., CLIFFORD BRANGWYNNE, Chemical & Biological Engineering, Princeton Univ. — The cytoskeleton of living cells is a composite material consisting of a network of biopolymers including f-actin and microtubules (MTs). MTs are able to bear significant compressive loads in cells as a result of reinforced short wavelength buckling, due to the surrounding actin network. However, the length scale of compressive force propagation, even for macroscopic rods, remains poorly understood. Here we propose a minimal theory that incorporates elastic restoring forces from the surrounding network, elucidating the compressive force-dependence of the buckled rod shape. We identify a threshold length as the effective distance stresses can propagate in such network, and show that the decay length is tunable by modifying the longitudinal mechanical coupling coefficients. We test these predictions with experiments in macroscopic rods, and show that the degree of mechanical coupling directly controls the penetration depth of buckling, in agreement with theoretical and numerical predictions. Our results suggest that the length scale over which mechanical signals are transduced in cells may be actively controlled, and could provide design principles for novel types of fiber composite materials based on biomimetic control of the longitudinal coupling coefficients.

10:24AM H52.00011 Undulatory buckling of a rod constrained by an elastic matrix, JIA LIU, TIANXIANG SU, Harvard University, OSCAR LOPEZ-PAMIES, UIUC, PEDRO REIS, MIT, KATIA BERTOLDI, Harvard University — Elastic instabilities of rods constrained by an elastic matrix and subjected to axial compression have long been recognized as essential for structural applications in the context of failure mitigation and, more recently, towards exploitation of functionality. Relevant fields for this class of problems include drilling, biomedical instrumentation and root growth in plants. We explore the two possible scenarios observed when, above a threshold load, compression is applied to a rod constrained by a matrix: i) the rod can develop a planar oscillatory solution (sinusoidal buckling) or ii) it can take the configuration of a helix (helical buckling). We identify the principal parameters of this system, perform a systematic parametric study and rationalize the phase diagram through a hybrid of theoretical and numerical analyses. Particular attention is devoted to the effect of the mechanical properties of the constraining matrix which is found to have a critical influence on this buckling scenario.

10:36AM H52.00012 Slack, stress, and noisy structures in inertial strings, JAMES HANNA, CHRISTIAN SANTANGELO, Department of Physics, University of Massachusetts - Amherst — Strings and chains are inextensible filaments with negligible bending and twist resistance. Local arc length conservation is enforced by the stress, a Lagrange multiplier field screened by curvature. Uniform stress fields are generated by a wide class of inertial motions that includes travelling waves of curvature and torsion, while gradients in stress result in more complicated dynamics. We will discuss a theoretical example inspired by experimental and numerical observations of the growth of an arch in a straightening chain, involving the amplification, rectification, and advection of slack.

10:48AM H52.00013 Sinusoidal to helical buckling of an elastic rod under a cylindrical constraint, TIANXIANG SU, Harvard University, JAMES MILLER, ARNAUD LAZARUS, Massachusetts Institute of Technology, NATHAN WICKS, JAHIR PABON, Schlumberger-Doll Research, KATIA BERTOLDI, Harvard University, PEDRO REIS, Massachusetts Institute of Technology — We investigate the buckling and post-buckling behavior of an elastic rod loaded under cylindrical constraint. Our precision desktop-scale experiments comprise of axially compressing a hyper-elastic rod inside a transparent acrylic pipe. These experiments are also modeled using a discrete elastic rod simulation that includes frictional effects. Under imposed displacement, the initially straight rod first buckles into a sinusoidal mode and eventually undergoes a secondary instability into a helical buckling regime. The buckling and post-buckling behavior is found to be highly dependent on the systems' geometry, in particularly the aspect ratio of the rod to pipe diameter. We quantify the wavelength and pitch of the periodic patterns through direct digital imaging and record the reaction forces at both ends of the pipe. The observed behavior is rationalized through scaling arguments and captured by numerical simulations.

Tuesday, February 28, 2012 8:00AM - 11:00AM —

Session H53 GSNP: Focus Session: Continuum Descriptions of Discrete Materials 153B

8:00AM H53.00001 Failure of a loose packing of grains , GREG FARRELL, NARAYANAN MENON, UMass-Amherst

— One-sided repulsive interactions and history-dependent friction forces can cause the mechanics of real granular systems to deviate significantly from that of cohesive solids. Marked deviations from elastic behavior can be seen in the mechanical response and structure of sedimented loose packings of frictional spheres even for very delicate perturbations. In our experiments, particles' displacements are observed with 3D fluorescent imaging as a shear plane is displaced through the packing. As anticipated, we find the shear force is approximately linear with the displacement between discrete yielding events. However, even in this apparently linear region, structural aging continues to occur for the smallest displacements that we can apply. This suggests the inaccessibility of a reversible shear deformation regime in loose packings of granular material. We present a spatial characterization of the particle motion that distinguishes between these continuous instances of irreversibility and the larger discrete failure events.

8:12AM H53.00002 Jamming in Hopper Flows: Analysis of Survival Times¹ , MICHAL DICHTER, Brandeis

University, SHUBHA TEWARI, Western New England University, BULBUL CHAKRABORTY, Brandeis University — Many granular systems experience a transition from a fluid-like state to a solid-like state characterized by a sudden arrest in dynamics, or “jamming.” Recent experiments by the Behringer Group at Duke University suggest a probabilistic model of jamming in hopper flows. We will show the results of numerical simulations of dense, gravity-driven, granular flows in a two-dimensional hopper with a tapered outlet [PRE 79, 011303 (2009)]. We will present results for the statistics of mass flow at the outlet, and the probability of survival without a jam. We will correlate the survival times with velocity and density distributions near the hopper opening.

¹This project is funded by NSF.

8:24AM H53.00003 Experimental analysis on how grain properties affect the performance of jammed granular systems for variable stiffness robotic applications¹ , NADIA CHENG, KARL IAGNEMMA, ANETTE HOSOI, KATY GERO, Massachusetts Institute of Technology

— Jamming of granular media has become increasingly utilized as a variable stiffness mechanism for industrial and robotic applications. The goal of our work is to better understand how grain properties affect jamming so that granular systems can be designed to fulfill the requirements of a given application. We have primarily focused on experimental studies to analyze how certain grain properties—such as shape, surface roughness, size distribution, and shape distribution—affect the performance of granular systems. Potential applications that utilize jamming would typically require that a contained granular system transition between effective solid states (e.g., when particular shape or strength needs to be maintained) and effective liquid states (e.g., when the system needs to be compliant such that it can be shaped or actuated by its environment). Therefore, we are interested in quantifying 1) the strength of compacted granular systems in their effective solid states and 2) the “ease of flow” and compliance of granular systems in their effective liquid states.

¹The work presented here is supported by the DARPA M3 program

8:36AM H53.00004 Shear-Transformation-Zone Theory of Glassy Diffusion, Stretched Exponentials, and the Stokes-Einstein Relation , JAMES LANGER, University of California, Santa Barbara

— The success of the shear-transformation-zone (STZ) theory in accounting for broadly peaked, frequency-dependent, glassy viscoelastic response functions is based on the theory's first-principles prediction of a wide range of internal STZ transition rates. Here, I propose that the STZ's are the dynamic heterogeneities frequently invoked to explain Stokes-Einstein violations and stretched-exponential relaxation in glass-forming materials. I find that, to be consistent with observations of Fickian diffusion near T_g , an STZ-based diffusion theory must include cascades of correlated events, but that the temperature dependence of the Stokes-Einstein ratio is determined by an STZ-induced enhancement of the viscosity. Stretched-exponential relaxation of density fluctuations emerges from the same distribution of STZ transition rates that predicts the viscoelastic behavior.

9:12AM H53.00005 A granular flow law based on nonlocal fluidity , KEN KAMRIN, MIT, GEORG KOVAL, INSA Strasbourg

— A general, three-dimensional law to predict granular flow in an arbitrary geometry has been an elusive goal for decades. Recently, an elasto-plastic continuum model has shown the ability to approximate steady flow and stress profiles in multiple inhomogeneous flow environments. However, the model does not capture some phenomena observed in the slow, creeping flow regime. As normalized flow-rate decreases, granular stresses are observed to become largely rate-independent and a dominating length-scale emerges in the mechanics. This talk attempts to account for these effects using the notion of nonlocal fluidity, which has proven successful in treating nonlocal effects in emulsions. The idea is to augment the usual granular fluidity law with a diffusive second-order term scaled by the particle size that spreads flowing zones accordingly. Below the yield stress, the local contribution vanishes and the fluidity becomes rate-independent, as we require. We implement the modified law in multiple geometries and validate its predictions for velocity, shear-rate, and stress against discrete particle simulations.

9:24AM H53.00006 Rheology of discontinuously shear thickening suspensions beyond simple shear , PAWEL ZIMOCZ, GARETH MCKINLEY, ANETTE HOSOI, Massachusetts Institute of Technology

— The behavior of discontinuously shear thickening suspensions in flows other than simple shear is not well understood, in part due to unresolved experimental challenges. For example, such suspensions thicken most easily close to rigid boundaries due to the no-slip condition. This makes experiments highly dependent on the shape and size of the container used. We show that by placing a lubricating layer of oil between the suspension and the container we can generate flows where thickening is nearly independent of rigid boundaries. This method is particularly useful in creating quasi one- and two-dimensional flows, which can be easily visualized. We use this method to conduct capillary breakup experiments with thickening suspensions of silica and cornstarch particles, in which we observe the formation of beads-on-a-string morphologies with multiple satellite and sub-satellite bead generations, similar to the morphologies observed in breakup of viscoelastic fluids. Using a one-dimensional continuum model, we show how nonlinear rheology of thickening suspensions results in the creation of these complex morphologies.

9:36AM H53.00007 Activated processes in a stress landscape: a rheological model for dense driven granular materials¹ , BULBUL CHAKRABORTY, DAPENG BI, Brandeis University

— We model (Phil. Trans. R. Soc. A 2009 367) the rheological behavior of granular materials based on a stress-based statistical ensemble and the Soft Glassy Rheology framework (SGR). It takes into account the disordered nature of granular packings and the metastability of jammed states, as well as spatial heterogeneity and intermittency. In this model, mesoscopic subregions of a driven granular material undergo activated processes in a *stress* landscape with a broad distribution of barrier heights. Due to the athermal nature of granular materials, the activated processes are induced not by the thermodynamic temperature, but by a temperature-like quantity which is a measure of the fluctuation of stresses. Results and predictions of the model have been successfully applied to analyze experiments in a Couette geometry. We will discuss applications of the stress-activated framework in, for example, recent experiments that study non-local rheology in dense flows (PRL 106 108301(2011)).

¹This work has been supported by NSF.

9:48AM H53.00008 Shear-transformation-zone theory of plasticity in hard-sphere materials, CHARLES K.C. LIEOU, JAMES S. LANGER, AHMED E. ELBANNA, JEAN M. CARLSON, Department of Physics, University of California, Santa Barbara — The dynamics of sheared, dense granular materials exhibits features, such as a dynamic yield stress and a glass transition, similar to those of other amorphous solids. However, strictly granular, hard-sphere systems fundamentally differ from traditional glassy and colloidal systems because at microscopic scales their dynamics and interaction energies are insensitive to thermal temperature. In this talk we present a theory of plasticity for sheared, granular materials that combines Shear Transformation Zone (STZ) theory with Edwards' statistical theory of granular materials. We find that the dynamics of a strictly granular system, like other amorphous solids, can be captured statistically in terms of entropic mechanisms. In our analysis of sheared hard spheres, the volume V replaces the energy E as a function of entropy S in conventional statistical mechanics. In place of an effective disorder temperature, a central feature of the STZ theory for traditional glassy systems, the compactivity $X = \partial V / \partial S$ characterizes the internal state. We derive the STZ equations of motion for a granular material accordingly, and predict its macroscopic properties such as shear viscosity and macroscopic frictional coefficient under different shearing conditions.

10:00AM H53.00009 Width of Shear Zones in Gravity-Driven Granular Flows, SHUBHA TEWARI, Western New England University, BULBUL CHAKRABORTY, Brandeis University — Gravity-driven granular flow in a vertical hopper exhibits a flow profile that consists of a plug near the center and a shear zone near the boundary walls. It has been observed that the width of the shear zone is a few particle diameters and is independent of the channel width, however, the mechanism by which the width is selected remains unclear. Using event-driven simulations of granular flow in a two-dimensional hopper, we investigate the width of the shear zone as a function of the channel width and the boundary conditions at the wall. We focus on the role played by fluctuations in the stress as the source of activated slips near the wall as a candidate mechanism for the shear zone.

10:12AM H53.00010 From streamline jumping to strange eigenmodes: Learning from simple continuum models of granular mixing¹, IVAN C. CHRISTOV², JULIO M. OTTINO, RICHARD M. LUEPTOW, Robert R. McCormick School of Engineering and Applied Science, Northwestern University — Simple continuum models of granular flow can provide fundamental insight into how and why granular materials mix. Though a similar kinematic framework can be used to study both fluid and granular mixing, there are striking differences that we explore through a computational-experimental study of granular flow in a slowly rotating quasi-two-dimensional polygonal container. In the Lagrangian frame, for small numbers of revolutions, we show that the mixing pattern is captured by a model termed "streamline jumping." This minimal model, arising at the limit of a vanishingly-thin surface flowing layer, possesses no intrinsic stretching or streamline crossing in the usual sense, yet it can lead to complex particle trajectories that resemble chaos. In the Eulerian frame, meanwhile, we show the presence of naturally-persistent granular mixing patterns ("strange" eigenmodes) for intermediate numbers of revolutions. Unlike fluid mixing, however, strong diffusive effects (due to particle collisions in granular flows) result in fast decay of these transient patterns in monodisperse mixtures. Meanwhile, segregation leads to permanent excitation of eigenmodes in bidisperse mixtures.

¹This work was supported, in part, by NSF Grant CMMI-1000469.

²Current affiliation: Department of Mechanical and Aerospace Engineering, Princeton University.

10:24AM H53.00011 From liquid to stone: a polydispersive colloidal model for cement setting¹, ENRICO MASOERO, ROLAND PELLENG, FRANZ-JOSEF ULM, SIDNEY YIP, Massachusetts Institute of Technology, EMANUELA DEL GADO, ETH Zurich — The main binding phase of cement is the nano-porous C-S-H gel, (calcium-silicate-hydrate). Here we investigate the temporal evolution of the mechanical properties of cement across the rigidity transition from liquid paste to solid stone, due to the precipitation of C-S-H. This transition is named "setting" and occurs several hours after mixing cement powder with water. We present a numerical model of random insertion of colloidal C-S-H nano-particles in the Monte Carlo framework. The particles interact with each other according to a generalized Lennard-Jones potential. Depending on the particle size polydispersity, the packing fraction of the final assemblies ranges between 0.64 and 0.73. The mechanical properties of the assemblies indicate that the packing fraction is the key parameter for continuum mechanics models at larger scales. In fact, both the stiffness and the strength of the assemblies increase with the packing fraction, while the ductility decreases. On the other hand, the evaluation of the specific surface requires an additional parameter fixing the length scale, for example, the characteristic size of the nano-pores. We finally show the relevance of our results for cement setting with a simple semi-analytical model of micro-pore filling.

¹Supported by Schlumberger and by the Swiss SNSF

10:36AM H53.00012 Effect of randomness on wave propagation in granular systems, MOHITH MANJUNATH, AMNAYA P. AWASTHI, PHILIPPE H. GEUBELLE, Department of Aerospace Engineering, University of Illinois at Urbana-Champaign — Granular systems have been shown to possess energy absorbing and potential wave mitigation characteristics due to the flexibility in tuning the properties of the particles. The present study focuses on the impact of randomness on wave propagation in 1D and 2D lattices of spherical particles where the randomness is associated with either the mass, Young's modulus or radius of the spheres. The 1D study (motivated by M. Manciau et. al. (2001)) reveals the presence of two distinct regimes of decay in peak compressive force with distance for any level of randomness. The transition between the regimes of exponential and power-law decay is shown to occur when the amplitude of the leading pulse reduces below that of the scatter. Investigation into the ensemble kinetic and potential energies of the system as a function of time shows the gradual transfer of energy from potential to kinetic with increase in the level of randomness. In 2D square packed systems simulated with a modified version of the molecular dynamics package LAMMPS, we note that the decay in peak compressive force is present due to dimensionality as well as randomness. Normalization is then used to quantify the decay due to randomness alone and we investigate the anisotropy of the randomness induced decay.

10:48AM H53.00013 Continuum Representation of the Mechanics of Random Fiber Networks, ALI SHAHSAVARI, CATALIN PICU, Rensselaer Polytechnic Institute — Solving boundary value problems over large domains of random fiber networks is important in the design of fiber-based engineering materials and in the understanding of the biophysics of biological materials. In most of these applications, systems contain a very large number of fibers, which renders nearly impossible solving boundary value problems while resolving every fiber in the problem domain. Therefore, developing a continuum model for the discrete system is desirable. This presentation focuses on conditions under which this mapping can be performed and the minimum size of the problem beyond which the continuum representation is valid. Random fiber networks are highly heterogeneous and exhibit non-affine deformation with correlated fields at different observation length scales. The scale of transition from the discrete to the continuum model must be large enough to capture all the statistically independent subdomains of the network. This scale cannot be determined exclusively based on geometric considerations (e.g. based on fiber density). These considerations, along with a constitutive model for the small deformation of continuum models of fiber networks are discussed in this talk.

Tuesday, February 28, 2012 8:00AM - 11:00AM —

Session H54 GSNP: Focus Session: Complex and co-evolving networks - Dynamics on Networks

8:00AM H54.00001 Robustness and Assortativity for Diffusion-like Processes in Scale-free Networks¹, ANTONIO SCALA, CNR-ISC, Uos “La Sapienza”, GREGORIO D’AGOSTINO, ENEA - CR “Casaccia”, VINKO ZLATIĆ, Theoretical Physics Division, Rudjer Boskovic Institute, GUIDO CALDARELLI, IMT Lucca Institute for Advanced Studies — By analyzing the diffusive dynamics of epidemics and of distress in complex networks, we study the effect of the assortativity on the robustness of the networks. We first determine by spectral analysis the thresholds above which epidemics/failures can spread; we then calculate the slowest diffusional times. Our results show that disassortative networks exhibit a higher epidemiological threshold and are therefore easier to immunize, while in assortative networks there is a longer time for intervention before epidemic/failure spreads. Moreover, we study by computer simulations a diffusive model of distress propagation (financial contagion). We show that, while assortative networks are more prone to the propagation of epidemic/failures, degree-targeted immunization policies increases their resilience to systemic risk.

¹FET Open Project “FOC” nr. 255987, European project “MOTIA” JLS-2009-CIPS-AG-C1-016

8:12AM H54.00002 Time scales and dynamical processes in activity driven networks, NICOLA PERRA, BRUNO GONCALVES, Northeastern University, ROMUALDO PASTOR-SATORRAS, UPC, ALESSANDRO VESPIGNANI, Northeastern University — Network science has undergone explosive growth in the last ten years. This growth has been driven by the recent availability of huge digital databases, which has facilitated the analysis and construction of large-scale networks from real data and the identification of statistical regularities and structural principles common to many systems. Network modeling has played an essential role in this endeavor; however models are chiefly constructed by considering as relevant ingredients only the connectivity and statistical properties of the networks, while disregarding the actual agents' behavior. Here we address this challenge by measuring the agents' interaction activity in real-world networks and defining a minimal model capable of reproducing the intrinsically additive nature of connectivity patterns obtained from time-aggregated network representations. Additionally, we demonstrate that processes such as epidemic and information spreading in highly dynamical networks can be better characterized in terms of agent social activity than by connectivity based approaches

8:24AM H54.00003 Network growth dynamics of fire ant (*Solenopsis invicta*) nests, NICK GRAVISH, School of Physics, Georgia Tech, MICHAEL A.D. GOODISMAN, School of Biology, Georgia Tech, DANIEL I. GOLDMAN, School of Physics, Georgia Tech — We study the construction dynamics and topology of fire ant (*Solenopsis invicta*) nests. Fire ants in colonies of hundreds to hundreds of thousands create subterranean tunnel networks through the excavation of soil. We observed the construction of nests in a laboratory experiment. Workers were isolated from focal colony and placed in a quasi 2D, vertically oriented arena with wetted soil. We monitored nest growth using time-lapse photography. We found that nests grew linearly in time through tunnel lengthening and branching. Tunnel path length followed an extended power law distribution, $P(l - l_0)^\beta$. Average degree of tunnel nodes was $k = 2.17 \pm 0.40$ and networks were cyclical. In simulation we model the nest growth as a branching and annihilating levy-flight process. We study this as a function of dimensionality (2D and 3D space considered) and step length distribution function $P(l_s)$. We find that in two-dimensions path length distribution is exponential, independent of the functional form of $P(l_s)$ consistent with a poisson spatial process while in three-dimensions $P(l) = P(l_s)$. Comparing simulation and experiment we attribute the slower than exponential tail of $P(l)$ in experiment as a result of a behavioral component to the ant digging program.

8:36AM H54.00004 The Impact of Time Delays in Network Synchronization in a Noisy Environment¹, G. KORNISS, RPI — Coordinating, distributing, and balancing resources in networks is a complex task and it is very sensitive to time delays. To understand and manage the collective response in these coupled interacting systems, one must understand the interplay of stochastic effects, network connections, and time delays. In synchronization and coordination problems in coupled interacting systems individual units attempt to adjust their local state variables (e.g., pace, orientation, load) in a decentralized fashion. They interact or communicate only with their local neighbors in the network, often with explicit or implicit intention to improve global performance. Applications of the corresponding models range from physics, biology, computer science to control theory. I will discuss the effects of nonzero time delays in stochastic synchronization problems with linear couplings in an arbitrary network. Further, by constructing the scaling theory of the underlying fluctuations, we establish the absolute limit of synchronization efficiency in a noisy environment with uniform time delays, i.e., the minimum attainable value of the width of the synchronization landscape.² These results have also strong implications for optimization and trade-offs in network synchronization with delays.

¹Supported in part by DTRA, ARL, and ONR.

²D. Hunt, G. Korniss, and B.K. Szymanski, Phys. Rev. Lett. 105, 068701 (2010).

9:12AM H54.00005 Predicting the origin of contagion processes on complex, multi-scale networks, RAFAEL BRUNE, CHRISTIAN THIEMANN, DIRK BROCKMANN, Northwestern University — Contagion phenomena in space often exhibit complex, multiscale spatio-temporal patterns driven by the interaction of non-local dispersal and nonlinear dynamics. A key challenge is the prediction of dynamic patterns based on information on human interactions, mobility and initial conditions. The development of computational models has thus received considerable attention. However, in many realistic situations, a process has already evolved for some period before detection and identifying the spatial origin is difficult. Surprisingly, this “inverse problem” has received little attention in the past. We show in a paradigmatic model for human disease dynamics that despite the spatial complexity of dynamic patterns, the origin of outbreak can be predicted with high fidelity. Based on the technique of shortest path trees in strongly heterogeneous, multi-scale human mobility networks we show that at any point in time the spatial origin can be reconstructed reliably. This novel perspective on complex spatio-temporal dynamics can be applied to systems beyond human disease dynamics for instance the reconstruction of neolithic diffusion of agriculture into Europe and related migration driven historic phenomena.

9:24AM H54.00006 Influence and structural balance in social networks, P. SINGH, S. SREENIVASAN, B. SZYMANSKI, G. KORNISS, RPI — Models on structural balance have been studied in the past with links being categorized as friendly or antagonistic [Ref- T. Antal et al., Phys. Rev. E 72, 036121 (2005)]. However no connection between the nature of the links and states of the nodes they connect has been made. We introduce a model which combines the dynamics of the structural balance with spread of social influence. In this model, every node is in one of the three possible states (e.g. leftist, centrist and rightist) [Ref- F. Vazquez, S. Redner, J. Phys A, 37 (2004) 8479-8494] where links between leftists and rightists are antagonistic while all other links are friendly. The evolution of the system is governed by the rules of structural balance and opinion spread takes place as a result of structural balance process. The dynamics can lead the system to a number of fixed points (absorbing states). We study how the initial density of centrists n_c affects the dynamics and probabilities of ending up in different absorbing states. We also study the scaling behavior of the expected time to converge to one of the absorbing states as a function of the initial density of centrists and under some variations of our basic model.

9:36AM H54.00007 Majority-vote model on a dynamic small-world square lattice, THOMAS E. STONE, Husson University, SUSAN R. MCKAY, University of Maine — Majority-vote models are often used to study consensus building, coarsening dynamics, and phase transitions, among other phenomena. In addition to the microscope rules governing a particular model, it is well known that the relevant properties of each system depend crucially on the underlying lattice structure. Here we investigate a majority-vote with noise model on a square lattice with dynamic small-world rewiring via Monte Carlo simulation and finite size scaling analyses. We construct the order-disorder phase diagram and find the critical exponents associated with the continuous phase transition. We compare our results to those obtained from two-dimensional static small-world networks, as well as the isotropic lattice and mean-field limiting cases.

9:48AM H54.00008 Underlying mechanisms for commuting and migration processes , FILIPPO SIMINI, ALBERT-LASZLO BARABASI, Northeastern University, JAMES BAGROW, Northwestern University — Both frequent commuting and long-term migration are complex human processes that strongly depend on socio-demographic, spatial, political, and even economic factors. We can describe both processes using weighted networks, in which nodes represent geographic locations and link weights denote the flux of individuals who commute (or migrate) between locations. Although both processes concern the movements of individuals, they are very different: commuting takes place on a daily (or weekly) basis and always between the same two locations, while migration is a rare, one-way displacement. Despite these differences, a recently proposed stochastic model, the Radiation model, provides evidence that both processes may be successfully described by the same underlying mechanism. For example, quantities of interest for either process, such as the distributions of trip length and destination populations, appear remarkably similar to the model's predictions. We explore the similarities and differences between commuting and migration both empirically, using census data for the United States, and theoretically, by comparing these commuting and migration networks to the predictions given by the Radiation model.

10:00AM H54.00009 A quantitative measure for organization of complex and co-evolving networks , GEORGI GEORGIEV, Assumption College and Tufts University — To define evolution and self-organization in complex networks a quantitative measure for organization is necessary. Two systems should be numerically distinguishable by their degree of organization and their rate of self-organization. Here we apply as a measure for quantity of organization the inverse of the average sum of physical actions of all elements in a system per unit motion multiplied by the Planck's constant. The meaning of quantity of organization here is the number of quanta of action per one unit motion of an element. For example, a unit motion for electrons on a computer chip is the one necessary for one computation. This definition can be applied to the organization in any complex system. Systems self-organize to decrease the average action per element per unit motion in them. This is the attractor for a dynamical, nonlinear system evolving in time. Constraints increase this average action, so constraint minimization is a basic mechanism for action minimization. Increase of quantity of elements in the network, leads to faster constraint minimization through grouping, decrease of average action per element and motion and therefore faster self-organization and evolution.

10:12AM H54.00010 Identification of Interventions to Control Network Crises , JIE SUN, SAGAR SAHASRABUDHE, ADILSON MOTTER, Northwestern University — Large-scale crises in financial, social, infrastructure, genetic and ecological networks often result from the spread of disturbances that in isolation would only cause limited damage. Here we present a method to identify and schedule interventions that can mitigate cascading failures in general complex networks. When applied to competition networks, our method shows that the system can often be rescued from global failures through actions that satisfy restrictive constraints typical of real-world conditions. However, under such constraints, interventions that can rescue the system from a propagating cascade exist over specific periods of time that do not always include the early postperturbation period, suggesting that scheduling is critical in the control of network cascades.

10:24AM H54.00011 Effect of degree correlations on controllability of complex networks , MARTON POSFAI, YANG LIU, Center for Complex Network Research and Department of Physics, Northeastern University, Boston, Massachusetts 02115, USA, JEAN-JAQUES SLOTINE, Non-linear Systems Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139, USA, ALBERT-LASZLO BARABASI, Center for Complex Network Research and Department of Physics, Northeastern University, Boston, Massachusetts 02115, USA — While significant effort was made during the past decade to understanding the structure, evolution and function of complex networks, little is known about our ability to control them. A system is considered controllable if by imposing appropriate external signals on a set of its nodes, called driver nodes, the system can be driven from any initial state to any desired final state in finite time. The controllability of a network can be quantified by calculating the minimal number of driver nodes needed to obtain complete control. We study the effect of degree correlations on network controllability via both numerical simulations and analytical calculations. Numerical simulations are performed by systematically adding correlations to model networks using appropriate rewiring schemes inspired by simulated annealing. Analytical results are derived using the cavity method originally developed in spin glass theory. The numerical and analytical results enable us to give qualitative predictions of controllability for any networks based on their degree correlation profiles. We test our predictions on several real networks and find consistent results.

10:36AM H54.00012 Control Capacity in Complex Networks , TAO JIA, YANG-YU LIU, CCNR, Northeastern University, JEAN-JACQUES SLOTINE, Massachusetts Institute of Technology, ALBERT-LASZLO BARABASI, CCNR, Northeastern University — By combining tools from control theory and network science, an efficient methodology was proposed to identify the minimum sets of driver nodes, whose time-dependent control can guide the whole network to any desired final state. Yet, this minimum driver set (MDS) is usually not unique, but one can often achieve multiple potential control configurations with the same number of driver nodes. Given that some nodes may appear in some MDSs but not in other, a crucial question remain unanswered: what is the role of individual node in controlling a complex system? We first classify a node as critical, redundant, or ordinary if it appears in all, no, or some MDSs. Then we introduce the concept of control capacity as a measure of the frequency that a node is in the MDSs, which quantifies the importance of a given node in maintaining Controllability. To avoid impractical enumeration of all MDSs, we propose an algorithm that uniformly samples the MDS. We use it to explore the control capacity of nodes in complex networks and study how it is related to other characteristics of the network topology.

10:48AM H54.00013 Controlling Complex Networks with Compensatory Perturbations , SEAN CORNELIUS, Northwestern University, Department of Physics and Astronomy, WILLIAM KATH, Northwestern University, Department of Engineering Sciences and Applied Mathematics, ADILSON MOTTER, Northwestern University, Department of Physics and Astronomy — The response of complex networks to perturbations is of critical importance in areas as diverse as ecosystem management, power system design, and cell reprogramming. These systems have the property that localized perturbations can propagate through the network, causing the system as a whole to change behavior and possibly collapse. We will show how this same mechanism can actually be exploited to prevent such failures and, more generally, control a network's behavior. This strategy is based on counteracting a deleterious perturbation through the judicious application of additional, compensatory perturbations—a prospect recently demonstrated heuristically in metabolic and food-web networks. Here, we introduce a method to identify such compensatory perturbations in general complex networks, under arbitrary constraints that restrict the interventions one can actually implement in real systems. Our method accounts for the full nonlinear time evolution of real complex networks, and in fact capitalizes on this behavior to bring the system to a desired target state even when this state is not directly accessible. Altogether, these results provide a new framework for the rescue, control, and reprogramming of complex networks in various domains.

Tuesday, February 28, 2012 11:15AM - 2:15PM –
Session J1 GIMS: Focus Session: Advances in Scanned Probe Microscopy II: High Frequencies & Optical Techniques 203

11:15AM J1.00001 Towards Magnetic Resonance Imaging of Semiconducting and Biological Nanostructures, D.P. WEBER, FEI XUE, P. PEDDIBHOTLA, M. POGGIO, University of Basel, Switzerland — In recent years a technique combining nuclear magnetic resonance (NMR) and sensitive force microscopy has emerged as a viable method for doing magnetic resonance imaging (MRI) on the nanometer scale [1]. This method, known as magnetic resonance force microscopy (MRFM), has the potential to create three-dimensional (3D), non-destructive, sub-surface images of the density of particular nuclear magnetic moments with isotopic contrast. Resolution better than 10 nm has been achieved with ^1H in a single virus particle [2]. Here we discuss the application of this technique to nanobiological samples, such as viruses, small bacteria, or cell membranes, and to various semiconductor nanostructures including quantum wells (QWs) and nanowires (NWs). In particular, we focus on the sample preparation challenges presented by these samples. Transfer and attachment of these sub-micrometer samples to our micrometer-sized force sensor includes the use of a focused ion beam (FIB) technique and manual micromanipulators used together with optical microscopy.

[1] Nanotechnology 21, 342001 (2010).

[2] Proc. Nat. Acad. Sci. U.S.A. 106, 1313 (2009).

11:27AM J1.00002 Nanoscale MRI of electron spins at millikelvin temperatures, GEERT WIJTS, ANDREA VINANTE, OLEKSANDR USENKO, ARTHUR DEN HAAN, LAURENS SCHINKELSHOEK, TJERK OOSTERKAMP, Leiden University — Magnetic Resonance Imaging by Atomic Force Microscopy (MRI-AFM) combines the non-destructive subsurface sensitivity of an MRI scanner with the high spatial resolution of an Atomic Force Microscope. It is a powerful technique to detect a small number of spins that relies on force detection by an ultrasoft, magnetically tipped cantilever and selective magnetic resonance manipulation of the spins. In order to minimize the thermomechanical noise of the cantilever and to increase spin polarization, MRI-AFM should be carried out at ultralow temperatures. Therefore, we developed a SQUID-based detection technique, which avoids heating of the cantilever and the spin sample. Using this technique, we demonstrate the manipulation and detection of dangling bond paramagnetic centers on a silicon surface at temperatures as low as 30 millikelvin. The fluctuations of these unpaired electron spins are supposedly linked to $1/f$ magnetic noise and decoherence in SQUIDs as well as in several superconducting and single spin qubits. We find evidence that spin diffusion plays a key role in the dynamics of spins at low temperatures.

11:39AM J1.00003 ESR induced anomalous polarization in Magnetic Resonance Force Microscopy, LEI CHEN, ERIC MOORE, JONILYN LONGENECKER, JOHN MAROHN, Cornell University — Mechanically detecting electron spin resonance has opened up new avenues of performing magnetic resonance detection and imaging to an individual spin-labeled macromolecule. The large gradient field from the magnetic tipped cantilever creates selective resonance conditions for each spin label in the macromolecule. The detection is made through the shifts in the cantilever self-oscillating frequency due to the back action on to the cantilever from the resonating spin polarization. In order to improving the detection sensitivity, great efforts have been made to transfer polarization of electron spins to nearby nuclear spins. Here, we reported an anomalous frequency shift in our mechanically detected ESR experiment. This ESR induced anomalous frequency shift, however is larger in amplitude and slower in relaxation time than ESR frequency shift. We will discuss that this anomalous polarization are potentially due to the dynamic nuclear polarization (DNP) mechanism.

11:51AM J1.00004 Nanomechanical detection of nuclear magnetic resonance using a silicon nanowire oscillator, JOHN NICHOL, University of Illinois at Urbana-Champaign — “Bottom-up” nanomechanical devices such as nanowires, nanotubes, and grapheme oscillators have previously been proposed as next-generation scanning probe force and mass sensors because of their potential for ultralow mechanical dissipation. Here, we report the use of a radio frequency silicon nanowire mechanical oscillator as a nuclear magnetic resonance force sensor to detect the statistical polarization of ^1H spins in polystyrene. Using a specialized scanning probe microscope, as well as a polarization-enhanced fiber-optic interferometer, we operate the nanowire as a force sensor at cryogenic temperatures. Nanowires of the type we study have very low intrinsic dissipation, and they experience negligible increase in dissipation as close as 10 nm from a surface. In order to couple the ^1H spins to the nanowire oscillator, we have developed a magnetic resonance force detection protocol which utilizes a nanoscale current-carrying wire to produce large time-dependent magnetic field gradients as well as the rf magnetic field. Under operating conditions, the nanowire exhibited an ultralow force noise of $1.9 \text{ aN}^2/\text{Hz}$ in the measurement quadrature. Further progress toward nanometer scale magnetic resonance imaging using this technique is discussed.

12:27PM J1.00005 Mechanism for Edge-enhanced Optical Response of Tip Induced Plasmonic Emission¹, GUO LI, Univ. of Sci. & Tech. of China; Institute of Physics, CAS, China, LIUGUO CHEN, CHAO ZHANG, ZHENCHAO DONG, Univ. of Sci. & Tech. of China; ZHENYU ZHANG, Univ. of Sci. & Tech. of China; Harvard University — In the investigation of tip induced plasmonic emission supplemented by STM, molecular layers are always viewed as spacers suppressing the induced emission. However, our nanoscale photo mapping of $\text{H}_2\text{TBPP}/\text{Ag}(111)$ strikingly showed enhanced emission at the molecule-island edge, which is even remarkable higher than that on the bare Ag surface. To understand this intriguing phenomenon, DFT calculations have been carried out. We found that when an organic molecule is adsorbed on Ag surface, its HOMO couples with the Ag states around the Fermi level, and forms an inelastic tunneling channel. The involved states of this channel accumulate in the interface and around the phenyl groups. Therefore, when the STM tip locates at the edge of the molecular island, the proportion of the inelastic tunneling current increases and the photo emission is enhanced. We also found that this edge-enhanced photo response is generic; the investigations of other molecule/metal systems demonstrate similar results.

¹Supported by NBRP of China, CAS, the NSF of China, and National “973” programs of China.

12:39PM J1.00006 Adiabatic Plasmon Nanofocusing for Ultrashort Pulses and Spectroscopy, JOANNA ATKIN, SAMUEL BERWEGER, ROBERT OLMON, XIAOJI XU, MARKUS RASCHKE, University of Colorado at Boulder — The simultaneous control of optical fields on both nanometer spatial and femtosecond time scales would enable direct spectroscopic access to the elementary electronic and vibrational excitations in matter. Here, we utilize adiabatic surface plasmon polariton (SPP) nanofocusing on free-standing 3D tapered metal tips in order to generate nanometer confined field localization at the tip apex. Using the second harmonic generation (SHG) at the tip apex we perform MIIPS pulse optimization and frequency-resolved optical gating (FROG) characterization of the nanofocused pulses. With the combination of high bandwidth coupling using a chirped grating, pulse-shaping, and low-dispersion nanofocusing, we can achieve full optical control on the nanoscale, from $< 16 \text{ fs}$ pulse duration to arbitrary optical waveforms. This technique enables linear and non-linear plasmon-enhanced spectroscopy, with the simultaneous temporal control over ultrashort pulses opening the possibility for true time-resolved scanning-probe imaging. We demonstrate this capability for background-free probing of individual molecular and nanocrystalline systems.

12:51PM J1.00007 Near-Field Enhanced UV Resonance Raman Spectroscopy Using an Aluminum Bow-tie Nano-antenna, LING LI, SHUANG FANG LIM, ROBERT RIEHN, HANS HALLEN, North Carolina State University — An aluminum bow-tie nano-antenna is combined with the resonance Raman effect in the deep UV to dramatically increase the sensitivity of Raman spectra to a small volume of material, such as benzene used here. By carefully choosing the right geometric parameters for the nano-antenna, we achieved a gain of a half million in signal intensity from the near field enhancement due to the surface plasmon resonance in the aluminum nanostructure. The on-line resonance enhancement contributes another factor of several thousands, limited by the laser line width. Thus, an overall gain of billions is achieved. We also demonstrated that the strong electric field gradients inside the bow-tie gap induce gradient-field Raman peaks for several strong IR modes.

1:03PM J1.00008 Multimodal Imaging of Heterogeneous Materials, WEI LIU, JIANYONG YANG, WITec Instruments, THOMAS DIENG, UTE SCHMIDT, WITec GmbH — New materials for highly specified applications can either have mono-atomic flat surfaces or a roughness of several hundred micro- or millimeter. In the past two decades, AFM was the main techniques used to characterize the morphology of nano-materials. On the other hand, Raman spectroscopy is known to be used to unequivocally determine the chemical composition of a material. By combining Raman spectroscopy with high resolution confocal optical microscopy, the analyzed material volume can be reduced below $0.02 \mu\text{m}^3$, thus leading to the ability to acquire Raman images with diffraction limited resolution. The combination of confocal Raman microscopy with Atomic Force Microscopy (AFM) is a breakthrough in microscopy. Using such a combination, the high spatial and topographical resolution obtained with an AFM can be directly linked to the chemical information provided by confocal Raman microscopy. True Surface Microscopy, allows confocal Raman imaging guided by the surface topography obtained by an integrated non-contact optical profilometer. Large-area topographic coordinates from the chromatic confocal profilometer can be precisely correlated with the large area confocal Raman imaging data. This allows true surface Raman imaging on heavily inclined or rough surfaces, with the sample surface held in constant focus, while maintaining highest confocality. In summary, the combination of confocal Raman microscopy with AFM and true surface microscopy allows the characterization of materials at high, submicron resolution, as well as on mm-rough surfaces across large areas.

1:15PM J1.00009 Local 2D-2D tunneling in high mobility electron systems, MATTHEW PELLICCIONE, ADAM SCIAMBI, JOHN BARTEL, DAVID GOLDBERGER-GORDON, Stanford University, LOREN PFEIFFER, KEN WEST, Princeton University, MICHAEL LILLY, Sandia National Laboratory, SETH BANK, University of Texas, Austin, ARTHUR GOSSARD, University of California, Santa Barbara — Many scanning probe techniques have been utilized in recent years to measure local properties of high mobility two-dimensional (2D) electron systems in GaAs. However, most techniques lack the ability to tunnel into the buried 2D system and measure local spectroscopic information. We report scanning gate measurements on a bilayer GaAs/AlGaAs heterostructure that allows for a local modulation of tunneling between two 2D electron layers. We call this technique Virtual Scanning Tunneling Microscopy (VSTM) [1,2] as the influence of the scanning gate is analogous to an STM tip, except at a GaAs/AlGaAs interface instead of a surface. We will discuss the spectroscopic capabilities of the technique, and show preliminary results of measurements on a high mobility 2D electron system.
[1] A. Sciambi, M. Pelliccione *et al.*, Appl. Phys. Lett. **97**, 132103 (2010).
[2] A. Sciambi, M. Pelliccione *et al.*, Phys. Rev. B **84**, 085301 (2011).

1:27PM J1.00010 Infrared Phonon Fingerprinting of Nanocrystals through Broadband Near-Field Spectroscopy, ALEXANDER S. MCLEOD, University of California, San Diego, GERARDO DOMINGUEZ, California State University, San Marcos, PRISCILLA KELLY, MARK THIEMENS, University of California, San Diego, LINGFENG M. ZHANG, University of California, San Diego; Boston University, ALEX RODIN, MICHAEL M. FOGLER, University of California, San Diego, FRITZ KEILMANN, Max Planck Institute of Quantum Optics and Center for NanoScience, D.N. BASOV, University of California, San Diego — Near-field infrared spectroscopy has recently been demonstrated with the capability to resolve optical properties of sub-wavelength sample areas across a broad range of infrared frequencies. This method holds promise for the direct identification of sub-wavelength chemical composition in nanostructured and heterogeneous samples. We apply this technique to the study of phonon-resonant silicon carbide nanocrystals tens of nanometers in size using an apertureless scanning near-field optical microscope (SNOM) coupled to a pulsed broadband infrared laser source and FTIR spectrometer. We present measurements of nanocrystal near-field spectra in the range of $700\text{--}1200 \text{ cm}^{-1}$ evaluated in comparison with the near-field spectra of bulk silicon carbide, calibrated using ellipsometry. A detailed analytic model of the probe-sample near-field interaction is applied for the identification of nanoscale resonant size effects. These techniques provide a powerful method for identifying and characterizing sub-wavelength nanocrystals in heterogeneous samples via near-field infrared “phonon fingerprinting.”

1:39PM J1.00011 Creation of Electron Trap States in Silicon Dioxide By Local Electron Injection¹, DUSTIN WINSLOW, CLAYTON WILLIAMS, University of Utah — Over a decade ago, the Scanning Tunneling Microscope was shown capable of desorbing single hydrogen atoms from the surface of hydrogen terminated silicon.² The resultant dangling bonds can act as atomic scale quantum dots.³ Electrons trapped in such dangling bond states at the surface of crystalline silicon have short retention times at room temperature, due to the proximity of the occupied state energy level to the conduction band. Here we report on a method for creating electron trap states at the surface of a silicon dioxide film by electron injection from a metalized Atomic Force Microscope probe tip. Single Electron Tunneling Force measurements⁴ are employed to examine the existence of trap states in the silicon dioxide surface before and after the electron injection. Evidence for electron trap state creation, without topographic modification of the silicon dioxide surface, will be presented. The trap states created by this process have electron retention times which are greater than one second at room temperature. The methodology for trap state creation and detection will be presented.

¹Work supported by ARO Grant No. W911 NF-1 0-1-0315

²T.C. Shen *et. al.* Science 268, 1590 (1995).

³M. B Haider *et. al.* PRL 102, 046805 (2009).

⁴E. Bussmann, *et. al.* Appl. Phys. Lett., 85, 13 (2004).

1:51PM J1.00012 Nm-scale Mapping of Thermally-Activated Trap Emission in an AlGaIn/GaN High Electron Mobility Transistor, D. CARDWELL, A.R. AREHART, S.A. RINGEL, J.P. PELZ, The Ohio State University — AlGaIn/GaN high electron mobility transistors (HEMTs) are intrinsically ideal for high frequency and high power applications, but have degraded performance due to charge trapping. Nm-scale AFM-based electrical measurements sensitive to the emission of trapped charge, such as scanning Kelvin probe microscopy (SKPM), can, in principle, be used to determine the energies, cross sections, and densities of electrically-active traps with high spatial resolution. Using SKPM, we obtain nm-scale surface potential transient (SPT) maps over the entire surface of an AlGaIn/GaN HEMT. Surprisingly, we find significant SPTs near the edges of the device that are similar to conductance transients, and whose time constants vary with temperature, indicating thermally-activated emission. Comparison of nm-scale measurements and electrostatic simulations will be discussed to quantify the spatial distribution of trapped charge near the edge of the device. Work supported by ONR-DRIFT (P. Maki).

2:03PM J1.00013 Stochastic switching of microcantilever motion¹, WARNER VENSTRA, HIDDE WESTRA, HERRE VAN DER ZANT, Kavli Institute of Nanoscience — Fluctuation-induced transitions between two stable states of a strongly driven microcantilever are studied. Intrinsic geometric and inertial nonlinearities of the cantilever give rise to an amplitude-dependent resonance frequency, and at a critical point bifurcation occurs. Two states are stable, represented by vibration at a low and a high amplitude. Adding noise facilitates transitions between the states. The transition rate rises upon increasing noise intensity, as expected for noise-activated escape from a dynamic double well. Further increasing the noise intensity causes a parametric change in the dynamic double well, and results in a decay of the switching rate. Close to the onset of spontaneous transitions, the bistable cantilever is very sensitive. We demonstrate the noise-enhanced detection of weak modulations of the bistable cantilever, resulting in an optimum signal-to-noise ratio at non-minimum noise intensity.

¹Financial support: FOM Program 10: Physics for Technology

Tuesday, February 28, 2012 11:15AM - 2:15PM –

Session J2 FEd: Invited Session: K-12 Science Education: Closing the Gap with the Leading Nations 204AB

11:15AM J2.00001 A Framework for K-12 Science Education, HELEN QUINN, Stanford University — I will discuss the content and purpose of the NRC study report “a framework for K-12 science education” and report on the ongoing project led by Achieve, in which over 20 states are engaged to develop science standards based on this document.

11:51AM J2.00002 The Globalization of Science Education, GEORGE DEBOER, AAAS Project 2061 — Standards-based science education, with its emphasis on clearly stated goals, performance monitoring, and accountability, is rapidly becoming a key part of how science education is being viewed around the world. Standards-based testing within countries is being used to determine the effectiveness of a country's educational system, and international testing programs such as PISA and TIMSS enable countries to compare their students to a common standard and to each other. The raising of standards and the competition among countries is driven in part by a belief that economic success depends on a citizenry that is knowledgeable about science and technology. In this talk, I consider the question of whether it is prudent to begin conversations about what an international standards document for global citizenship in science education might look like. I examine current practices to show the areas of international agreement and the significant differences that still exist, and I conclude with a recommendation that such conversations should begin, with the goal of laying out the knowledge and competencies that international citizens should have that also gives space to individual countries to pursue goals that are unique to their own setting.

12:27PM J2.00003 Physics For All – yes, it's real physics, ARTHUR EISENKRAFT, University of Massachusetts Boston — Can “all” students learn “real” physics? We want to provide instruction to a wider segment of the population including those students who will not go into STEM (Science, Technology, Engineering, Math) careers. We also want to maintain the integrity of physics, challenge all students, and not compromise the rigor of our courses. Accomplishing this requires a research guided approach to instruction, curriculum and assessment. Physics First and Physics for All have become a success story for thousands of students in urban, suburban, and rural districts. At the same time, the International Physics Olympiad and other competitions have raised the expectation of what the most motivated students can achieve. Many physics educators are exploring ways to set higher goals for our most gifted students while also providing physics instruction to students previously excluded from our physics classes. Many of the same issues that K-12 educators are struggling with are equally important to the college community as colleges try to educate both future physicists and an educated citizenry. Great novels and symphonies are accessible to people of different backgrounds and levels of expertise. We should develop strategies that enable us to share an understanding of physics with all students because everyone deserves an opportunity to reflect on the wondrous workings of our universe.

1:03PM J2.00004 An Introduction to the new AP Physics algebra-based program: A new focus on best practices¹, GAY STEWART, University of Arkansas, Fayetteville — Advanced Placement (AP) credit was always designed to represent good college courses. After a call from the NRC, the College Board undertook a redesign of the AP Science courses to improve the quality of teaching and learning in the nation's high schools, modeling best practices at the college level. The Physics Redesign has focused on the AP Physics B course, the equivalent of the algebra-based introductory college physics course. This talk will focus on the background to this undertaking, the process that was followed, and the resulting courses. The impact these changes will have on current teaching practices will be discussed. Currently, Physics B is supposed to follow a preparatory course. Now, the material is divided up and deepened to make each year a stand-alone, rigorous, conceptual and problem-solving course. The significantly deeper conceptual level for the newly designed course allows teachers more time for inquiry-based, student-centered learning. Because of the two-course design, the first year will be accessible to more students. These can be placed flexibly into a school's curriculum; examples will be discussed. Examples from the new curriculum framework for these courses will be presented.

¹Thanks to the NSF for support in the early phases of the redesign.

1:39PM J2.00005 The Role of Pre-College Preparation in College Physics Success¹, PHILIP SADLER, Harvard-Smithsonian Center for Astrophysics — There is no shortage of, often contradictory, opinions concerning how best to prepare students for college physics, but personal experience is a poor substitute for rigorous investigation. After collecting data from 11,000 science students and their instructors at randomly chosen colleges and universities, we can offer a more universal picture of the middle school to college learning progression in physics. Using epidemiological methods to mine the backgrounds of students taking introductory physics courses, we find predictors of performance and persistence while controlling for demographic differences. I will report on our findings on the value of middle school physical science preparation, lab experiences, technology use, classroom demonstrations, coverage, block scheduling, Advanced Placement, Physics First, project work, and facility in mathematics.

¹The work has been supported by NSF projects: GSE/RES 624444 Persistence Research in Science and Engineering and 635090, Synthesis of Research on Advanced High School Coursework in Science and Mathematics.

Tuesday, February 28, 2012 11:15AM - 2:15PM –

Session J3 GQI DCMP: Invited Session: Quantum Computing with Superconducting Circuits 205AB

11:15AM J3.00001 Continuous High-Fidelity Monitoring of a Superconducting Qubit: From Quantum Jumps to Feedback¹, I. SIDDIQI, QNL, University of California, Berkeley — Great advances have been made in superconducting qubit technology since the first demonstration of coherent oscillations more than 10 years ago. Continuous, high-fidelity monitoring of the qubit state, however, has remained an elusive target. We demonstrate this functionality by using a wide-bandwidth superconducting parametric amplifier operating near the quantum noise limit to read out the state of a transmon qubit coupled to a linear resonant cavity. Depending on the qubit-cavity detuning and the cavity photon occupation, two different measurement regimes can be accessed. In the strong measurement regime, the qubit states are fully resolved in a time much shorter than T_1 . This permits the observation of quantum jumps between qubit states in real time, and enables the study of the quantum Zeno effect and measurement non-idealities. In the weak measurement regime, information is extracted slowly and the measurement is no longer projective on short time scales. However, the measurement record is still highly correlated with the qubit dynamics and can be used to steer the qubit state using feedback. We demonstrate this idea by phase-locking Rabi oscillations to a classical reference. This allows the oscillations to persist indefinitely, albeit with a reduced amplitude indicative of the efficiency of the feedback protocol.

¹This research is supported by the ARO QCT program.

11:51AM J3.00002 Observation of the dynamical Casimir effect in a superconducting circuit, CHRISTOPHER WILSON, Chalmers University — Modern quantum theory predicts that the vacuum of space is not empty, but instead teeming with virtual particles flitting in and out of existence. While initially a curiosity, it was quickly realized that these vacuum fluctuations had measurable consequences, for instance producing the Lamb shift of atomic spectra and modifying the magnetic moment for the electron. This type of renormalization due to vacuum fluctuations is now central to our understanding of nature. 40 years ago, Moore suggested that a mirror undergoing relativistic motion could convert virtual photons into directly observable real photons. This effect was later named the dynamical Casimir effect (DCE). Using a superconducting circuit, we have observed the DCE for the first time. The circuit consists of a coplanar transmission line with an *electrical length* that can be changed at a substantial fraction of the speed of light. The length is changed by modulating the inductance of a superconducting quantum interference device (SQUID) at high frequencies (> 10 GHz). In addition to observing the creation of real photons, we observe two-mode squeezing of the emitted radiation, which is a signature of the quantum character of the generation process.

12:27PM J3.00003 Towards a scalable superconducting qubit architecture, MATTHIAS STEFFEN, IBM — I will review IBM's current approach towards building a scalable superconducting qubit architecture. The goal is to build a system using quantum error correction schemes based on two-dimensional surface codes, which are predicted to have a remarkably low fault tolerant threshold. I will briefly outline the particular skew-square lattice configuration and describe the concept of logical qubits and gates. On the experimental side, I will show recent advances towards implementing such surface code. This includes improvements in qubit coherence times, now exceeding $T_1=5\mu s$ reliably, achieved by shielding the sample from infrared radiation confirming other recent results. Additional approaches leading to even longer coherence times are reviewed. With improved coherence times we show improved gate fidelities of two-qubit gates based the cross-resonance effect – an all microwave approach towards implementing two-qubit gates. I will conclude by reviewing some interesting future engineering challenges that should be addressed on our way towards building a quantum computer.

1:03PM J3.00004 The Photon Shell Game and the Quantum von Neumann Architecture with Superconducting Circuits¹, MATTEO MARIANTONI, Department of Physics and California NanoSystems Institute, University of California, Santa Barbara, CA 93106-9530, USA — Superconducting quantum circuits have made significant advances over the past decade, allowing more complex and integrated circuits that perform with good fidelity. We have recently implemented a machine comprising seven quantum channels, with three superconducting resonators, two phase qubits, and two zeroing registers. I will explain the design and operation of this machine, first showing how a single microwave photon $|1\rangle$ can be prepared in one resonator and coherently transferred between the three resonators. I will also show how more exotic states such as double photon states $|2\rangle$ and superposition states $|0\rangle + |1\rangle$ can be shuffled among the resonators as well [1]. I will then demonstrate how this machine can be used as the quantum-mechanical analog of the von Neumann computer architecture, which for a classical computer comprises a central processing unit and a memory holding both instructions and data. The quantum version comprises a quantum central processing unit (quCPU) that exchanges data with a quantum random-access memory (quRAM) integrated on one chip, with instructions stored on a classical computer. I will also present a proof-of-concept demonstration of a code that involves all seven quantum elements: (1), Preparing an entangled state in the quCPU, (2), writing it to the quRAM, (3), preparing a second state in the quCPU, (4), zeroing it, and, (5), reading out the first state stored in the quRAM [2]. Finally, I will demonstrate that the quantum von Neumann machine provides one unit cell of a two-dimensional qubit-resonator array that can be used for surface code quantum computing. This will allow the realization of a scalable, fault-tolerant quantum processor with the most forgiving error rates to date.

[1] M. Mariantoni *et al.*, Nature Physics 7, 287-293 (2011.)

[2] M. Mariantoni *et al.*, Science 334, 61-65 (2011).

¹Matteo Mariantoni acknowledges support from an Elings Postdoctoral Fellowship. This work was supported by IARPA under ARO award W911NF-08-1-0336 and W911NF-09-1-0375.

1:39PM J3.00005 Realization of Three-Qubit Quantum Error Correction with Superconducting Circuits, MATTHEW REED, Yale University — Quantum computers promise to solve certain problems exponentially faster than possible classically but are challenging to build because of their increased susceptibility to errors. Remarkably, however, it is possible to detect and correct errors without destroying coherence by using quantum error correcting codes. The simplest of these are the three-qubit codes, which map a one-qubit state to an entangled three-qubit state and can correct any single phase-flip or bit-flip error of one of the three qubits, depending on the code used [1]. The fidelity of a process in which errors can occur on all qubits, where there is the possibility of an uncorrectable double or triple error, should therefore decrease only quadratically with error probability. I will first introduce how the three-qubit encoded state can be produced in our superconducting architecture by employing interactions with non-computational qubit states, as previously demonstrated [2]. I will then discuss how these non-computational interactions can be generalized to produce a novel three-qubit conditional-conditional NOT (CCNot) or Toffoli gate, which implements the correcting step of an error correction algorithm. Finally, I will explain how, by combining these ingredients, we have performed a single pass of both quantum bit- and phase-flip error correction and have demonstrated the predicted first-order insensitivity to errors.

[1] M. A. Nielsen and I. L. Chuang, Cambridge University Press, 2000.

[2] L. DiCarlo, et al. Nature 467, 574 (2010).

Tuesday, February 28, 2012 11:15AM - 2:15PM – Session J4 DAMOP: Non-Equilibrium Dynamics with Quantum Gases 205C

11:15AM J4.00001 Non Equilibrium Quantum Criticality: an intuitive approach, EMANUELE DALLA TORRE, EUGENE DEMLER, Department of Physics, Harvard University, THIERRY GIAMARCHI, DPMC-MaNEP, University of Geneva, Switzerland, EHUD ALTMAN, Department of Condensed Matter Physics, Weizmann Institute of Science, Israel — Since their discovery in 1976, equilibrium quantum critical points have attracted continuous interest, due to their universality (i.e. the independence from the microscopic details of the systems). In two recent papers [1,2] we have extended these concepts to non-equilibrium systems, by studying the universal properties of quantum systems driven by time-dependent noise. We were able to demonstrate that [1] they can show a new class of non-equilibrium quantum criticality, and [2] small perturbations around the critical point lead to new physical phenomena, such as the spontaneous generation of an effective temperature and an effective dissipation. To this end, we developed a real-time renormalization group (RG) in the Keldysh path-integral formalism, which may however appear cryptic to the non-experts. In this talk, I will show how the main conclusions of the RG approach can be understood by simpler arguments based on circuit theory and fluctuation-dissipation relations.

[1] E.G. Dalla Torre, et al. "Quantum critical states and phase transitions in the presence of non-equilibrium noise," Nature Physics 6, 806 (2010)

[2] E.G. Dalla Torre, et al. "Dynamics and universality in noise driven dissipative systems," arXiv: 1110.3678 (2011)

11:27AM J4.00002 Dynamics of noise correlations of ultracold bosons in an optical lattice, KHAN W. MAHMUD, EITE TIESINGA, Joint Quantum Institute, NIST and University of Maryland, USA — We study second order correlations of ultracold bosons in an optical lattice for superfluid and Mott insulating phases. Starting with a superfluid ground state, a sudden increase in the lattice depth projects it into a non-equilibrium state. We examine the subsequent dynamics of the system - analyzing noise correlations of the atomic cloud after time-of-flight expansion. We also investigate the effects of three and higher-body interactions on noise correlations in deep lattices.

11:39AM J4.00003 Stability of Counterflow Superfluidity¹ , NOAH BRAY-ALI, CARL WILLIAMS, Joint Quantum Institute, NIST and University of Maryland, 100 Bureau Drive, Stop 8423, Gaithersburg, MD 20899-8423, USA, EUGENE DEMLER, Department of Physics, Harvard University, Cambridge MA 02138 — We examine the stability of the counterflow superfluid state in two component mixtures of ultracold atoms in optical lattices. Using a Gutzwiller mean-field approach, we find a sharp boundary separating stable counterflow from a dynamically unstable regime. As the inter-component interaction strength increases, the critical counterflow rate drops, falling to zero when interactions are strong enough to induce phase separation of the two components. Going beyond mean-field theory, we compute the decay rate of counterflow within the stable regime due to phase slips. The results agree well with numerically exact simulations and are calculated in a regime of parameters relevant to current experiments on mixtures of ultracold alkali atoms.

¹NBA acknowledges support from the National Research Council Postdoctoral Research Associateship

11:51AM J4.00004 Fermion Dynamics from Gross-Pitaevskii-like Equations , MICHAEL FORBES, Institute for Nuclear Theory, University of Washington, RISHI SHARMA, TRIUMF — The dynamics of condensed fermions (i.e. the Unitary Fermi Gas) play a key role in understanding a range of physical systems, from dynamics in rotating traps of cold atoms, to explaining pulsar glitches in neutron stars. Density functional theory (DFT) provides a powerful tool for modeling these dynamics, but unfortunately, simulating even a few vortices requires the use of leadership class computing. This talk will address the efficacy of using modified Gross-Pitaevskii (GP) like equations to model the dynamics of Fermi systems. These GP-like equations are significantly easier to solve, yet still capture much of the relevant physics. We shall advocate an approach of using fermionic DFT to adjust the form of the modified GP-like equations, and then using the latter to model more complicated phenomena beyond the capability of the fermionic DFT. The dynamics of vortices pinned on defects will serve as an example.

12:03PM J4.00005 Expansion of Bose-Hubbard Mott insulators in optical lattices¹ , MARK JREIS-SATY, Department of Mechanical Engineering, Columbia University, New York NY 10025, USA, JUAN CARRASQUILLA, Department of Physics, Georgetown University, Washington DC 20057, USA, F. ALEXANDER WOLF, Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, Augsburg University, D-86135 Augsburg, Germany, MARCOS RIGOL, Department of Physics, Georgetown University, Washington DC 20057, USA — We present a study of the expansion of bosonic Mott insulators in the presence of an optical lattice after switching off a confining potential. We use the Gutzwiller mean-field approximation and consider two different setups. In the first one, the expansion is restricted to one dimension. We show that this leads to the emergence of two condensates with well-defined momenta, and argue that such a construct can be used to create atom lasers in optical lattices. In the second setup, we study Mott insulators that are allowed to expand in all directions in the lattice. In this case, a simple condensate is seen to develop within the mean-field approximation. However, its constituent bosons are found to populate many nonzero momentum modes. An analytic understanding of both phenomena in terms of the exact dispersion relation in the hard-core limit is presented.

¹This work was supported by the US Office of Naval Research.

12:15PM J4.00006 Protection of dissipative quantum state preparation by interlacing the control with dynamical decoupling pulses¹ , Z.R. GONG, WANG YAO, Department of Physics, and Center for Theoretical and Computational Physics, The University of Hong Kong — Various dissipative processes have recently been exploited for preparing quantum state with multipartite entanglement between many qubits. Most such schemes are applicable only to an ensemble of identical qubits, and inhomogeneous broadening will reduce the state preparation fidelity. Here we show that by interlacing the dynamical decoupling pulse sequence with the dissipative state preparation control, the errors resulting from the inhomogeneous broadening can be suppressed up to certain order of the pulse interval and the desired entangled states can be prepared with high fidelity. We give two examples where sequence of π pulses interlaced with dissipative control realize high fidelity preparation of cluster states and many-body singlets of atomic qubits.

¹The work was supported by the Research Grant Council of Hong Kong under Grant No. HKU 706711P.

12:27PM J4.00007 ABSTRACT MOVED TO L4.00008 —

12:39PM J4.00008 Periodically and almost periodically driven quantum system , LUCA D'ALESSIO, ANATOLI POLKOVNIKOV, Boston University — When a quantum system is driven periodically in time it can display dynamical localization, i.e its energy grows extremely slowly and may saturate at a value smaller than the infinite temperature limit. We show that by making the period of the perturbation longer this phenomenon is destroyed and the energy of the system grows quickly and saturates at the infinite temperature limit. We argue that this process is related to the breaking down of a particular form of perturbation theory (in the duration in of driving) and can be interpreted as a transition from a local to a long-range effective Hamiltonian. We discuss how robust our findings are against small aperiodicity in the driving. We finally discuss how realize this interesting non-equilibrium physics in cold atom experiments.

12:51PM J4.00009 Cold bosons in noisy optical lattices , JOHANNES SCHACHENMAYER, Department of Physics and Astronomy, University of Pittsburgh, HANNES PICHLER, PETER ZÖLLER, Institute for Theoretical Physics, University of Innsbruck, and Institute for Quantum Optics and Quantum Information, Innsbruck, ANDREW DALEY, Department of Physics and Astronomy, University of Pittsburgh — Cold atoms in optical lattices open the possibility to experimentally study strongly interacting many-body quantum systems with controllable parameters. A key challenge to prepare interesting quantum states in these systems is to achieve sufficiently low temperatures. At these temperatures a deep theoretical understanding of possible heating processes and how they affect the characteristics of the quantum state becomes essential. In every realistic experiment there exist many sources of noise that cause phase and amplitude fluctuations in the standing laser waves that form the optical lattice potential. This classical noise can lead to heating and a significant change of the quantum state. We study the stochastic many-body non-equilibrium dynamics of bosons in an optical lattice and determine how the state changes depending on the characteristics of the noise. We do this by solving time-dependent stochastic many-body Schrödinger equations, both analytically and numerically.

1:03PM J4.00010 Many-body Landau-Zener Transition in Cold Atom Double Well Optical Lattices , YINYIN QIAN, MING GONG, CHUANWEI ZHANG, Washington State University — Ultra-cold atoms in optical lattices provide an ideal platform for exploring many-body physics of a large system arising from the coupling among a series of small identical systems whose few-body dynamics are exactly solvable. Using Landau-Zener (LZ) transition of bosonic atoms in double well optical lattices as an experimentally realizable model, we investigate such few to many body route by exploring the relation and difference between the few-body (in one double well) and many-body (in double well lattice) non-equilibrium dynamics of cold atoms in optical lattices. We find the many-body coupling between double wells greatly enhances the LZ transition probability, while keeping the main features of the few-body dynamics. Various experimental signatures of the many-body LZ transition, including atom density, momentum distribution, and density-density correlation, are obtained.

1:15PM J4.00011 Quasi steady-states, spin statistics, and interaction-induced transport of ultra-cold atoms in 1D optical lattices¹, CHIH-CHUN CHIEN, Los Alamos National Laboratory, MICHAEL ZWOLAK, Oregon State University, MASSIMILIANO DI VENTRA, University of California, San Diego — We consider several non-equilibrium scenarios where ultra-cold atoms are initially loaded into the ground state of a 1D optical lattice. The system is then set out of equilibrium either by inducing a density imbalance or by imposing time-dependent inhomogeneous interactions. To monitor the dynamics, we have implemented the micro-canonical approach to transport [1] which has been previously used to study electron dynamics in nanoscale systems. We have found that by removing particles on the right half of the lattice, fermions form a quasi steady-state current, which can be observed as a plateau in the current as a function of time. In contrast, the bosonic current oscillates and decays to zero in the thermodynamic limit [2]. The difference appears in uniform lattices as well as lattices with a harmonic trap. Further, when light-induced interactions are applied to half of the lattice, we have found, using a Hartree-Fock approximation, a conducting-nonconducting transition in the fermionic case as the interaction increases. Our studies are relevant to recent experiments on transport of ultra-cold atoms and address fundamental issues in nanoscale electronic transport.

[1] Di Ventra and Todorov, J. Phys. Cond. Matt. 16, 8025 (2004).

[2] Chien, Zwolak, Di Ventra, arXiv: 1110.1646.

¹Work supported in part by DOE.

1:27PM J4.00012 Spin Caloritronics in Noncondensed Bose Gases, CLEMENT WONG, HEDWIG VAN DRIEL, RAKPONG KITTINARADORN, HENK STOOF, REMBERT DUINE, Utrecht University — We consider coupled spin and heat transport in a two-component, atomic Bose gas in the noncondensed state. We find that the transport coefficients show a temperature dependence reflecting the bosonic enhancement of scattering, and discuss experimental signatures of the spin-heat coupling in spin accumulation and total dissipation. Inside the critical region of Bose-Einstein condensation, we find anomalous behavior of the transport coefficients, and in particular, an enhancement for the spin caloritronics figure of merit that determines the thermodynamic efficiency of spin-heat conversion.

1:39PM J4.00013 Universal energy fluctuations in thermally isolated driven systems, GUY BUNIN, Department of Physics, Technion, LUCA D'ALESSIO, Department of Physics, Boston University, YARIV KAFRI, Department of Physics, Technion, ANATOLI POLKOVNIKOV, Department of Physics, Boston University — When an isolated system is brought in contact with a heat bath, its final energy is random and follows the Gibbs distribution—this finding is a cornerstone of statistical physics. The system's energy can also be changed by performing non-adiabatic work using a cyclic process. Almost nothing is known about the resulting energy distribution in this set-up, which is in particular relevant to recent experimental progress in cold atoms, ion traps, superconducting qubits and other systems. Here we show that when the non-adiabatic process consists of many repeated cyclic processes, the resulting energy distribution is universal and different from the Gibbs ensemble. We predict the existence of two qualitatively different regimes with a continuous second-order-like transition between them. We illustrate our approach by performing explicit calculations for both interacting and non-interacting systems.

1:51PM J4.00014 Lie-algebraic Approach to Dynamics of Closed Quantum Systems and Quantum-to-Classical Correspondence¹, VICTOR GALITSKI, Joint Quantum Institute and Physics Department, University of Maryland — I will briefly review our recent work on a Lie-algebraic approach to various non-equilibrium quantum-mechanical problems, which has been motivated by continuous experimental advances in the field of cold atoms. First, I will discuss non-equilibrium driven dynamics of a generic closed quantum system. It will be emphasized that mathematically a non-equilibrium Hamiltonian represents a trajectory in a Lie algebra, while the evolution operator is a trajectory in a Lie group generated by the underlying algebra via exponentiation. This turns out to be a constructive statement that establishes, in particular, the fact that classical and quantum unitary evolutions are two sides of the same coin determined uniquely by the same dynamic generators in the group. An equation for these generators - dubbed dual Schrödinger-Bloch equation - will be derived and analyzed for a few of specific examples. This non-linear equation allows one to construct new exact non-linear solutions to quantum-dynamical systems. An experimentally-relevant example of a family of exact solutions to the many-body Landau-Zener problem will be presented. One practical application of the latter result includes dynamical means to optimize molecular production rate following a quench across the Feshbach resonance.

¹This work was supported by NSF-CAREER award and US-ARO.

2:03PM J4.00015 Visibility of the Amplitude (Higgs) Mode in Condensed Matter and Cold Atomic Systems, DANIEL PODOLSKY, ASSA AUERBACH, Physics Department, Technion - Israel Institute of Technology, DANIEL P. AROVAS, Department of Physics, University of California at San Diego — The amplitude mode is a ubiquitous collective excitation in condensed matter systems with broken continuous symmetry. It is expected in antiferromagnets, short coherence length superconductors, charge density waves, and lattice Bose condensates. Its detection is a valuable test of the corresponding field theory, and its mass gap measures the proximity to a quantum critical point. However, since the amplitude mode can decay into low energy Goldstone modes, its experimental visibility has been questioned. Here we show that the visibility depends on the symmetry of the measured susceptibility. We discuss various experimental setups for measuring the scalar susceptibility. We show that the optical conductivity of the O(2) theory (relativistic superfluid) displays a threshold behavior at the Higgs mass.

Tuesday, February 28, 2012 11:15AM - 1:51PM –

Session J5 DMP: Focus Session: Interfaces in Complex Oxides - Electronic Structure 206A

11:15AM J5.00001 Angle resolved photoemission spectroscopy of the electronic structure of complex oxide interfaces, KYLE SHEN, Cornell University — Engineering interfaces between complex oxides has proven to be a powerful technique for tuning their electronic and magnetic properties. To fully understand how these interfaces can control these electronic properties, one requires advanced spectroscopic tools to uncover their electronic structure. Angle-resolved photoemission spectroscopy (ARPES) is the leading tool for probing energy and momentum resolved electronic structure. To understand the physics of these complex oxide interfaces, we have developed an approach which combines state-of-the-art oxide molecular beam epitaxy with high-resolution ARPES. As one example, we describe our work on oxide superlattices $[\text{LaMnO}_3]_{2n} / [\text{SrMnO}_3]_n$ with alternating LaMnO_3 and SrMnO_3 blocks. Our ARPES measurements reveal that as a function of separation between the LaMnO_3 - SrMnO_3 interfaces, the interfacial quasiparticle states evolve from a quasi-three-dimensional ferromagnetic metal, to a two-dimensional spin-polarized electron liquid, and ultimately to a pseudogapped ferromagnetic insulator with increasing superlattice thickness, n . I will also describe our work on other oxide thin films SrTiO_3 and Sr_2TiO_4 -based interfaces where the quasiparticle interactions can be tuned as a function of dimensionality, and work on cuprate and ruthenate thin films.

11:51AM J5.00002 Spectral and spatial redistribution at the $\text{LaAlO}_3/\text{SrTiO}_3$ interface, T. GUENTER, A. RUBANO, T. FINK, HISKP, University Bonn, Germany, D. PAPARO, F. MILETTO GRANOZIO, U. SCOTTI DI UCCIO, L. MARRUCCI, Dip. di Scienze Fisiche, University Naples, Italy, J. MANNHART, MPI for Solid State Research, Stuttgart, Germany, M. FIEBIG, Materials Department, ETH Zürich, Switzerland — A conductive two-dimensional electron liquid (2DEL) appears at the $\text{LaAlO}_3/\text{SrTiO}_3$ (LAO/STO) interface for a LAO thickness of $n \geq 4$ unit cells. Despite the tremendous research interest, many questions regarding the origin and characteristics of the 2DEL have to be addressed yet. In particular, this includes the electronic structure of the “buried interface.” Optical second harmonic generation (SHG) is an ideal tool for studying interfaces, since it is sensitive to the interfacial symmetry breaking along the stacking direction. Using SHG with frequency-tunable amplified femtosecond laser pulses we obtain information about the structural reorganization of the interfacial STO conduction band for SHG photon energies up to 6.2 eV. A massive spectral weight redistribution is present for $n \geq 3$, indicating a global reorganization of the conduction band structure. At low temperatures the spectral resolution is enhanced which alleviates the distinction of interfacial electronic transitions. Additionally, we discuss the modification of the interfacial states by variation of the STO surface termination. Our data are supported by a theoretical framework based on symmetry selection rules that allows a specific assignment of interfacial $\text{O}(2p)\text{-Ti}(3d)$ transitions to the SHG spectrum.

12:03PM J5.00003 Electronic properties of $\text{LaAlO}_3/\text{SrTiO}_3$ superlattices: interface charge density, Fermi surfaces, plasmon and optical spectra¹, SE YOUNG PARK, ANDREW J. MILLIS, Columbia University — We present calculations of the charge density profile, Fermi surface topology, plasmon and optical excitation spectra of the electron gas at the $\text{LaAlO}_3/\text{SrTiO}_3$ interface. The calculations are based on a self-consistent Hartree/RPA approximation and a tight binding parametrization of the band structure. The subband occupancy is determined as a function of polar discontinuity magnitude and dielectric constant. The number of occupied xy bands changes significantly whereas for all reasonable polar discontinuity and dielectric constant profiles only one yz and one xz bands are occupied. These yz and xz band give dominant contributions to the long-distance tail of the interface charge. The plasmon and optical absorption spectra are determined. The results are compared with experimental data.

¹Support: DOE ER-046169 and the Kwanjeong education foundation

12:15PM J5.00004 Direct observations of the band alignment of $\text{LaAlO}_3/\text{SrTiO}_3$ using scanning tunneling microscopy, Y.P. CHIU, B.C. HUANG, P.C. HUANG, Department of Physics, National Sun Yat-sen University, Kaohsiung, 804, Taiwan, V.T. TRA, J.Y. LIN, Institute of Physics, National Chiao Tung University, Hsinchu, 300, Taiwan, J.C. YANG, Y.H. CHU, Department of Materials Science and Engineering, National Chiao Tung University, HsinChu, 300, Taiwan — In this work, by using cross-sectional scanning tunneling microscopy, local and direct evidence of the electronic information across the $\text{LaAlO}_3/\text{SrTiO}_3$ hetero-interfaces are investigated. A combination of scanning tunneling spectroscopy and analysis with atomic resolution across the hetero-interface reveals how the oppositely charged atomic planes undergo electronic reconstructions and introduce a built-in electric field across the polar LaAlO_3 thin films grown on SrTiO_3 substrates. With the consideration of the tip-induced band bending effect, the magnitude of the built-in field across LaAlO_3 , the band bending on SrTiO_3 side, and the decay length of the band downshift of SrTiO_3 side at the hetero-interface are directly observed.

12:27PM J5.00005 Multi-orbital subband structure of transition-metal oxide 2DEGs, PHIL D.C. KING, University of St Andrews, W. MEEVASANA, Suranaree University of Technology, H.Y. HWANG, Z.-X. SHEN, Stanford University, F. BAUMBERGER, University of St Andrews — We demonstrate the creation and control of two-dimensional electron gases (2DEGs) in the 3d and 5d transition metal oxides SrTiO_3 and KTaO_3 . These 2DEGs, of the form usually generated by interface engineering, are created here at the bare oxide surfaces. This permits their detailed spectroscopic investigation using angle-resolved photoemission (ARPES), and we employ this to directly image the d-orbital subband structure of the 2DEGs. We find that quantum confinement lifts the degeneracy of the bulk band structure, driving orbital ordering of the 2DEG. We measure the resulting ladder of light d_{xy} subbands, which co-exist at lower binding energies with heavy d_{xz}/d_{yz} -derived states. The electronic structure revealed by ARPES is in quantitative agreement with our model tight-binding calculations. While the strong spin-orbit coupling of KTaO_3 promotes substantial orbital mixing, our calculations predict only a small Rashba splitting of the 2DEG states, consistent with our experimental measurements where any spin splitting is too small to be resolved. The polar nature of the $\text{KTaO}_3(100)$ surface plays a striking role in mediating formation of the 2DEG as compared to non-polar $\text{SrTiO}_3(100)$, reminiscent of the polar catastrophe at $\text{LaAlO}_3/\text{SrTiO}_3$ interfaces.

12:39PM J5.00006 A Universal Critical Density Underlying the Physics of Electrons at the $\text{LaAlO}_3/\text{SrTiO}_3$ Interface, ARJUN JOSHUA, S. PECKER, J. RUHMAN, E. ALTMAN, S. ILANI, Weizmann Institute of Science — The two-dimensional electron system formed at the interface between the insulating oxides LaAlO_3 and SrTiO_3 exhibits ferromagnetism, superconductivity, and a wide range of unique magnetotransport properties. A key challenge is to find a unified microscopic mechanism that underlies these emergent phenomena. Here we show that a universal Lifshitz transition between d-orbitals lies at the core of the observed transport phenomena in this system. Our measurements find a critical electronic density at which the transport switches from single to multiple carriers. This density has a universal value, independent of the LaAlO_3 thickness and electron mobility. The characteristics of the transition, its universality, and its compatibility with spectroscopic measurements establish it as a transition between d-orbitals of different symmetries. A simple band model, allowing for spin-orbit coupling at the atomic level, connects the observed universal transition to a range of reported magnetotransport properties. Interestingly, we also find that the maximum of the superconducting transition temperature occurs at the same critical transition, indicating a possible connection between the two phenomena. Our observations demonstrate that orbital degeneracies play an important role in the fascinating behavior observed so far in these oxides. Ref: arxiv.org/abs/1110.2184

12:51PM J5.00007 Localization of the Two-dimensional Electron Gas in $\text{LaAlO}_3/\text{SrTiO}_3$ Heterostructures, TOMAS HERNANDEZ, CHUNG WUNG BARK, CHANG-BEOM EOM, MARK S. RZCHOWSKI, University of Wisconsin-Madison — We use low temperature magnetotransport measurements to compare the quasi 2-dimensional electron gas (2DEG) at the $\text{LaAlO}_3/\text{SrTiO}_3$ interface in heterostructures grown on $(\text{LaAlO}_3)_{0.3}\text{-(Sr}_2\text{AlTaO}_6)_{0.7}$ (LSAT) substrates to the 2DEG at the $\text{LaAlO}_3/\text{single crystal SrTiO}_3$ interface. All heterostructures were grown by pulsed laser deposition with *in-situ* reflection high-energy electron diffraction. For the samples on LSAT, we find that increasing the carrier concentration by growing at lower oxygen partial pressures changes the conductivity mechanism, from strongly localized transport at low carrier concentrations to metallic conductivity with indications of weak localization at higher concentrations. We interpret this as an increasing occupation of Ti 3d bands of layers near the interface, changing the spatial extent of the conduction region and its susceptibility to localization by disorder and point defects at the interface. On the other hand, the 2DEG of similarly grown LaAlO_3 on single crystal SrTiO_3 shows metallic behavior and low temperature measurements display Kohler scaling of the out-of-plane magnetoresistance, consistent with classical orbital transport.

1:03PM J5.00008 Localized electron states and phase separation at the $\text{LaAlO}_3/\text{SrTiO}_3$ interface, S. SATPATHY, K.V. SHANAVAS, Department of Physics & Astronomy, University of Missouri — Even though the 2D electron gas at the polar interfaces of LAO/STO has been studied extensively, an explanation for the observed magnetic centers or the coexistence of magnetism and superconductivity is still lacking. Earlier density-functional calculations have indicated the presence of multi-bands and two types of electrons at the interface [1]. Here we propose that a combination of lattice disorder, octahedral rotations, and Jahn-Teller distortion can lead to some of these electrons to be localized near the interface and form lattice polarons. Evidence for this is presented from detailed density-functional calculations, which indicate that the energy gain associated with JT distortion and impurity or disorder induced local potentials can offset the kinetic energy cost of localization. Our model studies [2] also show the possible existence of a phase separation, thereby providing a natural explanation for the coexistence of magnetism and superconductivity [3].

[1] Z. S. Popović, S. Satpathy and R. M. Martin *Phys. Rev. Lett.*, **101**, 256801 (2008)

[2] B. R. K. Nanda and S. Satpathy *Phys. Rev B*, **83**, 195114 (2011)

[3] L. Li *et. al. Nature Physics*, **7**, 762 (2011); J. A. Bert *et. al. ibid*, 767 (2011);

1:15PM J5.00009 Electronic structure, Fermi surfaces, and electron-phonon coupling in La-doped Sr_2TiO_4 and SrTiO_3 ¹, YUEFENG NIE, SHOUVIK CHATTERJEE, BULAT BURGANOV, ERIC MONKMAN, JOHN HARTEY, DANIEL SHAL, Laboratory of Atomic and Solid State Physics, Department of Physics, Cornell University, Ithaca, NY 14853, USA, CHE-HUI LEE, DARRELL SCHLOM, Department of Materials Science and Engineering, Cornell University, Ithaca, New York 14853, USA, KYLE SHEN, Laboratory of Atomic and Solid State Physics, Department of Physics, Cornell University, Ithaca, NY 14853, USA — Sr_2TiO_4 is a quasi-two-dimensional Ruddlesden-Popper structure analogue to SrTiO_3 , and is isostructural with the cuprate parent compound La_2CuO_4 . Although the electronic structure of SrTiO_3 has been well-explored due to its importance in oxide electronics, little is known about the electronic properties of Sr_2TiO_4 . To investigate this, we synthesized epitaxial La doped Sr_2TiO_4 and SrTiO_3 films on (100) LSAT substrates by molecular beam epitaxy (MBE) and investigated the electronic structure using angle-resolved photoemission spectroscopy (ARPES). The electronic structure of 5% La doped Sr_2TiO_4 shows a single electron like band with mostly Ti-3d_{xy} character dispersing across the Fermi surface which corresponds well with LDA calculations. This is in contrast to doped SrTiO_3 where all three t_{2g} bands are degenerate. We also observed signatures of strong electron-phonon coupling in the quasi-two-dimensional Sr_2TiO_4 materials which appear to be absent in three-dimensional SrTiO_3 .

¹The work is supported by the Cornell Center for Materials Research through the National Science Foundation.

1:27PM J5.00010 Theory of SrTiO_3 2DEGs, GURU KHALSA, ALLAN MACDONALD, The University of Texas at Austin — There has been much recent interest in oxide 2DEGS - in particular those involving SrTiO_3 . In spite of the simple conduction band structure of the parent material, there has been no quantitative understanding of the physical properties of these systems. We have built a model, informed by experiment, that is sufficiently realistic to describe defect free surface/interface states in SrTiO_3 . The model is able to account for non-local dielectric screening and the orbital dependence of quantum confinement effects. Preliminary results of the model will be compared with experiment.

1:39PM J5.00011 Conducting band structure in $\text{LaTiO}_3/\text{SrTiO}_3$ interfaces¹, YOUNG JUN CHANG, Advanced Light Source (ALS), LBNL & Fritz-Haber-Institut, LUCA MORESCHINI, AARON BOSTWICK, Advanced Light Source (ALS), LBNL, ANDREW L. WALTER, Advanced Light Source (ALS), LBNL & Fritz-Haber-Institut, KARSTEN HORN, Fritz-Haber-Institut, ELI ROTENBERG, Advanced Light Source (ALS), LBNL — Oxide interfaces between insulating hosts show unexpected conducting carriers, which can be useful for next-generation electronic applications. However, the fundamental understanding of the conducting interfaces remains elusive. Here we report *in situ* angle-resolved photoemission spectroscopy (ARPES) studies in the $\text{LaTiO}_3/\text{SrTiO}_3$ heterostructures, of which layer thicknesses were precisely prepared by pulsed laser deposition in the BL7.0, ALS. We found that the interface generates a high-density electron gas over few unit cells from the junction. We further discuss the orbital characteristics of the interface electronic states with comparison to the recent theoretical calculations. Based on the unit-cell layer resolved electronic structure of the $\text{LaTiO}_3/\text{SrTiO}_3$ interface, we discuss the conducting carriers comparing to the $\text{LaAlO}_3/\text{SrTiO}_3$ interfaces.

¹The ALS is supported by the director of the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under contract DE-AC02-05CH11231. Y. J. C., A. L. W., and K. H. acknowledge the support by the Max Planck Society.

Tuesday, February 28, 2012 11:15AM - 2:15PM –
Session J6 DMP: Focus Session: van der Waals Bonding in Advanced Materials - Layered Structures & Mechanical Properties 206B

11:15AM J6.00001 Improved Description of Soft Layered Materials with van der Waals Density Functional Theory, GABRIELLA GRAZIANO, London Centre for Nanotechnology and Department of Chemistry, University College London, ISIS Facility, Rutherford Appleton Laboratory, JIRI KLIMES, London Centre for Nanotechnology and Department of Chemistry, University College London, FELIX FERNANDEZ-ALONSO, ISIS Facility, Rutherford Appleton Laboratory, Department of Physics, University College London, ANGELOS MICHAELIDES, London Centre for Nanotechnology and Department of Chemistry, University College London — The accurate description of dispersion forces with approaches based on density functional theory has long been a coveted goal and is currently one of the most active areas of research in computational physics/chemistry. We have tested two new functionals, the optimized Becke88 van der Waals (optB88-vdW) and optimized PBE van der Waals (optPBE-vdW) [1, 2] to describe materials where van der Waals interactions dominate. Structural (bond length and interlayer distance) and energetic parameters (atomization and interlayer binding energies) of graphite and hexagonal-boron nitride have been calculated using these functionals and we show that our calculations are in very good agreement with experiments and higher level theoretical calculations. From these calculations it is possible to conclude that optB88- vdW and optPBE-vdW are promising functionals for the accurate description of systems held together mainly by dispersion forces.

[1] Klimeš *et al.*, J. Phys.: Condens. Matter **22**, 022201 (2010).

[2] Klimeš *et al.*, Phys. Rev. B **83**, 195131 (2011).

11:27AM J6.00002 Moiré pattern of a single layer MoS₂ grown on Cu(111)¹, DUY LE, TALAT S. RAHMAN, University of Central Florida — We present results of first principles calculations of the geometric and electronic structures of a single layer of Molybdenum disulfide (MoS₂) on Cu(111) utilizing the van der Waals density functional [1]. The lowest energy Moiré structure consists of (4 × 4) MoS₂ on (5 × 5) Cu(111), in agreement with experimental observation [2]. Examination of the local density of electronic states and charge redistribution shows that the layer is not purely physisorbed on the surface, rather there exists a chemical interaction between it and the Cu surface atoms. Interestingly the MoS₂ film is found to be not appreciably buckled, while the atoms in the top Cu layer gets reorganized and vertically disordered. The sizes of Moiré patterns for a single layer of MoS₂ adsorbed on several other close packed metal surfaces are estimated by minimizing the lattice mismatch between the film and the substrate.

[1] M. Dion *et al*, Phys. Rev. Lett. **92**, 246401 (2004)

[2] D. Kim *et al*, Langmuir **27**, 11650 (2011)

¹Work supported in part by U.S. Department of Energy under grant DE-FG02-07ER15842

11:39AM J6.00003 Observation of tightly bound charged excitons in monolayer MoS₂, KELIANG HE, Case Western Reserve University, KIN FAI MAK, Columbia University, CHANGGU LEE, Sumgkyunkwan University, Suwon, Korea, JIM HONE, TONY HEINZ, Columbia University, JIE SHAN, Case Western Reserve University — Recent advances in the development of atomically thin layers of materials have opened up many new research opportunities. In particular, the transition metal-dichalcogenide molybdenum disulfide (MoS₂) has been shown to cross over from a dark indirect semiconductor to a highly luminescent direct gap material in the limit of monolayer thickness.¹ Here we report results of studies of the optical absorption and photoluminescence of a monolayer MoS₂ field-effect transistor (FET) at 10 K. In the limit of very low doping, the optical properties are dominated by an excitonic feature at ~ 1.9 eV. As the doping density is increased, a new resonance emerges on the low-energy side of the exciton. This feature has been identified as a trion, the bound state of an exciton and an additional electron (or hole). The absorbance and photoluminescence of both the trion and exciton can be tuned by electrostatic doping. A large trion binding energy, exceeding room temperature, is inferred. Our observation can be understood in terms of the dynamical many-body response of a 2D electron gas to the optically created hole and reflects the unusually strong many-body interactions in this 2D system.

¹Mak et al. *Phys. Rev. Lett.* **105**, 136805 (2010); Splendiani et al. *Nano Letters* **10**, 1271-1275, (2010).

11:51AM J6.00004 Beyond graphene: atomic scale structure of quasi-2D van der Waals materials, CHRISTOPHER GUTIERREZ, LIUYAN ZHAO, KIN FAI MAK, PAUL CADDEN-ZIMANSKY, DMITRI EFETOV, TONY F. HEINZ, GEORGE W. FLYNN, PHILIP KIM, ABHAY PASUPATHY, Columbia University, ROBERT J. CAVA, Princeton University — Graphene, a single atomic layer of graphite, has attracted much attention for its unique electronic and mechanical properties. But what role does reduced dimensionality play in other 2D atomic crystals? In this talk we present scanning tunneling microscopy (STM) measurements of the atomic scale structure and spectroscopy of related quasi-2D materials including the transition metal dichalcogenides (TMDs), and their heterostructures with graphene.

12:03PM J6.00005 Here to stay: Stability and structure of (6√3×6√3)-R30° graphene on SiC(111) by all-electron DFT including van der Waals effects, VOLKER BLUM, LYDIA NEMEC, PATRICK RINKE, MATTHIAS SCHEFFLER, Fritz-Haber-Institut, D-14195 Berlin, Germany — SiC is a favorite growth substrate for mono- and few-layer graphene by Si sublimation. On the Si side, large ordered graphene areas can be obtained as commensurate (6√3×6√3)-R30° ("6√3") periodic films [1]. From a thermodynamic perspective, graphene formation competes with several other phases, including graphite on one side, and several Si-rich reconstructions on the other. The question whether 6√3 graphene on SiC(111) is thermodynamically or just kinetically stabilized could be answered by density functional theory (DFT) calculations but for two challenges: (1) The needed surface slab systems are extremely large (up to 2000 atoms in this work), and (2) most standard DFT functionals do not include van der Waals effects. We here show by all-electron DFT including van der Waals effects (PBE+vdW [2]) that the 6√3 graphene-like phases on SiC(111) are thermodynamically stable compared to competing surface phases, and obtain the full structure including the substrate-induced graphene corrugation. The impact of strain in smaller-cell approximants and that of possible graphene defects is discussed. [1] K. Emtsev *et al.*, Nature Materials **8**, 203 (2009). [2] A. Tkatchenko, M. Scheffler, PRL **102**, 073005 (2009).

12:15PM J6.00006 Edge-Edge interactions in stacked graphene, EDUARDO CRUZ-SILVA, University of Massachusetts Amherst, XIAOTING JIA, Massachusetts Institute of Technology, MAURICIO TERRONES, The Pennsylvania State University, MILDRED DRESSELHAUS, Massachusetts Institute of Technology, VINCENT MEUNIER, Rensselaer Polytechnic Institute — Graphene is often considered as the ultimate material for nanoscale electronics due to its unique structure-dependent properties. It has recently been shown that edge reconstruction and reshaping using combined electron irradiation and Joule heating could be used to control graphene properties towards nanodevice design. For instance, HRTEM experiments on few-layered graphene have revealed the presence of small graphene patches and platelets over larger graphene domains. While these platelets usually move freely over the larger graphene surface, they sometimes get locked in positions close to the edges of the larger sheet, thereby modifying the local electronic environment. We modeled this behavior with extensive density functional calculations using the van der Waals functional of Dion *et al.* Local interactions at the edges are found to be sufficiently strong to explain the presence of stacking configurations (e.g. AA) that are known to be energetically unfavorable in 2D graphene. Our results explain the observed dynamics of these stacked platelets and provide a deeper understanding of graphene edge reconstruction.

12:27PM J6.00007 Influence of water on the electronic structure of metal supported graphene: Insight from van der Waals density functional theory¹, JI FENG, XIAO LI, ENGE WANG, Peking University, China, SHENG MENG, Institute of Physics, China, JIRI KLIMES, ANGELOS MICHAELIDES, University College London — We investigate the interaction between water and metal supported graphene through van der Waals density functional theory calculations. Our results show a systematic increase in the adsorption energy of water on graphene in the presence of underlying metal substrates. In addition, we find that the electronic nature of the graphene-metal contacts behave differently upon water adsorption: in the case of a weak, physical graphene-metal contact, the charge carrier doping level of graphene is tuned by water, resulting in a Fermi level shift on the order of 100 meV. In the case of a strong chemical graphene-metal contact, the ? and ?* bands of graphene are hardly perturbed by water adsorption. These results illustrate the correlated nature of the interactions between water, graphene, and metal substrates, and show that the electronic structure and the doping level of graphene can be controlled by water deposition.

¹This work was supported by NSFC Projects 10974238, 91021007, 11174009 of China

12:39PM J6.00008 Alkanes adsorbed on graphene: a vdW-DF study, ELISA LONDERO, EMMA KARLSON, MARCUS LANDAHL, DIMITRI OSTROVSKII, JONATAN RYDBERG, ELSEBETH SCHROEDER, Chalmers University of Technology — Studies of small chains of molecules adsorbed on graphene are important for application of graphene in possible devices, not least its use as a gas sensor for the detection of single molecules. In this work we present a density functional theory study of the first ten n-alkanes adsorbed on graphene using the vdW-DF functional. We compare our adsorption energies to temperature programmed desorption measurements finding a similar linear scaling with the number of carbon atoms in the chain. The presence of an offset when extrapolating to the case of no molecules on the surface is also confirmed.

12:51PM J6.00009 To wet or not to wet? Dispersion forces tip the balance for water ice on metals, JAVIER CARRASCO, Instituto de Catal sis y Petroleoqu mica, CSIC, Marie Curie 2, E-29049 Madrid, Spain, BISWAJIT SANTRA, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany, JIRI KLIMES, ANGELOS MICHAELIDES, London Centre for Nanotechnology and Department of Chemistry, University College London, London WC1E 6BT, UK — For almost 30 years now, density functional theory (DFT) has been used to explore the molecular level details of water-metal interfaces. However, since the typical generalized gradient approximation exchange-correlation functionals used in these studies do not account for van der Waals (vdW) dispersion forces, the role dispersion plays in water adsorption remains unclear. Here, we tackle this issue head on applying a newly developed non-local functional [J. Klimeš *et al.*, J. Phys.: Condens. Matter **22**, 022201 (2010)] to two of the most widely studied water-ice adsorption systems, namely water on Cu(110) and Ru(0001). We show that non-local correlations contribute substantially to the water-metal bond and that this is an important factor in governing the relative stabilities of wetting layers and 3D bulk ice [J. Carrasco *et al.*, Phys. Rev. Lett. **106**, 026101 (2011)]. Due to the greater polarizability of the substrate metal atoms, non-local correlations between water and the metal exceed those between water within ice. This sheds light on a long-standing problem, wherein common DFT exchange-correlation functionals incorrectly predict that none of the low temperature experimentally characterized ice-like wetting layers are thermodynamically stable.

1:03PM J6.00010 Understanding the magnetic properties present at hybrid organic-ferromagnetic interfaces and the role of the van der Waals interaction, NICOLAE ATODIRESEI, VASILE CACIUC, Peter Gr nberg Institut (PGI) and Institute for Advanced Simulation (IAS), Forschungszentrum J lich and JARA, 52425-J lich, Germany, PREDRAG LAZIĆ, Massachusetts Institute of Technology, Cambridge, 02139 Massachusetts, USA, STEFAN BL GEL, Peter Gr nberg Institut (PGI) and Institute for Advanced Simulation (IAS), Forschungszentrum J lich and JARA, 52425-J lich, Germany — The design of nanoscale spintronic elements in multifunctional devices relies on a clear theoretical understanding of the physics at the electrode-organic system interfaces and in particular, the functionality of specific molecules in a given organic-metal surface environment. The density functional theory provides a framework where a realistic understanding of these systems with predictive power can be expected. However, only very recent functionals describe the exchange correlation of the organic molecule-metal interface reliably including the van der Waals interaction. We show that this has a great influence in particular on specific flat adsorbed π -conjugated electron systems. Our first-principles calculations performed for several organic molecules containing $\pi(p_z)$ electrons adsorbed onto a magnetic substrate show that the magnetic properties such as the local spin polarization, molecular magnetic moments and their spatial orientation can be specifically tuned by using substituents with different electronegativities. References: [1] N. Atodiresei *et al.*, PRL **102**, 136809 (2009); [2] J. Brede *et al.*, PRL **105**, 047204 (2010); [3] N. Atodiresei PRL **105**, 066601 (2010); [4] C. Busse *et al.*, PRL **107**, 036101 (2011). [5] N. Atodiresei *et al.*, PRB **84**, 172402 (2011).

1:15PM J6.00011 Simultaneous conductance and mechanical measurements on single molecule junctions reveal enhanced binding due to van der Waals interactions¹, SRIHARSHA V. ARADHYA, MICHAEL FREI, Columbia University, MARK S. HYBERTSEN, Brookhaven National Laboratory, LATHA VENKATARAMAN, Columbia University — Quantitative measurement of Van der Waals (vdW) interactions at the single molecule level remains challenging in experiments and its accurate inclusion in first principles theory is also complex. Here we report simultaneous measurement of force and electrical conductance across Au-molecule-Au junctions using a conducting atomic force microscope (AFM) for 4,4'-bipyridine (BP) and 1,2-bis(4-pyridyl)ethylene (BPE) molecules. For each of these molecules two distinct molecular junction structures are observed with characteristic conductances, consistent with previous studies utilizing scanning tunneling microscopy (STM). These two structures are found to have very different mechanical properties. Specifically, we find that the higher conductance junctions have a significantly larger rupture force and stiffness than those that show the lower conductance. They also have a larger rupture force than Au point contacts, suggesting multiple points of contact. Density functional theory (DFT) calculations suggest that the rupture force for the low conductance structure is well characterized as arising from N-Au donor acceptor interaction. However, the large rupture force and stiffness of the high conductance structure is most naturally explained as being due to the vdW contributions.

¹Support: NSF CHE 07-44185 and The Packard Foundation

1:27PM J6.00012 Mechanical properties of van der Waals interactions at compositionally graded interfaces between metals and organic semiconductors¹, HUARUI SUN, Department of Mechanical Engineering, University of Michigan, VLADIMIR STOICA, Department of Physics, University of Michigan, MAX SHTEIN, Department of Materials Science and Engineering, University of Michigan, ROY CLARKE, Department of Physics, University of Michigan, KEVIN PIPE, Department of Mechanical Engineering, Department of Electrical Engineering and Computer Science, University of Michigan — Interfacial bonding plays an important role in energy transfer (e.g., electrical conduction, thermal transport, or acoustic coupling) in composite materials as well as electronic and optoelectronic devices. In this work we use an ultrafast laser to excite vibrational modes in a thin aluminum film that is in contact with a small molecular organic semiconductor (copper phthalocyanine, CuPc). From the measured acoustic dynamics, we derive the fundamental mechanical properties of the van der Waals bonding at the Al/CuPc interface, and further study how these mechanical properties change in a series of samples as the interface is compositionally graded. The implications of these results are discussed in the contexts of interfacial thermal resistance, organic optoelectronic devices, and thermoelectric energy conversion.

¹We gratefully acknowledge the support from the United States Air Force Office of Scientific Research.

1:39PM J6.00013 Benchmark data base for accurate van der Waals interaction in inorganic fragments¹, JAN BRNDIAR, IVAN STICH, Institute of Physics, Slovak Academy of Sciences — A range of inorganic materials, such as Sb, As, P, S, Se are built from van der Waals (vdW) interacting units forming the crystals, which neither the standard DFT GGA description as well as cheap quantum chemistry methods, such as MP2, do not describe correctly. We use this data base, for which we have performed ultra accurate CCSD(T) calculations in complete basis set limit, to test the alternative approximate theories, such as Grimme [1], Langreth-Lundqvist [2], and Tkachenko-Scheffler [3]. While none of these theories gives entirely correct description, Grimme consistently provides more accurate results than Langreth-Lundqvist, which tend to overestimate the distances and underestimate the interaction energies for this set of systems. Contrary Tkachenko-Scheffler appear to yield surprisingly accurate and computationally cheap and convenient description applicable also for systems with appreciable charge transfer.

[1] S. Grimme, J. Comp. Chem. **27**, 1787 (2006)

[2] K. Lee, *et al.*, Phys. Rev. B **82** 081101 (R) (2010)

[3] Tkachenko and M. Scheffler Phys. Rev. Lett. **102** 073005 (2009).

¹Financial support from APVT (ESF-EC-0007-07) under the Nanoparma ESF FANAS project is gratefully acknowledged. This research was supported in part by ERDFOPR&D, Project CE QUTE ITMS 26240120009, and via CE SAS QUTE.

1:51PM J6.00014 Interlayer binding energy of graphite: A mesoscopic determination from deformation¹, ZHE LIU, Department of Mechanical and Aerospace Engineering, Monash University, VIC 3800, Australia, ZE LIU, QUANSHUI ZHENG, Department of Engineering Mechanics and Center for Nano and Micro Mechanics, Tsinghua University, Beijing 100084, China, COMPUTATIONAL MATERIALS SCIENCE COLLABORATION, CENTER FOR NANO AND MICRO MECHANICS COLLABORATION — Despite the interlayer binding energy (BE) being one of the most important material properties of graphite, direct experimental determination is yet to be reported. In this talk, we present a novel experimental method to directly measure the interlayer BE of HOPG. By employing the self-retraction motion of a graphite flake in a graphite island (Phys. Rev. Lett. 100, 067205 (2008)), we assembled a graphite top flake spanning a graphite step, yielding a contact area ($\sim \mu\text{m}^2$) with a graphite platform. STM scan showed that the interface was atomically smooth. The deformation of the top flake should be determined by the BE with the graphite platform. Thus using a finite element model to simulate the top-flake height profiles measured by AFM, we determine the graphite BE as $0.19(\pm 0.01)\text{J/m}^2$, which can serve as a benchmark for other theoretical and experimental works. Our proposed method can be easily extended to measure the BEs between graphite/graphene and other types of substrates. It can also be used in other systems, particularly lamellar materials and thin films.

¹Funded by NSFC through Grant No. 10832005, the National Basic Research Program of China (Grant No. 2007CB936803), the National 863 Project (Grant No. 2008AA03Z302), and small grant from Engineering faculty at Monash University.

2:03PM J6.00015 Helium atom diffraction from a monolayer solid with a beam that penetrates to the substrate, LUDWIG BRUCH, Physics Dept; University of Wisconsin-Madison, FLEMMING HANSEN, Chemistry Dept., Technical University of Denmark — Diffraction of a thermal energy helium atomic beam is evaluated in the situation that the target monolayer lattice is so dilated that the atomic beam penetrates to the region between the monolayer and the substrate. Parameters are chosen to be representative of a hypothetical $p(1 \times 1)$ commensurate monolayer solid of $\text{H}_2/\text{KCl}(001)$. Depending on the spacing between the monolayer and the substrate and on the angle of incidence, there are cases where part of the incident beam is trapped in the interlayer region for times exceeding 50 ps. The methodology is a direct extension of the wave-packet propagation used for the scattering of helium from the quantum monolayer solid $\text{H}_2/\text{NaCl}(001)$.¹

¹L. W. Bruch, F. Y. Hansen and F. Traeger, J. Chem. Phys. **134**, 194308 (2011)

Tuesday, February 28, 2012 11:15AM - 2:15PM – Session J7 DMP: Focus Session: Graphene Devices 207

11:15AM J7.00001 Graphene-Superconductor based Bolometers, HELI VORA, PIRANAVAN KUMARAVADIVEL, BENT NIELSEN, XU DU, Department of Physics & Astronomy, Stony Brook University — Due to its small volume and linear energy dependence of electron density of states, graphene has very low electronic heat capacitance compared to what is found in metals with achievable volume. This makes it a promising material for applications requiring bolometric sensing of radiation with a fast response without compromising sensitivity. Here we report fabrication of graphene-superconductor tunnel junctions and characterization of their bolometric response. When radio frequency radiation is shone onto the junction, the electrons in graphene heat up and dynamic resistance within the superconducting gap changes. The relation between absorbed power and temperature rise is used to characterize heat conductance and thermal noise equivalent power.

11:27AM J7.00002 Microwave transport and noise in graphene devices, BERNARD PLACAIS, ANDREAS BETZ, EMILIANO PALLECCHI, GWENDAL FÈVE, JEAN-MARC BERROIR, Ecole Normale Supérieure, CHRISTIAN BENZ, ROMAIN DANNEAU, Karlsruhe Institute of Technology, ANTONELLA CAVANNA, ALI MADOURI, Laboratoire de Photonique et Nanostructures, MESOSCOPIC PHYSICS GROUP TEAM, PHY NANO TEAM, ANR MIGRAQUEL COLLABORATION — We report on microwave transport and noise in graphene sheets, capacitors and transistors. We achieved a transit frequency of 80 GHz in graphene-on-sapphire transistors [1]. This is close to the state-of-the art for a 200nm gate length. In order to investigate electronic diffusion in graphene we have realized 10 GHz bandwidth experiments in metal-oxide-graphene capacitors. The crossover from capacitor to skin-effect limited cavity regimes provides an accurate and direct measurement of the diffusion constant $D(\varepsilon)$. We find D to be energy independent, which points to a mass-disorder scenario [2]. Finally, we have measured the shot noise of CVD graphene in a broad range of bias up to 1V drain-source voltage. In our GHz-frequency measurements we observe a Fano factor exhibiting the three characteristic regimes of electron-impurity, electron-electron and electron-phonon interactions.

[1] E. Pallecchi et al, Appl. Phys. Lett. 99, 113502 (2011)

[2] E. Pallecchi et al, Phys. Rev. B 83, 125408 (2011)

11:39AM J7.00003 Anomalous noise characteristics in graphene p-n junctions¹, JANICE WYNN GUIKEMA, ATIKUR RAHMAN, NINA MARKOVIC, Johns Hopkins University — Graphene p-n junctions provide an interesting platform to study the Dirac nature of charge carriers, which gives rise to phenomena such as Klein tunneling and electron lensing. p-n junctions also play an important role in graphene nanodevices, but the ubiquitous low-frequency noise typically limits the device performance. It has been observed that the low-frequency noise for back-gated single layer and bilayer graphene decreases at the Dirac point, even though the resistance is maximal there. This decrease has been attributed to the effects of spatial charge inhomogeneity, and the noise in such devices decreases with decreasing temperature. We will present noise characteristics of dual-gated graphene p-n junction devices. At the Dirac point, the noise shows an “M” shape as a function of top gate voltage. Away from the Dirac point the shape changes depending on the back gate and top gate voltage. Unlike the low-frequency noise in graphene nanodevices, noise across the p-n junction decreases with increasing temperature. We also observed that the noise amplitude is larger in p-n-p or n-p-n devices than in p-p-p or n-n-n devices. We will discuss the mechanism that explains this anomalous noise behavior in graphene p-n junction.

¹This work is supported in part by NSF DMR-1106167

11:51AM J7.00004 Incidence Angle-dependent Transport across a Single Graphene $p-n$ Junction Formed by Buried Split-gates¹, SURAJIT SUTAR, EVERETT COMFORT, JIAN LIU, CNSE, University at Albany (SUNY), TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Tsukuba, Japan, JI UNG LEE, CNSE, University at Albany (SUNY), CNSE, UNIVERSITY AT ALBANY (SUNY) TEAM, NATIONAL INSTITUTE FOR MATERIALS SCIENCE COLLABORATION — Due to electron chirality effects, carrier transport across Graphene $p-n$ junctions (GPNJ) is predicted to have strong angular dependence [1]. This work reports evidence of such effects in a single GPNJ for various geometries created by the use of buried split-gates (SG). Standard processes are used to fabricate 2-terminal Graphene devices aligned to buried Polysilicon SG at different angles to the junction. Sweeping the SG biases V1 and V2 allows mapping the doping-dependent device resistance (R_t). For doping levels (V1,V2), subtracting the average unipolar resistance $R_t(V1,V1)$ from the bipolar resistance $R_t(V1,V2)$ gives the average junction resistance $R_j(V1,V2)$, subtracting out both contact and channel resistances. For bipolar doping, R_j shows a sharper peak for tilted channels than one that is normal to the junction, the peak being sharpest for 45° , the largest angle probed. This trend is observed for both exfoliated and CVD Graphene, especially for higher mobility and lower widths, consistent with theory. The ratio of the maximal R_j for 45° and 0° devices is about 2.5, significant for the modest Graphene mobilities of our devices. [1] V. Cheianov et al., **Science**, **315**, 2007, pp 1252.

¹This work was supported by the INDEX (SRC/NRI) center

12:03PM J7.00005 Gate-Controlled P-I-N Junction Switching Device with Graphene Nanoribbon, SHU NAKAHARAI, TOMOHIKO IJIMA, SHINICHI OGAWA, National Institute of Advanced Industrial Science and Technology, HISAO MIYAZAKI, SONGLIN LI, KAZUHIITO TSUKAGOSHI, National Institute for Materials Science, SHINTARO SATO, NAOKI YOKOYAMA, National Institute of Advanced Industrial Science and Technology — The concept of a novel graphene P-I-N junction switching device with a nanoribbon is proposed, and its basic operation is demonstrated in an experiment. The concept aims to optimize the operation scheme for graphene transistors toward a superior on-off property. The device has two bulk graphene regions where the carrier type is electrostatically controlled by a top-gate, and these two regions are separated by a nanoribbon which works as insulator. As a result, the device forms a (P or N)-I-(P or N) junction. The off state is obtained by lifting the band of the bulk graphene of the source side and lowering that of the drain side, so that the device forms a P-I-N junction. In this configuration, the leakage current is reduced more effectively than the conventional single gate transistors due to a high barrier height and a long tunneling length in the nanoribbon. The on state is obtained by flipping the polarity of the bias of either top-gate to form a P-I-P or N-I-N junction. An experiment showed that the drain current was suppressed in the cases of P-I-N and N-I-P compared to P-I-P and N-I-N, and all of the behaviors were consistent with what was expected from the device operation model. This research is granted by JSPS through FIRST Program initiated by CSTP.

12:15PM J7.00006 Fabrication of suspended graphene heterojunctions for exploring the intrinsic transport of Dirac fermions, PIRANAVAN KUMARAVADIVEL, XU DU, Stony Brook University — With linear energy dispersion and chirality, the quasiparticles in graphene differs from the conventional electrons in solid state systems in that the motions of the quasiparticles are governed by the Dirac Weyl equation. High quality of suspended graphene has made it possible to reach lower carrier densities and longer mean free paths and therefore has opened up the possibility of studying some of the unique, intrinsic properties of this Dirac electron system, which cannot otherwise be observed in conventional graphene devices on various substrates. To retain and exploit such properties of suspended graphene in heterojunction devices requires fabricating a contactless air top gate over the suspended graphene channel. Here we report on fabrication of such a device, which enable us to explore further, some interesting physics and transport of these Dirac fermions in graphene.

12:27PM J7.00007 Transport Properties of Gate Tunable Graphene-Based Tunnel Diodes, DAMON FARMER, VASILI PEREBEINOS, PHAEDON AVOURIS, IBM T.J. Watson Research Center — Due to its linear dispersion relation and unique physical properties, graphene has become a material of intense experimental and theoretical investigation. There has been rapid progress in the fabrication and understanding of graphene devices, particularly those based on the field effect transistor (FET) configuration. These three-terminal switches rely on a gate field to control electronic transport (diffusive or quasi-ballistic) in the graphene channel, where the field is perpendicular to the current flow. Here, a different type of three-terminal graphene device is demonstrated, one based on quantum tunneling. These devices build upon the convention two-terminal metal-insulator-metal (MIM) tunnel diode configuration by replacing one of the metal electrodes with graphene. Incorporation of a third (gate) electrode allows for modulation of the accessible density of states in the graphene electrode, thereby tuning the threshold voltage for tunneling in the diode. This tunable diode concept, where the gate field is parallel to the tunneling direction, is novel for a purely solid-state system. The device characteristics owing to the unique properties of graphene will be discussed, as will the underlying physics of device operation.

12:39PM J7.00008 Drain Current Saturation in Sub- μm Graphene Field Effect Transistors, SHU-JEN HAN, IBM TJ Watson Research Center, DHARMENDAR PALLE, IBM Research Labs, Austin, AARON FRANKLIN, ALBERTO VLADES-GARCIA, IBM TJ Watson Research Center — Recently, graphene field-effect transistors (FET) with high cut-off frequencies (f_T) were reported; however, the devices showed very weak drain current saturation, leading to an undesirably high output conductance. A crucial figure-of-merit for analog/RF transistors is the intrinsic gain (gm/gds). In this work, we show that by employing an embedded gate structure with an equivalent oxide thickness less than 2 nm, strong drain current saturation can be obtained for graphene FETs with short channels. The mechanism was not entirely due to velocity saturation, but rather the combination of a shift of the Dirac point in the voltage domain and a strong bias-dependent gate capacitance. The mechanisms are also verified with models.

12:51PM J7.00009 Self-aligned high transconductance CVD graphene transistor, YUCHI CHE, ALEXANDER BADMAEV, ZHEN LI, CHONGWU ZHOU, University of Southern California — Exceptional electronic properties of graphene make it a highly promising material for high-speed electronics. However, the design and practical realization of graphene transistors are still challenging, which limit the potential of graphene. In this work, we present a novel, practical, and highly scalable method for the fabrication of self-aligned graphene transistors. Large-area single-layer graphene films were grown on copper foil and were transferred onto 12 inch Si wafers. Furthermore, in order to achieve wafer-scale fabrication of graphene transistors with high yield, we developed a self-aligned fabrication approach by standard lithographical methods. The fabricated transistors with gate lengths in the range of 110 to 170 nm showed excellent performance with the peak current density of $1.3 \text{ mA}/\mu\text{m}$. The peak transconductance reaches $0.5 \text{ mS}/\mu\text{m}$, which is one of the best transconductance for CVD graphene transistor published up to date. Our novel fabrication method shows great potential toward practical implementation of graphene in high frequency devices and circuits.

1:03PM J7.00010 Graphene Enabled Vertical Field Effect Transistors, EVAN P. DONOGHUE, Physics, University of Florida, Gainesville, FL, MAXIME G. LEMAITRE, Material Science and Engineering, University of Florida, Gainesville, FL, MITCHELL A. MCCARTHY, BO LIU, Physics, University of Florida, Gainesville, FL, BILL R. APPLETON, MS&E, NIMET, Univrsity of Florida, Gainesville, FL, ANDREW G. RINZLER, Physics, University of Florida, Gainesville, FL — Vertical field effect transistors (VFETs) using a carbon nanotube source electrode have recently demonstrated state-of-the-art current densities at low operating voltages from comparatively low mobility organic semiconductors. Unlike in conventional thin film transistors, transconductance arises from a gate field modulation of the contact barrier at the organic semiconductor/nanotube interface (with the performance enhanced by nanotube Fermi level shifts allowed by their low density of electronic states). Graphene's low density of states near the Dirac point similarly makes it a good candidate source electrode in VFETs. We have now demonstrated such devices, facilitated by the use of a novel transfer technique that improves areal yields while avoiding both polymeric residue and the particulates that necessitate the use of thicker channel layers in nanotube VFETs. Critical to high performance is a facile method developed for perforating the graphene sheet with holes of a tunable size and density, allowing for a direct assessment of the role of self-screening effects in VFETs. These initial graphene enabled VFETs achieve on-current densities exceeding $250\text{mA}/\text{cm}^2$ at drive voltage swings of less than 4V with on/off current ratios larger than 10^6 .

1:15PM J7.00011 Transport/magnetotransport of high-performance graphene transistors on organic molecule-functionalized substrates, SHAO-YU CHEN, Academia Sinica, PO-HSUN HO, National Taiwan University, REN-JYE SHIUE, Academia Sinica, CHUN-WEI CHEN, National Taiwan University, WEI-HUA WANG, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan — We present the transport and magnetotransport of high-quality graphene transistors on conventional SiO_2/Si substrates by modification with organic molecule self-assembled monolayers (SAMs). Graphene devices on organic SAM-functionalized substrates exhibit high carrier mobility, low intrinsic doping, suppressed carrier scattering, and reduced thermal activation of resistivity at room temperature. Magnetotransport of graphene devices with pronounced quantum Hall effect and Shubnikov-de Haas oscillations also confirms the high quality of graphene on this ultrasmooth organic SAM-modified platform. The high-performance graphene transistors on the solution-processable SAM-functionalized SiO_2/Si substrates are promising for the future development of large-area and low-cost fabrications of graphene-based nanoelectronics.

1:27PM J7.00012 Quantum transport simulation of graphene transistors, YANG LU, JING GUO, University of Florida, COMPUTATIONAL NANOTECHNOLOGY TEAM — Owing to its unique electrical and thermal properties, graphene has attracted great interests as potential building blocks of next generation electronics, especially for RF applications. Due to lack of band gap, Klein tunneling plays an important role in sub-100nm graphene transistors. Inelastic phonon scattering introduced by intrinsic phonons of graphene and polarized substrate also affect device performance. We show that coupling between inelastic phonon scattering and Klein tunneling leads to different device physics of graphene transistors from common nanoscale transistors. The electron-phonon interaction and quantum transport in graphene transistors are modeled by the non-equilibrium green's function method within the self-consistent Born approximation. We evaluate the effect of inelastic process on both DC and RF performance of graphene transistors. We also briefly discuss the self-heating effects in graphene transistors introduced by inelastic phonon scattering.

1:39PM J7.00013 Pulse gating on graphene quantum dots, CHRISTIAN VOLK, CHRISTOPH NEUMANN, SEBASTIAN KAZARSKI, STEFAN FRINGES, STEPHAN ENGELS, BERNAT TERRES, JAN DAUBER, STEFAN TRELLENKAMP, UWE WICHMANN, CHRISTOPH STAMPFER, JARA-FIT and II. Institute of Physics B, RWTH Aachen, Aachen and Peter Gruenberg Institut (PGI-8/9), Forschungszentrum Juelich, Juelich, Germany — Graphene quantum devices have received increasing attention over the last years. Graphene quantum dots (QDs) are interesting systems for implementing spin qubits. Compared to well-established GaAs-based QDs, their smaller hyperfine and spin-orbit coupling promises more favorable spin coherence times. However, while the preparation, manipulation, and read-out of single spins have been demonstrated in GaAs, research on graphene QDs is still at an early stage. Although Coulomb blockade phenomena and excited state spectroscopy is now well established, experimental signatures allowing the identification of relaxation times have been hard to trace. Here we report on the current status of pulse gating experiments on graphene quantum devices and in particular we will present measurements of the charge relaxation rates in single-layer graphene QDs. The investigated devices consist of an island with a diameter of 120 nm, 4 lateral graphene gates and 2 charge detectors. From so-called diamond measurements we extract a charging energy of 11 meV and excited state level spacings on the order of 2-4 meV. The gates allow to individually tune the tunnelling-in and -out rates down to low MHz regime. Low-bias pulse gate measurements allow finally to extract relaxation rates on the order of 50 ns.

1:51PM J7.00014 Ultrafast conductivity measurements in CVD graphene¹, JAMES HEYMAN, YILIKAL AYINO, ROLAN MANDERSON-JONES, JACOB STEIN, Macalester College, Department of Physics and Astronomy — We study carrier dynamics in CVD graphene films on Al_2O_3 using time-resolved THz spectroscopy (TRTS). Excitation with a 50fs, 800nm pulse produces a conductivity change $\Delta\sigma$ which we measure as a decrease in transmission of an ultrafast THz pulse. Ongoing work seeks to investigate TRTS in a magnetic field to directly probe scattering rates of photogenerated carriers. At present we report zero field measurements. We observe different recovery dynamics for low ($\Delta\sigma \ll \sigma_0$) and high ($\Delta\sigma > \sigma_0$) pump powers. For pump fluence $\varphi < 10^{12}\text{photons cm}^{-2}$ ($\Delta\sigma \ll \sigma_0$) we find $\Delta\sigma \propto \varphi$ and observe a nearly exponential decay $\Delta\sigma \propto e^{-t/\tau}$ with decay time $\tau \approx 2\text{ps}$. At higher powers ($\Delta\sigma > \sigma_0$) $\Delta\sigma$ is sublinear in φ , and the decay rate decreases, with $\tau \approx 4\text{psat } \varphi \approx 5 \cdot 10^{13}\text{photons cm}^{-2}$. Graphene's unusual conductivity relation, $\sigma \propto \sqrt{n}$, predicts the observed behavior, since $\Delta\sigma \propto \sqrt{n_0 + n_{\text{photo}}} - \sqrt{n_0}$ is approximately linear for $n_0 \gg n_{\text{photo}}$, while $\Delta\sigma \propto \sqrt{n_{\text{photo}}}$ for $n_{\text{photo}} \gg n_0$. Here n_0 and σ_0 are the equilibrium carrier density and conductivity in these p-type films. At high pump powers we also observe a rapid initial recovery on $\sim 500\text{fs}$ timescale which is not described by this simple model.

¹Work supported by the National Science Foundation under Grant Nos. DMR-1006065 and DMR-0959341

2:03PM J7.00015 Delay Analysis of Graphene Field Effect Transistors and T-Gate Self-Aligned GFETs¹, HAN WANG, ALLEN HSU, KI KANG KIM, JING KONG, TOMAS PALACIOS, Massachusetts Institute of Technology — In this paper, we propose a new method for extracting the carrier transit delays in radio-frequency (RF) graphene field effect transistors (GFETs). This delay analysis not only gives deep physical insight into the carrier transport in the channel, but also provides valuable information that can guide the device engineers in optimizing the design of high performance RF GFETs. The contribution of this work is three-fold. First, GFETs are fabricated on sapphire substrate to reduce the parasitics from the GSG pads. This minimizes the error in measuring the S-parameter of the device and allows small-signal capacitances to be accurately extracted. Second, we present for the first time a detailed delay analysis of high frequency graphene transistors. Lastly, the simple and robust method proposed can accurately extract the intrinsic transit delay of the GFETs - the delay purely associated with the carrier transiting across the intrinsic gate region – and allows a new method for direct experimental extraction of the average carrier velocity in the channel. Based on the analysis, we propose a self-aligned device structure to minimize the parasitic delays in GFETs. This GFET structure uses a T-shape gate as the mask to allow the source and drain metals to be aligned to the edge of the gate. A T-gate self-aligned GFET with gate head of 300 nm and foot 50 nm is fabricated and its DC and RF characteristics are reported.

¹This work was partially supported by the ONR GATE MURI program, the MARCO MSD program and the Army Research Laboratory.

Tuesday, February 28, 2012 11:15AM - 2:15PM –
Session J8 DCMP GMAG: Quantum Magnetism, BEC, and Disorder 208

11:15AM J8.00001 Finite- T spectral function of the BEC quantum magnets¹, SUHAS GANGADHARIAH, University of Basel, Switzerland, SASHA CHERNYSHEV, UC Irvine — We discuss the momentum, frequency, and temperature dependence of the spectral function of interacting 3D bosonic excitations in the vicinity of the BEC quantum critical point. The relaxation rate is demonstrated to have a highly non-trivial ω -dependence with several asymptotic regimes that are studied in some detail. The spectral function is shown to exhibit, in a wide range of temperatures, an asymmetric quasiparticle peak and a shoulder, originating from the behavior of the self-energy. These spectral features should be readily observable in neutron-scattering experiments in the BEC quantum magnets. We also argue that this behavior of the spectral function must persist throughout the strong-coupling limit.

¹Supported by the DoE.

11:27AM J8.00002 ABSTRACT WITHDRAWN —

11:39AM J8.00003 Theory of magnetic Bose glass in Br-doped dichloro-tetrakis-thiourea-nickel (DTN)¹, STEPHAN HAAS, University of Southern California, RONG YU, Rice University, TOMMASO ROSCILDE, Ecole Normale Supérieure de Lyon - France — We will review here the microscopic model allowing to describe quantitatively the physics of Br-doped DTN. The magnetic Hamiltonian of Br-DTN describes $S=1$ spins coupled through bimodally distributed antiferromagnetic bonds, and with a correlated bimodal distribution of single-ion anisotropies. A spin-boson mapping leads to a description in terms of a Bose-Hubbard-like model with random hoppings and random on-site interactions for magnetic quasiparticles, whose density is controlled by the applied magnetic field. This model features an extended gapless and compressible Bose-glass phase in low fields, extending down to zero field, at which the compressibility vanishes, corresponding to a Mott-glass phase. We will present extensive quantum Monte Carlo results for the thermodynamic signatures of the Bose glass, and for the quantum critical signatures of the magnetic ordering transition occurring at stronger field, which corresponds to a remarkable realization of the Bose-glass/superfluid transition.

¹Numerical calculations have been supported by an INCITE award from the DOE.

11:51AM J8.00004 Magnetization and Specific Heat Investigations of the Bose Glass: Br-doped $\text{NiCl}_2\text{-4SC}(\text{NH}_2)_2$, FRANZISKA WEICKERT, CORNELIU MICLEA, ROMAN MOVSHOVICH, VIVIEN ZAPF, Los Alamos National Laboratory, RONG YU, Rice University Houston, TOMMASO ROSCILDE, ENSL, Lyon, France — $\text{NiCl}_2\text{-4SC}(\text{NH}_2)_2$ (DTN) is an insulating material, which shows field induced XY-AFM order between $H_{c1} = 2.1$ T and $H_{c2} = 12.6$ T. In boson language, the ground state of DTN can be described as a Mott insulator, and the ordered state as a Bose-Einstein condensation of magnons. Bond disorder is introduced by substituting Br atoms on Cl positions, which simultaneously changes the super exchange interaction along the c -direction on a local scale and leads to a Mott-glass ground state in zero field. Furthermore, the system develops a gapless Bose glass for magnetic fields $0 < H < H_{c1}$ and $H > H_{c2}$, followed by a Mott insulating state above the saturation field H_{sat} . Note, that the critical fields $H_{c1,2}$ and H_{sat} are shifted compared to those of pure DTN. In this talk, we report on measurements of the magnetization and specific heat at very low temperatures between 50 mK and 3 K in high magnetic fields up to 14 T on an 8% Br-doped single crystal DTN. We compare our data with the local gap model, which reduces the low-temperature and low-field behavior to those of an ensemble of individual three level systems with local magnetization $M_S = 0, \pm 1$ and a finite energy gap for $H = 0$.

12:03PM J8.00005 Magnetic Bose glass in Br-doped $\text{NiCl}_2\text{-4SC}(\text{NH}_2)_2$: Magneto-Electric Effect, LIANG YIN, JIAN-SHENG XIA, NEIL SULLIVAN, University of Florida, VIVIEN ZAPF, LANL, ARMANDO PADUAN-FILHO, Universidade de Sao Paulo — $\text{NiCl}_{1.85}\text{Br}_{0.15}\text{-4SC}(\text{NH}_2)_2$ is a candidate for Bose glass state of the magnetism at low temperatures, which is the bosonic analog of Anderson localization. Here we explore the glassy dynamics of the magnetization taking advantage of magneto-electric coupling in this material. We report measurements of the magneto-electric effect in $\text{NiCl}_{1.85}\text{Br}_{0.15}\text{-4SC}(\text{NH}_2)_2$ using two different experimental setups: (i) magnetic field-induced polarization and (ii) electric-field-induced magnetization. Both measurements show that the proposed Bose glass state in a high magnetic field is sensitive to the applied frequencies of AC magnetic and electric fields, with a maximum response between 700Hz and 1000Hz. This frequency-dependent behavior could provide information about the characteristic response time and the size of magnetic clusters.

12:15PM J8.00006 Disorder in a two-dimensional quantum spin liquid, DAN HUVONEN, MARTIN MANS-SON, SEVERIAN GVASALIYA, SHUANGYI ZHAO, ETH Zurich, TATIANA YANKOVA, Moscow State University, VASILIIY GLAZKOV, Kapitza Institute for Physical Problems, ERIC RESSOUCHE, Institut Laue-Langevin, CHRISTOF NIEDERMAYER, MARK LAVER, Paul Scherrer Institut, GEORG EHLERS, Oak Ridge National Laboratory, ANDREY ZHELUDEV, ETH Zurich — We discuss magnetic field induced phase transition to magnon Bose-Einstein condensate state in a disordered two-dimensional spin gap antiferromagnet. Disorder was introduced into piperazinium hexachlorodipicrate (PHCC) by chemically substituting up to 10% of exchange interaction mediating Cl ions for Br. We present specific heat, magnetization, susceptibility, elastic and inelastic neutron scattering results in fields up to 14T. Data reveals that disorder enlarges significantly the spin gap and induces nonzero susceptibility in the gapped phase. Reduction of magnon bandwidth and lifetime are evident from inelastic neutron scattering measurements. Although the phase transition seems to survive, the condensate wavefunction acquires a history dependence. In contrary to theoretical expectations, the extracted critical exponents show no changes within experimental accuracy.

12:27PM J8.00007 Dynamics of the Random-Field Ising Model, SPENCER TOMARKEN, DANIEL SILEVITCH, THOMAS ROSENBAUM, Department of Physics, The University of Chicago — Ising magnets with long, needle-like domains can be treated as single extended spins which interact via dipole-dipole forces. Typically such dipole interactions cancel out due to spatial symmetry, but the combination of randomly packed grains and the application of a magnetic field transverse to the easy axis of magnetization can break the symmetry. This results in a site-random-magnetic field that points along the easy axis and varies from grain to grain, described by the Random-Field Ising Model (RFIM). We report a series of magnetization measurements in longitudinal and transverse magnetic fields that demonstrate RFIM behavior in the room-temperature, rare-earth ferromagnet $\text{Nd}_2\text{Fe}_{14}\text{B}$, and analyze our data in terms of predicted scaling relations.

12:39PM J8.00008 Strong Disorder Renormalization Group for the Many Body Localization Transition, GIL REFAEL, California Institute of Technology, VADIM OGANESYAN, City University of New York, SHANKAR IYER, California Institute of Technology — The strong disorder renormalization group, originally devised by Ma and Dasgupta to study the random Heisenberg antiferromagnet, has subsequently been used to investigate the low energy physics and quantum phase transitions of a variety of strongly disordered systems. However, recent work by Basko, Aleiner, and Altshuler has focused attention on the many body localization transition, a dynamical quantum phase transition that involves the localization of highly excited eigenstates of a many body system in Fock space. Numerical results from an exact diagonalization study by Pal and Huse suggest that the many body localization transition may exhibit so-called infinite-randomness, a property that implies that a strong disorder renormalization group may be well-suited to study this transition. With the many body localization transition in mind, we therefore outline a strong disorder renormalization procedure that targets the least-localized eigenstate of a model. We then apply this procedure to study disordered quantum Ising and XXZ models. The latter model is similar to the one investigated by Pal and Huse and is expected to contain a dynamical transition between localized and ergodic phases; our principal aim is to use the strong disorder RG to characterize this transition.

12:51PM J8.00009 Evolution of magnetic order and fluctuations in Ni-V close to the disordered ferromagnetic quantum critical point¹, ALMUT SCHROEDER, RUIZHE WANG, S. UBAID-KASSIS, Kent State University, P.J. BAKER, F.L. PRATT, ISIS, S.J. BLUNDELL, T. LANCASTER, I. FRANKE, J.S. MOELLER, Oxford University — Muon spin rotation and magnetization data of the d-metal alloy $\text{Ni}_{1-x}\text{V}_x$ are presented at several vanadium concentrations x below and above the critical $x_c \approx 11\%$ where the onset of long-range ferromagnetic (FM) order is suppressed. Bulk magnetization shows signatures of a disordered quantum phase transition (QPT), most clearly in the paramagnetic regime: Above x_c the temperature dependence of the magnetic susceptibility is best described by simple non-universal power laws marking a quantum Griffiths phase. But the deviations from a clean FM in the ordered phase are more subtle to recognize in the bulk magnetization and are noticed only close to x_c . Muon data reveal a broad field distribution in the FM regime at even small x ($x \geq 4\%$). The evolution of the magnetic cluster distribution and dynamics from the pristine FM towards the paramagnetic regime will be presented. This adds new insight in this model system at a disordered QPT.

¹Part of this work supported by NSF DMR 0306766 and OBR 440653

1:03PM J8.00010 Unconventional spin-Peierls state in the quantum magnet TiOBr ¹, J.-P. CASTEL-LAN, Argonne National Laboratory, J.P. CLANCY, University of Toronto, J.P.C. RUFF, Advanced Photon Source, S. ROSENKRANZ, R. OSBORN, Argonne National Laboratory, B.D. GAULIN, McMaster University, F.C. CHOU, S.H. HUANG, National Taiwan University — The discovery of spin-Peierls transitions in inorganic materials such as CuGeO_3 with T_{sp} of 14K allowed for the growth of large single crystals. With the availability of large single crystals the opportunity arises to introduce both magnetic and nonmagnetic impurities and study the resulting perturbations from the ground state. Recently a new class of unconventional spin-Peierls materials were discovered TiOBr and TiOCl . TiOBr and TiOCl have been shown to exhibit dimerized singlet ground states and undergo not one but two successive phase transitions. We have performed x-ray scattering measurements on single crystals of TiOBr . These measurements reveal both commensurate and incommensurate spin-Peierls phases; below $T_{c2} \sim 48\text{K}$ incommensurate super-lattice reflections arise at $Q=[H\pm\delta, K+1/2\pm\epsilon, L]$ which persists down to the lock in transition at $T_{c1} \sim 27\text{K}$. We will report on the details of these successive transitions and the destruction of the long-range ordered spin-Peierls state with introduction of magnetic vacancies by doping with Sc.

¹Work supported by US DOE BES-MSED DE-AC02-06CH11357.

1:15PM J8.00011 Ashkin-Teller criticality and pseudo-first-order behavior in a frustrated Ising model on the square lattice¹, SONGBO JIN, ARNAB SEN, ANDERS SANDVIK, Boston University — We consider the square-lattice frustrated Ising model with first- and second-neighbor interactions, $J_1 < 0$ and $J_2 > 0$. Its thermal phase transition to “stripe” order when $g = J_2/|J_1| > 1/2$ has remained controversial despite many past studies. Using Monte Carlo simulations to investigate the order-parameter distribution and its Binder cumulant, we demonstrate Ashkin-Teller criticality for $g \geq g^*$, i.e., the critical exponents vary continuously between those of the 4-state Potts model at g^* and the Ising model for $g \rightarrow \infty$. The Potts point, below which the transition is first-order, is $g^* = 0.67 \pm 0.01$, much lower than previously believed. The system exhibits *pseudo first-order* behavior for $g^* \leq g \leq g'$ ($g' \approx 0.9$), which was previously misinterpreted as actual first-order behavior.

¹NSF Grant No. DMR-1104708.

1:27PM J8.00012 Quantum phase diagram of the spin ladder model with next-nearest neighbor interactions, YANCHAO LI, HAIQING LIN, Beijing Computational Science Research Center, Beijing 100084, People's Republic of China — By using the density matrix renormalization group technique, we investigate the quantum phase diagram of a two-leg spin-1/2 ladder with diagonal and in-chain next-nearest neighbor interactions for both anti-ferromagnetic and ferromagnetic frustrated cases. Through analyzing the correlation function and four-site entropy, the existence of the controversial columnar dimer phase is confirmed, and the phase transitions caused by the in-chain next-nearest neighbor interaction are presented for the anti-ferromagnetic frustrated case; meanwhile, for the ferromagnetic frustrated case, we find that the system possesses a tetramer phase, a ferromagnetic phase, and the states I and II, and the spin arrangements for I and II are determined.

1:39PM J8.00013 Majorana Spin Liquids on a two-leg ladder¹, HSIN-HUA LAI, OLEXEI MOTRUNICH, California Institute of Technology — We realize a gapless Majorana Orbital Liquid (MOL) using orbital degrees of freedom and also an $\text{SU}(2)$ -invariant Majorana Spin Liquid (MSL) using both spin and orbital degrees of freedom in Kitaev-type models on a 2-leg ladder. The models are exactly solvable by Kitaev's parton approach, and we obtain long-wavelength descriptions for both Majorana liquids. The MOL has one gapless mode and power law correlations in energy at incommensurate wavevectors, while the $\text{SU}(2)$ MSL has three gapless modes and power law correlations in spin, spin-nematic, and local energy observables. We study the stability of such states to perturbations away from the exactly solvable points. We find that both MOL and MSL can be stable against allowed short-range parton interactions. We also argue that both states persist upon allowing $\mathbb{Z}_2$ gauge field fluctuations, in that the number of gapless modes is retained, although with an expanded set of contributions to observables compared to the free parton mean field.

¹National Science Foundation through grant DMR-0907145 and A. P. Sloan Foundation.

1:51PM J8.00014 Static and dynamic properties of a strong-leg spin ladder, DAVID SCHMIDIGER, SEBASTIAN MUEHLBAUER, SEVERIAN GVASALIYA, ANDREY ZHELUEV, Neutron Scattering and Magnetism Group, ETH Zurich, Laboratory for Solid State Physics, PIERRE BOUILLLOT, DPMC-MaNEP, University of Geneva, CORINNA KOLLATH, Departement de Physique Theorique, University of Geneva, THIERRY GIAMARCHI, DPMC-MaNEP, University of Geneva — Static and dynamic properties of the strong-leg $S = 1/2$ Heisenberg spin ladder system $(\text{C}_7\text{H}_{10}\text{N})_2\text{CuBr}_4$ are studied using inelastic neutron scattering and neutron diffraction experiments, as well as bulk magneto-thermodynamic measurements. The leg-odd excitation channel is dominated by long-lived single-magnon states in the entire Brillouin zone, which supports a symmetric-ladder model for this material [1]. In the leg-even channel, a considerable fraction of the spectral weight is contained in a novel long-lived two-magnon bound state. Contrary to reports by other authors, in applied magnetic fields we observe a Bose-Einstein condensation of magnons that manifests itself if 3D long-range antiferromagnetic ordering. The latter emerges beyond $H_c=2.8$ T and is due to weak inter-chain interactions. The field-temperature phase diagram showing the spin liquid, Tomonaga-Luttinger spin liquid and BEC phases is mapped out. The experimental results are in spectacular agreement with DMRG calculations. The latter provide additional insight on certain spin ladder properties specific to the strong-leg regime.

[1] D. Schmidiger, S. Mühlbauer, S. N. Gvasaliya, T. Yankova, and A. Zheludev Phys. Rev. B 84, 144421 (2011).

2:03PM J8.00015 Sign problem free quantum Monte Carlo simulations of spin density wave transitions in metals, EREZ BERG, Harvard University, MAX METLITSKI, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, SUBIR SACHDEV, Harvard University — We present a version of the spin-fermion model for spin density wave (SDW) transitions in metals, which can be simulated using the determinant quantum Monte Carlo method with no sign problem. The sign problem is eliminated by generalizing the model to include two orbitals which are coupled through the SDW field. The resulting model has a pseudo-time reversal symmetry that guarantees that the minus signs resulting from integrating out the fermions cancel, resulting in a real effective action for the SDW bosonic field. We present preliminary results for the SDW and pairing susceptibilities and the fermion Green's function near the quantum critical point.

Tuesday, February 28, 2012 11:15AM - 2:15PM –
Session J9 GMAG DMP: Focus Session: Magnetic Oxide Thin Films And Heterostructures -
Multiferroic Thin Films 209

11:15AM J9.00001 Electric-field induced magnetization reversal using multiferroics, MORGAN TRASSIN, Department of Materials Science and Engineering, University of California, Berkeley, CA 94720 — Controlling magnetism using solely electric fields is interesting not only from a fundamental standpoint, but presents great potential for ultimately low energy consumption logic and memory. The evidence of the electrically controllable antiferromagnetic ordering in the multiferroic magnetoelectric bismuth ferrite (BiFeO₃) drew an increasing interest in the pursuit for new emerging devices. To use such functionality for device applications, deterministic control not only of antiferromagnetism, but also ferromagnetism is essential. To achieve this goal, a ferromagnet/multiferroic heterostructure has been proposed based on the combination of magnetoelectric coupling in BiFeO₃ and exchange coupling between magnetic materials and offers a new pathway for the electrical control of magnetism. By combination of a piezoresponse force microscopy, photoemission electron microscopy and anisotropic magnetoresistance measurements, we demonstrated the non-volatile reversal of a CoFe layer magnetization induced solely by the application of an electric field at room temperature. This 180 degree rotation of the magnetization of the ferromagnetic layer is mediated by a strong interfacial coupling. The correlation between the ferroelectric state in the multiferroic layer and the CoFe ferromagnetic domain architecture is evidenced. The projection of this strong magnetoelectric coupling in an out-of-plane configuration, allowing the reduction by an order of magnitude of voltage required, will be discussed. Our results show the high potential of magnetoelectric-based heterostructures for future low energy consumption data storage devices.

11:51AM J9.00002 Properties of LuFe₂O₄ Films Grown by Molecular-Beam Epitaxy, R. MISRA, C.M. BROOKS, The Pennsylvania State University, University Park, PA, J.A. MUNDY, T. HEEG, Cornell University, NY, J. SCHUBERT, Peter Grunberg Institute (PGI 9-IT), Julich, Germany, Z.K. LIU, The Pennsylvania State University, University Park, PA, D. MULLER, D.G. SCHLOM, Cornell University, NY, P. SCHIFFER, The Pennsylvania State University, University Park, PA — LuFe₂O₄ is an exotic material with a simultaneous existence of ferroelectricity and ferrimagnetism at the highest temperature (240 K) of any known material [1]. 25 nm thick films of this unusual multiferroic were grown by MBE on MgAl₂O₄, MgO, and SiC substrates. XRD shows that the LuFe₂O₄ films are single-phase and epitaxial. Film stoichiometry was regulated using an adsorption controlled growth process by depositing LuFe₂O₄ in an iron rich environment at pressures and temperatures where the excess iron desorbs from the film surface during growth. STEM images reveal the layered structure of LuFe₂O₄ and a clean substrate-film interface free of second phases. The magnetization data exhibits a rapid increase in magnetization below 240 K consistent with the bulk paramagnetic to ferrimagnetic phase transition. On further cooling, the zero field cooled (ZFC) branch of the magnetization displays a peak at 205 K that is suggestive of a glassy transition, which is also seen in bulk samples. At 100 K and 70 kOe, we observe a saturation magnetization of 2.4 μ_B /f. u. (theoretical value of 3 μ_B /f. u.)

[1] Ikeda *et. al.*, Nature **436** (2005) 1136–1138.

12:03PM J9.00003 Growth and Characterization of Magnetoelectric Fe₂TeO₆ Thin Films¹, JUNLEI WANG, PETER DOWBEN, CHRISTIAN BINEK, University of Nebraska-Lincoln — Promising spintronic concepts such as Cr₂O₃ based voltage-controlled exchange bias systems [1] employ electric controlled boundary magnetization. Symmetry arguments reveal that equilibrium boundary magnetization is a generic property of magnetoelectric antiferromagnets [2]. However, experimental evidence of boundary magnetization is scarce and microscopic evidence has only been provided for the Cr₂O₃ (0001) surface [3]. In order to bring the concept of boundary magnetization into a broader experimental context we prepare the magnetoelectric antiferromagnet Fe₂TeO₆ with tri-rutile structure. We use two distinct approaches for the thin film growth, RF sputtering and pulsed laser deposition (PLD). Both methodologies start from targets which we prepare from sintered powder of Fe₂TeO₆ produced in a solid-state reaction. We characterize the magnetoelectric thin film of Fe₂TeO₆ structurally, magnetically and magnetoelectrically using XRD, SQUID, RHEED, LEED and MOKE. Our investigation aims on an experimental test of the predicted generality of the equilibrium boundary magnetization in magnetoelectric antiferromagnets.

[1] He, Xi *et al.*, Nature Materials **9**, 579 - 585 (2010)

[2] Belashchenko, K.D., Phys. Rev. Lett. **105**, 147204 (2010)

[3] Wu N. *et al.*, Phys. Rev. Lett. **106**, 087202 (2011)

¹This project is supported MRSEC DMR 0213808 and by the NRC/NRI supplement to MRSEC.

12:15PM J9.00004 Probing of ferroelectric and antiferromagnetic orders of multiferroic YMnO₃ via second harmonic generation¹, SRINIVAS POLISETTY, MIKEL HOLCOMB, CAMERON KEENAN, FELIO PEREZ, DAVID LEDERMAN, West Virginia University — The ferroelectric and antiferromagnetic properties of epitaxial, hexagonal (0001) YMnO₃ thin films grown on GaN/Al₂O₃ substrates were studied using second harmonic generation. A Ti:sapphire laser with a 15 W Nd:YVO₄ pump was used to generate the second harmonic signal. Above the Néel temperature, ferroelectric ordering was clearly observed as deduced from angular plots of the incoming and outgoing polarization of the second harmonic generation (SHG) signals. Additional antiferromagnetic order was identified below the Néel temperature. The ferroelectric-magnetic coupling studied via SHG will be discussed.

¹This work was supported in part by the Office of Naval Research and the National Science Foundation

12:27PM J9.00005 Investigation of Electric Field Control of Antiferromagnetic Domains in Epitaxial BiFeO₃ Thin Films Using Neutron Diffraction, W. RATCLIFF, National Institute of Standards and Technology, Gaithersburg, MD 20899, V. ANBUSATHIAH, T. GAO, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20424, P.A. KIENZLE, National Institute of Standards and Technology, Gaithersburg, MD 20899, I. TAKEUCHI, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20424 — BiFeO₃ (BFO) is a multiferroic which displays both ferroelectric and magnetic order at room temperatures. Thin films possess a simple G-type antiferromagnetic order. In the bulk, this ordering takes on an additional long-wavelength modulation in the form of a spiral [1]. Recent neutron diffraction results have revealed that it is possible to recover a modulated magnetic structure in thin films which is strongly dependent on the orientation of the substrate on which the film is grown [1]. Based on this, BFO thin films were deposited on a vicinal SrTiO₃ substrate. PFM measurements demonstrate that a ferroelectric monodomain was achieved. New neutron diffraction results show that it is possible to change the population of magnetic domains in such films through the application of an electric field (which also switches the ferroelectric domain state). Based on these results, magneto optic Kerr effect (MOKE) measurements were performed on patterned pads of exchanges coupled Co film deposited on top of the BFO films. The results of these measurements will be discussed in the context of device applications. [1] Lee Seongsu; Choi Taekjib; Ratcliff W. II; *et al.*, Phys. Rev. B **78**, 100101 (2008); Ratcliff William II; Kan Daisuke; Chen Wangchun; *et al.*, Advanced Functional Materials **21**, 1567 (2011).

12:39PM J9.00006 Antiferromagnetic and structural phase transitions in tetragonal-like BiFeO₃, H.M. CHRISTEN, G.J. MACDOUGALL, W. SIEMONS, Oak Ridge National Laboratory, J.H. NAM, Korea Institute of Ceramic Engineering and Technology, J.L. ZARESTKY, M.D. BIEGALSKI, S. LIANG, E.R. DAGOTTO, S.E. NAGLER, Oak Ridge National Laboratory — The recent observation that strain stabilizes a tetragonal-like (“T-like”) polymorph of BiFeO₃ has illustrated how epitaxial constraints can fundamentally alter the properties of this multiferroic material. We performed detailed temperature-dependent neutron and x-ray scattering experiments on epitaxial BiFeO₃ films on different substrates (SrTiO₃, LaAlO₃, YAlO₃) to study the nature of the monoclinic crystal structure and of the antiferromagnetic (AFM) order. In agreement with Monte Carlo simulations for a classical Heisenberg model, we observe a much lower Néel temperature in the T-like morph ($T_N \simeq 325\text{K}$) than in less-strained (“R-like”) films ($T_N \simeq 645\text{K}$), and additionally a low-temperature coexistence of C-type and G-type AFM. Independent of the antiferromagnetic transition, at $T \simeq 375\text{K}$ we also observe a structural phase transition from one type of monoclinic distortion to a different one. In combination, these measurements shed light on the complexity of the phase diagram of BFO, and provide routes to explore how the material’s properties can be tuned by external parameters. Research supported by the U.S. DOE, BES, MSED (H.M.C., W.S., S.L., E.D., H.M.C) and SUFD (M.D.B., G.J.M, J.L.Z, S.E.N.).

12:51PM J9.00007 Reversible switching of magnetic easy axis in Co/BiFeO₃ thin film heterostructures¹, TIEREN GAO, ANBUSATHIAH VARATHARAJAN, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20424, WILLIAM RATCLIFF, NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA, ICHIRO TAKEUCHI, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20424, UNIVERSITY OF MARYLAND TEAM, NIST COLLABORATION — We are investigating the magnetic properties of a thin Co layer deposited on top of and exchange coupled to (001) BiFeO₃ (BFO) thin films. 5 nm Co layer is evaporated and patterned into 100 micron x 100 micron pads. We measure angular dependent magnetic hysteresis loop of the Co layer using the magneto-optical Kerr effect and by sweeping the direction of the external magnetic field. We find that exchange-coupled Co layer always develops a magnetic easy axis along the [100] or [010] direction of BFO. As electric field pulses are applied between the Co pad and the bottom electrode (SrRuO₃), non-volatile changes in the magnetic properties are observed in the Co layer. For a particular Co/BFO configuration, application of an electric field corresponding to the ferroelectric coercive field of the BFO film switches the magnetic easy axis by 45°. Upon application of the opposite electric field pulse, the easy axis switches back to the original direction. Subsequent applications of the alternating electric field pulses result in repeating reversible switching between the initial easy axis direction and the 45° rotated direction.

¹This work is funded by NSF MRSEC at UMD.

1:03PM J9.00008 Probing interface reconstructions in multiferroic BiFeO₃ and charge ordered La_{0.5}Ca_{0.5}MnO₃ heterostructures, GUNEETA SINGH-BHALLA, MORGAN TRASSIN, YING-HAO CHU, RAMMAMOORTHY RAMESH, Berkeley — Spurred by the potential for device structures with multiple tuning parameters, recent explorations of carefully engineered oxide interfaces have highlighted intriguing possibilities. A famous example includes the LaAlO₃/SrTiO₃ heterostructure where the individual layers are insulating but an electron gas appears at the interface. In similar fashion, the atomically engineered interface between antiferromagnetic BiFeO₃ and ferromagnetic manganite [La,Sr]MnO₃ results in the formation of a ferromagnetic state in BiFeO₃ at the interface. Here we explore the interface between BiFeO₃ and the charge ordered manganite, La_{0.5}Ca_{0.5}MnO₃. The insulating nature of La_{0.5}Ca_{0.5}MnO₃ and BiFeO₃ allows us to directly probe the electronic properties of the interface via transport measurements. A combination of capacitance and field effect measurements combined with structural probes shed new light on the charge ordered manganite and multiferroic interface. We explore the effects of cross-plane ferroelectric switching in BiFeO₃ on charge ordering in La_{0.5}Ca_{0.5}MnO₃, and hence the electronic and magnetic properties of La_{0.5}Ca_{0.5}MnO₃ near the interface. We discuss our results and implications.

1:15PM J9.00009 Promise of new multiferroics: Synthesis and characterization of epitaxial NiTiO₃ films, TAMAS VARGA, EMSL at PNNL, Richland, WA, TIMOTHY DROUBAY, PNNL, Richland, WA, MARK BOWDEN, EMSL at PNNL, Richland, WA, SCOTT CHAMBERS, PNNL, Richland, WA, BERND KABIUS, WILLIAM SHELTON, PONNUSAMY NACHIMUTHU, VAITHIYALINGAM SHUTTHANANDAN, EMSL at PNNL, Richland, WA, EMSL INTRAMURAL TEAM — In a search for new multiferroic materials where the direction of magnetization can be switched by an applied electric field, we have looked for materials in which polarization and magnetization are strongly coupled. Recent theory calculations predicted that the family of compounds MTiO₃ (M = Mn, Fe, Ni), in a certain polymorphic structure (acentric *R3c*), are promising candidates where a polar lattice distortion can induce weak ferromagnetism. Guided by these insights, a rhombohedral phase of NiTiO₃ has been prepared in epitaxial thin film form, whose structure is very close to that predicted to be a multiferroic. The synthesis of such new epitaxial films, their full structural characterization and physical property measurements along with our first-principles DFT calculations to predict the desired NiTiO₃ structure and its stability are reported.

1:27PM J9.00010 Structural Control of Magnetic Anisotropy in a Multiferroic EuTiO₃ Thin Film, J.W. FREELAND, Argonne National Laboratory, X. KE, Oak Ridge National Laboratory, P.J. RYAN, J.W. KIM, J.-H. LEE, Argonne National Laboratory, R. MISRA, P. SCHIFFER, Pennsylvania State University, T. BIROL, C.J. FENNIE, D.G. SCHLOM, Cornell University — Strain control of EuTiO₃ has been shown under tensile strain the system converts to a multiferroic groundstate with ferromagnetic and ferroelectric order[1]. Here we present a study of the magnetic order in thin films of EuTiO₃ grown on DyScO₃(110) substrates by reactive molecular-beam epitaxy (MBE). Neutron scattering and magnetic measurements show the magnetic moment orders with an easy axis along only one of the (110) pseudocubic axis of the unit cell. Such an easy axis is connected to the uniaxial crystal structure that evolves from cubic to tetragonal with octahedral tilting, which agrees well with the strain dependent structure predicted under biaxial tensile strain. The magnetic anisotropy for Eu is attributed to an asymmetric crystal field due to the uniaxial symmetry of the Eu-O coordination. Work at Argonne, including the Advanced Photon, is supported by the U.S. Department of Energy, Office of Science, and Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. [1] J.-H. Lee et al. Nature 466, 954 (2010).

1:39PM J9.00011 Growth and Optical Properties of Multiferroic LuFe₂O₄ Thin Films, R.C. RAI, A. DELMONT, A. SPROW, Department of Physics, SUNY College at Buffalo, NY 14222, B. CAI, M. NAKARMI, Department of Physics, Brooklyn College and Graduate Center of the CUNY, Brooklyn, NY 11210 — We present surface, structural, electronic, and optical properties of multiferroic LuFe₂O₄ thin films grown on single crystal (0001) sapphire, (111) YSZ, and (001) LiNbO₃ substrates using electron-beam deposition. LFO thin films have been deposited on substrates at temperature 750 °C in an oxygen environment and post-deposition annealed at temperatures ranging from 600 to 800 °C to improve the stoichiometry and the crystal quality. We have used AFM and XRD for surface and structural characterization of the LFO thin films. To investigate the charge order phenomenon and the electronic properties, we carried out variable temperature (78 – 450 K) optical and resistivity measurements on the LFO thin films. The absorption spectra of LFO thin films show strong electronic excitations with the energy gap of ~2.18 eV at 300 K. Further, the energy gap of LFO displays strong temperature dependence, exhibiting a ferrimagnetic transition at ~240 K and a charge-order transition at ~350 K, respectively. We will also discuss the electronic excitations of the LFO thin film in the energy range 0.5 – 5.0 eV and their correlations with different magnetic and charge-ordered states.

1:51PM J9.00012 Exchange bias in BiFeO₃/CoFe₂O₄ heterostructure, YONGHANG PEI, Physics Department, University of Virginia, JIWEI LU, RYAN COMES, Department of Materials Science and Engineering, University of Virginia, STUART WOLF, Physics Department, University of Virginia — Room temperature multiferroics BiFeO₃ (BFO), both ferroelectric and antiferromagnetic, has been extensively investigated as a part of exchange bias structures since it promises the electrical field control over the exchange bias. This work focuses on the exchange interaction between ferromagnet CoFe₂O₄ (CFO) and BFO. Bilayer films CFO and BFO were first grown on SrTiO₃ (STO) by Pulsed Electron Deposition (PED) and then field cooled in magnetic field. XRD showed single phase CFO and BFO were grown epitaxially on STO single crystal substrates, and the typical thickness was 21nm for BFO and 3.6~18nm for CFO. In the bilayer structure, we observed that the coercive field increased 100% at 300K and 30 % at 50K, comparing to these of CFO single layer. Also in the bilayer structure, a noticeable exchange bias field (Hex) increased from ~30 Oe at 300 K to ~ 60 Oe at 50 K. We will discuss the impact of the film thickness and the roughness of interface on exchange bias.

2:03PM J9.00013 Magnetic and ferroelectric properties of patterned multiferroic CoFe₂O₄-BiFeO₃ nanocomposites¹, RYAN COMES, University of Virginia, Department of Materials Science and Engineering, MIKHAIL KHOKHLOV, Guilford College, HONGXUE LIU, JIWEI LU, STUART WOLF, University of Virginia, Department of Materials Science and Engineering — CoFe₂O₄ (CFO) offers unique properties as a magnetoelectric material due to its large magnetoelastic response when strained. Previous work has shown that when CFO is co-deposited with BiFeO₃ (BFO) nanostructured phase segregation occurs with CFO pillars forming in a BFO matrix and electrical control of the magnetic anisotropy is possible.[1] Such a system offers unique possibilities for an electrically-controlled spintronic logic scheme.[2] We have recently demonstrated the ability to control the location of the CFO pillars in CFO-BFO nanocomposites using e-beam lithography patterning of uniform CFO films grown on Nb-doped SrTiO₃. Square arrays of pillars with spacings as small as 100 nm have been grown in nanocomposites using pulsed electron deposition. Piezoresponse force microscopy (PFM) measurements show clear ferroelectric response in the BFO matrix. The out-of-plane piezoelectric response, d_{33} , has been measured via PFM within the BFO matrix and is in good agreement with published results for BFO. Magnetic force microscopy (MFM) shows in-plane magnetic anisotropy in the pillars due to compressive in-plane strain. [1] F. Zavaliche, et al. *Nano Lett.* **7** (2007). [2] S.A. Wolf, et al. *Proc. IEEE* **98** (2010).

¹Funding from Nanoelectronics Research Initiative, NSF (DMR-08-19762), DARPA (HR-0011-10-1-0072) and NDSEG.

Tuesday, February 28, 2012 11:15AM - 2:15PM —

Session J10 DCOMP: Invited Session: How Reliable are Computed Electronic Properties? 210A

11:15AM J10.00001 Validation of Atomic, Molecular and Condensed Matter Calculations, ERIC SHIRLEY, NIST — The advances in calculational techniques have brought first-principles calculations to a state of frequently having their results for various physical properties agreeing well with measured results for the same properties. Validation of computational results can therefore be an important undertaking in the overall scheme of first-principles work. Along these lines, such validation does not refer to the appropriateness of approximations made in calculations which are necessary to have a practicable methodology. Rather, such validation refers to whether calculations are implemented correctly given whatever approximations one assumes. Three areas are to be discussed in turn to illustrate issues that may arise. These include density-functional total-energy calculations in atoms and ions, in which as many as four atomic-structure programs were tested (and corrected) to permit reasonably high-precision comparisons of results. Second, calculations of dielectric properties and excitation spectra of solids shall be discussed, to illustrate the myriad of choices one might be required to make in terms of approximations, and how various approximations' results can only be compared if numerical methodologies used in conjunction with the respective approximations are sufficiently similar. Third, as a point of reference, brief consideration shall be given to the progress in the calculational validation area made within the quantum chemistry community.

11:51AM J10.00002 New Tools for the Verification and Validation of Electronic Structure Calculations¹, FRANCOIS GYGI, Department of Computer Science, University of California Davis, Davis CA 95616 — First-principles electronic structure calculations are playing an increasingly important role in the prediction of materials properties and in the interpretation of experimental data. Numerous simulation codes including various levels of approximations and various numerical approaches are now readily available to users. The complexity of first-principles calculations and the large number of input parameters needed in a simulation make it challenging to obtain high quality, reproducible data. Results obtained with different electronic structure codes are difficult to compare as they involve a multitude of data formats, making the process of verification and validation (V&V) of electronic structure data complex and error prone. In order to facilitate V&V activities, we have introduced ESTEST [1,2], a web-based framework that allows for automatic comparison and post-processing of results obtained with six electronic structure codes. Recent developments make it possible to extend this functionality to a decentralized network of servers. We discuss general issues related to the process of verification and validation of electronic structure data and outline requirements for the development of future V&V tools.

[1] G. Yuan and F. Gygi, *Computational Science & Discovery* **3**, 015004 (2010) doi:10.1088/1749-4699/3/1/015004G

[2] <http://estest.ucdavis.edu>

¹Supported by NSF OCI 0749217 and DOE SciDAC DE-FC02-06ER25794.

12:27PM J10.00003 Single-electron excitations of molecules and solids — reliability and robustness of density-functional theory and *GW* calculations, MATTHIAS SCHEFFLER¹, Fritz-Haber-Institut der MPG — State-of-the-art theory addresses single-electron excitations in molecules and condensed matter by linking density-functional theory (DFT) with many-body perturbation theory. Experimentally such results correspond to measurements by direct or indirect photoemission. In actual calculations it is common to employ the pseudopotential approach, where pseudo-wave-functions enter the calculation of the selfenergy, and the core-valence interaction is treated at the DFT level. Furthermore, calculations are typically not done selfconsistently but as a first-order perturbation on some starting point. The latter may be DFT with LDA, GGA, LDA+*U*, HF, or hybrid functionals. Unfortunately, these different starting points can give noticeably different results. In this talk I will evaluate the various approximations, by comparing and analyzing pseudopotential and all-electron calculations. I will also emphasize the need for selfconsistency either by an iterative solution of the Dyson equation or by properly adjusting the zero-th order exchange-correlation functional.

¹Work done in collaboration with V. Atalla, F. Caruso, C. Draxl, R. Gomez-Abal, H. Jiang, R. Ramprasad, X. Ren, P. Rinke, A. Rubio.

1:03PM J10.00004 Role of Validation and Predictions in Modeling: Specific Examples from Semiconductor Industry Applications, SADASIVAN SHANKAR, Intel Corporation Santa Clara, California, USA — With the advent of newer non-Silicon materials, using modeling to estimate properties are becoming necessary for process technology development. Since these materials are integrated as part of larger devices, interfaces and material domains are increasingly modulating properties of materials. Unlike in bulk materials, electronic and thermodynamic properties are difficult to characterize in these material structures as the device sizes overlap with material domains. We will illustrate specific cases from semiconductor processing and property estimation on the importance of verification of models for internal consistency and validation with experimental data. Given the discrepancy of scales between predictions and measurement, techniques need to bridge them. In addition, models that are developed need to be modular with open interfaces for cross-checking and integration across scales as indicated in the recently announced Materials Genome Initiative.

[1] President's initiative on Materials Genome Initiative for Global Competitiveness, June 2011

[2] S. Shankar, B. V. McKoy, W. L. Morgan, "Self-Consistent Modeling of Weakly Ionized Plasmas-Challenges in Quantum and Classical mechanics," Sixth U.S. National Congress on Computational Mechanics, U.S. Association for Computational Mechanics, Dearborn, Michigan, (2001)

1:39PM J10.00005 Materials by design, GERBRAND CEDER, Massachusetts Inst of Tech-MIT — No abstract available.

Tuesday, February 28, 2012 11:15AM - 2:15PM —

Session J11 DMP: Focus Session: Graphene Structure, Stacking, Interactions: Density Functional Theory 210B

11:15AM J11.00001 Electronic structure, electron-phonon coupling and superconductivity in metal-doped few-layer graphene, SERDAR OGUT, University of Illinois at Chicago, XUHUI LUO, University of Illinois at Chicago & National Institute of Standard and Technology, TANER YILDIRIM, National Institute of Standard and Technology & University of Pennsylvania — We systematically investigate from first-principles how the electronic properties and electron-phonon (el-ph) coupling change in metal (Ca, Li) doped graphene as we tune the number of graphene layers from single layer to three layers and to the case of bulk graphite. We find that the Fermi level and el-ph constant can be tuned by the number of layers. In particular, the number of graphene layers has a large effect on the inter-layer metal free-electron-like states, which give rise to large el-ph constant in these systems. Surprisingly, the el-ph coupling in Ca intercalated tri-layer graphene system is stronger than one in the superconducting Ca-doped graphite. Our results suggest the possibility of high T_c superconductivity in metal doped few-layer graphene for nanodevice applications.

11:27AM J11.00002 First-principles investigation of lithium doped of bilayer graphene and Lithium Intercalated Carbon Nanotubes, OGUZ GULSEREN, HUSEYIN SENER SEN, Bilkent University — We have performed first-principles calculations based on density-functional theory for understanding of the structural and electronic properties of Li doped bilayer graphene and Li intercalated CNTs especially addressing the controversial charge transfer state between Li and C. We have checked the possible adsorption, substitution and intercalation of Li by using a bilayer graphene system both with AB stacking (12 different initial configurations) and AA stacking (8 different initial configurations). All calculations are repeated both with LDA and GGA exchange-correlation potential, even though the values of binding energies are different, their order and corresponding physical picture are same from both of the functionals as well as the stackings. In conclusion, we can summarize that Li prefers the hollow site adsorption geometry and it prefers intercalation but not the substitution. In these adsorption modes, almost 0.9 electron of Li atom is transferred to neighboring carbon atoms network leaving positively charged core behind.

11:39AM J11.00003 Ab Initio Study of the Interactions between Dopant Atoms in Graphene¹, IGOR VASILIEV, NABIL AL-AQTASH, TAREK TAWALBEH, KHALDOUN AL-TARAWNEH, New Mexico State University — We present a first-principles computational study of the interactions between the boron (B) and nitrogen (N) dopant atoms in graphene. Our calculations are carried out using density functional theory combined with the generalized gradient approximation for the exchange-correlation functional. The total energies, equilibrium geometries, electronic charge distributions, and densities of states of doped graphene sheets are examined in cases of B-B, N-N, and B-N co-doped graphene. We find the B-B and N-N interactions to be repulsive and the B-N interaction to be attractive. In all cases studied, dopant-dopant interactions appear to have a relatively short range. The interaction energy between the two dopant atoms is found to be inversely proportional to the square of the separation distance. We interpret these results in terms of structural relaxation and electronic charge transfer.

¹Supported by NSF CHE-1112388.

11:51AM J11.00004 Ab Initio Study of the Interactions between Dopant Atoms and Point Defects in Graphene¹, TAREK TAWALBEH, IGOR VASILIEV, New Mexico State University — We apply a first-principles computational method based on density functional theory to study the interaction of substitutional boron and nitrogen atoms with Stone-Wales defects and vacancies in graphene. Our calculations are carried out using a pseudopotential technique combined with the generalized gradient approximation for the exchange-correlation functional implemented in the SIESTA electronic structure package. Graphene sheets are modeled by periodic supercells containing up to 160 atoms. The equilibrium geometries, total energies, electronic structures, and densities of states of doped and defective graphene sheets are examined as a function of the separation distance between dopant atoms and point defects in graphene. The results of our study demonstrate the presence of attractive interaction between dopant atoms and point defects in graphene. The interaction energy decreases rapidly with increasing the dopant-defect separation distance.

¹Supported by NSF CHE-1112388.

12:03PM J11.00005 Many-body study of cobalt adatoms adsorbed on graphene¹, YUDISTIRA VIRGUS, WIRAWAN PURWANTO, HENRY KRAKAUER, SHIWEI ZHANG, College of William and Mary — Interest in the adsorption of transition metal adatoms on graphene has grown rapidly. The interaction between magnetic adatoms and graphene may have applications in designing spintronics devices. Several theoretical and experimental studies have examined Co adatoms on graphene. Calculations of Co-graphene systems have largely been done at the density functional theory (DFT) level, with local or semi-local functionals and with an empirical Hubbard on-site repulsion U (LDA+ U). We use auxiliary-field quantum Monte Carlo (AFQMC), in combination with DFT and quantum chemistry methods, to examine the effects of electron correlation in Co-graphene systems, without adjustable parameters. Binding energy curves for Co-graphene and model structures will be presented, and their implications on the electronic and structural properties will be discussed.

¹DOE, ONR, and NSF

12:15PM J11.00006 Adsorption of group VA atoms in single and double vacancy of graphene, SHYAM KATTEL, BORIS KIEFER, Physics Department, New Mexico State University, PLAMEN ATANASSOV, Chemical and Nuclear Engineering Department, University of New Mexico — Dopants can greatly affect the electronic structure of graphene. In this study we report on the effect of group VA elements associated with single vacancy (SV) and double vacancy (DV) on the electronic structure of graphene. The results of our density-functional-theory (DFT) computations predict strong and exothermic chemisorption of group VA atoms to SV and DV in graphene ($M@SV/DV$, where $M=N, P, As, Sb, \text{ or } Bi$) which leads to large, systematic and diverse effects on its electronic structure. We find that $N@SV$ has a small band gap below Fermi level (E_F) and $P@SV$ has semiconducting and magnetic properties consistent with previous studies. Our preliminary band structure computations show that $As@SV$ induces $\sim 100\%$ spin polarization close to E_F while $Sb@SV$ and $Bi@SV$ are metallic. In contrast, $N@DV$ has a large spin polarization near E_F while all other DV defects are predicted to be metallic. These results suggest that especially $As@SV$ and $N@DV$ may have interesting applications in spintronics and nanoelectronics.

12:27PM J11.00007 ABSTRACT WITHDRAWN —

12:39PM J11.00008 Stability and electronic structure of the functionalized graphene layers¹, JACEK A. MAJEWSKI, KAROLINA MILOWSKA, MAGDALENA BIROWSKA, MAGDALENA WOJNSKA, University of Warsaw — We present results of extensive ab initio calculations in the framework of the density functional theory of the graphene layers (GLs) doped with nitrogen and boron, and also functionalized with simple OH, COOH, NH_n , and CH_n molecules. We calculate binding energies, heat of formation, resulting local deformations (characteristic sp^3 rehybridization of the bonds induced by fragments), electronic structure, elastic properties (Young's modulus and Poisson ratio), and conductance of doped and functionalized GLs as a function of the density of the functionalizing systems. Generally, the stability of the functionalized graphene layers decreases with the growing concentration of functionalizing molecules and we determine the critical density of the molecules that can be chemisorbed on the surface of GLs. We find out that the GLs functionalization leads in many cases to the opening of the graphene band gap and can be therefore utilized in graphene devices. In particular, the zero band gap in K-point of the pristine single GL increases to 0.11, 0.12, 0.25, and 0.24 eV for the GL functionalized with OH, NH, NH_2 , and COOH, respectively.

¹The studies were carried out within the SiCMAT Project financed under the European Funds for Regional Development (Contract No. UDA-POIG.01.03.01-14-155/09).

12:51PM J11.00009 Band Structures of bilayer graphene with experimentally measured twisting angles, HOULONG L. ZHUANG, Department of Materials Science and Engineering, Cornell University, ROBIN W. HAVENER, School of Applied and Engineering Physics, Cornell University, JIWOONG PARK, Department of Chemistry and Chemical Biology, Cornell University, RICHARD G. HENNIG, Department of Materials Science and Engineering, Cornell University — Using density functional theory (DFT) and tight binding calculations, we study the band structure of bilayer graphene as a function of twisting angles and compare the results to spectroscopic measurements. To test the accuracy of DFT, we first compare the band structure with DFT and the G_0W_0 approximation for several bilayer graphene systems with special twisting angles. Our DFT results agree with previous DFT calculations for the weak coupling between the two layers and the band structure. Calculations of the quasiparticle dispersion using the G_0W_0 approximation show that DFT underestimates the Fermi velocity of bilayer graphene and the bandgap away from the K' point. Scaling of the DFT band structure by an empirical parameter that depends on the twist angle accounts for most of the difference between the DFT and the G_0W_0 approximation. Based on the G_0W_0 calculations, we fit a set of tight-binding parameters for the interlayer coupling Hamiltonian. Using this tight-binding model we study the band structure of bilayer graphene for twist angles that closely match experimental systems and have larger unit cells. The results of these band structure calculations explain the experimentally observed G band resonance in Raman spectroscopy for specific twist angles.

1:03PM J11.00010 From graphene to graphite: A first-principles study¹, BI-RU WU, Department of Nature Science, Center for General Education, Chang Gung University — The multilayer graphene and graphite are systematic studied via a first-principles method based on density functional theory and general gradient approximation. The hexagonal, Bernal and rhombohedral stacking types are considered. The total energy, the electronic structure and the strength of the multilayer graphene and graphite are analyzed to study the process of graphene to graphite. We predict the number of graphene multilayers shall be greater than 15 layers to behave as a graphite bulk.

¹This work was supported by the National Science Council of the Republic of China and Chang Gung University.

1:15PM J11.00011 Accurate computational studies of carbon doped two-dimensional boron-nitride¹, HYOUNGKI PARK, AMITA WADEHRA, JOHN W. WILKINS, Department of Physics, The Ohio State University, ANTONIO H. CASTRO NETO, Graphene Research Centre, National University of Singapore, Singapore and Department of Physics, Boston University — Advances in development of atomic-layer crystals with a plethora of new materials are greatly extending the range of possible applications of these two-dimensional (2D) materials. One of these materials is the hexagonal structure of boron nitride (h-BN). Hexagonal BN has a wide band gap and a lattice constant similar to that of graphene. We show that even small quantities of C atoms can offer new functionalities and transform h-BN to be an amazing playground for 2D physics. Large-scale accurate density-functional-theory calculations with the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional reveal the electronic and the magnetic properties of h-BN with substitutionally embedded carbon atoms. Results of local magnetic moments induced by substitution and their interactions are presented for low C concentrations. We also show the electronic structures of quantum dots made of carbon nano-domains for applications in optics and opto-electronics.

¹Supported by DOE-Basic Energy Science DOE-BES-DMS (DEFG02-99ER45795). AHCN acknowledges DOE grant DE-FG02-08ER46512, ONR grant MURI N00014-09-1-1063, and the NRF-CRP award (R-144-000-295-281). Computing resources are provided by NERSC and OSC.

1:27PM J11.00012 Electronic and Structural Properties of Graphene Dots in h-BN, ZHAOHUI HUANG, JAMES CHELIKOWSKY, University of Texas at Austin — A major challenge for graphene-based applications is the creation of a tunable electronic band gap as would be present for traditional semiconductor alloys. Since hexagonal boron nitride has a very similar structure to graphene, it is a natural candidate to modify the electronic structure of graphene by forming a hybrid phase sheet containing domains of graphene and hexagonal boron nitride, as has been done experimentally. Here we investigate the properties of such hybrid sheets by using pseudopotential-density functional theory implemented in real space. We find for a graphene dot comparable in size to those observed in experiment, the band gap of the sheet is not significantly modified. Moreover, when the size of graphene dot decreases below $\sim 13\text{\AA}$, strong structural instabilities of the graphene domain occur.

1:39PM J11.00013 Hybrid density functional study of 2D graphene-boron nitride (BCN) nanostructures¹, AMITA WADEHRA, HYOUNGKI PARK, JOHN W. WILKINS, The Ohio State University, ANTONIO H. CASTRO NETO, Graphene Research Centre, National University of Singapore and Boston University — Graphene has attracted enormous research interest in the last few years because of its intriguing physics as well as application potential. Recent synthesis of BCN nanostructures by doping graphene with a wide bandgap insulator boron nitride (BN) has unveiled new possibilities for this material [1]. BCN nanostructures are semiconductors and possess interesting properties that are distinct from the parent compounds. Reliable theoretical estimates can predict the feasibility and usefulness of still largely unexplored BCN nanostructures, and provide a route to engineer their properties. We study electronic structures of a variety of 2D BCN nanostructures using hybrid functional HSE in density functional theory (DFT). We show that their properties can be gradually tuned and are sensitive to composition and the type of configurations. In agreement with experimental observation, a strong tendency to phase-segregate exists for low concentration of BN in graphene. We also investigate magnetic properties of graphene containing substitutional nitrogen atoms, and their suitability for magnetic devices.

[1]. L. Ci et al., *Nature Materials* 9, 430 (2010).

¹Supported by DOE grants DE-FG02-99ER45795 and DE-FG02-99ER45795, ONR grant MURI N00014-09-1-1063, and NRF-CRP award R-144-000-295-281. Computational resources: NERSC and OSC.

1:51PM J11.00014 First-principles and Tight-binding Investigations of Graphene-like Systems¹, X.W. SHA, E.N. ECONOMOU, D.A. PAPACONSTANTOPOULOS, George Mason University, M. PEDERSON, M.J. MEHL, Naval Research Laboratory, M. KAFESAKI, University of Crete — We have performed first-principles calculations of graphene-like systems with large unit cells of the order of 100 atoms. These are mostly quasi-circular pieces of graphene with or without hydrogen atoms to passivate dangling bonds. We have also introduced nitrogen replacements of carbon atoms to explore possibilities of creating a quantum-mechanical analog of the split-ring resonator used in negative refractive index metamaterials. In addition, vibrational spectra were calculated to check the stability of the small flakes. Furthermore, we have used the NRLMOL DFT code with extensions to treat an AC magnetic field coupled to spin and orbital moments. We simulate the graphene-like system to a circuit model to show the cancellation of individual loop currents and the emergence of an edge ballistic current. A tight-binding Hamiltonian was fitted to our NRLMOL results using the NRLTB method. The TB approach starts with an exact fit to the benzene molecule and the resulting TB parameters are transferable to the larger molecules matching well the HOMO-LUMO gap found by the DFT. The NRLTB scheme allows to calculate the electronic spectra of much bigger systems, and examples with results for systems with more than a thousand atoms will be presented.

¹This work is supported by the Air Force and ONR.

2:03PM J11.00015 Quasiparticle Band Gaps of Graphene and Graphene on Hexagonal Boron Nitride Substrate, NEERAV KHARCHE, SAROJ NAYAK, Computational Center for Nanotechnology Innovations, Department of Physics, Rensselaer Polytechnic Institute — Graphene holds great promise for post-silicon electronics; however, it faces two main challenges: opening up a band gap and finding a suitable substrate material. Graphene on hexagonal boron nitride (hBN) substrate provides a potential system to overcome these challenges. While theoretical studies suggested a possibility of a finite band gap of graphene on hBN, recent experimental studies find no band gap. We have studied graphene-hBN system using the first-principles density functional method and the many-body perturbation theory within GW approximation [1]. A Bernal stacked graphene on hBN has a band gap on the order of 0.1 eV, which disappears when graphene is misaligned with respect to hBN. The latter is the likely scenario in realistic devices. In contrast, if graphene supported on hBN is hydrogenated, the resulting system (graphene) exhibits band gaps larger than 2.5 eV. The graphene band gap is due to chemical functionalization and is robust in the presence of misalignment, however, it reduces by about 1 eV due to the polarization effects at the graphene/hBN interface.

[1] N. Kharche and S. K. Nayak, *Nano Lett.*, DOI: 10.1021/nl202725w, (2011).

Tuesday, February 28, 2012 11:15AM - 2:03PM –
Session J12 DMP: Focus Session: Graphene: Growth, Mechanical Exfoliation, and Properties
- Strain and Structure 210C

11:15AM J12.00001 Growth-induced electronic properties of epitaxial graphene¹, PHILLIP FIRST, School of Physics, Georgia Institute of Technology — The growth of epitaxial graphene on silicon carbide is challenging to understand and control, yet rife with scientific and technological opportunities. This is due in part to different growth-induced structures such as the “moiré” alignment of graphene layers in multilayer epitaxial graphene on SiC(0001) and the formation of sidewall ribbons at natural and lithographically-defined SiC(0001) step-bunches (nanofacets). We apply scanning tunneling microscopy (STM) and spectroscopy (STS) to probe the local energy bands of such growth-induced structures. STS at cryogenic temperatures and large magnetic fields creates a comb of discrete Landau level energies that we use to quantitatively characterize the local electronic properties.

¹Work done in collaboration with NIST-CNST; supported by NSF and NRI-INDEX.

11:51AM J12.00002 Colossal Corrugations in Freestanding Graphene Observed with STM¹, P.M. THIBADO, P. XU, Y. YANG, S.D. BARBER, M.L. ACKERMAN, J.K. SCHOELZ, SALVADOR BARRAZA-LOPEZ, L. BELLAICHE, Department of Physics, University of Arkansas, IGOR A. KORNEV, Propriétés et Modélisation des Solides, France — The discovery of graphene, a unique two-dimensional electron system with extraordinary physical properties, has ignited tremendous research activity in both science and technology. Graphene interactions with a substrate, such as SiO₂/Si, are known to significantly degrade the electrical performance of graphene devices. Alternatively, suspending a graphene device eliminates the substrate interaction, thereby yielding a 10-fold increase in mobility. However, a detailed investigation on the microscopic scale explaining the origin of these improvements has yet to be completed. In this talk, we present for the first time atomic-resolution STM images of a freestanding graphene membrane. Samples were prepared by direct CVD growth and by large graphene sheet transfer, both onto a 2000-mesh copper grid. Atomic-scale corrugation amplitudes were observed in perfect registry with, yet 50 times larger than the expected electronic corrugations. Density functional theory revealed that charge localization occurs directly beneath the STM tip due to bond angles rotating away from sp² hybridization as graphene flexes in response to the electrostatic attraction. A detailed model of the 3-way interaction which accounts for the observed behavior will be discussed.

¹Support provided by ONR N00014-10-1-0181, N00014-08-1-0915, NSF 0855358, 0701558, DoE 46612.

12:03PM J12.00003 Melon: A carbon-nitride analog to graphene, JOEL THERRIEN, YANCEN LI, ECE U. Mass Lowell, DANIEL SCHMIDT, Plastics Eng U Mass Lowell — Although graphene remains the premier 2-D material, many others have been shown to exist. A close analog to graphene would be a two-dimensional sheet composed of carbon and nitrogen, known as melon. Bulk melon, also known as graphitic carbon-nitride, has been successfully synthesized and shown to be an organic semiconductor with a band-gap around 2.7 eV. We report on the successful synthesis of single layer and few layer melon. The physical and electrical characteristics of this close cousin to graphene will be presented along with the synthesis method.

12:15PM J12.00004 AB-stacked multilayer graphene synthesized via chemical vapor deposition: a characterization by hot carrier transport, DEBTANU DE, CARLOS DIAZ-PINTO, Department of Physics and the Texas Center for Superconductivity, University of Houston, Houston, Texas 77204, VIKTOR HADJIEV, The Texas Center for Superconductivity, University of Houston, Houston, Texas 77204, HAIBING PENG, Department of Physics and the Texas Center for Superconductivity, University of Houston, Houston, Texas 77204 — We report the synthesis of AB-stacked multilayer graphene via ambient pressure chemical vapor deposition on Cu foil. Four-terminal devices were fabricated from such graphene and characterized by hot carrier transport at temperatures down to 240 mK and in magnetic fields up to 14 T. The differential conductance (dI/dV) shows a characteristic dip at longitudinal voltage bias $V=0$ at low temperatures, indicating the presence of hot electron effect due to a weak electron-phonon coupling. Under magnetic fields, the magnitude of the dI/dV dip diminishes through the enhanced intra-Landau level cyclotron phonon scattering. Our results provide new perspectives in obtaining and understanding AB-stacked multilayer graphene, important for future graphene-based applications.

12:27PM J12.00005 Signatures of indentation strain in graphene conductance, MATTHEW BARR, MARIO BORUNDA, ERIC HELLER, Harvard University — We investigate effects on the conductance of a graphene sheet of electron scattering from a localized indentation. Strain in graphene creates effective magnetic fields, and the scattering from a radial strain profile is distinct from other short range scatterers. Through tight-binding calculations, we examine the expected conductance in several experimental geometries, including within graphene nano-ribbons and suspended graphene.

12:39PM J12.00006 Transport in Suspended graphene under strain, HANG ZHANG, JHAO-WUN HUANG, JAIRO VELASCO, DAVID DUNG TRAN, KEVIN MYHRO, ZENG ZHAO ADAM, FENGLIN WANG, YONGJIN LEE, WENZHONG BAO, CHUN NING (JEANIE) LAU, None — Suspended graphene devices with graphene flakes were fabricated using acid etching approach, and strained via application of gate voltage. The stretching procedure was observed and verified by in situ SEM imaging. We observe a change in the devices' minimum conductance and mobility values. Latest experimental results will be compared with theoretical models.

12:51PM J12.00007 Suppression of Weak-Localization Effect in Strained CVD -grown Graphene¹, XIAOCHANG MIAO, SEFAATTIN TONGAY, ARTHUR F. HEBARD, Department of Physics, University of Florida, Gainesville, FL 32611 — We investigate the magnetic field and temperature-dependent transport properties of CVD-grown graphene subjected to different strains. The graphene is transferred to kapton substrates to which a blending force can be applied. In zero magnetic field, the prefactor to the logarithmic-in-temperature conductivity correction decreases by an approximate factor of 3 for strains as high as 0.6 %. There is also a concomitant decrease in diffusivity by a factor of 7. At 5 K we observe negative magnetoresistance for fields up to 0.2 Tesla followed by positive magnetoresistance at higher fields. We attribute the low field negative magnetoresistance to weak-localization and find that it is well described by theory. The strains resulting from the applied blending force inhibit the intervalley scattering rate more than an order of magnitude, thereby leading to a suppression of weak-localization.

¹This work is funded by NSF and ONR.

1:03PM J12.00008 Probing Mechanical Properties of Chemical Vapor Deposition Graphene Membranes Using Indentation Methods, GWAN-HYOUNG LEE, Department of Mechanical Engineering, Columbia University, (And) Samsung-SKKU Graphene Center (SSGC), RYAN COOPER, SUNGJOO AN, AREND VAN DER ZANDE, NICHOLAS PETRONE, Department of Mechanical Engineering, Columbia University, SUNWOO LEE, Department of Electrical Engineering, Columbia University, ALEX HAMMERBERG, Department of Mechanical Engineering, Columbia University, CHANGGU LEE, Department of Mechanical Engineering, Sungkyunkwan University, BRYAN CRAWFORD, Nanomechanics Inc., JEFFREY KYSAR, JAMES HONE, Department of Mechanical Engineering, Columbia University — Recent experimental studies have shown that two-dimensional pristine graphene is the strongest material ever measured. We used Atomic Force Microscopy (AFM) and Agilent G200 nanoindenter to measure the mechanical properties of graphene films obtained by Chemical Vapor Deposition (CVD). CVD graphene with different grain size and number of layers were produced in controlled synthetic conditions and transferred onto silicon dioxide substrate with holes of various diameters. Nano-indentation measurement revealed that stiffness and fracture strength of CVD graphene membranes are similar to those of pristine graphene membranes under the condition that suspended graphene membrane is within a single grain boundary without defects. Furthermore, elastic modulus and fracture strength of multi-layer graphene membranes increase with respect to the number of layers.

1:15PM J12.00009 Electron transport measurement of graphene under one-dimensional local strain, A. KANDA, H. TOMORI, Y. NUKUI, Y. TOYOTA, H. KARUBE, S. NIHEI, University of Tsukuba and CREST-JST, Y. OOTUKA, University of Tsukuba, K. TSUKAGOSHI, MANA-NIMS and CREST-JST, M. HAYASHI, Akita University, H. YOSHIOKA, Nara Women's University — Introducing a nonuniform strain is a promising technique for controlling electron transport in graphene. Theories have predicted the formation of band gaps with properly designed strain; however, reports on experimental transport properties of strained graphene are quite limited. In this presentation, we report the measurement of electron transport in graphene under one-dimensional local strain. The local strain was introduced by inserting a one-dimensional dielectric nanorod between a graphene film and its substrate, using a technique reported in [1]. We found that the conductivity across the strained region decreases around the Dirac point in comparison with the unstrained graphene attached to the substrate, although the mobility far from the Dirac point is almost unchanged. The results cannot be explained by the change of the capacitance between the graphene film and the gate electrode, indicating that the strain affects the electron transport. The experimental results on strained and unstrained graphene devices from the same graphene film as well as the numerical results will be discussed.

[1] H. Tomori *et al.*, Appl. Phys. Express 4, 075102 (2011).

1:27PM J12.00010 Introducing designed local strain to graphene using dielectric nanostructures, H. TOMORI, A. KANDA, H. GOTO, Y. NUKUI, Y. TOYOTA, H. KARUBE, S. NIHEI, University of Tsukuba and CREST-JST, Y. OOTUKA, University of Tsukuba, K. TSUKAGOSHI, MANA-NIMS and CREST-JST, M. HAYASHI, Akita University, H. YOSHIOKA, Nara Women's University — Strain engineering is a promising method for controlling electron transport in graphene. In this presentation, we report a simple and easy method for inducing designed local strain in graphene films [1]. Nanostructures made of a dielectric material (electron beam resist) are placed between graphene and the substrate, and graphene sections between nanostructures are attached to the substrate. The strength and spatial pattern of the strain can be controlled by the size and the separation of nanostructures. Application of strain is confirmed by the Raman spectroscopy as well as from scanning electron microscope (SEM) images. The Raman 2D peak shows spatially nonuniform downshift, which corresponds to the positions of the resist nanostructures. From SEM images, the maximum stretch of the graphene film reaches about 20%. This technique can be applied to formation of band gaps in graphene.

[1] H. Tomori *et al.*, Appl. Phys. Express 4, 075102 (2011).

1:39PM J12.00011 ABSTRACT WITHDRAWN —

1:51PM J12.00012 Mechanical-Electric-Magnetic Coupling Effects in Black and White Graphenes, WANLIN GUO, Key Lab of Intelligent Nano Materials and Devices of MOD, Institute of Nano Science, Nanjing University of Aeronautics & Astronautics — Nanoscale multifield couplings can turn very common materials such as carbon and boron nitride into promising functional materials for many device applications. We recently found that the magnetism in graphene nanoribbons on silicon substrates can be tuned linearly by applied bias voltage (*Phys.Rev.Lett.* **103**, 187204, 2009), and this novel magnetoelectric effect is robust to material and geometry variations. Adsorbed graphene nanoribbons can also create tunable magnetism on silicon surface (*Phys.Rev.B* **82**, 235423, 2010). Strain tunable magnetism has also been found in defect graphene (*ACS Nano* **4**, 2124, 2010; *Phys. Rev. B* **82**, 085425, 2010). Contrast to the zero-gap graphene, Hexagon-BN layers (white graphene) and rolled-up nanotubes are generally insulating, we show that the wide gap in them can be tuned into semiconducting range, even closed in BN nanoribbons by electric fields and narrowed by reduced tube diameter or local curvature radius (*Nano Lett.* **10**, 5049, 2010; *Phys. Rev. B* **82**, 035412, 2010). What is more, our recent experiments have demonstrated that flow-induced-voltage in graphene can be 20 folds higher than in graphite (*Appl.Phys.Lett.* **99**, 073103 (2011)). Such extraordinary mechanical-electric-magnetic coupling effects in graphene and BN systems open up new vistas in functional devices compatible with silicon-based technology for efficient energy conversion and novel functional systems.

Tuesday, February 28, 2012 11:15AM - 2:15PM –
Session J13 DMP GMAG: Focus Session: Magnetic Nanostructures - Thin Films, Surfaces and Interfaces 211

11:15AM J13.00001 A Symmetry Microscope for Disordered Materials, DANIEL PARKS, Department of Physics, University of Oregon, KEOKI SEU, Advanced Light Source, Lawrence Berkeley National Lab, RUN SU, Department of Physics, University of Oregon, ERIC FULLERTON, ERIK SHIPTON, Electrical and Computer Engineering, UC San Diego, SUJOY ROY, Advanced Light Source, Lawrence Berkeley National Lab, STEVE KEVAN, Department of Physics, University of Oregon — We use position-resolved coherent speckle patterns in concert with rotational x-ray autocorrelation analysis to uncover “hidden” ordering at specific length scales in labyrinthine magnetic domains. Central to this measurement is understanding how finite-size effects influence the statistics of rotational cross-correlations. To this end, we present numerical simulations of domain configurations whose speckle patterns display rotational ordering similar to experimental candidates, and examine how the real-space structure of ordered and disordered domains differs. In a scanning measurement, we observe what appears to be an island of ordering in an otherwise disordered perpendicular magnetic thin film.

11:27AM J13.00002 New Magnetic State In Thin-Film Antiferromagnets and Uncompensated Magnetization¹, IGOR V. ROSHCIN, K.E. BADGLEY, Texas A&M University, K.D. BELASHCHENKO, University of Nebraska-Lincoln, MIKHAIL ZHERNENKOV, MICHAEL R. FITZSIMMONS, Los Alamos National Laboratory — We observe a new magnetic state, for which the origin ($M(H=0)=0$ point) is outside the major hysteresis loop, which means that zero magnetization at zero applied field cannot be reached isothermally. We observe this in antiferromagnet-only, (110)-FeF₂ grown on MgF₂ samples. The surface is responsible for the macroscopically broken time-reversal symmetry, uncompensated magnetization (UM) in a nominally compensated antiferromagnet, and, ultimately, for the new magnetic state. We argue that it is an equilibrium state. Magnetometry and polarized neutron reflectivity (PNR) measurements indicate that the UM is present in this AF. We report rather unusual properties of this UM, including the “intrinsic exchange bias.” While its manifestation in a shift of the hysteresis loop is similar to that of the “classical” exchange bias observed in bilayers, here, it is observed in a single layer material. We discuss the implications of the origin of the UM on the exchange bias mechanism.

¹Work is supported by Texas A&M University, TAMU-CONACYT Collaborative Research Program, DOE.

11:39AM J13.00003 Existence of Ferromagnetism in Stacked Bilayers of Pd/C₆₀¹, SIDDHARTHA GHOSH, SEFAATTIN TONGAY, ARTHUR F. HEBARD, Department of Physics, University of Florida, Gainesville, FL 32611 USA, HASAN SAHIN, SALIM CIRACI, UNAM-Institute of Materials Science and Nanotechnology, Bilkent University, 06800 Ankara, Turkey — We report on an experimental and theoretical study of the magnetic properties of multilayer structures fabricated by alternating layers of sputter-deposited Pd and thermally-sublimated C₆₀. Auger Electron Spectroscopy and SEM techniques have been used to characterize samples for which magnetic measurements in a commercially available SQUID have been made. The magnetization measurement reveals ferromagnetism in the Pd/C₆₀ system, which has Curie temperature $T_C \sim 450K$, modified Bloch coefficient $P \sim 2.7$ and a temperature-independent coercive field of 50 Oe. The observed ferromagnetism is surprising since both C₆₀ and Pd are non-ferromagnetic in the non-interacting limit. Density functional theory (DFT) calculations show that while the C₆₀ molecules are nonmagnetic unless polymerized, Pd films have a degenerate ground state that can become ferromagnetic with a weak perturbation. Though the calculated charge transfers of ~ 0.06 e between C₆₀ and Pd are not the cause of ferromagnetism, DFT shows that ferromagnetism can be associated with Pd clusters or an interaction of C₆₀ molecules with sharp edges of the Pd thin film.

¹This work is supported by the National Science Foundation (NSF) under Contract Number 1005301 (AFH) and by TUBITAK through Grant No:108T234 (SC).

11:51AM J13.00004 Spin-Wave Transmission in Ferromagnetic Thin Films: Flexoelectric Control and Spin-Wave Drag¹, TIANYU LIU, GIOVANNI VIGNALE, University of Missouri, Columbia, MICHAEL FLATTE, University of Iowa — Spin waves in insulating ferromagnets have recently emerged as an effective low-dissipation carrier of spin currents. In this work we explore a novel form of control of spin waves by *flexoelectric interactions*, which couple an electric field to the spatial gradient of the magnetization. We show that not only the short-wavelength exchange spin waves, but also the long-wavelength magnetostatic spin waves in a thin-film of magnetic insulator can be effectively controlled by an electric field. In fact, the relative electric-field-induced phase shift is even larger for magnetostatic spin waves than for exchange spin waves. We further show that spin waves in an insulating ferromagnetic film can excite a spin current in an adjacent conducting or insulating film, by way of long-ranged dipole-dipole interaction between the layers, in a magnetic analogue of the electronic Coulomb drag.

¹Work supported by ARO Grant No. W911NF-08-1-0317

12:03PM J13.00005 Impact of preparation conditions on the magnetocaloric properties of Gd thin films, H.F. KIRBY, D.D. BELYEA, J.T. WILLMAN, University of South Florida, C.J. HENDRYX, Newsome High School, C.W. MILLER, University of South Florida — The impact of the deposition temperature and gettering were investigated on Ta(5nm)/Gd(30nm)/Ta(5nm) thin films' magneto caloric(MCE) properties. The samples were grown by magnetron at temperatures up to 600 °C, with and without gettering. Structure of the samples was investigated by X-ray diffraction and ray reflectivity. The isothermal magnetization of the samples was above and below the Curie temperature of the Gd. The entropy change associated with the second order phase was calculated from M(H,T) using the thermodynamic Maxwell. Increasing the deposition temperature generally improves entropy peak (magnitude, FWHM, and temperature of the peak), but leads to significant oxidation. The ungettered sample grown at 00 °C was purely GdO (111). Gettering the chamber by sputtering the walls of the chamber for 30 minutes prior to deposition this oxidation issue, and increased the relative cooling power RCP) of films grown at elevated temperatures. The RCP values of the sample set were increased by as much as 42% over ungettered. Supported by AFOSR and NSF.

12:15PM J13.00006 Chiral modulations in MnSi thin films, THEODORE MONCHESKY, ERIC KARHU, Dalhousie University, ULRICH RÖBLER, ALEXEI BOGDANOV, Institut für Festkörper- und Werkstoffforschung Dresden, SAMER KAHWAJI, Dalhousie University, BRIAN KIRBY, NIST Center for Neutron Research, HELMUT FRITZSCHE, Canadian Neutron Beam Centre, Chalk River, MICHAEL ROBERTSON, Acadia University, CHARLES MAJKRZAK, NIST Center for Neutron Research — We present an investigation of the magnetic textures present in MnSi thin films grown on Si(111) by molecular beam epitaxy. The magnetic structure is investigated with SQUID magnetometry and polarized neutron reflectometry (PNR). For an out-of-plane magnetic field, a conical phase is formed with a reduced wavelength of $2\pi/Q = 13.9$ nm that has both left-handed and right-handed chirality due to the presence of inversion domains in the films. We show that the epitaxially induced tensile stress in the MnSi thin films creates an easy-plane uniaxial anisotropy. The magnetoelastic coefficient is obtained from SQUID measurements in combination with transmission electron microscopy and x-ray diffraction data. The agreement between density functional calculations of the coefficient with the experimental value support the conclusion that the uniaxial anisotropy originates from the magnetoelastic coupling. For an in-plane magnetic field, theoretical calculations based on a Dzyaloshinskii model that includes an easy-plane anisotropy predict a variety of modulations to the magnetic order that are not observed in bulk MnSi crystals. Evidence for these states is found in the SQUID and PNR measurements.

12:27PM J13.00007 Stabilization of surface magnetism by organic-acid adsorption¹, J. GÁZQUEZ, Instituto de Ciencia de Materiales Barcelona, Spain, J. SALAFRANCA, Universidad Complutense de Madrid, Spain, N. PÉREZ, A. LABARTA, Universitat de Barcelona, Spain, S.T. PANTELIDES, Vanderbilt University, TN, S.J. PENNYCOOK, Oak Ridge National Laboratory, TN, X. BATLLE, Universitat de Barcelona, Spain, M. VARELA, Oak Ridge National Laboratory, TN — Magnetically-disordered layers at the surface of nanoparticles and low dimensionality magnetic oxides significantly reduce the magnetization density with respect to bulk values. However, high crystal quality Fe₃O₄ nanoparticles capped with non-magnetic organic acid molecules display a surprisingly high magnetization, of unknown origin. Here, we present a real space structural, chemical and magnetic characterization of oleic-acid-capped Fe₃O₄ nanoparticles with nanometer resolution, demonstrating the presence of a strong magnetic surface layer. In combination with theoretical calculations, we establish the key role of the nanoparticle/organic-acid bond. Magnetization is restored in the surface layer because the bonding with the acid's O atoms partially lifts the surface reconstruction, resulting in surface O-Fe atomic configuration and distances close to the bulk values. Our findings have implications for the optimization of magnetic properties of nanoparticles and thin films.

¹Acknowledgements: European Research Council Starting Investigator Award program (JS, JG), Spanish MICINN and Catalan DIUE (NP, AL, XB) and the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division (MV, SJP).

12:39PM J13.00008 Surface Structure of L1₀-MnGa(111) Ultra-Thin Films Studied Using Scanning Tunneling Microscopy and First Principles Calculations¹, REYES GARCIA DIAZ, KANGKANG WANG, Ohio University Nanoscale and Quantum Phenomena Institute, NOBORU TAKEUCHI, Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, ARTHUR SMITH, Ohio University Nanoscale and Quantum Phenomena Institute — Manganese gallium alloys have drawn lots of attention recently for their many desirable properties such as high spin polarization and low damping terms. Furthermore, the magnetic properties depend sensitively on the Mn:Ga stoichiometry, ranging from ferromagnetic for MnGa, to ferrimagnetic for Mn₂₋₃Ga, and antiferromagnetic for Mn₃Ga, giving this material great magnetic tune-ability. In this talk, we will focus on the stoichiometric L1₀-structured MnGa(111) surface and study its atomic, electronic, and magnetic properties. Ultra-thin MnGa films (< 10 nm) are grown on GaN(0001) substrates using molecular beam epitaxy, and transferred *in-situ* to the analysis chamber for room-temperature scanning tunneling microscopy studies. Atomic resolution images reveal the existence of both 1×1 and 2×2 surface structures. We investigate these structures using periodic, spin-polarized density functional theory with the generalized gradient approximation (GGA), Vanderbilt ultra-soft pseudo-potentials, and a repeated slab geometry. The parameters are optimized to achieve the lowest-energy configuration. Results from these calculations and their comparison with the STM images will be reported.

¹Authors gratefully acknowledge support from the U.S. DOE and the NSF.

12:51PM J13.00009 Surface Ferromagnetism in Pt films, PUSHKAL THAPA, Dept. of Physics, Wayne State University, Detroit, MI 48201, USA, PARASHU KHAREL, Dept. of Physics, Univ. of Nebraska, Lincoln, Nebraska 68588, USA, RENAT SABIRIANOV, Nebraska Center for Materials and Nanoscience, Univ. of Nebraska, Lincoln, Nebraska 68588, USA, MOHAMMAD FAIZ, Dept. of Physics, Wayne State University, Detroit, MI 48201, USA, JULIE BORCHERS, NIST Center for Neutron Research, Gaithersburg, MD, 20899, USA, DAVID SELLMYER, Dept. of Physics and Astronomy, Univ. of Nebraska, Lincoln, Nebraska 68588, USA, BORIS NADGORNÝ, Dept. of Physics, Wayne State University, Detroit, MI 48201, USA — It has long been recognized that Pt as well as some other noble metals are on the verge of being magnetic, with ferromagnetism in these metals readily detected in nanoparticles. Here we report the observation of surface ferromagnetism in Pt thin films. Both sputtered and e-beam evaporated Pt films of various thicknesses (from 10 ~ 100 nm) have been studied. Detailed SQUID measurements indicate that the film magnetization is largely independent of its thickness. This result is consistent with the neutron scattering data, indicating the presence of a magnetic moment near the top Pt surface, and with the spin polarization measurements by point contact Andreev reflection spectroscopy, demonstrating a sizable spin polarization. Our experimental observations are supported by the first principle density functional calculations showing that certain configurations of Pt atoms on Pt (111) surface exhibit a magnetic moment of up to 1.1 μ_B per Pt atom. We argue that magnetism in this system is due to band narrowing, related to reduced coordination numbers of Pt atoms located at the surface.

1:03PM J13.00010 TiO₂ as an electrostatic template for epitaxial growth of EuO on MgO(001) by reactive molecular beam epitaxy, ADRIAN SWARTZ, JARED WONG, IGOR PINCHUK, ROLAND KAWAKAMI, UC Riverside — Interfacial electrostatics play a key role in determining epitaxial quality in the heteroepitaxy of ionic rock salt materials. We investigate the initial growth modes and the role of interfacial electrostatic interactions of EuO epitaxy on MgO(001) by reactive molecular beam epitaxy. A TiO₂ interfacial monolayer is employed to alleviate electrostatic interactions between the ions of the EuO and MgO to produce high quality epitaxial growth of EuO on MgO(001) with a 45 degree in plane rotation. For comparison, direct deposition of EuO on MgO, without the TiO₂ layer, is discussed. A key difference of EuO epitaxy on TiO₂/MgO is the ability to form EuO by substrate assisted oxidation and without the introduction of external oxygen to the interface. Such ultrathin films are shown to have bulk like magnetic properties

1:15PM J13.00011 Magnetic Thin Films of Inorganic Nanosheets, TAKASHI YAMAMOTO, HIROAKI NAMBA, YASUAKI EINAGA, Department of Chemistry, Keio University, JST-CREST TEAM — Molecule-based magnets have been fascinating materials because of the potential applications in information storage, electronic and spintronic devices. However, such applications would require arraying the active materials on a substrate or interfacing with other components. Here, we focus on fabricating multi-functional magnetic films using inorganic nanosheets as a building block. The thin films could be prepared by the modified Langmuir-Blodgett, LB, technique or the layer-by-layer, LbL, method, which are representative wet-processings for film preparation. As the magnetic LB film, we chose semiconductive titania nanosheets and magnetic Prussian Blue. Upon band gap excitation of titania nanosheets, electron injection into Prussian Blue was achieved with scavenging interlayer water molecules, leading to photoreduction to Prussian White. As the magnetic LbL film, we chose magnetic layered double hydroxide, LDH, nanosheets and non-magnetic smectite nanosheets. In powdered LDH, a coercivity increased with expanding the interlayer spacing. On the other hand, despite the larger interlayer spacing for the LbL film, a coercivity was less than that of the comparative powdered LDH. It is indicated LDH nanosheets are integrated in an anisotropic manner in the LbL films.

1:27PM J13.00012 Suppression and Revival of Magnetic Correlations at Interfaces, AXEL EUVERTE, FREDERIC HEBERT, GEORGE BATROUNI, Institut Non-Lineaire de Nice, SIMONE CHIESA, College of William & Mary, RICHARD SCALETTAR, UC Davis — We study a model of metal-insulator interfaces consisting of a multilayer, repulsive Hubbard Hamiltonian in which the interaction is nonzero on one set of layers and zero on another. As the interface hybridization is tuned, the magnetism and spectral functions in the correlated layers undergo an evolution in which the signatures of strong interaction are first reduced and subsequently revived due to the formation of an interfacial spin liquid phase. The penetration into the correlated layers of the suppression of magnetic order is found to be 4-6 layers.

1:39PM J13.00013 Effects of inhomogeneous strain on the magnetization behavior of magnetic nanostructures in $\text{BiFeO}_3/\text{CoFe}_2\text{O}_4$ composite, NICOLAS AIMON, MARK MASCARO, FRANK LIU, MIT DMSE, MARKUS BUEHLER, MIT Mechanical Engineering Department, CAROLINE ROSS, MIT DMSE — In $\text{CoFe}_2\text{O}_4/\text{BiFeO}_3$ (CFO/BFO) nanostructured thin films, where ferromagnetic nanopillars are embedded in a ferroelectric matrix, electric field induced rotation of the easy axis of the ferrimagnetic nanopillars has been demonstrated experimentally [Zavaliche et al. 2005]. However, for applications where the magnetic pillars would be used to store information, electric control of the magnetization has to be achieved at the scale of a single pillar, without disturbing the neighbors, and the effects of local strain on the magnetic reversal is therefore of interest. We carried out finite element simulations of the strain state of an arrangement of CFO pillars when the BFO matrix surrounding one of them is under piezoelectric strain. Because of stress relaxation at the top free surface of the thin film, the strain is highly inhomogeneous along the pillar. The position-dependent strain was imported into a micromagnetic simulation, giving a position-dependant magnetoelasticity, to predict the switching behavior of the CFO pillars and estimate the feasibility of electric control of a single magnetic bit in this system. The reversal of the pillars was found to be highly incoherent, showing that the pillars cannot be treated as a macrospin.

1:51PM J13.00014 Magnetic field dependencies of dielectric and ferroelectric properties in $\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3/\text{La}_3/8\text{Ca}_5/8\text{MnO}_3$ multiferroic thin films, YI-PING YAO, YU-KUAI LIU, SI-NING DONG, XIAO-GUANG LI, University of Science and Technology of China — In this work, the temperature and magnetic field dependencies of dielectric and ferroelectric properties were investigated for $\text{Au}/\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3/\text{La}_3/8\text{Ca}_5/8\text{MnO}_3$ (PZT/LCMO) thin films grown on (001)-oriented SrTiO_3 substrates. The results indicate there exists a large magnetodielectric effect up to 30% at $T = 220$ K, $f = 1$ MHz and $H = 0.8$ T in these multi-layer films, which is promising for practical application as compared with conventional multiferroics demanding large magnetic fields and low temperatures. From the electric polarization hysteresis loops, it is found that with increasing temperature at $H = 0$ T the coercive field E_c of PZT decreases at low temperature range, and then starts to increase till the Curie temperature of LCMO ($T_c \sim 220$ K) where a maximum appears. This peak is obviously suppressed and shifted to a higher temperature with increasing magnetic fields, which may be related to the depolarization field which is affected by the change of the carrier concentration in LCMO. As for the variation of remnant polarization P_r , it increases with increasing temperatures from 50 K to 300 K, but decreases with increasing magnetic fields around T_c . This magnetoelectric effect implies that the strain effect due to the magnetostriction of LCMO may also have some impact on the variation of hysteresis loops. These findings provide potential for multifunctional devices in spintronics.

2:03PM J13.00015 Tailored inter and intra layer exchange coupled superlattices for optimized magnetocaloric effect¹, TATHAGATA MUKHERJEE, S. MICHALSKI, R. SKOMSKI, D.J. SELMYER, CH. BINEK, Department of Physics & Astronomy and the Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE, 68588-0111 — We explore Magnetocaloric (MC) properties of Fe/Cr superlattices with tailored inter- and intra-layer interaction using simple 3d metals. Our multilayers are fabricated by pulsed-laser deposition with emphasis on maximizing magnetic entropy changes near room temperature. Nanostructuring² allows tailoring ferromagnetic and antiferromagnetic coupling. This in concert with finite size scaling of the ferromagnetic Fe films has the potential to lead to optimized MC materials. Thermodynamic and MC properties of such Fe/Cr superlattices are studied with the help of SQUID magnetometry. Entropy changes are deduced via the Maxwell relation in single phase regions, X-ray diffraction and X-ray reflectivity are used to correlate structural data with the magnetic properties.

¹Financial support by NRI, and NSF through EPSCoR, Career DMR-0547887, and MRSEC Grant No. 0820521.

²T. Mukherjee, S. Sahoo, R. Skomski, D. J. Sellmyer, and Ch. Binek, Phys. Rev. B **79**, 144406 (2009).

Tuesday, February 28, 2012 11:15AM - 2:15PM — Session J14 GMAG DMP FIAP: Focus Session: Spins in Semiconductors - Spin-Orbit Coupled Electrons and Holes in Semiconductors 212

11:15AM J14.00001 Spin-dependent transport of spin-orbit coupled holes in GaAs nanostructures, ALEX HAMILTON, University of New South Wales — In undergraduate physics, we are often taught that holes in the valence band are just positively charged heavy electrons. But valence band holes are spin-3/2 particles, and this gives them very different properties to spin-1/2 electrons, particularly when confined to low dimensions. These differences show up as highly anisotropic spin properties, which can be directly probed with conventional transport measurements. We have fabricated high quality hole quantum wires that show clean and stable quantized conductance plateaus [1]. In contrast to 1D electron quantum systems, the spin-splitting in these hole wires is highly anisotropic [2], and depends only on the orientation of the in-plane magnetic field relative to the quantum wire [3]. However the orientation and k -dependence of the spin-splitting cannot be reconciled with existing theories, suggesting that more theoretical work is needed before we understand the physics of spin-3/2 holes, even on “simple” (100) surfaces. We have also studied spin-3/2 holes in quantum dots, which show characteristic signatures of Kondo physics. A clear zero-bias peak is observed in the differential conductance, which splits with an applied in-plane magnetic field. The splitting is twice as large as the splitting for the lowest one-dimensional subband, consistent with Kondo physics. Unlike electrons this splitting is highly anisotropic with magnetic field, due to the strong spin-orbit coupling [4].

[1] O. Klochan et al., Appl. Phys. Lett. **89**, 092105 (2006).

[2] R. Danneau et al., Phys. Rev. Lett. **97**, 026403 (2006).

[3] J C H Chen et al, New Journal of Physics **12**, 033043 (2010).

[4] O. Klochan et al, Phys. Rev. Lett. **107**, 076805 (2011).

11:51AM J14.00002 Quantum-confined holes: More spin for your buck!¹, ULRICH ZUELICKE, Victoria University of Wellington, New Zealand — The physical properties of charge carriers in crystalline solids are dictated largely by the material's band structure. Typically, band electrons from the (lowest) conduction band behave very similarly to free electrons in vacuum, only with parameters such as their mass and g -factor adjusted. In contrast, holes from the (upper-most) valence band show a much richer behavior owing to their intrinsic spin-3/2 degree of freedom and this spin's strong coupling to the crystal momentum of holes. In a two-dimensional (2D) quantum well, size quantisation induces an energy splitting between heavy-hole (HH) and light-hole (LH) subbands. The existence of this HH-LH *splitting* makes it tempting to consider HH and LH degrees of freedom separately, in particular in situations where only the highest (generally HH-like) 2D hole subband is occupied. In my talk, I will focus on how such an approach overlooks intriguing differences in the mesoscopic and many-particle properties exhibited by quantum-confined holes as compared with their conduction-electron counterparts. Recent results on the density response [1] and spin susceptibility of 2D holes will be presented to illustrate the ramifications of ubiquitous HH-LH *mixing*. I will also discuss how the temporal modulation of Rashba spin splitting in hole nanostructures generates larger-magnitude spin currents than in corresponding band-electron systems [2]. Finally, Andreev reflection of holes in a p-type-semiconductor – superconductor hybrid system will be considered [3], which also exhibits novel behavior due to band mixing.

[1] T. Kernreiter, M. Governale, and U. Zulicke, New J. Phys. **12**, 093002 (2010).

[2] T. Kernreiter, M. Governale, A. R. Hamilton, and U. Zulicke, Appl. Phys. Lett. **98**, 152101 (2011).

[3] D. Futterer, M. Governale, U. Zulicke, and J. Konig, Phys. Rev. B **84**, 104526 (2011).

¹Work supported by the MacDiarmid Institute for Advanced Materials and Nanotechnology.

12:27PM J14.00003 Spin-electric stripes: electric voltage generated by spin current¹, YULI LYANDAGELLER, Department of Physics Purdue University — At the boundaries of the two-dimensional conductor, stripes arise with an electric field transverse to the flowing electric current, and with 100% electron spin polarization perpendicular to the 2D plane. In these boundary stripes, the magnitudes of spin polarizations are the same, the magnitudes of transverse electric fields are the same, but the directions of electric fields and orientations of spins are opposite. If the spin relaxation is negligible, the magnitudes of the electric fields are directly related to the spin current. The stripes at boundaries are separated by a center-stripe, in which the magnitude and direction of the electric field depend on the ratio of the skew scattering and side jump spin currents. The spin polarization is zero on the centerline and reaches +1 or -1 at the boundaries between the central and periphery stripes if spin relaxation of the z-component of spin normal to the 2D plane is absent. Weak spin relaxation modifies the magnitudes of the spin polarization and electric fields, with +1 or -1 spin polarization persisting at the edges of the sample. Favorable experimental settings, in which electron or hole spin relaxation of the z-component of spin is suppressed but the spin current is not, are discussed.

¹arXiv:1107.3121; Support from NSF under the grant # ECCS-0901754 is gratefully acknowledged.

12:39PM J14.00004 Spin-orbit or Aharonov-Casher edge states in semiconductor two-dimensional systems, L.L. XU, J.J. HEREMANS, Virginia Tech, C.K. GASPE, S. VIJAYARAGUNATHAN, T.D. MISHIMA, M.B. SANTOS, University of Oklahoma — In semiconductors with spin-orbit interaction we experimentally search for edge states induced by the Aharonov-Casher vector potential or Rashba-type spin-orbit interaction. The Aharonov-Casher effect is electromagnetically dual to the Aharonov-Bohm effect and is predicted to lead to a possibly helical edge state structure at two-dimensional sample edges. We use InGaAs/InAlAs heterostructures patterned into mesoscopic side-gated channel structures, where the edge states can be induced, and where backscattering between edge states can be experimentally measured in the resistance. Sweeping side-gate voltage, low temperature resistances are measured across such mesoscopic closed-path structures at either low applied magnetic field, in-plane or normal to the plane, or at fixed magnetic filling factors of 5, 6, 7, and 8 to obtain states of defined spin. Resistance oscillations are observed at low magnetic fields and around filling factor 6 as function of side-gate voltage, and we analyze the oscillations in the light of the search for the edge states (DOE DE-FG02-08ER46532, NSF DMR-0520550).

12:51PM J14.00005 Spin orbit coupling induced splitting in excitations of high mobility 2DESs¹, ALBERT F. RIGOSI, URSULA WURSTBAUER, ARON PINCZUK, Columbia University, JOHN WATSON, SUMIT MONDAL, MICHAEL J. MANFRA, Purdue University, KEN W. WEST, LOREN N. PFEIFFER, Princeton University — Spin orbit interaction (SOI) induces a splitting of the conduction bands in two-dimensional electron systems (2DES) in GaAs. We study the impact of zero-field spin-splitting on excitations of ultra high mobility 2DESs by resonant inelastic light scattering experiments. To distinguish between splitting caused by bulk inversion asymmetry (Dresselhaus) and structure inversion asymmetry (Rashba), we studied symmetric (two-side modulation doped) and asymmetric (single-side modulation doped) quantum wells grown along (001) and (110) crystallographic directions. We probe the excitation modes as a function of transferred momentum for different crystallographic directions in the plane of the QW. At large wave vectors we find a complex splitting of the single-particle intersubband excitation mode that is strongly dependent on the combination of Dresselhaus and Rashba SOI. The observed mode splitting is a result of effective SOI fields in both, ground and first excited subband. Suitable choices of crystallographic orientations yield Dresselhaus and Rashba terms.

¹Supported by NSF and AvH

1:03PM J14.00006 Current-induced spin polarization along spin orbit fields in strained InGaAs¹, BENJAMIN M. NORMAN, C.J. TROWBRIDGE, Department of Physics, University of Michigan, Ann Arbor, J. STEPHENS, A.C. GOSSARD, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, V. SIH, Department of Physics, University of Michigan, Ann Arbor — Current-induced spin polarization is a phenomenon in which electron spins undergo a momentum-dependent net spin polarization², but the mechanism and how material parameters govern the magnitude of this effect remains an open question. Conductive channels are etched into strained n-doped InGaAs samples along the [110], $\bar{1}\bar{1}0$, [100] and [010] crystal axes with ohmic contacts at either end to allow control of electrical current. While the spin polarization direction is found to align along the direction of the measured spin-orbit effective magnetic fields³, the magnitude of the spin polarization is not proportional to the magnitude of the spin-orbit fields. Surprisingly, crystal axes with the smallest spin-orbit fields appear to have the largest net spin polarization. Our measurements suggest that the longer spin dephasing time for smaller spin-orbit interactions may play a significant role.

¹Work supported by the NSF

²Y. K. Kato, R. C. Myers, A. C. Gossard, and D. D. Awschalom, Phys. Rev. Lett. **93**, 176601 (2004)

³B. M. Norman, C. J. Trowbridge, J. Stephens, A. C. Gossard, D. D. Awschalom, and V. Sih, Phys. Rev. B. **82**, 081304(R) (2010)

1:15PM J14.00007 Thermodynamic compressibility and spin-splitting in one-dimensional quantum wires, LUKE W. SMITH, University of Cambridge, U.K., A.R. HAMILTON, University of New South Wales, Australia, K.J. THOMAS, Sungkyunkwan University, Korea, M. PEPPER, University College London, U.K., I. FARRER, D. ANDERSON, G.A.C. JONES, D.A. RITCHIE, University of Cambridge, U.K. — We study spin-splitting and the much-debated 0.7 structure in GaAs quantum wires using compressibility measurements that directly probe the thermodynamic density of states. Two quantum wires are simultaneously defined in the upper and lower well of a GaAs/AlGaAs double quantum well heterostructure, using midline-gated split-gate devices [1]. The lower wire probes the ability of the upper wire to screen the electric field from a biased surface gate. The technique is sensitive enough to resolve spin splitting of the 1D subbands in the presence of an in-plane magnetic field. The compressibility response of the 0.7 structure is measured, and its evolution with increasing temperature and magnetic field is studied [2]. Despite the sensitivity of our measurements we see no evidence of the formation of the quasibound state predicted by the Kondo model of the 0.7 structure. Instead our data are more consistent with theories which predict that the 0.7 structure arises as a result of spontaneous spin polarization.

[1] I.M. Castleton *et al*, Physica B 249, 157 (1998).

[2] L.W. Smith *et al*, Phys. Rev. Lett. 107, 126801 (2011)

1:27PM J14.00008 Spin-orbit effects in two-dimensional hole systems on hydrogen-terminated silicon (111) surfaces, BINHUI HU, TOMASZ M. KOTT, BRUCE E. KANE, University of Maryland — We have studied spin-orbit effects in two-dimensional hole systems (2DHSs) on hydrogen-terminated Si(111) surfaces using Shubnikov-de Haas (SdH) oscillations. The device has a vacuum field-effect transistor structure [1], and the 2DHS is induced on the H-Si(111) surface. Hole concentrations up to $8 \times 10^{11} \text{ cm}^{-2}$ are obtained, and the peak hole mobility is about $15,000 \text{ cm}^2/\text{Vs}$ at $T = 1.5 \text{ K}$. SdH oscillations show that the heavy hole subband is spin split due to spin-orbit effects. Both frequencies and beating node locations of the SdH oscillations are used to characterize the spin-orbit effects. The spin-splitting energy is measured as a function of the hole concentration, and the underlying physics will be discussed. Heavy-hole effective mass is determined by the temperature dependence of the SdH oscillations, and the relationship between the effective mass and the hole concentration will be presented. [1] K. Eng, R. N. McFarland, and B. E. Kane, Appl. Phys. Lett. 87, 052106 (2005)

1:39PM J14.00009 Quasiparticle velocities in 2D electron/hole liquids with spin-orbit coupling¹, DAVID AASEN, STEFANO CHESI, BILL COISH, McGill University — We study the influence of spin-orbit interactions on quasiparticle dispersions in two-dimensional electron and heavy-hole liquids in III-V semiconductors. To obtain closed-form analytical results, we work within the screened Hartree-Fock approximation, valid in the high-density limit. For electrons having a linear-in-momentum spin-orbit interaction, we confirm known results based on the random-phase approximation and we extend those results to higher order in the spin-orbit coupling. For hole systems, with a leading nonlinear-in-momentum spin-orbit interaction, we find two important distinctions. First, the group velocities associated with the two hole-spin branches acquire a significant difference in the presence of spin-orbit interactions, allowing for the creation of spin-polarized wavepackets in zero magnetic field. Second, we find that the interplay of Coulomb and spin-orbit interactions is significantly more important for holes than for electrons and can be probed through the quasiparticle group velocities. These effects should be directly observable in magnetotransport, Raman scattering, and femtosecond-resolved Faraday rotation measurements.

¹preprint arXiv:1110.6661v1

1:51PM J14.00010 Spin Coulomb drag and optical excitations in low dimensional systems, IRENE D'AMICO, University of York, CARSTEN ULLRICH¹, University of Missouri — Within the remit of new quantum technologies, an intense effort is devoted to improving our understanding of spin dynamics, with the aim of building novel spintronics devices. In this context the theory of spin Coulomb drag (SCD) was recently developed. It shows that Coulomb interactions are an intrinsic decay mechanism for spin currents. As confirmed by experiments, SCD can be substantial in semiconductors, and it is bound to become one of the most serious issues in spin polarized transport, since, due to its intrinsic nature, it cannot be avoided even in the purest material. More recently the influence of SCD on optical spin-injection and spin-resolved optical experiments has been considered. Here we report on SCD effects on intersubband optical spin excitations in III-V quantum wells, where SCD may contribute substantially to the linewidth of spin plasmons. By going beyond the usual local density functional approximation and properly including the effects due to the inhomogeneity of the system in the growth direction, we show that the quantization of states in the growth direction may strongly reduce the intrinsic plasmon linewidth.

¹Supported by DOE Grant DE-FG02-05ER46213.

2:03PM J14.00011 Theory of Helical Fermi liquids, ALI ASHRAFI, DMITRII MASLOV, University of Florida — We extend the Landau Fermi Liquid (FL) theory to include spin-orbit coupling (SOC). In particular, the Rashba SOC is chosen as an example. It is shown that although “charge-part” quantities, such as the charge susceptibility and effective mass, are determined solely by the quasi-particles, “spin-part” quantities, such as the spin susceptibility, have contributions from the damped states in between the two Fermi surfaces induced by the SOC. However, contributions to the lowest order in the SOC can still be extracted from the theory. The nature of the instabilities of such spin-orbit coupled FL is discussed.

Tuesday, February 28, 2012 11:15AM - 1:51PM –
Session J15 DMP FIAP GMAG: Focus Session: Spins in Metals - Spin Transport in Novel Devices and Structures 213

11:15AM J15.00001 An Alternative Approach for Fabricating Ring-shaped Spin-transfer Torque RAM Devices, ROBERT BURKE, ALAN EDELSTEIN, Army Research Laboratory — Several techniques have been investigated to fabricate spin-torque transfer RAM (STT RAM) devices with ring-shaped geometries. In-plane STT RAM devices with ring-shaped geometries are advantageous in that the magnetization is confined to the ring structure, eliminating the demagnetization field. This, in turn, reduces the critical current needed to switch the magnetization. To date, the most popular fabrication technique of ring-shaped STT RAM involves a combination of electron beam lithography and ion beam milling. A significant issue with ion beam milling, however, involves the redeposition of the MTJ material on the ring-shaped surface, which leads to shorting of the devices. In our study, we seek an alternative method for forming the ring-shaped devices which eliminates the shorting problem. As a result, we are using a nanopillar and cap structure template to define the ring-shaped geometry of the devices. The nanopillar and cap structure template is fabricated using a combination of a bilayer resist and electron beam lithography to either create a mold for the deposition of a nanopillar and cap structure via ion beam deposition or a resist-based nanopillar and cap structure. This study will report on the results of this process and its prospects as an alternative to ion beam milling.

11:27AM J15.00002 Spin dependent tunneling and possible spin torque effects in magnetic nanoparticle tunnel junctions , CHEN WANG, HSIN-WEI TSENG, ROBERT A. BUHRMAN, DANIEL C. RALPH, Cornell University — It has been predicted that electron tunneling between two magnetic electrodes via a magnetic nanoparticle can exhibit enhanced magnetoresistance at low temperature due to a coherent tunneling mechanism in the Coulomb blockade regime. This has been qualitatively demonstrated for large ensembles of nanoparticles. It has also been predicted that the tunneling current in such a system might exert spin transfer torque with quantum behaviors associated with the discrete energy level of the nanoparticles. Here we report the fabrication and measurement of sub-100 nm nano-pillar tunnel junctions with the layer structure CoFeB/MgO/(CoFeB nanoparticles)/MgO/CoFeB with the dual goal of 1) probing the spin-dependent coherent tunneling associated with the magnetization of a single or very few nanoparticles and 2) exploring the potential for magnetization switching and current-driven dynamics in the nanoparticles induced by spin transfer torque.

11:39AM J15.00003 What determines the sign of magnetoresistance in a molecular tunnel junction? , SUBHASISH MANDAL, RANJIT PATI, Michigan Technological University — The recent observations of both positive and negative sign of tunneling magnetoresistance (TMR) in the same organic spin-valve structure has mystified researchers working in organic spintronics. In this article, we resolve this puzzle by exploring the role of interfacial metal-molecule coupling on TMR in a single molecular spin-valve junction. A planar organic molecule sandwiched between two nickel electrodes is used to build a prototypical spin-valve junction. A parameter-free, single particle Green's function approach in conjunction with a posteriori density functional theory involving a hybrid orbital dependent functional is used to calculate the spin-polarized current. The effect of external bias is explicitly included to investigate the spin-valve behavior. Our calculations show that only a 3% change in the interfacial distance at the metal-molecule junction can alter the sign of the TMR from a positive to a negative value.

11:51AM J15.00004 Spin-dependent inertial force and spin current in accelerating systems , MAMORU MATSUO, Kyoto university, JUN'ICHI IEDA, Japan Atomic Energy Agency, EIJI SAITOH, Tohoku university, SADAMICHI MAEKAWA, Japan Atomic Energy Agency — In the frontier of spintronics, much attention is paid on the control of spin currents. Due to the recent progress of nanoelectromechanics, mechanical manipulation of spins will increase in importance. We discuss theoretically the generation of spin currents in both rotationally and linearly accelerating systems. The explicit form of the spin-dependent inertial force acting on electrons in accelerating systems in the presence of electromagnetic fields is derived from the generally covariant Dirac equation. It is shown that the force is responsible for the generation of spin currents by mechanical rotation and vibration in the first order of the spin-orbit coupling. We also investigate $SU(2) \times U(1)$ gauge theory in accelerating systems, which allows us to extend the spintronic theory in inertial frame to non-inertial frame.

12:03PM J15.00005 Anomalous Magneto Transport in amorphous TbFeCo thin films¹ , NATTAWUT ANUNIWAT, Physics Department, University of Virginia, MARC COSTANTINE, JIWEI LU, Materials Science Department, University of Virginia, MANLI DING, JOSEPH POON, Physics Department, University of Virginia — TbFeCo has attracted some interests because of its high perpendicular anisotropy and tunable magnetic properties for nanomagnetic and spintronics application. In this study, we report a strong size dependence of the coercive field in 30 nm-thick $Tb_{30}Fe_{63.5}Co_{6.5}$ films with MgO capping. Magneto Optical Kerr effect (MOKE) and Vibrating Sample Magnetometer are performed on unpatterned films. The films exhibited strong PMA characteristics with $M_S \sim 200$ emu/cc, $H_C \sim 6000$ Oe, and $K_U \sim 5 \times 10^6$ erg/cc. The films were then fabricated into Hall bars with 500 nm, 50 μm and 500 μm in width. From anomalous Hall effect (AHE), H_C was determined for these patterned films. For Hall bars with the width less than 50 μm , an increase in the coercivity field (~ 1.4 Tesla) was observed at room temperature. The temperature dependent of AHE was characterized from 50K to 300K. The thickness and composition dependent will also be studied and discussed.

¹This work is supported by DARPA and DTRA.

12:15PM J15.00006 Anisotropic Magnetoresistance in single-crystalline Ag/NiO/Fe₃O₄/MgO(001) sample , JIA LI, ALI SUCIPT TAN, JIM SON, ERIC JIN, ZI Q. QIU, Department of Physics, University of California at Berkeley — Anisotropic Magnetoresistance (AMR) is a well-known phenomenon in ferromagnetic (FM) materials that the resistivity exhibit different values as the electric current flows parallel and perpendicular to the magnetization direction, respectively. Recognizing that the AMR depends on the spin axis rather than spin direction, we propose that AMR effect should also exist in antiferromagnetic (AFM) materials. In this presentation, we will report the AMR effect in single crystalline Ag/Fe₃O₄/NiO/MgO(001) films in which the electrical current is mainly carried by the nonmagnetic Ag film. By changing the FM Fe₃O₄ magnetization direction with an external magnetic field, the AFM NiO spin axis direction can be changed through the Fe₃O₄/NiO coupling. We observe a non-zero AMR effect in Ag and that the AMR value depends sensitively on the Ag thickness, suggesting that the observed AMR comes from the spin-dependent NiO/Ag interfacial scattering. Moreover, the magnitude of the AMR effect at 1nm thick Ag in Ag/Fe₃O₄/NiO/MgO(001) is comparable to the AMR value from single Fe film.

12:27PM J15.00007 AIP Prize for Industrial Applications of Physics Lecture: Controlled exchange in recording media and spintronic devices , ERIC FULLERTON, University of California, San Diego — Controlled exchange in recording media and spintronic devices Eric Fullerton University of California, San Diego New functionality and performance advantages have been achieved in magnetic recording media by the formation of complex heterostructures and have helped delay predicted recording limits that arise from thermal instabilities in the media [1]. Example media structures include antiferromagnetically coupled (AFC) media [2] and exchange-spring media structures [3, 4] which emerged in longitudinal and perpendicular recording products and have helped to extend recording densities [1]. In this presentation I will review the implementation of exchange-coupled media, the surprising physics that emerged and its impact on hard-drive products. I will further discuss how similar approaches can be used in emerging recording technologies such as heat assisted magnetic recording [4] and bit patterned media [5, 6] as well as many spintronic devices [7,8].

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- [3]. A. Berger, et al., Appl. Phys. Lett. **93**, 122502 (2008).
- [4]. J.-U. Thiele, S. Maat and E. E. Fullerton, Appl. Phys. Lett. **82**, 2859 (2003).
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- [6]. M. V. Lubarda et al., IEEE Trans. Magn. **47**, 18 (2011).
- [7]. S. Mangin, et al., Nature Materials **5**, 210 (2006).
- [8]. I. Yul'ayev et al., Appl. Phys. Lett. **99**, 132502 (2011).

1:03PM J15.00008 Influence of the exchange bias on the magnetic losses in CoFeB/MgO/CoFeB tunnel junctions¹, RYAN STEARRETT, W.G. WANG, XIAOMING KOU, L.R. SHAH, J.Q. XIAO, E.R. NOWAK, University of Delaware — We report the influence of the exchange bias on the low-frequency magnetic losses of the reference layer in CoFeB/MgO/CoFeB tunnel junctions near maximum resistance susceptibility. The phase lag associated with the magnetic losses in the reference layer, ε , is field-dependent during its magnetic reversal, being largest around the antiparallel state and slowly decreasing with higher applied fields. Such behavior would indicate a direct influence of the exchange bias strength. Its strength is determined by the magnitude of the reference layer switching field, H_{ref} . This is defined as the field at which the magnetoresistance-sensitivity product exhibits its maximum. Devices with the strongest exchange bias tend to have the thickest seed layers and exhibit elevated values for H_{ref} and ε . However, ones with weakened exchange bias due to prolonged annealing show a reduction in H_{ref} and ε with increased annealing time. A comparison between top and bottom pinning configurations is also discussed along with its impact on double-barrier magnetic tunnel junctions.

¹Supported by DOE under Award No. DE-FG02-07ER46374 and NASA Space Grant Fellowship

1:15PM J15.00009 ABSTRACT WITHDRAWN —

1:27PM J15.00010 Magneto-optical properties of Fe thin films in an external electric field¹, KOHJI NAKAMURA, TORU AKIYAMA, TOMONORI ITO, Mie University, MICHAEL WEINERT, University of Wisconsin - Milwaukee, ARTHUR FREEMAN, Northwestern University — Controlling magnetic properties by an external electric field (E -field) is a key challenge in magnetic physics. Previously, from first-principles calculations,² we demonstrated the E -field-driven magnetocrystalline anisotropy modification in Fe thin films and at the Fe/MgO interface. Here, we extend our investigations to treat the magneto-optical properties of Fe thin films in an E -field. Calculations were carried out using the film-FLAPW method³, in which an E -field is incorporated and the conductivity tensor is obtained by applying the Kubo formula of linear response theory. Results predict that for an Fe monolayer, when the E -field is introduced over $1\text{V}/\text{\AA}$, the calculated interband conductivity in the low energy region (less than about 2eV from E_F) are modified compared to that in zero field, due to a magnetization reorientation from out-of-plane to in-plane. The calculated plasma frequency is also found to be reduced by 7%, which suggests an E -field-driven magnetoresistance.

¹Work at Northwestern University was supported by the U.S. Department of Energy (DE-FG02-88ER45372).

²Nakamura, Shimabukuro, Fujiwara, Akiyama, Ito, Freeman, PRL**102**, 187201(2009); Nakamura, Akiyama, Ito, Weinert, Freeman, PRB**81**, 220409R(2010)

³Wimmer, Krakauer, Weinert, Freeman, PRB**24**, 864(1981); Weinert, Wimmer, Freeman, PRB**26**, 4571(1982)

1:39PM J15.00011 Spin transport in metal-oxide switching devices, CURT A. RICHTER, Semiconductor and Dimensional Metrology Div, NIST Gaithersburg, MD, H.-JAE JANG, Semiconductor and Dim. Metrology Div, NIST and Dept. of Physics, Wake Forest University, OLEG KIRILLOV, Semiconductor and Dimensional Metrology Div, NIST Gaithersburg, MD, OANA JURCHESCU, Department of Physics, Wake Forest University, Winston-Salem, NC — Metal-oxide-based devices in which resistive switching occurs, often referred to as memristors or resistive-RAM (random oxide memory), show promise for use in technologically exciting applications such as high-density non-volatile memories, electronically reconfigurable logic, and neural networks. We report on electron spin transport through electrochemically precipitated copper filaments formed in TaO_x memristive devices consisting of $\text{Co}(60\text{ nm})/\text{TaO}_x(16\text{ nm})/\text{Cu}(5\text{ nm})/\text{Py}(60\text{ nm})$ with crossbar-type electrode geometry. These metal-oxide switching devices with ferromagnetic electrodes show memristive behavior having a typical OFF/ON resistance ratio of 10^5 . Magnetoresistance measurements performed by sweeping an external magnetic field display evidence of spin transport in the low-resistance ON-state at 77 K. Spin transport vanishes in the OFF-state. These data are strong evidence that the fundamental switching mechanism in these metal-oxide devices is the creation of Cu filaments in the ON-state that completely span the 16 nm thick TaO_x and form a continuous metallic conduction path. In addition to helping elucidate the conduction pathway in these intriguing structures, our findings can advance electronics combining spintronic and electronic functions.

Tuesday, February 28, 2012 11:15AM - 2:15PM —
Session J16 DCMF: Vanadium Dioxide; Nano and Devices 251

11:15AM J16.00001 M2 phase in free-standing single-crystalline nanostructures of VO_2 at ambient conditions¹, E. STRELCOV, Southern Illinois University Carbondale, Carbondale, IL, A. TSELEV, I.N. IVANOV, Oak Ridge National Laboratory, Oak Ridge, TN, J. ZHANG, Southern Illinois University Carbondale, Carbondale, IL, J.D. BUDAI, J.Z. TISCHLER, S.V. KALININ, Oak Ridge National Laboratory, Oak Ridge, TN, A. KOLMAKOV, Southern Illinois University Carbondale, Carbondale, IL — A significant drawback of a promising material for realization of an ultrafast switch based on a metal-insulator transition (MIT) - VO_2 - is the inherent linkage between the MIT and lattice transformation from tetragonal to monoclinic with a lattice contribution in the band gap formation in the stable monoclinic M1 structure. On the other hand, the metastable M2 phase exhibits a pure Mott MIT and was shown to be driven metallic without the structural change. Existence of this phase at ambient conditions was reported for Cr and Al-doped VO_2 and nanostructures doped with oxygen vacancies. Here we report stabilization of the M2 phase in VO_2 single-crystalline nanoplatelets (NPLs) doped with Al during the growth process via two new methods. Development of these methods came from our recent in situ studies of the NPL growth mechanism. We reconstructed temperature-doping phase diagram for the NPLs. Electrical properties of the NPLs were also studied as functions of doping level and temperature.

¹Work at SIUC was funded through NSF 772 ECCS-0925837 and SISGR-DOE ERKCM67. Work at ORNL's CNMS was sponsored by DSUF OBES, U.S. DOE. J.D.B. and J.Z.T. were supported by MSED OBES, U.S. DOE.

11:27AM J16.00002 Photocurrent in Vanadium Dioxide¹, T. SERKAN KASIRGA, DONG SUN, JAE H. PARK, JAMES COY, XIAODONG XU, DAVID H. COBDEN, University of Washington — We investigate the photoresponse of VO_2 using scanning photocurrent microscopy below and above the metal-insulator transition at 67°C . To avoid complications of nonuniform strain and twinning boundaries we focus on single-crystal suspended nanobeams, where the strain is either minimal or well controlled. At intermediate temperatures the metallic and insulating phases coexist and a photocurrent and photoconductance associated with the boundary between them is seen. The magnitude and profile of the photoresponse above and below the transition demonstrates a photothermal mechanism, with fast electron-lattice relaxation and absence of built-in electric fields in the insulating phase consistent with strong electron-electron correlations and a short screening length.

¹Supported by Department of Energy BES DE-SC0002197 and Army Research Office 48385-PH.

11:39AM J16.00003 Electronic phases in vanadium dioxide nanowires observed by scanning tunneling spectroscopy, JOHN HATCH, Department of Physics, SUNY at Buffalo, LUISA WHITTAKER, Department of Chemistry, SUNY at Buffalo, TAI-LUNG WU, ADAM STABILE, G. SAMBANDAMURTHY, Department of Physics, SUNY at Buffalo, SARBAJIT BANERJEE, Department of Chemistry, SUNY at Buffalo, HONG LUO, Department of Physics, SUNY at Buffalo — The electronic behavior of vanadium dioxide around its metal-insulator transition has been the focus of many experimental and theoretical investigations, concerning transition mechanisms. In this work, we present our experimental investigation of the temperature driven metal-insulator transition in individual single crystal vanadium dioxide nanowires with scanning tunneling spectroscopy. The local density of states is studied at temperatures around the transition temperature. We observe three distinct electronic phases: the insulating phase and two metallic phases with different density of states, both in terms of conductivity and in the complexity of the density-of-states spectra. Vanadium dioxide nanowires doped with tungsten were also studied and will be discussed.

11:51AM J16.00004 Current-induced metastable states in single-crystalline VO₂ nanoplatelets¹, ALEXANDER TSELEV, J.D. BUDAI, Oak Ridge National Laboratory, Oak Ridge, TN, E. STRELCOV, Southern Illinois University Carbondale, Carbondale, IL, J.Z. TISCHLER, Oak Ridge National Laboratory, Oak Ridge, TN, A. KOLMAKOV, Southern Illinois University Carbondale, Carbondale, IL, S.V. KALININ, Oak Ridge National Laboratory, Oak Ridge, TN — The metal-insulator transition (MIT) in VO₂ occurs close to ambient temperature, $T_c = 68^\circ\text{C}$, which can be reduced by doping. The phase transition results in a few orders of magnitude change of electrical conductivity and is accompanied by a change of the lattice from tetragonal to monoclinic, which is associated with lattice expansion of $\sim 1\%$ along the tetragonal c-axis of the metallic phase. We observed that, in suspended single-crystalline VO₂ nanoplatelets (NPLs) carrying a sufficiently strong electrical current, Joule heating leads to formation of metal-semiconductor domains, which are self-organized in chains providing a path for the current flow. This results in NPL bending depending on the current strength, which can be used for electrically controlled actuator action. The observed domain structures should be interpreted as distinct metastable states in freestanding and end-clamped quasi-1D VO₂ samples. We analyze the stability conditions for the heterophase domains patterns and main prerequisites for the realization of current-controlled nanoactuators based on the proposed concept.

¹Work at SIUC was funded through NSF 772 ECCS-0925837 and SISGR-DOE ERKCM67. Work at ORNL's CNMS was sponsored by DSUF OBES, U.S. DOE. J.D.B. and J.Z.T. were supported by MSED OBES, U.S. DOE.

12:03PM J16.00005 Hydrogen stabilization of metallic VO₂ in single-crystal nanobeams¹, JIANG WEI, HENG JI, WENHUA GUO, ANDRIY NEVIDOMSKYY, DOUGLAS NATELSON, Rice University — Vanadium dioxide (VO₂) is a strongly correlated material with a metal-insulator transition at 67°C from a high temperature, rutile metal to a lower symmetry insulating state. Substitutional doping can alter the properties of VO₂, but is irreversible. Using individual microcrystals and nanobeams, we show that spillover may dope VO₂ reversibly with atomic hydrogen. Raman and optical microscopy show a stabilized metallic state, consistent with single-crystal electron diffraction and scanning electron microscopy that demonstrate a post-hydrogenation structure similar to the rutile state. Electronic transport shows that the energy band gap of insulating phase can be reversibly tuned towards the metallic phase upon different hydrogenation conditions and the metallic state may be stabilized down to cryogenic temperatures. Electronic structure calculations agree that a hydrogen-containing distorted rutile structure is energetically favored over the monoclinic state.

¹Supported by Robert A. Welch Foundation and Department of Energy award DE-FG02-06ER46337

12:15PM J16.00006 Identifying the Role of Domains in Metal-Insulator Transitions in Individual Nanowires of Tungsten-Doped VO₂, ADAM STABILE, SUJAY SINGH, TAI-LUNG WU, Department of Physics, SUNY at Buffalo, LUISA WHITTAKER, Department of Chemistry, SUNY at Buffalo, PAYAM TAHERIROSTAMI, Department of Physics, SUNY at Buffalo, SARBAJIT BANERJEE, Department of Chemistry, SUNY at Buffalo, G. SAMBANDAMURTHY, Department of Physics, SUNY at Buffalo — Though it is well known that the metal-insulator transition (MIT) in VO₂ can be achieved by a variety of external parameters, an understanding of how different parameters drive such a transition has remained relatively unknown. We report transport and Raman spectroscopic characteristics on voltage (V)- and temperature (T)-driven MIT in individual, single-crystal, tungsten-doped VO₂ nanowires. From transport analyses we discuss the T -dependent features in I vs V curves; specifically hysteresis gaps and resistance jump features seen in sub-micron devices. From Raman spectroscopic analyses we discuss the Raman intensity of A_g modes while driving the temperature and voltage across the transition. We conclude that driving T supports a slow transition to the rutile (R) metallic phase with a wide temperature range of mixed insulating, monoclinic (M1) and R states due to the population of metallic domains. V -driven transition does not appear evolve via the formation of domains, but is activated when V is sufficiently large above a T -dependent threshold.

12:27PM J16.00007 Ionic Liquid Gated Vanadium Oxide Three Terminal Devices: Chemical Stability and Field Effect¹, YOU ZHOU, ZHENG YANG, SHRIRAM RAMANATHAN, Harvard University — Understanding electrostatic field effect in correlated oxides is one approach to uncovering mechanisms leading to metal-insulator transition and further is of great interest in oxide-based device technologies. We have fabricated ionic liquid gated VO₂ three-terminal devices. The VO₂/IL interface properties were systematically studied with emphasis on electrochemical stability, gate capacitance and charging/discharging using photoelectron spectroscopy, impedance spectroscopy and other electrical characterization. We have observed a large modulation of VO₂ channel conductance at room temperature with polarity dependence. Interestingly, the conductance modulation also exhibits a time-dependent response to external gate bias and possible mechanisms will be discussed.

¹We acknowledge Office of Naval Research Grant N00014-10-1-0131 for financial support

12:39PM J16.00008 Gating Effect on VO₂ nanowire by Ionic Liquid¹, HENG JI, JIANG WEI, DOUGLAS NATELSON, Rice University — VO₂ is a well-known strongly correlated material with insulator-to-metal phase transition at 68°C . Below this temperature, VO₂ is an insulating material whose temperature dependence behaves like a semiconductor with 0.6 eV band gap. However, such material cannot be gated by traditional method. In our experiment, we applied a new technique, using ionic liquids, to provide a much stronger transverse electric field on the VO₂ nanowire. We did not observe obvious gating effect on VO₂, but in the meantime, we found that VO₂ is sensitive to hydrogen. The hydrogen produced by electrochemistry when applying voltage on the electrolyte (an ionic liquid with water contamination, in this case) can dramatically change the conductance of VO₂.

¹Robert A. Welch Foundation and Department of Energy award DE-FG02-06ER46337

12:51PM J16.00009 Strain control of the metal-insulator transition in vanadium dioxide nanobeams¹, JAE HYUNG PARK, SERKAN KASIRGA, JAMES COY, XIAODONG XU, DAVID COBDEN, University of Washington, NANODEVICE LAB COLLABORATION — To be able perform systematic studies at the metal-insulator transition in VO₂, we have developed a platform for applying axial strain to suspended single-crystal nanobeams while carrying out optical and transport measurements. The nanobeams are positioned on a piezo-actuated silicon structure using a nanomanipulator. The strain can be used to control the transition temperature, because the metallic and insulating phases have different c-axis lattice constants, or to move the interphase boundary between metal and insulator in coexistence. We report transport, Raman and photoconductance measurements as the transition is tuned in this way.

¹Supported by Department of Energy grant BES DE-SC0002197 and Army Research Office grant 956073-PH.

1:03PM J16.00010 Investigation of switching behavior of two-terminal devices on VO₂¹, IULIANA P. RADU, Katholieke Universiteit Leuven and IMEC, Belgium, KOEN MARTENS, BOGDAN GOVOREANU, SOFIE MERTENS, XIAOPING SHI, MALGORZATA JURCZAK, IMEC, Belgium, STEFAN DE GENDT, Katholieke Universiteit Leuven and IMEC, Belgium, ANDRE STESMANS, Katholieke Universiteit Leuven, JORGE A. KITTL, IMEC, Belgium, MARC HEYNS, Katholieke Universiteit Leuven and IMEC, Belgium — Vanadium dioxide undergoes an insulator to metal transition at about 68 °C. Two-terminal devices fabricated on VO₂ show a steep decrease of resistance when the current or voltage applied are large enough. This switching has been largely attributed to a field effect even in two-terminal devices but controversy still exists. We fabricate devices with an array of electrode separations and widths and study how the dc switching voltage and current depend on device size. The data obtained from these devices are most consistent with a Joule heating mechanism governing the switching. Additionally we perform an ac investigation of these devices and find that the switching to the low resistance state can happen faster than 5ns (the time resolution of the measurement set-up) while the switching to the high resistance state is of the order of hundreds of nanoseconds, consistent with the estimated heat dissipation time. In spite of the Joule heating mechanism which is expected to induce device degradation, we find that the devices can be switched for more than 10¹⁰ cycles making VO₂ a promising material for memory applications.

¹We acknowledge support from the IMEC core partners program, FWO, and a Marie Curie grant.

1:15PM J16.00011 Local thermal heating in VO₂ electric-field-induced metal insulator transition, A. ZIMMERS, L. AIGOUY, Laboratoire de Physique et d'Etude des Matériaux (LPEM), ESPCI-ParisTech-UPMC-CNRS, Paris, France, A. SHARONI, Dept. of Physics and Institute of Nanotechnology, Bar Ilan University, Ramat Gan, Israel, S. WANG, Department of Physics and Materials Science and Engineering and Center for Advanced Nanoscience, UCSD, La Jolla, CA, USA, J.G. RAMIREZ, Department of Physics and Center for Advanced Nanoscience, UCSD, La Jolla, CA, USA, I.K. SCHULLER, Department of Physics and Materials Science and Engineering and Center for Advanced Nanoscience, UCSD, La Jolla, CA, USA — Over recent years, the insulator to metal transition (IMT) of the vanadium dioxide (VO₂) Mott insulator has been revisited revealing an electric-field-induced resistance switching. Whether this feature is purely due to an electrical field effect or due to some Joule heating is still under debate. Here we report a local temperature measurement in a 10μm and a 20μm VO₂ junction while going through the resistance switching. The sample was placed at ΔT=15K below 340K (the thermally induced insulator to metal transition). When ramping up the voltage across the junction we find that the local heating inside the VO₂ junction is close to 15K. This data suggests that in these temperature, current and voltage ranges, the field induced IMT can be explained by local Joule heating. Work supported by the French ANR-09-BLAN-0388-01 and the US DOE and AFOSR.

1:27PM J16.00012 Electrical properties of vanadium dioxide – dielectric – metal structures and the metal-insulator transition¹, KOEN MARTENS, KULeuven ESAT department / IMEC, IULIANA RADU, KULeuven Physics department / IMEC, SOFIE MERTENS, XIAOPING SHI, MARC SCHAEKERS, IMEC, STEFAN DE GENDT, KULeuven Chemistry department / IMEC, MARC HEYNS, KULeuven Materials Science department / IMEC, JORGE KITTL, IMEC — VO₂ and its metal-to-insulator transition (MIT) are of interest for memory and logic nanoelectronic devices due to its very fast transition, its full volume transition implying good scalability and reliability and relatively large resistance on/off ratio of 2-5 orders of magnitude. In this work the equivalent of the heart of MOS (metal-oxide-semiconductor) technology, the MOS capacitor is investigated for the VO₂ case in which the Si is replaced by VO₂. Thermally oxidized VO₂ with a HfO₂ or Al₂O₃ dielectric grown on top with Atomic Layer Deposition were used to form MOS structures. The MOS capacitor electrical properties are analyzed such as the gate current and capacitance behavior with special regard to the MIT. The influence of the MIT on gate dielectric tunneling is shown and modeled as well as RRAM phenomena and an evaluation of the field effect. Implications for the field-induced metal-insulator transition and for device applications are discussed.

¹The FWO is acknowledged for funding.

1:39PM J16.00013 Field-effect modulation of conductance in VO₂ nanobeam transistors with HfO₂ as the gate dielectric, SHAMASHIS SENGUPTA, Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai, KEVIN WANG, KAI LIU, Department of Materials Science and Engineering, University of California, Berkeley, AJAY BHAT, SAJAL DHARA, Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai, JUNQIAO WU, Department of Materials Science and Engineering, University of California, Berkeley, MANDAR M. DESHMUKH, Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai — Field-effect transistors have been fabricated from VO₂ nanobeams using HfO₂ as the gate dielectric. When heated up from low to high temperatures, VO₂ undergoes an insulator-to-metal transition. We observe a change in conductance (6 %) of our devices induced by gate voltage when the system is in the insulating phase. The response is reversible and hysteretic, and the area of the hysteresis loop becomes larger as the rate of gate sweep is slowed down. A phase lag exists between the response of the conductance and the gate voltage. This indicates the existence of a memory of the system involving a timescale of a few minutes. The origin of such slow processes may lie in the coupling between the dipolar arrangement and the strain state of the VO₂ crystal.

1:51PM J16.00014 Metal-to-insulator transition in a columnar nanocomposite oxide¹, ZHAOLIANG LIAO, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70810, USA, PENG GAO, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI 48109, USA, SHANE STADLER, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70810, USA, XIAOQING PAN, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI 48109, USA, RONGYING JIN, E. WARD PLUMMER, JIANDI ZHANG, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70810, USA — The capability of tuning lattice strain, composition, and dimensionality in epitaxial film growth provide a new avenue of exploring new functionality in correlated electron materials. Here we demonstrated a chemical ratio controlled metal-insulator transition in the nanocomposite films of V₂O₃-La_{2/3}Sr_{1/3}MnO₃ (LSMO) grown on LaAlO₃ (111) substrate through alternative deposition of LSMO and V₂O₃. A V-Mn ion exchange between V₂O₃ and LSMO occurs during the growth and results in the formation of nanoscale and vertically columnar-like insulating Mn₂O₃ and metallic La_{1-x}Sr_xVO₃ composite, as qualitatively revealed by scanning transmission electron microscopy. As determined by transport measurement, a metal-insulator transition is found in the composite films, which depends on the ratio of deposition time of V₂O₃ to LSMO.

¹Supported by U.S. DOE under Grant No. DOE DE-SC0002136.

2:03PM J16.00015 Avalanches in sub-micron V_2O_3 devices¹, SIMING WANG, Department of Physics and Center for Advanced Nanoscience, Materials Science and Engineering Program, University of California San Diego, GABRIEL RAMIREZ, Department of Physics and Center for Advanced Nanoscience, University of California San Diego, IVAN SCHULLER, Department of Physics and Center for Advanced Nanoscience, Materials Science and Engineering Program, University of California San Diego — Systematic resistance versus temperature measurements were performed on micron and sub-micron V_2O_3 devices. Instead of smooth R-T curves reported previously, multiple jumps in resistance are observed through the temperature driven metal-insulator transition. These jumps range over 3 orders of magnitude in resistance. A power law distribution of the jump sizes indicates that the metal-insulator transition in V_2O_3 occurs through a series of avalanches. The power law exponent in V_2O_3 devices is very close to that found in similar VO_2 devices.² This indicates that the phase transition in VO_2 and V_2O_3 are similar and occur through phase separation, percolation and avalanches. The effect of magnetic field on the avalanches in V_2O_3 will be discussed.

¹This work has been supported by the US Department of Energy, Office of Basic Energy Sciences, and Division of Materials Sciences under Award FG03-87ER-45332.

²A. Sharoni, J. G. Ramirez, and I. K. Schuller, Phys. Rev. Lett. **101**, 026404 (2008).

Tuesday, February 28, 2012 11:15AM - 2:15PM – **Session J17 DMP: Focus Session: Surfaces and Interfaces in Nonoxide Nanostructures: Growth, Structure, and Characterization - Organic/Inorganic Interfaces & Quantum Dots 252A**

11:15AM J17.00001 Current at Metal-Organic Interfaces, KLAUS KERN, Max Planck Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart + Ecole Polytechnique Federale de Lausanne - EPFL, CH-1015 Lausanne — Charge transport through atomic and molecular constrictions greatly affects the operation and performance of organic electronic devices. Much of our understanding of the charge injection and extraction processes in these systems relies on our knowledge of the electronic structure at the metal-organic interface. Despite significant experimental and theoretical advances in studying charge transport in nanoscale junctions, a microscopic understanding at the single atom/molecule level is missing. In the present talk I will present our recent results to probe directly the nanocontact between single molecules and a metal electrode using scanning probe microscopy and spectroscopy. The experiments provide unprecedented microscopic details of single molecule and atom junctions and open new avenues to study quantum critical and many body phenomena at the atomic scale. Implications for energy conversion devices and carbon based nanoelectronics will also be discussed.

11:51AM J17.00002 Temperature dependence in metal/organic heteroepitaxy, GEOFFREY ROJAS, XUMIN CHEN, DONNA KUNKEL, University of Nebraska-Lincoln, MATHIAS BODE¹, Argonne National Laboratory, AXEL ENDERS, University of Nebraska-Lincoln, UNIVERSITY OF NEBRASKA-LINCOLN COLLABORATION, ARGONNE NATIONAL LABORATORY COLLABORATION — The nucleation and growth of 2D single layers of tetraphenyl porphyrin molecules on Ag(111) are studied with variable temperature scanning tunneling microscopy. The heteroepitaxy of the organic/metal thin film occurs in strict analogy with known processes of metal heteroepitaxy. A similar hierarchy of energetic barriers to diffusion along edges and around corners is established. Temperature is the key component to selectively activating these barriers and determining shape of the adislands, from fractal-like shapes at low temperature to compact shape at high temperatures. Using existing models of metal heteroepitaxy, the terrace diffusion and binding energies of tetraphenyl porphyrin are approximated from measurement of island size as a function of temperature. This study provides evidence of the validity of using existing models of metal heteroepitaxy for the description of organic/metal heteroepitaxial systems.

¹now at Universität Würzburg

12:03PM J17.00003 Scanning Tunneling Microscopy investigation of the assembly of diF-TES-ADT on Ag(111)¹, SHAWN HUSTON, Appalachian State University, JIUYANG WANG, North Carolina State University, MARSHA LOTH, JOHN ANTHONY, University of Kentucky, BRAD CONRAD, Appalachian State University, DANIEL DOUGHERTY, North Carolina State University — Over the past two decades organic molecules have shown increasing promise as active layers in electrical devices such as field effect transistors, organic light emitting diodes, and organic photovoltaic devices. The suitability of organic molecules for use in these devices is governed by several properties, chief among them being the ability to self-organize into a film showing high carrier mobility. Organic thin film transistors (OTFT) partially composed of solution processed 2,8-difluoro-5,11-bis(triethylsilyl)ethynyl-anthradithiophene have shown high performance. To date these OTFTs have been constructed solely by solution processing. As such, we have chosen to investigate the possibility of vapor deposition as an alternative. Our investigation of the viability of vapor deposition of this promising molecule begins with deposition on Ag(111) as a model system. Preliminary STM results will be presented and discussed.

¹BC wishes to acknowledge the Ralph E. Powe Junior Faculty Enhancement Award for generous support.

12:15PM J17.00004 DFT study of metal/organic interfaces; optimizing morphology and energy levels for maximum Voc, MICHELLE TOMASIK, ALEXIE KOLPAK, JEFFREY GROSSMAN, MIT — Metal/organic interfaces are important for understanding the electronic properties of any device incorporating organic molecules, although these interfaces have been much less studied than their metal/inorganic counterparts. Using density functional theory, we examine the electronic structure of the interfaces of three metals: silver, aluminum, magnesium, and an organic molecule, Alq3, which is utilized in organic light emitting diodes. We calculate properties of interfaces with a clean metal surface as well as ones with small metal particles injected close to the organic. The effects of the different metals are to charge the Alq3 to varying degrees and perturb the energy levels as the metal states mix with the organic molecule. Insights into the energy level alignment and morphology at these interfaces as a function of the electrode workfunction will be discussed, with the goal of maximizing the open circuit voltage through the choice of metal and deposition process.

12:27PM J17.00005 DFT based modeling of C₆₀/Dichloropentacene/Au OPV heterojunctions, JUN WANG, JIAN-MING TANG, KARSTEN POHL, University of New Hampshire — The co-assembly of functionalized pentacenes (electron-donor materials) and fullerenes (electron-acceptor materials) on metal substrates provides a model for studying the structural and electronic properties for novel organic photovoltaic (OPV) heterojunctions. Our previous STM experimental results show C₆₀ to form single, double and triple nano chains on an intact single-domain, brick-wall structured 6,13-dichloropentacene (DCP) monolayer adsorbed on stepped Au(788). Here, we present theoretical DFT calculations of the geometric and electronic structure, and the charge transfer in this interacting three-component system. Our calculations show that single C₆₀ molecules prefer to either absorb on top of the DCP molecules (slightly shifted off the Cl center) or in between the DCP rows of the brick-wall structure. When adsorbing chains of C₆₀ they will align with either the troughs in between the DCP rows or the top of the DCP rows, in agreement with experiment. Compared to the isolated DCP molecules, the HOMO and LUMO levels move up towards the vacuum level by about 1 eV upon monolayer formation, resulting in charge transfer to C₆₀.

12:39PM J17.00006 Acetophenone on Si(001) with STM and DFT¹, STEVEN SCHOFIELD, ADAM RAHNEJAT, London Centre for Nanotechnology and Department of Physics and Astronomy, UCL, London, UK, OLIVER WARSCHKOW, Centre for Quantum Computation and Communication Technology, University of Sydney, Australia, DANIEL BELCHER, MARIAN RADNY, PHILLIP SMITH, School of Mathematical and Physical Sciences, University of Newcastle, Australia — Organic molecules are likely to play an important role in future technologies, e.g., in novel devices where individual molecules are incorporated as active elements, and in extending the functionality of existing technologies. A detailed, atomic-scale understanding of the structural and electronic properties of molecules on surfaces is key to the development of these technologies. Here we present scanning tunnelling microscopy (STM) and density functional theory (DFT) data of the surface binding configurations of acetophenone adsorbed to Si(001). Topographic and spectroscopic tunnelling experiments were performed at 77 K and room temperature in the limit of very low coverage. We find in analogy to other similar molecules such as acetaldehyde [1], acetone [2,3] and acetic acid [4], acetophenone molecules covalently bond to the Si(001) surface in a variety of configurations that can be directly manipulated using the STM tip. In its most stable configuration, the adsorbate stands upright on the surface, attached via the C and O atoms of its acetyl group, producing a geometry that is robust and attractive for molecular electronics applications. [1] JCP 131, 104707 (2010), [2] PCCP 11, 2747 (2009), [3] JACS 129, 11402 (2007), [4] PRB 84, 153302 (2011).

¹SRS acknowledges an EPSRC Fellowship (EP/H003991/1)

12:51PM J17.00007 Contact Angle Behavior for Fullerene/Porphyrin Mixtures on Si surfaces¹, MIRIAM CEZZA, ROMAINE A. ISAACS, Department of Materials Science and Engineering, University of Maryland, MD, 20742, QIAN SHAO, Department of Chemistry and Biochemistry, University of Maryland, College Park, MD, 20742, SHY-HAUH GUO², LOURDES G. SALAMANCA-RIBA, Department of Materials Science and Engineering, University of Maryland, MD, 20742, JANICE REUTT-ROBEY, Department of Chemistry and Biochemistry, University of Maryland, College Park, MD, 20742, RAYMOND J. PHANEUF, Department of Materials Science and Engineering, University of Maryland, MD, 20742 — Fullerene/porphyrin mixtures are of great interest in bulk heterojunction organic solar cells. Here we study the morphology of the phase separation which occurs when [6,6]-phenyl-C₆₁-butyric acid methyl ester (PCBM) and tetranitro-zinc phthalocyanine (tn-ZnPc), are deposited onto silicon (111) substrates, including the individual domain length scales, shapes and wetting angles. tn-ZnPc forms small clusters on the Si surface with a contact angle of approximately 15°, while PCBM forms compact clusters on broad (~0.5 µm diameter) “wetting-layer” disks, with the cluster contact angle of ~19°. Interestingly, a 50% mixture shows topography qualitatively similar to that for PCBM, but with a larger contact angle of 22°, indicating that the mixture wets the interface less than either pure component alone.

¹Work supported by the NSF-MRSEC at the University of Maryland #DMR0520471.

²The Laboratory for Physical Sciences, College Park, MD, 20740

1:03PM J17.00008 ABSTRACT WITHDRAWN —

1:15PM J17.00009 Molecular nanostructures on graphite, ANDREAS RIEMANN, LINDA GRABILL, BRANDON OWENS, ERIC KREBS, Western Washington University — The self-assembly of different amino acids on graphite has been studied using Scanning Tunneling Microscopy. Experiments involving the amino acid methionine have shown that the molecules arrange themselves in well-ordered molecular wires with equidistant spacing tunable by the amount of adsorbate concentration on the surface. This behavior can be explained by an attractive interaction of the amino and carboxyl groups with each other, whereas the side chains exhibit repulsive interactions. Experiments using other amino acids with different side chains, like tyrosine and histidine, show adsorption behavior which lead to densely packed films of well-ordered amino acids, but no molecular wire structure. The repulsive interactions of the side chains can not be experimentally observed. This interesting phenomenon of inter-molecular interaction was further investigated using molecular mechanics calculations for these molecules.

1:27PM J17.00010 Spontaneous Formation of Quantum Height Manganese Gallium Islands and Atomic Chains on N-polar Gallium Nitride (0001)¹, ARTHUR R. SMITH, ABHIJIT CHINCHORE, KANGKANG WANG, MENG SHI, YINGHAO LIU², Ohio University Nanoscale and Quantum Phenomena Institute — Significant interest has been shown over the last 15+ years in the growth of 2-D island nanostructures of special heights on semiconductor surfaces due to quantum size effects, often referred to as ‘electronic growth.’ Recently, there has been much interest in growth of magnetic metal layers on gallium nitride surfaces, but electronic growth in this system was not reported, until now. Surprisingly, we find that deposition of manganese onto gallium-rich, GaN(0001) results in the spectacular formation of 2-D quantum-height MnGa island structures. Two unique island heights, differing by just one atomic layer, are observed - one being 0.93 nm (5 atomic layers), the other 1.13 nm (6 atomic layers). The 0.93 nm high islands are unstable against the completion of the next atomic layer (0.93 + 0.20 nm), so a single quantum thickness is preferred (1.13 nm). A row structure at the surface of the islands is also revealed, with atomic resolution images suggesting a mixture of Mn and Ga. Auger electron spectroscopy confirms a significant surface Mn content. In addition, growth of 1-D atomic chains at the surface of the completed 1.13 nm high islands is also seen, indicating strongly anisotropic diffusion. The observed behavior is consistent with a quantum size effect driven growth.

¹Authors gratefully acknowledge support from the U.S. DOE and NSF.

²present address: MPA-CINT, MS K771, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

1:39PM J17.00011 Wavelength tunable high quality positioned InAs quantum dots grown on patterned GaAs (001) substrates, AYESHA JAMIL, University of Cambridge, JOANNA SKIBA-SZYMANSKA, Toshiba Research Europe Ltd., IAN FARRER, University of Cambridge, MARTIN WARD, Toshiba Research Europe Ltd., JONATHAN GRIFFITHS, GEB JONES, University of Cambridge, ANDREW SHIELDS, Toshiba Research Europe Ltd., DAVE RITCHIE, University of Cambridge, TOSHIBA RESEARCH EUROPE LTD. COLLABORATION — Semiconductor quantum dots serve as ideal contenders in the domains of quantum optics, quantum cryptography and quantum information processing. The decisive factor about their possible applications is their peak emission energy. Naturally grown quantum dots suffer from the problem of random nucleation behavior and non-uniform dot sizes. Here we report on the growth of site-controlled InAs quantum dots on pre-patterned GaAs(001) substrates with adjustable wavelengths. Interplay of the dot growth parameters, particularly growth temperature and Indium deposition amount, as well as the size of the initial template has been employed. With a 20 nm thick GaAs spacer layer grown between the regrowth interface and the quantum dot layer, uniform arrays of quantum dots have been achieved with emission wavelengths covering a spectral window ranging from 900 nm to 1200 nm. This has been achieved without risking the single dot occupancy per nucleation site measured to be > 60% for all of the investigated samples. To ensure better quality of dots, wafer cleanliness is monitored throughout the process. The dots thus show bright emission lines with no spectral jittering.

1:51PM J17.00012 Investigation of spatial correlation of type-II ZnTe quantum dots embedded in ZnCdSe barriers, UTTAM MANNA, ISMAIL NOYAN, GERTRUDE NEUMARK, APAM, Columbia University, SIDDHARTH DHOMKAR, BIDISHA ROY, IGOR KUSKOVSKY, Queens College of CUNY, The Graduate Center of CUNY, RICHARD MOUG, City College of CUNY, LE PENG, MARIA TAMARGO, City College of CUNY, The Graduate Center of CUNY — Doped and undoped multilayered structures of ZnTe type-II quantum dots (QDs) embedded in a ZnCdSe matrix have been grown in order to investigate the formation of an intermediate band, lying within the ZnCdSe band gap, with the aim of absorbing photons with energies below ZnCdSe bandgap. These materials may be useful for intermediate bandgap solar cells. The reciprocal space map (RSM) of the ZnTe/ZnCdSe multilayer QD structure consisting of periodic superlattice peaks in the q_x direction have been studied for two different ZnCdSe spacer thicknesses ($d_A \approx 3.5$, $d_B \approx 1.5$ nm). The ZnTe QDs give rise to diffuse scattering in RSM, which is found to be elongated in the q_x direction for both samples indicating a vertical correlation of the QDs. From the widths of the diffuse maxima in the q_z direction, we found that 16% and 40% of QDs are correlated vertically for $d_A \approx 3.5$ nm and $d_B \approx 1.5$ nm, respectively. With increasing correlation, the pairing probability of the dots increases, leading to a larger average QD size. This conclusion is supported by a smaller blue-shift (26 vs 36 meV) of the photoluminescence peak position with increasing excitation intensity, over five orders of magnitude, for the structure with narrower spacers.

2:03PM J17.00013 Characterization of quantum dot chains using transmission electron microscopy, TYLER PARK, JOHN COLTON, JEFFREY FARRER, Brigham Young University, HAEYEON YANG, South Dakota School of Mines and Technology — We report on the growth and characterization of InGaAs self-assembled quantum dots which form into chains through an altered Stranski-Krastanov method. The methods we are using to study these quantum dot chains include imaging and chemical analysis using a transmission electron microscope (TEM). In order for the quantum dot chains to be characterized using the TEM, the samples must be cut and thinned to allow enough electrons to pass through the sample for our techniques. We are making cross-section and plan view cuts which allow us to get information about the chemical composition, indium segregation, size and spacing, contaminants and other aspects of the dots.

Tuesday, February 28, 2012 11:15AM - 2:15PM –

Session J18 DMP: Focus Session: Nanostructures and Metamaterials, Growth, Structure, and Characterization – New Fabrication Techniques 252B

11:15AM J18.00001 Large Area 3D Negative Index Metamaterials Formed by Printing, JOHN ROGERS, University of Illinois — Negative index metamaterials (NIMS) are man-made structures with values of permittivity and permeability that are simultaneously negative over some range of frequencies. Although advanced lithographic techniques can form the necessary three dimensional (3D) nanoscale features for NIMS, such methods can be applied only over small areas (100's of μm^2) on specialized substrates, with low throughput. This talk summarizes a 3D transfer printing method that can yield 3D-NIMS with excellent optical characteristics, in ways that are scalable to arbitrarily large areas and are compatible with manufacturing. We demonstrate 3D-NIMS with 11-layers and sub-micron unit cell dimensions, over areas $> 75 \text{ cm}^2$, corresponding to $> 10^5 \times 10^5$ unit cells, all with excellent uniformity and minimal defects. These areas and numbers of unit cells both correspond to increases of more than 2×10^7 times, over previous results. Multiple cycles of printing with a single stamp demonstrate use in a manufacturing mode at throughputs that are $\sim 10^8$ times higher than those possible with state-of-the-art focused-ion beam lithography systems (~ 2.5 s per unit cell). Optical measurements show negative index of refraction in the NIR spectral range, with values as large as $\text{Re}(n) \sim -7$ at $\lambda = 2.4 \mu\text{m}$ and high figures of merit (FOM) of ~ 8 at $\lambda = 1.95 \mu\text{m}$ indicating low loss operation. Related approaches can be used to form similar classes of 3D-NIMS with operation in the visible regime.

11:51AM J18.00002 Optical metamaterials with different metals and wedge demonstration of negative refraction with fishnet metamaterials at visible wavelengths¹, NIAN-HAI SHEN, THOMAS KOSCHNY, Ames Lab/Iowa State University, MARIA KAFESAKI, FORTH, COSTAS M. SOUKOULIS, Ames Lab/Iowa State University and FORTH — We investigate the influence of different metals on the electromagnetic response of fishnet metamaterials in the optical regime. We found that, instead of using a Drude model, metals with a dielectric function from experimentally measured data should be applied in order to correctly predict the behavior of optical metamaterials. Through comparison of the performance for fishnet metamaterials made with different metals, i.e., gold, copper, and silver, we found silver is the best choice for the metallic parts compared to other metals, because silver allows for the strongest negative-permeability resonance and, hence, for optical fishnet metamaterials with a high figure-of-merit. We push the negative-index metamaterials to the visible regime and our improved wedge setup provides an unambiguous demonstration of negative refraction for the designed optical metamaterial.

¹Work at Ames Laboratory was supported by the Department of Energy (Basic Energy Sciences) under contract No. DE-AC02-07CH11358. This was partially supported by the European Community Project NIMNIL (Contract No. 228637).

12:03PM J18.00003 Subwavelength imaging of plasmonic nano-bubble cavity probed by Cathodoluminescence, JUN XU, MIT, HYUNGJIN MA, UIUC, NICHOLAS FANG, MIT — Concentrating light into a deep-subwavelength volume is big challenge in conventional optics due to the diffraction limit. In recent years, plasmonics, the interaction of light and metallic nanostructures, offers new opportunities in manipulating light-matter interaction at a subwavelength scale. Because of a strong localized resonant response of the, the field can be confined in a plasmonic cavity with an ultra-small mode volume and a high Purcell factor. Plasmonic light sources at the nanoscale have been demonstrated by utilizing an active medium. However, such light sources are characterized based on either a diffraction-limited technique or a spatially-averaged lifetime measurement, neither of which show subwavelength information. Here, we present a method, cathodoluminescence (CL) that shows a subwavelength resolution image of nanoscale air bubbles trapped in between thin amorphous silicon and silver. A novel multiple-fringe pattern, with a strong dependence on the air gap width, is observed due to an enhanced luminescence. A simple model, based on an oscillating electric dipole, is applied to explain the phenomena. Both the plasmonic and conventional cavity effect of the light interacting with the novel nano-bubble system are considered. The plasmonic nano-bubbles may provide a new approach to generate localized light from a continuous thin film layer with high efficiency, for the application in ultra-compact optical device, molecular imaging, etc.

12:15PM J18.00004 Direct laser writing of three dimensional metal nanostructures using a femtosecond laser and various chemistries, SEUNGYEON KANG, KEVIN VORA, SHOBHA SHUKLA, ERIC MAZUR, Harvard University — Metal nanostructures play important role in various areas such as catalysts or in plasmonics and especially for metamaterial applications. To generate these structures, most fabrication techniques can allow mass production but are either non-controllable, suffer from high cost and low throughput or are limited in two dimensions. Direct laser writing technique resolves these problems but has been mainly used to fabricate polymeric structures. We direct laser write 3D metal structures of tunable dimensions ranging from hundreds of nanometers to micrometers. With computer-controlled translation stage and by utilizing nonlinear optical interactions between chemical precursors and femtosecond pulses, we can limit the metal-ion photo-reduction process to a focused spot smaller than that of the diffraction-limit to create metal nanostructures in a focal volume. We study the chemistry that effects the photo induced metal growth to generate desirable metal structures. By varying the types of solvent, polymer and the concentration ratios of chemicals, we demonstrate our control over the morphology of the resulting metal structures and other features such as flexibility and conductivity. We plan to create diverse metal nanostructures for a wider range of metamaterial applications.

12:27PM J18.00005 Self-assembly of metallic nanoparticles into macroscopic, high-density, monolayer films, JAKE FONTANA, NRC-NRL Postdoctoral Resident at Naval Research Laboratory, RON RENDELL, JAWAD NACIRI, BANAHALLI RATNA, Naval Research Laboratory — A vital element of bringing pragmatic optical metamaterials to fruition is the ability to produce and characterize macroscopic, self-assembled, high-density, ensembles of nanoparticles. We have developed a method that functionalizes metallic nanoparticles with thiol-ene ligands, self-assembles the nanoparticles into high-density, monolayer, centimeter size domain films using phase separation, transports the films onto substrates using surface tension gradients, and crosslinks, via click chemistry, the nanoparticles together into a solid film. We have determined the real and imaginary parts of the phase shift for the films using a Mach-Zehnder interferometer and spectrophotometer and compare the measurements to simulations. We discuss the implications of this self-assembly process for the construction of macroscopic optical metamaterials.

12:39PM J18.00006 Designing Phoxonic Metamaterials with Fractal Geometry, SISI NI, Institute for Soldier Nanotechnologies, Department of Materials Science and Engineering, Massachusetts Institute of Technology, CHEONG YANG KOH, Defense Science Organization, Singapore, STEVE KOOL, EDWIN THOMAS, Institute for Soldier Nanotechnologies, Department of Materials Science and Engineering, Massachusetts Institute of Technology, — Recently, the concepts of fractal geometry have been introduced into electromagnetic and plasmonic metamaterials. With their self-similarity, structures based on fractal geometry should exhibit multi-band character with high Q factors due to the scaling law. However, there exist few studies of *phoxonic* metamaterials based on fractal geometry. We use COMSOL to investigate the wave propagation in two dimensional systems possessing fractal geometries. The simulations of these systems, guided by our recently developed general design framework, help to understand the role of design in determining the phononic properties of the structures. Proposed structures are being fabricated via standard lithographic or 3D printing techniques. The wave behavior of the structures can be characterized using Brillouin Light Scattering, Scanning Acoustic Microscope and Near-field Scanning Optical Microscopy. Due to their sparse spatial distribution, fractal phononic structures show potential for "smart skin", where multifunctional components can be fabricated on the same platform.

12:51PM J18.00007 Plasmon Enhanced Transparency of a Metallic Film on Silicon, TIANYI SUN, Department of Physics, Boston College, YANG WANG, School of Physics and Telecommunication Engineering, South China Normal University, ZHIFENG REN, KRZYSZTOF KEMPA, Department of Physics, Boston College — Low electrical resistivity and high optical transparency are highly desirable for thin films employed in various applications in electronics, optics, solar photovoltaics. In subwavelength scales, plasmon resonance can help electromagnetic waves to propagate through porous metallic films. In this work, we first employ a theory of effective dielectric response, and then quantitative simulations based on finite-difference-frequency-domain (FDFD) and finite-difference-time-domain (FDTD) methods, to understand and demonstrate physics of this effect. We show, that a nanoscopically perforated, yet continuous planar metallic film on silicon, can be designed to be highly transmissive in the entire visible range.

1:03PM J18.00008 Enhancing optical gradient forces with metamaterials¹, VINCENT GINIS, Vrije Univ. Brussel, PHILIPPE TASSIN, Vrije Univ. Brussel and Ames Lab/Iowa State Univ., IRINA VERETENNICOFF, Vrije Univ. Brussel — The transfer of linear momentum from electromagnetic waves to matter and the associated optical forces allow to dynamically manipulate the geometry of nanophotonic components with electromagnetic fields. In recent years, it has been proposed to use optical gradient forces for all-optical actuation of nanophotonic systems. This would open up the possibility for information processing inside nanoscale devices. Despite many efforts to increase these forces in integrated systems, they remain too small for most practical applications. In this contribution, we demonstrate how optical gradient forces can be enhanced significantly with the use of metamaterials. By implementing the techniques of transformation optics, we show how a metamaterial slab allows for the magnification of optical forces over several magnitudes, even when realistic losses are included.

¹Work at VUB was supported by the Research Foundation Flanders (FWO-Vlaanderen) and the Belgian Science Policy Office (Grant No. IAP VI/10). Work at ISU was supported by Ames Laboratory (U.S. DOE).

1:15PM J18.00009 Terahertz composite right/left-handed transmission-line metamaterial surfaces¹, ZHIJUN LIU, PHILIP HON, AMIR TAVALLAEI, TATSUO ITOH, BENJAMIN WILLIAMS, Electrical Engineering Department, University of California, Los Angeles, California 90095, USA, UCLA TERAHERTZ DEVICES AND INTERSUBBAND NANOSTRUCTURES LABORATORY TEAM, UCLA MICROWAVE ELECTRONICS LAB TEAM — We present terahertz metamaterial waveguides based on the concept of composite right/left-handed (CRLH) transmission-lines implemented in a metal-dielectric-metal geometry. The waveguides are fabricated with spin-coated Benzocyclobutene sandwiched between a ground plane and photolithographically defined top capacitive metal pads. Angle-resolved reflection spectroscopy measurement is used to map the dispersion of this metamaterial surface, which reveals strong resonant absorptions for both right-handed and left-handed (backward wave) propagating modes within the leaky-wave bandwidth. Tuning of the waveguide dispersion is demonstrated by varying the integrated lumped element capacitive geometry. The incident polarization provides selection of different waveguide modes, exhibiting either fully right/left handed, or right-handed only propagation. Analysis based on full-wave finite element method simulations as well as lumped circuit models will be presented.

¹This work was supported by NSF under Grant No. ECCS-0901827.

1:27PM J18.00010 Metamaterial Single Polarization Grid: Moving Towards the Dynamic Selective Polarizer, COREY SHEMELYA, THOMAS VANDERVELDE, Tufts University — Ongoing interest in active metamaterial devices has increased due to their scalability, tunability, and, more importantly, the ability to turn them on or off. A dynamic metamaterial polarizer has unique applications for identifying manmade objects anywhere in the IR. This work describes a single layer metamaterial polarization grid. The metamaterial grid is immediately scalable to many different wavelengths. The polarization grid has been designed for conversion to a dynamic metamaterial polarizer with simulated on/off ratios of 9 to 1. To this end, samples have been fabricated using varying doping concentrations of Si in GaAs grown epitaxially on Sapphire. Au metamaterials along with contact grids were then patterned and deposited. This design allows for potential dynamic responses as well as monolithic integration to create an active, metamaterial-stack, selective polarizer.

1:39PM J18.00011 A new theoretical model for enhanced optical transmission through thin films¹, ELI LANSEY, ISROEL MANDEL, Department of Physics, Graduate Center and City College of the City University of New York, JONAH GOLLUB, Phoebus Optoelectronics, DAVID CROUSE, Department of Electrical Engineering, City College of the City University of New York — We present a new theoretical approach for modeling the resonant properties and transmission through subwavelength apertures penetrating metal films. We show that standard cavity mode theory can be applied to an effective resonant cavity whose dimensions are determined by the aperture dimensions in conjunction with the evanescent decay lengths of the diffracted waves. This method predicts the dependence on variation in both the periodicity of the holes and the film thickness over a wide range of values. It further provides a physical mechanism for the enhanced transmission observed in periodic aperture arrays.

¹This material is based upon work supported by the DOD/DARPA SBIR PROGRAM under Contract No. W31P4Q-10-C-0074. It has been approved for public release, distribution unlimited.

1:51PM J18.00012 Enhanced second harmonic generation from aperiodic arrays of gold nanoparticles, ANTONIO CAPRETTI, ECE Dept. and Photonics Center Boston University & DIETL University of Naples Federico II, GARY WALSH, ECE Dept. and Photonics Center Boston University, JACOB TREVINO, Div. of MSE Boston University, GIOVANNI MIANO, DIETL University of Naples Federico II, LUCA DAL NEGRO, ECE Dept. and Photonics Center Boston University & Div. of MSE Boston University — Second harmonic generation (SHG) from planar arrays of metal nanoparticles has been investigated in the last years for several configurations of particle shape and excitation-collection directions. In particular L-shaped particles have been employed to remove centrosymmetry. In this work we study SHG dependence on the array geometry, by comparing the generation efficiency of periodic arrays with that of deterministic aperiodic ones, namely Fibonacci and Golden Angle Spiral, lacking planar centrosymmetry. Two excitation-collection configurations are employed to test fabricated arrays. The whole range of average particle separation is explored, from closed spaced particles (plasmonic regime) to far spaced particles (photonic regime). We observe that SHG efficiency can be increased by arranging centrosymmetric particles in aperiodic arrays without inversion symmetry, both in the plasmonic regime and in the photonic one. We also demonstrate that Fibonacci and Golden Angle Spiral arrays perform differently in respect of the average interparticle separation and the collection direction, allowing the tunability of SHG extraction.

2:03PM J18.00013 Plasmonic Coupling Effects in Large-area High-enhancement, Periodically-Arrayed Nanopillars, FRANCISCO BEZARES, JOSHUA CALDWELL, OREST GLEMBOCKI, Naval Research Laboratory, MAARIT KARINIEMI, JAAKKO NIINISTÖ, TIMO HATANPÄÄ, University of Helsinki, RONALD RENDELL, Naval Research Laboratory, MARAIZU UKAEGBU, Howard University, MIKKO RITALA, University of Helsinki, SHARKA PROKES, Naval Research Laboratory, CHARLES HOSTEN, Howard University, MARKKU LESKELA, University of Helsinki — Periodically arrayed Si nanopillars, coated with a thin layer of Ag, have been shown to produce large-area (~1 mm or more), uniform enhancement of the electromagnetic (EM) field near the surface of such arrays, thus suggesting suitability for the development of next-generation chem/bio-sensors. Although short-range plasmonic coupling effects are expected to increase the enhancement factor of these arrays several orders of magnitude, limitations in current lithographic techniques prohibit the fabrication of closely spaced nanopillars where such coupling effects become significant. Here we show experimentally that the use of Atomic Layer Deposition of Ag allows for the fabrication of Ag-coated Si nanopillar arrays with interpillar spacings of a few nanometers (~2 nm) resulting in 1-2 orders of magnitude increase in EM enhancement observed throughout the whole array area. Experimental observations that provide insight into the nature of the different coupling phenomena contributing to the overall enhancement of the EM field in these systems will also be discussed.

Tuesday, February 28, 2012 11:15AM - 2:15PM – Session J19 DCMP DAMOP: Invited Session: Strongly Interacting Cold Fermi Gases 253AB

11:15AM J19.00001 From ultracold Fermi Gases to Neutron Stars, CHRISTOPHE SALOMON, LKB, Ecole Normale supérieure — Ultracold dilute atomic gases can be considered as model systems to address some pending problem in Many-Body physics that occur in condensed matter systems, nuclear physics, and astrophysics. We have developed a general method to probe with high precision the thermodynamics of locally homogeneous ultracold Bose and Fermi gases [1,2,3]. This method allows stringent tests of recent many-body theories. For attractive spin 1/2 fermions with tunable interaction (^6Li), we will show that the gas thermodynamic properties can continuously change from those of weakly interacting Cooper pairs described by Bardeen-Cooper-Schrieffer theory to those of strongly bound molecules undergoing Bose-Einstein condensation. First, we focus on the finite-temperature Equation of State (EoS) of the unpolarized unitary gas. Surprisingly, the low-temperature properties of the strongly interacting normal phase are well described by Fermi liquid theory [3] and we localize the superfluid phase transition. A detailed comparison with theories including recent Monte-Carlo calculations will be presented. Moving away from the unitary gas, the Lee-Huang-Yang and Lee-Yang beyond-mean-field corrections for low density bosonic and fermionic superfluids are quantitatively measured for the first time. Despite orders of magnitude difference in density and temperature, our equation of state can be used to describe low density neutron matter such as the outer shell of neutron stars.

[1] S. Nascimbène, N. Navon, K. Jiang, F. Chevy, and C. Salomon, *Nature* **463**, 1057 (2010)

[2] N. Navon, S. Nascimbène, F. Chevy, and C. Salomon, *Science* **328**, 729 (2010)

[3] S. Nascimbène, N. Navon, S. Pilati, F. Chevy, S. Giorgini, A. Georges, and C. Salomon, *Phys. Rev. Lett.* **106**, 215303 (2011)

11:51AM J19.00002 Spin-Imbalance in One and Three-Dimensional Fermi Gases¹, RANDALL HULET², Rice University — The FFLO modulated superconductor state was independently proposed by Fulde and Ferrell, and Larkin and Ovchinnikov, as a way of accommodating the excess spin in a spin-polarized superconductor. The pairs in the FFLO state have non-zero center-of-mass momentum, which can produce a periodic structure with a spatially-modulated order parameter. Although there is some evidence for FFLO pairing in certain heavy fermion compounds that are able to accommodate both magnetic and superconducting order, conclusive experimental proof remains elusive. Motivated by the search for exotic paired states, we have performed experiments with spin-imbalanced ultracold atomic Fermi gases in both 3D and 1D. We use two hyperfine levels of ^6Li to emulate the spin-up and down states. The *s*-wave pairing interactions are controlled via a magnetically-tuned collisional (Feshbach) resonance. In 3D, we find that the gas phase separates into an evenly paired BCS-like core, surrounded by the excess spin-up atoms [1]. For the 1D experiment, a two-dimensional optical lattice was used to create an array of 1D tubes that are each filled with ~200 atoms. The weak axial confinement again produces a phase separation, but in contrast to 3D we find a partially-polarized central core surrounded by either fully-paired or fully-polarized wings, depending on the degree of overall spin-polarization [2]. Theory predicts that the partially-polarized phase is an FFLO superfluid. We are currently trying to obtain direct evidence for FFLO pairing, which may be revealed in the pair momentum distribution found by releasing the atoms axially and allowing them to expand in time-of-flight. We are also exploring the 1D-3D dimensional crossover that occurs when the coupling between tubes is reduced.

[1] G.B. Partridge *et al*, *Science* **311**, 503 (2006).

[2] Y.A. Liao *et al*, *Nature* **467**, 567 (2010).

¹Supported by the ARO with funds from the DARPA OLE program, ONR, and the NSF.

²In collaboration with Y.A. Liao, G.B. Partridge, Wenhui Li, A.S. Rittner, M. Revell, T. Paprotta, S.K. Baur, and E.J. Mueller.

12:27PM J19.00003 Many-body physics with ultracold alkali-earth fermions in optical lattices, JUN YE, University of Colorado at Boulder and NIST — No abstract available.

1:03PM J19.00004 Onset of a Pseudogap Regime in Ultracold Fermi Gases¹, AUREL BULGAC, University of Washington — We show, using an ab initio approach based on Quantum Monte Carlo technique, that the pseudogap regime emerges in ultracold Fermi gases close to the unitary point. We locate the onset of this regime at a value of the interaction strength slightly to the BCS side of the unitary point. We determine the evolution of the gap as a function of temperature and interaction strength in the Fermi gas around the unitary limit and show that our results exhibit a remarkable agreement with the recent wave-vector resolved radio frequency spectroscopy data. Our results indicate that a finite temperature structure of the Fermi gas around unitarity is complicated and involves the presence of preformed Cooper pairs, which however do not contribute to the long range order.

¹Support is acknowledged from the DOE under grants DE-FG02-97ER41014 and DE-FC02-07ER41457, from the Polish Ministry of Science under contract N N202 128439. Calculations were performed on the UW Athena cluster and at the Interdisciplinary Centre for Mathe

1:39PM J19.00005 Strongly Repulsive Quantum Gases¹ , TIN-LUN HO, Physics Department, The Ohio State University — Advances in cold atom experiments have shown that the properties of repulsive Fermi and Bose gases are far more intricate than generally expected, as these systems can produce molecules even in the weakly interacting regime. Recent experiments, however, reveal some general yet puzzling properties of these gases in the strongly repulsive regime. In this talk, we show that these properties are direct consequences of statistics, and are fundamental properties of quantum gases [1]. We shall also discuss the related issue of itinerant ferromagnetism, and discuss the physical settings in which ferromagnetism can be found.

[1] V. B. Shenoy and Tin-Lun Ho, arXiv: 1106.0960, to appear in Physical Review Letters

¹Supported by NSF DMR-0907366 and by DARPA W911NF-07-1-0464, W911NF0710576.

Tuesday, February 28, 2012 11:15AM - 2:15PM –

Session J20 COM CSWP: Invited Session: Sexual and Gender Diversity Issues in Physics 253C

11:15AM J20.00001 The State of Higher Education for STEM LGBTQQ Faculty/Staff¹ , SUSAN RANKIN, The Pennsylvania State University — It has long been understood—an understanding that has been well supported by research-based evidence—that institutional “climate” has a profound effect on any academic community’s ability to carry out its tripartite mission of teaching, research, and service (Bauer, 1996; Boyer, 1990; Peterson & Spencer, 1990; Rankin, 1998; 2003; 2010; Rankin & Reason, 2008; Tierney & Dilley, 1996). With the acknowledgment that institutions differ in the level of attention and emphasis on issues campus climate, it is safe to say that a campus climate offering equitable learning opportunities for all students, academic freedom for all faculty, and fairness in employment for all staff and administrators is one of the primary responsibilities of institutions of higher education. The research also suggests that a challenging campus climate exists for LGBTQQ students, faculty and staff. Based on the literature, a challenging climate leads to decreased productivity, decreased sense of value to the community, decreased retention, and negatively influences educational outcomes (Settles, et al. 2006; Trower & Chait (2002); Pascrell & Terenzini, 2005; Whitt, Edison, Pascarella, Terenzini, & Nora, 2001). Little is available in the literature on LGBTQQ faculty in the STEM fields. This program will engage participants in a review of the results of the 2010 project with regard to the experiences of LGBTQQ faculty and staff in the STEM fields.

¹Project supported by Campus Pride.

11:51AM J20.00002 Shattering the Lavender Ceiling: Sexual Minorities in Physics , MICHAEL RAMSEY-MUSOLF, University of Wisconsin-Madison — I will discuss some of the challenges experienced by sexual minorities in physics, from both a personal and broader perspective. I will also comment on the opportunities for the field to become more inclusive, supportive, and scientifically stronger by addressing these challenges.

12:27PM J20.00003 Why Awareness of LGBT issues in the Physics Community Makes Sense , JANICE HICKS, National Science Foundation — A thriving innovation ecology requires diversity of perspective and knowledge. We want to attract and retain the best possible talent to Science and Engineering, particularly after expensive investments in training of faculty, postdoctoral fellows and students. Participants who bring their authentic identity to work are much more efficient, as it takes a lot of energy to stay in the closet. It is a concern that so few S&E faculty are out of the closet – we don’t know the numbers and they are difficult to obtain. This makes it difficult for the younger generation of students to relate as they do not see sexual orientation as an obstacle. It is also important for LGBT people to be visible in order to benefit from workplace policies such as family leave and other benefits. There are some activities to promote a positive view of LGBT people in S&E. The National Organization of Gay and Lesbian Scientists and Technical Professionals (NOGLSTP) has been in existence since 1983, and holds receptions and symposia at the AAAS meeting and other professional society meetings, as well as a symposium called “Out to Innovate,” next to be held October 13-14, 2012 at Ohio State University. The American Chemical Society started an LGBT subdivision of its Division of Professional Relations in 2010. Much more needs to be done to educate leaders so they can speak knowledgeably about LGBT issues. Their ability to do so can affect their success in hiring and retaining top talent.

1:03PM J20.00004 Physics Climate as Experienced by LGBT+ Physicists , ELENA LONG, Kent State University — In 2009, Elena Long created the LGBT+ Physicists website (<http://lgbtphysicists.x10hosting.com>) as a warehouse for resources useful for sexual and gender minorities working in physics. This resource has grown to include networking resources, lists of LGBT-friendly universities and localities, recommendations for enacting positive change in physics communities, and out-reach to other STEM-oriented LGBT organizations. This has been possible in large part by the dynamic community of LGBT+ physicists and allies looking to make physics more welcoming towards our community. In 2011, Elena used her position as Member at Large on the executive committee of the Forum of Graduate Student Affairs (FGSA) to conduct a climate survey that included, among other things, the first serious look at LGBT+ demographics in physics. The survey focused particularly on issues of language heard and harassment experienced by physicists and was broken down into categories based on race, physical and mental ability, gender, and sexuality. Furthermore, it examined the outcomes of experienced harassment and the reasons for when harassment was not reported. Due to the nature of the study, overlapping demographics, especially “multiple minorities,” were also explored. This talk will give a brief history of the LGBT+ Physicists resource as well as an overview of the FGSA study.

1:39PM J20.00005 TBA , THEODORE HODAPP, American Physical Society APS — No abstract available.

Tuesday, February 28, 2012 11:15AM - 2:03PM –

Session J21 DMP: Focus Session: Search for New Superconductors: New Theories and Experiments 254A

11:15AM J21.00001 The Challenge of Unconventional Superconductivity¹ , MICHAEL NORMAN, Materials Science Division, Argonne National Laboratory — In the past few decades, several new classes of superconductors have been discovered. Most of these are unconventional in that they do not appear to be related to traditional superconductors where the order parameter is more or less spatially isotropic. As a consequence, it is felt by many (but not all!) that the cause of superconductivity arises from a different source than the electron-ion interactions that are at the heart of conventional superconductivity. But developing a rigorous theory for any of these classes of materials has proven to be a difficult challenge, and will continue to be one of the major problems in physics in the decades to come. This is particularly true in that if history is any guide, even more dramatic discoveries of unconventional superconductors await us in the future.

¹Work supported by the US DOE, Office of Science, under Contract No. DE-AC02-06CH11357 and by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the US DOE, Office of Science, under Award No. DE-AC02-98CH10.

11:51AM J21.00002 Transport properties of layered Ba(Pb,Bi)O₃ thin films, G.W.J. HASSINK, K. MUNAKATA, R.H. HAMMOND, M.R. BEASLEY, Geballe Laboratory for Advanced Materials, Stanford University, Stanford, CA 94305 — Doped BaBiO₃ is a 3D oxide superconductor with a maximum T_c of 30 K for Ba_{0.6}K_{0.4}BiO₃. There has been a lot of discussion on whether this high T_c can be explained purely by electron-phonon coupling with a high coupling constant λ . In addition, the presence of real-space paired 6s² electrons in the parent compound raise intriguing questions about whether there is an electron-electron coupling interaction as well. This possible negative-U interaction might be used to implement the suggestion by Berg, Orgad and Kivelson [Phys.Rev.B 78, 094509] that for a two-layer system where one layer provides electron pairing interaction and the other layer is conducting, the whole can be superconducting with a high T_c. Here we discuss the transport properties of BaPbO₃/BaBiO₃ bilayers, where the BaBiO₃ layer is thought to act as the pairing layer, while the BaPbO₃ acts as the conducting layer. The transport behavior changes to insulating upon decreasing the metallic BaPbO₃ layer thickness at values that single films are expected to still be metallic.

12:03PM J21.00003 Control of Two-Dimensional Multi-Component Superconductivity in SrTiO₃ Heterostructures by Interlayer Coupling, HISASHI INOUE, MINU KIM, SLAC National Accelerator Laboratory, University of Tokyo, CHRISTOPHER BELL, YASUYUKI HIKITA, SLAC National Accelerator Laboratory, HIROSHI OKAMOTO, University of Tokyo, HAROLD HWANG, Stanford University, SLAC National Accelerator Laboratory, University of Tokyo — Two-dimensional (2D) superconductivity (SC) in the clean limit is of particular interest since novel phases such as the Fulde-Ferrell-Larkin-Ovchinnikov state [1,2], and Landau-quantized SC [3] are suggested theoretically. In an attempt to approach this limit experimentally, SC was confined in a narrow δ -doped region of SrTiO₃ [4]. 2D subbands (SBs) were observed as well as 2D SC. Building on these results, we have explored the coupling between two 2D superconducting layers in structures with two δ -doped layers, with variable interlayer coupling controlled by their spacing. We observe multiple components of the SC in the temperature and angular dependent upper critical field plots. These data suggest that the SB structure in the doped and interlayer regions directly impact the SC, and may play an important role for the design and investigation of multi-component SC. [1] P. Fulde *et al.*, *Phys. Rev.* **135**, A550 (1964). [2] A. I. Larkin *et al.*, *Sov. Phys. JETP* **20**, 762 (1965). [3] M. Rasolt *et al.*, *Rev. Mod. Phys.* **64**, 709 (1992). [4] Y. Kozuka *et al.*, *Nature* **462**, 487 (2009).

12:15PM J21.00004 Electric field induced superconductivity in a layered transition metal chalcogenide, J.T. YE, Y.J. ZHANG, Y. MASTUHASHI, Y. IWASA, Department of Applied Physics, The University of Tokyo — Recent developments in electric double layer transistors (EDLTs) are attracting growing interests because of its stronger field effect orders of magnitude larger than other transistor techniques. This method provides unique abilities to reach the high carrier densities required for inducing superconductivity in several kinds of materials. Among them, layered materials are convenient examples to work with since high quality surface suitable for transistor channel could be easily obtained after mechanical cleavage. Especially, after the introduction of graphene techniques, high quality atomically flat surface can be routinely fabricated on a broad range of layered materials. Combining EDL with novel materials processing techniques on layered materials provides new opportunities in manipulating their electronic properties. We can achieve high carrier density up to 10¹⁴ cm⁻² electrostatically in layered materials and induce metal insulator transitions. Superconductivity, similar as that shown in ZnI EDL transistor, could be observed when we cool down the system to low temperature after inducing a metal insulator transition with large amount of accumulated carriers. The versatility of this combination shows its potential as a protocol to study varieties of layered materials for broader scope of possibilities in accessing their superconductivities. And hopefully, this method could also facilitate to induce superconductivity in new materials.

12:27PM J21.00005 Fano resonances in multigap Fe based superconductors and complexity for material design, ANTONIO BIANCONI, Physics Dept., Sapienza University of Rome — The Fano resonance in the superconducting gaps (or “shape resonance” or “Feshbach resonance”) in multigap superconductors [A Bianconi *Sol. State Commun.* **89**, 933 (1994)] has been proposed as the mechanism for high T_c in Fe-based superconductors and related compounds [D Innocenti *et al Supercond. Sci. Technol.*, 015012 (2011)] near the Lifshitz transition for a vanishing Fermi surface in a superlattice of layers or wires, in the proximity of a lattice, electronic, magnetic instability with competing interactions that give complex systems. The multiscale phase separation from nano-scale to micron scale in K0.8Fe1.6Se2. [A Ricciet *al Phys. Rev.B* **84**, 060511 (2011)] has been detected by a mixed real space and momentum space probe: scanning nano focused X-ray diffraction like in La2CuO4+y [M. Fratini, *et al Nature* **466**, 841 (2010) and [N. Poccia *et al Nature Materials* **10**, 733 (2011)] showing scale free structural organization of dopants favoring in the high T_c phase. The results on KFeSe show phase separation, percolating superconductivity, competing with percolating magnetism and shape resonances in the superconducting gaps.

12:39PM J21.00006 Ordering of dopants and potential increase of Tc to near room temperature, STUART WOLF, University of Virginia, VLADIMIR KRESIN, Lawrence Berkeley Laboratory — This talk will describe a novel method to increase the resistive Tc of cuprate superconductors to values that might approach room temperature, especially if applied to the underdoped region of the Tc versus carrier concentration phase diagram. This is the part of the so-called pseudogap region that exhibits energy gaps and a small Meissner effect well above the maximum resistive transition [1]. The method proposed here involves ordering of the dopants that provide the itinerant holes in the copper oxygen planes. These dopants also act as pair breakers since they are defects in the structure. The strategy we are proposing here is to separate the regions with dopants which provide the itinerant carriers in the cuprate planes from the metallic but dopant free regions nearby, but far enough away to be not seriously affected by the proximity effect. If this separation can be carried out appropriately and we will describe how this will be done in the talk, there will be fully connected high Tc regions that can fully span a sample and present a very high temperature resistive transition, approaching room temperature for some of the cuprates.

[1] V.Z. Kresin and S.A. Wolf, ArXiv 1109.0341

12:51PM J21.00007 Inhomogeneous superconducting state and the intrinsic Tc: Near room temperature superconductivity in the cuprates, VLADIMIR KRESIN, Lawrence Berkeley National Laboratory, STUART WOLF, University of Virginia — Doped cuprates are inhomogeneous superconductors and exhibit properties strongly affected by this inhomogeneity. The notion of an intrinsic critical temperature whose value greatly exceeds the resistive Tc is supported by a number of experimental studies and these will be reviewed in this talk. In particular the anomalous diamagnetism observed above the resistive transition is a manifestation of the presence of superconducting clusters embedded in a normal metallic matrix. The value of intrinsic critical temperature, that reflects the onset of superconductivity in the highest transition temperature clusters, is in some cuprates near room temperature. The transition to the fully superconducting state is percolative in nature and is strongly dependent on the inhomogeneities. Some consequences of such a system, including the ac response will be described.

1:03PM J21.00008 A Kohn Luttinger perspective on topological superconductivity¹, RONNY THOMALE, Stanford University, CHRISTIAN PLATT, WERNER HANKE, Universitaet Wuerzburg — On the basis of an orbital angular momentum and point group symmetry analysis, we argue that electron-driven fluctuations from the viewpoint of a Fermi surface instability generically provide a propensity towards topological superconductivity when the irreducible lattice representations associated with the Cooper pairs are multi-dimensional. For illustration, we explicate our generation recipe of topological superconductivity for the cases of ruthenates, cobaltates, and graphene doped to van Hove filling, i.e. representatives for square, triangular, and honeycomb lattice pairing.

¹Ronny Thomale acknowledges support by the SITP postdoctoral fellowship at Stanford. The authors are supported by DFG-SPP 1458/1.

1:15PM J21.00009 X-ray photoelectron spectroscopy of Single Crystals of intercalated Bismuth Selenide¹, SOMADITYA SEN, JOHN A. DUDEK, University of Wisconsin Milwaukee, WI, YING ZOU, Shanghai Institute of Applied Physics, China, MARY SEVERSON, MARK BISSEN, Synchrotron Radiation Center, Stoughton, WI, PRASENJIT GUPTASARMA², University of Wisconsin Milwaukee, WI — The possibility of superconductivity in topological insulators is likely to yield new physics, especially because the insulating normal state is highly unconventional. However, before moving on to microscopic theory, it is important to characterize and study basic systems available today. Here, we present XPS studies of intercalated single crystals of Bi₂Se₃ and Sb₂Se₃. Core level spectroscopy, combined with infra-red and Raman spectroscopy, yield details of the nature of bonding of atoms at the cleaved surface.

¹Work Supported by AFOSR-MURI

²Author for correspondence: pg@uwm.edu

1:27PM J21.00010 Search for Superconductivity in Single Crystals of Topological Insulators¹, PRASENJIT GUPTASARMA², SOMADITYA SEN, JOHN DUDEK, University of Wisconsin Milwaukee, WI, MARY SEVERSON, MARK BISSEN, Synchrotron Radiation Center, Stoughton, WI — Observation of superconductivity in Cu-intercalated Bi₂Se₃, and in Bi₂Te₃ under pressure, open up the possibility of occurrence of superconductivity in other similarly modified structures. Here, we present detailed studies from a comprehensive search for superconductivity in selenides and tellurides of Bismuth and Antimony. High-quality single crystals were intercalated with a number of different elements using both in situ and ex situ techniques, then scanned for a resistive or magnetic transition to superconductivity. With an intent to understand the nature of intercalation in these compounds, we discuss results from our search for superconductivity, together with crystal structure analysis and detailed optical and x-ray photoelectron spectroscopy studies of the cleaved surface.

¹Work supported by AFOSR-MURI

²Author for correspondence: pg@uwm.edu

1:39PM J21.00011 Surface Andreev Bound States of Topological Superconducting Phase in Doped Semiconductors: Application to Cu_xBi₂Se₃¹, TIMOTHY HSIEH, MIT, LIANG FU, Harvard — The recently discovered superconductor Cu_xBi₂Se₃ is a candidate for three-dimensional time-reversal-invariant topological superconductors, which is predicted to have robust surface Andreev bound states hosting massless Majorana fermions. In this work, we present an analytical and numerical study of the surface Andreev bound state wavefunction and dispersion. We find the topologically protected Majorana fermions at $k = 0$, as well as a new type of surface Andreev bound states at finite k . We relate our results to a recent point-contact spectroscopy experiment.

¹TH is supported by the U.S. DOE under cooperative research agreement Contract Number DE-FG02-05ER41360 and the NSF Graduate Research Fellowship under Grant No. 0645. LF is supported by the Harvard Society of Fellows.

1:51PM J21.00012 Functional renormalization group and variational Monte Carlo studies of the electronic instabilities in graphene near 1/4 doping, FA WANG, Department of Physics, MIT, QIANG-HUA WANG, National Lab of Solid State Microstructures, Nanjing University, China, FAN YANG, Department of Physics, Beijing Institute of Technology, China, DUNG-HAI LEE, Department of Physics, UC Berkeley; Materials Sciences Division, LBNL — We study the electronic instabilities of near 1/4 electron doped graphene using the functional renormalization group (FRG) and variational Monte-Carlo method. A modified FRG implementation is utilized to improve the treatment of the von Hove singularity. At 1/4 doping the system is a chiral spin density wave state exhibiting the anomalous quantized Hall effect, or equivalently a Chern insulator. When the doping drops below 1/4, the $d_{x^2-y^2} + id_{xy}$ Cooper pairing becomes the leading instability. Our results suggest near 1/4 electron- or hole-doped graphene is a fertile playground for the search of Chern insulators and superconductors.

Tuesday, February 28, 2012 11:15AM - 2:15PM –
Session J22 DMP DCOMP: Focus Session: Fe-based Superconductors - Nodal and Nodeless Superconductivity 254B

11:15AM J22.00001 Evolution of symmetry and structure of the gap in Fe-based superconductors with doping and interactions, ANDREY CHUBUKOV, SAURABH MAITI, University of Wisconsin-Madison, MAXIM KORSHUNOV, Russian Academy of Sciences, Siberian branch, THOMAS MAIER, Oak Ridge National Lab., PETER HIRSCHFELD, University of Florida — We present a detailed study of the symmetry and structure of the pairing gap in Fe-based superconductors. We treat them as quasi-2D systems, decompose the pairing interaction into s -wave and d -wave channels and into contributions from scattering between different Fermi surfaces and analyze how each scattering evolves with doping and input parameters. We verify that each interaction is well approximated by the lowest angular harmonics and use this simplification to analyze the interplay between the interaction with and without spin-fluctuation components, the origin of the attraction in the $s\pm$ and $d_{x^2-y^2}$ channels, the competition between them, the nature of angular dependence of the $s\pm$ gaps along the electron Fermi surface, the conditions under which $s\pm$ gap develops nodes, and the origin of superconductivity in heavily electron- or hole-doped systems, when only Fermi surfaces of one type are present. In particular, we find that with increased electron and hole doping, the competition from d -wave grows. In the case of strong hole doping, there is some ambiguity over the leading solution, but in the case of strong electron doping, d -wave emerges as clear winner.

11:27AM J22.00002 Non-Fermi liquid behavior in overdoped iron-pnictides, JOHNPierre PAGLIONE, KEVIN KIRSHENBAUM, SHANTA SAHA, TYLER DRYE, University of Maryland — Electrical transport, magnetic susceptibility and heat capacity data are presented on a series of single-crystal iron-based intermetallic compounds with the ThCr₂Si₂ structure with transition metal substitution used to heavily over-dope the system. We will present observations of unusual temperature dependences in transport, susceptibility and electronic specific heat that indicate an unexpected deviation from Fermi liquid behavior that persists to milliKelvin temperatures.

11:39AM J22.00003 Probing the Superconducting Order Parameter of Co-doped BaFe₂As₂ by Josephson Interferometry¹, JUAN ATKINSON, DALE VAN HARLINGEN, University of Illinois at Urbana-Champaign, PAUL CANFIELD, Ames Laboratory and Iowa State University — We probe the superconducting order parameter in Co-doped BaFe₂As₂ (Ba122) single crystals via measurements of the critical current of Josephson junctions fabricated on polished faces orthogonal to the c-axis. The modulation of the critical current as a function of magnetic flux applied along the c-axis is different for junctions fabricated on different points on a circularly polished face of the Ba122 crystal since each junction probes an effective order parameter of the crystal through an angle in k-space. These modulations map the phase anisotropy and test for the proposed $\pm$ mode pairing symmetry. We will present preliminary results of these studies and compare to existing theoretical models.

¹Work supported by the Department of Energy grant BNL-150252 through the DOE- Energy Frontier Research Center for Emergent Superconductivity.

11:51AM J22.00004 Nodal structure and quantum critical point beneath the superconducting dome of BaFe₂(As_{1-x}P_x)₂, YUJI MATSUDA, Kyoto University — Among BaFe₂As₂ based materials, the isovalent pnictogen substituted system BaFe₂(As_{1-x}P_x)₂ appears to be the most suitable system to discuss many physical properties, because BaFe₂(As_{1-x}P_x)₂ can be grown with very clean and homogeneous, as evidenced by the quantum oscillations observed over a wide doping range even in the superconducting dome giving detailed knowledge on the electronic structure. We investigate the structure of the superconducting order parameter in BaFe₂(As_{0.67}P_{0.33})₂ ($T_c = 31$ K) with line nodes by the angle-resolved thermal conductivity measurements in magnetic field. The experimental results are most consistent with the closed nodal loops located at the flat part of the electron Fermi surface with high Fermi velocity. The doping evolution of the penetration depth indicates that nodal loop is robust against P-doping. Moreover, the magnitude of the zero temperature penetration depth exhibits a sharp peak at $x=0.3$, indicating the presence of a quantum phase transition deep inside the superconducting dome.

This work has been done in collaboration with T. Shibauchi, K. Hashimoto, S. Kasahara, M. Yamashita, T. Terashima, H. Ikeda (Kyoto), A. Carrington (Bristol), K. Cho, R. Prozorov, M. Tanatar (Ames), A.B. Vorontsov (Montana) and I.Vekhter (Louisiana).

12:27PM J22.00005 London penetration depth in single crystals SrFe₂(As_{0.65}P_{0.35})₂, CHARLES P. STREHLOW, K. CHO, M.A. TANATAR, R. PROZOROV, Ames Laboratory, T. KOBAYASHI, S. MIASAKA, S. TAJIMA, Dept. of Physics, Osaka University, Osaka, Japan — In a contrast to a fully-gapped charge-doped (Ba,K)Fe₂As₂ and Ba(Fe,T)₂As₂ [1], isoelectron - substituted BaFe₂(As,P)₂ exhibit nodal superconducting gap [2]. To explore possible universality, low-temperature variation of the London penetration depth, $\Delta\lambda(T)$, was measured in optimally - doped SrFe₂(As_{0.65}P_{0.35})₂ with $T_c=29$ K. $\Delta\lambda(T)$ revealed notable deviations from the exponential temperature dependence, expected for a fully-gapped superconductors. Instead the data are best fit with a power-law function, $\Delta\lambda = AT^n$. The analysis of the data below $1/3T_c$ over a variable fitting temperature range produced exponents $n \leq 2$ which suggests the presence of nodes in the superconducting gap, similar to the P - doped Ba122 compounds.

[1] R. Prozorov and V. G. Kogan, Rep. Prog. Phys. **74**, 124505 (2011).

[2] K. Hashimoto, *et. al.* Phys. Rev. B **81**, 220501(R) (2010).

12:39PM J22.00006 London penetration depth in heavily over-doped Ba(Fe_{1-x}Co_x)₂As₂, JASON MURPHY, H. KIM, M.A. TANATA, A. THALER, P.C. CANFIELD, The Ames Laboratory, U. WELP, W.K. KWOK, Argonne National Laboratory, R. PROZOROV, The Ames Laboratory — The low-temperature variation of London penetration depth, $\Delta\lambda(T)$, has been previously studied in heavily over-doped Ba(Fe_{1-x}Ni_x)₂As₂ [1] and the authors suggested the development of line nodes. Similar conclusion was made from thermal conductivity measurements in Ba(Fe_{1-x}Co_x)₂As₂ [2]. However, $\Delta\lambda(T)$ in this system has only been measured for $x \leq 0.102$ [3], which is not far enough from optimal doping. Here we report tunnel - diode resonator (TDR) measurements in heavily overdoped single crystals of Ba(Fe_{1-x}Co_x)₂As₂ with Co content of $x = 0.108$ ($T_c=14.8$ K) and $x = 0.127$ ($T_c=9$ K). We found a robust power-law behavior of $\Delta\lambda = AT^n$ with $n = 2.5$ and $n = 2.11$ respectively. To test whether the nodes are symmetry imposed or accidental, samples were irradiated with heavy ions. The produced disorder, leads to a decrease in T_c and of the exponent n . These results effects will be discussed in a context of unconventional pairing in Fe-based superconductors.

[1] C. Martin *et. al.*, Phys. Rev. B **81**, 060505 (2010).

[2] J.-Ph. Reid *et. al.*, Phys. Rev. B **82**, 064501 (2010).

[3] R.T. Gordon *et.al.* Phys. Rev. B **82**, 054507 (2010).

12:51PM J22.00007 Specific Heat To H_{c2}: Evidence for Nodes or Deep Minima in the Superconducting Gap of Under- and Overdoped BaFe_{2-x}Co_xAs₂¹, G.R. STEWART, J.S. KIM, Department of Physics, Univ. Florida, Gainesville, FL, K. GOFRYK, F. RONNING, Los Alamos National Laboratory, Los Alamos, NM, A.S. SEFAT, Oak Ridge National Laboratory, Oak Ridge, TN, K.Y. CHOI, K.H. KIM, Department of Physics and Astronomy, Seoul National Univ., Seoul, South Korea — Low temperature specific heat, C , in magnetic fields up to H_{c2} is reported for BaFe_{1.91}Co_{0.09}As₂ (underdoped, H_{c2} $\approx$ 16 T, T_c=8 K), BaFe_{1.79}Co_{0.21}As₂ (overdoped, H_{c2} $\approx$ 27 T, T_c=17 K), and - for comparison - BaFe_{1.95}Ni_{0.05}As₂, which should have properties similar to the underdoped Co-sample. Previous measurements of thermal conductivity (as a function of temperature and field) and penetration depth on comparable composition samples gave some disagreement as to whether there was fully gapped/nodal behavior in the under-/overdoped materials respectively. The present work shows that the measured behavior of the specific heat γ ($\propto C/T$ as $T \rightarrow 0$, i. e. a measure of the electronic density of states at the Fermi energy) as a function of field obeys $\gamma \approx H^{0.6 \pm 0.1}$, similar to the Volovik effect for nodal superconductors, over the entire field range for both under- and overdoped Co samples as well as for the underdoped Ni sample. By comparison to theory, the possibility of two bands, one with line nodes and one fully gapped, being present in these materials is discussed.

¹Work at Florida supported by US DOE, contract no. DE-FG02-86ER45268, at Los Alamos by US DOE and LANL LDRD, at Oak Ridge by US DOE, at Seoul by NCRI grant no. 2010-0018300

1:03PM J22.00008 Nodal versus nodeless order parameters in LiFeP and LiFeAs superconductors, T. SHIBAUCHI, K. HASHIMOTO, S. KASAHARA, R. KATSUMATA, Y. MIZUKAMI, M. YAMASHITA, H. IKEDA, T. TERASHIMA, Y. MATSUDA, Kyoto University, A. CARRINGTON, University of Bristol — There is growing evidence that the superconducting gap structure is not universal in the iron-based superconductors. It is essential to determine experimentally what causes nodal and nodeless states. The 111 materials, LiFeAs and LiFeP provide a unique route to study this problem as both materials are superconducting, nonmagnetic, and importantly very clean, with long electronic mean-free paths. Here we report on high-precision measurements of magnetic penetration depth λ in clean single crystals of LiFeAs and LiFeP superconductors, which reveal contrasting low-energy excitations of quasiparticles. In LiFeAs the low-temperature $\lambda(T)$ shows a flat dependence indicative of a fully gapped state, which is consistent with previous studies. In contrast, LiFeP exhibits a T -linear dependence of superfluid density $\propto \lambda^{-2}$, indicating a nodal superconducting order parameter. A systematic comparison of quasiparticle excitations in the 1111, 122, and 111 families of iron-pnictide superconductors implies that the nodal state is induced when the pnictogen height from the iron plane decreases below a threshold value of ~ 1.33 Å.

1:15PM J22.00009 Inter-Layer Superconducting Pairing Induced c-axis Nodal Lines in Iron-based Superconductors, CHANDAN SETTY, Purdue University, YUEHUA SU, Yantai University, ZIQIANG WANG, Boston College, JIANGPING HU, Purdue University — A layered superconductor with a full pairing energy gap can be driven into a nodal superconducting (SC) state by inter-layer pairing when the SC state becomes more quasi-3D. We propose that this mechanism is responsible for the observed nodal behavior in a class of iron-based SCs. We show that the intra- and inter-layer pairings generally compete and the gap nodes develop on one of the hole Fermi surface pockets as they become larger in the iron-pnictides. Our results provide an explanation of the c-axis gap modulations and gap nodes observed by angle resolved photo emission spectroscopy. In addition, we predict that an anti-correlated c-axis gap modulations on the hole and electron pockets should be observable in the $s\pm$ -wave pairing state.

1:27PM J22.00010 Thermal-transport measurement of the nodal superconductor KFe_2As_2 , MINORU YAMASHITA, DAIKI WATANABE, TAKYUYA YAMASHITA, TAKASADA SHIBAUCHI, YUJI MATSUDA, Department of Physics, Kyoto University, HIDETO FUKAZAWA, TAKU SAITO, YOH KOHORI, Department of Physics, Chiba University, KUNIHIRO KIHIO, AKIRA IYO, HIROSHI EISAKI, AIST, Tsukuba — Hole-doped Fe-based superconductors, $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$, possess two different superconducting gap structures; a fully-gapped state near the optimally doped ($x \sim 0.5$) and a nodal gap state at the hole-dope end ($x = 1$). To investigate the detail gap structure, we performed thermal-transport measurements of KFe_2As_2 with very high purity ($\text{RRR} \sim 1,600$) down to 80 mK. From the temperature dependence of thermal conductivity at zero field, we find a finite residual of κ/T in the zero-temperature limit. This residual increases by magnetic field as $\propto \sqrt{H}$ in low fields, followed by a rapid increase near H_{c2} . Thermal conductivity measurements of different dopes ($x = 0.88, 0.93$) will be reported.

1:39PM J22.00011 Microwave Surface Impedance Measurements of $\text{SrFe}_2(\text{As,P})_2$ Single Crystals, HIDEYUKI TAKAHASHI, YOSHINORI IMAI, ATSUTAKA MAEDA, Department of Basic Science, the University of Tokyo, KENTARO KITAGAWA, KAZUYUKI MATSUBAYASHI, MASASHI TAKIGAWA, YOSHIYA UWATOKO, Institute for Solid State Physics, the University of Tokyo — Various pairing symmetries have been proposed concerning Fe-based superconductors both theoretically and experimentally. It was reported that LaFePO [1] and $\text{BaFe}_2(\text{As,P})_2$ [2] have line nodes in their superconducting gap. It is in sharp contrast to other Fe-based compounds such as LiFeAs [3] and $\text{Fe}(\text{Se,Te})$ [4]. To confirm whether line nodes in gap function is a common feature among P doped systems, we measured the microwave surface impedances of $\text{SrFe}_2(\text{As,P})_2$ single crystals ($T_c \sim 30\text{K}$). Single crystals were grown by self-flux method. The surface impedances were measured using a cavity perturbation technique. The imaginary part of surface impedance, which is proportional to London penetration depth in the superconducting state, shows a power law, $\lambda(T) - \lambda(0) \propto T^n$. The power law indicates low-energy quasiparticle excitation, and an exponent slightly smaller than 2 does not exclude the possibility of the existence of line nodes.

[1] J. D. Fletcher *et al.*, Phys. Rev. Lett. 102 (2009) 147001.
 [2] K. Hashimoto *et al.*, Phys. Rev. B 81 (2010) 220501(R).
 [3] Y. Imai *et al.*, J. Phys. Soc. Jpn. 80 (2011) 013704.
 [4] H. Takahashi *et al.*, Phys. Rev. B 84. (2011) 132503.

1:51PM J22.00012 Doping-induced line nodes in the superconducting gap of the iron arsenide $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ from thermal conductivity, R.T. GORDON, J.-PH. REID, X.G. LUO, H. SHAKERIPOUR, S. RENÉ DE COTRET, A. JUNEAU-FÉCTEAU, N. DOIRON-LEYRAUD, J. CHANG, LOUIS TAILLEFER, University of Sherbrooke, Canada, H. KIM, M.A. TANATAR, R. PROZOROV, Ames Laboratory and Iowa State University, USA, B. SHEN, H.-H. WEN, Nanjing University, China — The thermal conductivity κ of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ was measured down to 50 mK in magnetic fields up to 15 T, for heat current both parallel and perpendicular to the tetragonal c axis, across a range of K concentrations from optimal doping ($T_c = 38\text{K}$) down to $T_c = 7\text{K}$, deep into the region of coexistence with antiferromagnetic order. From optimal doping down to $T_c \simeq 15\text{K}$, well into the coexistence region, there is no residual linear term in $\kappa(T)$ as $T \rightarrow 0$, showing that there are no nodes in the superconducting gap anywhere on the Fermi surface. For concentrations in a narrow range such that $9\text{K} < T_c < 13\text{K}$, a large residual linear term appears, signaling the onset of nodes in the superconducting gap, most likely vertical line nodes running along the c axis. For $T_c < 9\text{K}$, the gap is again nodeless. We propose that these changes in the superconducting gap structure are triggered by changes in the Fermi surface as it is reconstructed by the growing antiferromagnetic order.

2:03PM J22.00013 Evidence for line nodes in the energy gap of overdoped $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$: A low-temperature specific heat study¹, GANG MU, Department of Physics, Graduate School of Science, Tohoku University, Japan, JUN TANG, YOICHI TANABE, JINGTAO XU, World Premier International Research Center, Tohoku University, Japan, SATOSHI HEGURI, Department of Physics, Graduate School of Science, Tohoku University, Japan, KATSUMI TANIGAKI, Department of Physics, Graduate School of Science and World Premier International Research Center, Tohoku University, Japan — We report the low-temperature specific heat (SH) study on $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ single crystals in a wide doping region under different fields. For the overdoped sample, we find the clear evidence for the presence of T^2 term in the electronic SH data, suggesting the presence of line nodes in the energy gap. This term is absent both for the underdoped and optimal doped samples. Moreover, the field induced electronic SH coefficient $\Delta\gamma(H)$ increases more quickly with the field for the overdoped sample than the underdoped and optimal doped ones, showing a large anisotropy of the gap for the overdoped sample. Our results suggest that the energy gap(s) in the present system may have different structures strongly depending on the doping regions.

¹The work is supported by Scientific Research on Priority Areas of New Materials Science Using Regulated Nano Spaces, the MEXT of Japan.

Tuesday, February 28, 2012 11:15AM - 2:15PM —
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11:15AM J23.00001 Phonon dispersions and structural transitions of CrO_2 under high pressure, SOORAN KIM, KYOO KIM, CHANG-JONG KANG, B.I. MIN, POSTECH — Phonon dispersions of chromium dioxide (CrO_2) are calculated to investigate the structural phase transitions as a function of pressure. The structural phase transition has been confirmed from the ground state tetragonal CrO_2 of rutile-type ($t\text{-CrO}_2$) to the orthorhombic CrO_2 of CaCl_2 -type ($o\text{-CrO}_2$). The ferromagnetic and half-metallic property is preserved even in $o\text{-CrO}_2$. The softening of Raman-active B_{1g} phonon mode, which is relevant to the above structural transition, is also obtained. We will discuss the possible more structural phase transitions from $o\text{-CrO}_2$ and the related phonon and magnetic properties at much higher pressure.

11:27AM J23.00002 Optimizing plasmonic properties of supported silver nanocube monolayers¹, ANATOLI IANOUL, ADAM BOTTOMLEY, NUR AHAMAD, Carleton University — The refractive index (RI) sensitivity of extinction spectra was compared experimentally for silver nanocubes in solution and in supported monolayers prepared by the Langmuir technique. The size of the nanocubes, RI of supporting dielectric substrate, and the monolayer surface pressure were used as variables in refractive index sensing (RIS) optimization. The dipolar plasmon modes of the colloidal nanocubes were found to have the highest RIS values of 176, 361 and 480 nm/RI units for 40, 80, and 130 nm cubes respectively. The largest figure of merit (FOM) of 4.55 was measured for a quadrupolar mode of 130 nm nanocubes. When compared to suspensions, RIS of supported nanocubes were reduced by ~50% and decreased with increasing monolayer surface pressure. RIS of 40 nm cube monolayers appeared to be sensitive to the substrate RI due to the RI dependent plasmon mode hybridization resulting in dipolar (D) and quadrupolar (Q) modes. RIS sensitivities of D and Q modes for silicon- supported nanocube monolayer were found to be 78 and 170 nm/RI units respectively. The FOM for the Q mode appeared to be 5.5. Intensity of this Q peak was found to increase with the angle of incident light. This work shows the use of high refractive index dielectric substrates, a passive molecular spacer, and large angles of incidence can significantly improve the detection of plasmonic response by supported nanocube monolayers.

¹NSERC, ERA

11:39AM J23.00003 Isotropic Structural Color of Nanostructured Metal Surfaces, SYLVANUS Y. LEE, Dept of Mechanical Engineering, Boston University, CARLO FORESTIERE, ALYSSA J. PASQUALE, GARY F. WALSH, Dept of Electrical and Computer Engineering, Boston University, MARCO ROMAGNOLI, PhotonIC Corp., LUCA DAL NEGRO, Dept of Electrical and Computer Engineering, Boston University — Engineering angularly insensitive (i.e., isotropic) structural coloration in metals without employing extrinsic materials have been a challenge due to the strong absorption properties of metals in the visible range. In this study, by combining plasmonic resonances of metallic nanoparticles and incoherent light scattering from deterministic arrays with isotropic and diffuse Fourier space, we demonstrate isotropic structural coloration of metal films with spatial uniformity and angular insensitivity. Specifically, we explore the angular scattering properties of aperiodic gold nanoparticle arrays with Pinwheel geometry and their hyperuniform counterpart (Delaunay-triangulated Pinwheel centroid, DTPC). The structures are designed by electromagnetic simulations based on the Coupled Dipole Method in partnership with three dimensional Finite Difference Time Domain modeling of plasmonic resonant nanoparticles on gold films. The experimental characterization is performed by measuring the far-field scattering spectra of the proposed arrays using angle-resolved reflection spectroscopy under white light illumination. The measured radiation diagrams of the fabricated plasmonic arrays demonstrate controllable and isotropic coloration of gold films. The proposed approach can potentially advance plasmonic applications to display, tagging and colorimetric sensing technologies.

11:51AM J23.00004 Ab-initio study of the free liquid Hg surface, LAZARO CALDERIN, Research Computing and Cyberinfrastructure, Penn State, University Park 16802, PA, USA, LUIS E. GONZALEZ, DAVID GONZALEZ, University of Valladolid, Valladolid, Spain — The free surface of liquid Hg at two temperatures (T=300 and 450 K) has been studied by using first principles molecular dynamics simulations. The calculated longitudinal ionic density profile shows an oscillatory shape extending several atomic diameters into the bulk and its wavelength is in good agreement with experiment. The associated self-consistent valence electronic density profile shows much weaker oscillations which are somewhat out of phase with the ionic ones. The calculated X-ray reflectivity shows a marked maximum at a wavevector transfer of $q_z \approx 2.2 \text{ \AA}^{-1}$ whose origin is related to the surface layering. Moreover, it shows a good agreement with the experimental reflectivity data.

12:03PM J23.00005 Noncontact technique for measuring the electrical resistivity and magnetic susceptibility of electrostatically levitated melts¹, G.E. RUSTAN, N.S. SPYRISON, A. KREYSSIG, R. PROZOROV, A.I. GOLDMAN, Iowa State University — Over the last two decades the popularity of levitation methods for studying equilibrium and supercooled melts has increased steadily. Measurements of density, viscosity, surface tension, and atomic structure have become well established. In contrast, measurements of electrical resistivity and magnetic susceptibility of levitated melts have been very limited. To fill this void, we have combined the tunnel diode oscillator (TDO) technique with electrostatic levitation (ESL) to perform inductively coupled measurements on levitated melts. A description of the basic operating principles of the TDO and ESL will be given, as well as a description of the implementation and performance characteristics of this technique. Preliminary measurements of electrical resistivity in the solid and liquid state will be presented for samples of Zr, Si, and Ge, as well as the measurements of ferromagnetic transitions in Fe and Co based alloys.

¹This work is supported by the National Science Foundation under grant DMR-08-17157

12:15PM J23.00006 Orientational ordering of tetrahedral clusters in CaCd_6 alloy, WOOSONG CHOI, Cornell University, MAREK MIHALKOVIC, Slovak Academy of Sciences, CHRIS HENLEY, Cornell University — In icosahedral CaCd quasicrystals and related alloy structures, each icosahedral cluster contains an innermost tetrahedral shell that is loosely coupled with its shell. We extract an effective potential for the pair interaction $V(\Omega, \Omega')$ of the orientations Ω of neighboring clusters, as mediated by the intervening atoms. Using the EAM potentials of Brommer et al., ¹we relax all atoms, with each tetrahedron constrained to a chosen (continuously variable) overall orientation but allowing distortions. Using singular value decomposition, the relaxed energies are represented as $V(\Omega, \Omega') = \sum_j A_j f_j(\Omega) f_j'(\Omega')$ where only a few terms are important and the f_j 's have simple sinusoidal forms (which can be understood physically). We thus obtain a fit with only a few parameters, in place of the 46-parameter fit of Brommer et al¹ based on 12 discrete orientations. By Monte Carlo simulations with the obtained interaction, we determine the pattern of the orientationally ordered state seen experimentally below ~90K, and check the ordering transition previously simulated only in small system sizes¹.

¹Brommer, Gähler, and Mihalković, Phil. Mag. 87, 2671 (2007)

12:27PM J23.00007 Electronic structure of Sr_2IrO_4 and its doped materials measured by angle-resolved photoemission spectroscopy, QIANG WANG, YUE CAO, J.A. WAUGH, S.R. PARK, University of Colorado at Boulder, TONGFEI QI, OLEKSANDR KORNETA, GANG CAO, University of Kentucky, D.S. DESSAU, University of Colorado at Boulder — The electronic structure of iridate Sr_2IrO_4 and its doped materials $\text{Sr}_2\text{Ir}_{1-x}\text{Rh}_x\text{O}_4$ and $(\text{Sr}_x\text{La}_{1-x})_2\text{IrO}_4$ were investigated by angle-resolved photoemission spectroscopy. For Sr_2IrO_4 , which is a $J_{\text{eff}}=1/2$ Mott insulator driven by strong spin-orbit coupling, the dispersion of the predominant Ir 5d bands has been successfully resolved and compared with theoretical calculations. The overall band structure is in line with LDA calculations with strong spin-orbit coupling and moderate electron correlation effects included. The detailed electronic structures of isovalent-doped $\text{Sr}_2\text{Ir}_{1-x}\text{Rh}_x\text{O}_4$ and electron-doped $(\text{Sr}_x\text{La}_{1-x})_2\text{IrO}_4$ are also obtained and compared with the electronic structure of the mother compound. These results help reveal the delicate interplay between charge, spin, orbit, and lattice degrees of freedom in iridates and other correlated electron systems.

12:39PM J23.00008 Electronic Structures of Oxygen-deficient PtO_2 ¹, YONG YANG, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, 305-0047, Japan, OSAMU SUGINO, 1. National Institute for Materials Science; 2. Institute for Solid State Physics, University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa 277-8581, Japan, TAKAHISA OHNO, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, 305-0047, Japan — We studied the electronic properties of beta-platinum dioxide ($\beta\text{-PtO}_2$), a catalytic material, based on density functional theory. Using the GGA+U method whose predicted band gap is verified by GW calculations, we found that the creation of an oxygen vacancy will induce local magnetic moment on the neighboring Pt and O atoms. The magnetism originates not only from the unpaired electrons that occupy the vacancy induced gap state, but also from the itinerant valence electrons. Because of antiferromagnetic (AF) coupling and the localized nature of gap states, the total magnetic moment is zero for charge-neutral state (V_{O}^0) and is $\sim 1 \mu_B$ for singly-charged states ($V_{\text{O}}^{\pm}$). Calculation of grand potential shows that, the three charge states (V_{O}^0 , $V_{\text{O}}^{\pm}$) are of the same stability within a small region, and the negatively charged state (V_{O}^-) is energetically favored within a wide range of the band gap. On this basis we discussed the implication on catalytic behavior.

¹Work is supported by the Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN) at Natl. Institute for Materials Science (NIMS). First-principles calculations were carried out by the supercomputer (SGI Altix) of NIMS.

12:51PM J23.00009 Theory of Non-Fermi Liquids, PATRICK O'BRIEN, Binghamton University — The focus of this project is to understand the simplest model needed to explain the physics of the material FeCrAs. The geometry of the FeCrAs crystal is used to perform crystal field splitting calculations, which in turn indicates a model that we will attempt to use to describe two of the main trends in the experimental data collected for the material. The model that we believe captures the physical character of FeCrAs for the resistivity and heat capacity measurements is the double exchange model. Next, we must find a way to describe an antiferromagnetic transition at 125K.

1:03PM J23.00010 Evolution between metastable strain glass state and stable martensitic phase in TiNi alloy, YUANCHAO JI, XIAOBING REN, National Institute for Materials Science, XIANGDONG DING, Los Alamos National Laboratory — Phase transitions occur when the thermodynamic free energy of one phase is not lowest for varying some external conditions, such as temperature, pressure, and others. However, metastable glass states that falls out of equilibrium may be observed on continued cooling. Some frozen metastable states can be further spontaneously transformed into thermodynamic stable ones. The corresponding inverse process, from low temperature stable phase to glass state then to another high temperature stable phase upon heating, seems proving the glass state like the metastable state like in chemical reactions. Here we report the inverse freezing (strain glass state) does not occur for the first time. The lower temperature B19' martensite directly transforms into the higher temperature B2 parent phase and the strain glass also transforms B2 phase in the heating process, although the glass state is in the intermediate between B2 and B19' phases in the cooling process in TiNi single crystal. Completely different transformation sequence reveals the inverse glass transition is not necessary between two stable phases and helps us further deepen the understanding of glass transition.

[1] X. Ren, et. al., Philos. Mag. A 90, 141(2010).

[2] X. Ren, et. al., MRS Bull. 34, 838(2009).

1:15PM J23.00011 Ab Initio Study of Phase-Change Materials Doped with magnetic Impurities, RICCARDO MAZZARELLO, YAN LI, RWTH Aachen University — Chalcogenide Phase-change materials are of great technological importance due to their ability to undergo reversible and fast transitions between the amorphous and crystalline phases upon heating. Recently, it was shown experimentally that $\text{Ge}_2\text{Sb}_2\text{Te}_5$ doped with Fe atoms exhibits phase-change behavior for low concentrations of Fe and that both the amorphous and the crystalline phases are ferromagnetic at low enough temperatures. Moreover, the two phases were found to have different saturation magnetization. This finding opens up the possibility of exploiting the phase-change behavior for fast magnetic switching in e.g. spintronic devices. We have investigated the structural, electronic and magnetic properties of Fe-doped $\text{Ge}_2\text{Sb}_2\text{Te}_5$ by first-principles simulations based on Density Functional Theory. Both amorphous and crystalline (hexagonal and cubic rocksalt) phases of $\text{Ge}_2\text{Sb}_2\text{Te}_5$ were considered. Our results show that in the amorphous phase, the magnitude of the magnetic moments of the Fe impurities is reduced with respect to the crystalline phases, due to the different local geometries and chemical environments, which explains the experimentally observed magnetic contrast between the two phases.

1:27PM J23.00012 Crystallization Times of $\text{Ge}_2\text{Sb}_2\text{Te}_5$ Nanostructures as a Function of Temperature, FARUK DIRISAGLIK, KADIR CIL, MAREN WENNBORG, ADRIENNE KING, MUSTAFA AKBULUT, University of Connecticut, YU ZHU, CHUNG LAM, IBM T. J. Watson Research Center, ALI GOKIRMAK, HELENA SILVA, University of Connecticut — Phase-change memory is a promising non-volatile memory technology in which a small volume of a phase change material is reversibly and rapidly switched between amorphous and crystalline phases by a suitable electrical pulse. Amorphization is achieved by fast cooling after a melting pulse while crystallization is achieved through electrical breakdown of the amorphous element that leads to heating above the crystallization temperature for a sufficient period. Significant difference between the crystallization behavior of phase-change materials in bulk, thin films and in nanostructures have been observed[1,2]. We have studied the crystallization times of nanoscale $\text{Ge}_2\text{Sb}_2\text{Te}_5$ line structures using 50-500 ns voltage pulses with a baseline offset in the 500 K to 625 K range under high-vacuum. The baseline voltage allows measurement of resistance before and after the pulse and crystallization time. Current and voltage were recorded with high time-resolution for amorphizing pulse and very long periods of time to observe the crystallization time. The crystallization time decreases for increasing temperature but it remains on the order of seconds even at elevated temperatures. [1] H. Wong et al., Proc IEEE 98, 2201, 2010. [2] T. Zhang et al., Scr. Mater. 58, 977, 2008.

1:39PM J23.00013 Electrical Resistivity of Liquid $\text{Ge}_2\text{Sb}_2\text{Te}_5$ in Patterned Nanostructures, KADIR CIL, FARUK DIRISAGLIK, MAREN WENNBORG, ADRIENNE KING, MUSTAFA AKBULUT, University of Connecticut, YU ZHU, CHUNG LAM, IBM T.J. Watson Research Center, HELENA SILVA, ALI GOKIRMAK, University of Connecticut — Phase change memory devices are based on the electrical resistivity contrast between the amorphous and the crystalline phases of chalcogenide materials [1]. Since melting is required to amorphize the material, knowledge of the liquid state properties is critical for device design. $\text{Ge}_2\text{Sb}_2\text{Te}_5$ (GST) is the most studied phase change material. However, the two experimental values reported to date for electrical resistivity of liquid GST (one on a thin film [2], the other in bulk [3]) differ by an order of magnitude. We have extracted the electrical resistivity of liquid GST from single pulse measurements on a large number of encapsulated GST line structures with varying lengths, widths and thicknesses. Each structure is self-heated to melt by the microsecond voltage pulse while voltage and current are monitored using an oscilloscope. The liquid state resistivity is calculated from slopes of liquid state resistance versus $1/\text{width}$, fitted as a function of length. The results we obtained for the liquid resistivity of GST in nanostructures are close to those obtained from measurements on bulk GST [3]. 1. H. Wong et al., Proc IEEE 98, 2201, 2010. 2. T. Kato and K. Tanaka, Jap. J. Appl. Phys. 44, 7340, 2005. 3. R. Endo et al., Jap. J. Appl. Phys. 49, 5802, 2010.

1:51PM J23.00014 3-D Numerical Study of Switching Dynamics in Nanoscale Phase Change Memory Devices¹, IBRAHIM CINAR, GULSEN KOSOGLU, OZGUR BURAK ASLAN, GULEN AKTAS, OZHAN OZATAY, Bogazici University, Department of Physics — Phase change memory (PCM) is currently regarded as a strong candidate technology to replace Flash memory in the market. In this work we report a detailed numerical study of the switching process in a nanoscale PCM cell, namely its switching dynamics during SET (turn on) and RESET (turn off) operations. A comprehensive picture of the electrical, thermal and phase change dynamics is obtained using a multiphysics approach with coupled differential equations in the framework of a three dimensional finite element model. The complexity of the problem was handled by constructing separate submodels; an electrical model which involves a temperature and phase dependent electrical conductivity, a thermal model where the joule heating from the electrical current serves as the heat source and involves temperature and phase dependent thermal conductivity and a phase change model. In this presentation we will concentrate on the electrical and thermal submodels in detail. The results of the phase change model taking into account homogeneous and heterogeneous nucleation kinetics will be discussed in another presentation. We will compare the numerical results with experimental data on GST based nanoscale phase change devices with various contact sizes and shapes.

¹This work has been supported by the European Commission FP7 Marie Curie IRG grant: PCM-256281, Bogazici University Infrastructure Research Fund: 6121, Turkish Academy of Sciences TUBA-GEBIP award.

2:03PM J23.00015 3-D Simulation Model of Phase Change and Percolation in Phase Change Memory¹, OZGUR BURAK ASLAN, IBRAHIM CINAR, GULSEN KOSOGLU, GULEN AKTAS, OZHAN OZATAY, Bogazici University, Department of Physics — Even though phase change memory (PCM) appears as a promising nonvolatile solid state memory with its high signal to noise ratio and superior scalability compared to other memory technologies, the complex nature of the phase change process necessitates advanced numerical modeling to optimize the performance of nanoscale memory cells. The phase change and the percolation processes of a nanoscale PCM cell during SET (turn on) and RESET (turn off) operations have been simulated based on a three dimensional finite element model. A multiphysics approach with coupled differential equations is used to observe and understand the phase change and percolation dynamics. The model to represent the PCM is divided into submodels consisting of an electrical, a thermal and a phase change model that affects nucleation kinetics of crystallites. Coupling the submodels in the framework of the multiphysics approach, this model allows us to predict threshold voltage and recrystallization temperature for switching by detecting the critical conditions for the formation of a conductive percolation path in phase change process. These results will be compared to the experimental results to be carried on. The subject of electrical and thermal model will be mentioned in another presentation.

¹This work has been supported by the European Commission FP7 Marie Curie IRG grant under contract number PCM-256281, Bogazici University Infrastructure Research Fund under contract number 6121 and Turkish Academy of Sciences TUBA-GEBIP award.

Tuesday, February 28, 2012 11:15AM - 2:15PM –

Session J24 DMP: Focus Session: Dopants and Defects in Semiconductors - Si and III-V 256

11:15AM J24.00001 Dislocation nucleation in Si – effect of Ge and vacancies, ZHI LI, CATALIN PICU, Rensselaer Polytechnic Institute — The presence of dislocations in Si devices is detrimental for their function. However, dislocations may nucleate during device processing from interfaces and from imperfections of the surface. In this work we study the conditions under which this may take place. Specifically, the activation energy for dislocation nucleation in pure Si is evaluated using an atomistic model and considering a corner stress concentrator. At lower temperatures, 60° dislocations nucleate in the shuffle set as half-hexagonal loops. The activation energy depends on the step height and on the spacing between steps. The effect of Ge on nucleation is evaluated using the same model and it is observed that the energy barrier decreases slightly in presence of these substitutional atoms. The presence of vacancies in the glide plane also decreases the activation energy. A low concentration of vacancies (0.5%) decreases the barrier for nucleation similarly with a large concentration of Ge (30%).

11:27AM J24.00002 Surface Charge Distribution on Hydrogen-Passivated Silicon Measured by UHV Kelvin Probe Microscopy, PAVEL NAGORNYKH, KRISTEN BURSON, WILLIAM CULLEN, BRUCE KANE, University of Maryland — A few years ago hydrogen-passivated silicon (H:Si) surfaces were used to observe high-mobility in FETs (100,000 cm²/Vs) [1]. This result is expected since chemical passivation of silicon produces an atomically flat surface with low density of defects. As chemical preparation can lead to creation of fixed charges on H:Si surface, one needs a method to get information about their distribution to further improve the quality of a process. This can be done by measuring electrostatic forces created by such charges with Kelvin Probe Microscopy (KPM), which obtains a voltage distribution map with a resolution of a few nm. We have used UHV KPM for our measurements, since UHV conditions are important for avoiding oxidation of H:Si surface as well as achieving its further depassivation/annealing. By annealing samples above depassivation temperature (500C), we have obtained data that provides more information about depassivation effect on charges that come from chemical residue on hydrogen and silicon itself. Preliminary results show standard deviations of voltage much smaller (by an order of magnitude) than ones measured previously on silicon oxide, consistent with high quality expected from chemical preparation.

[1] Robert N. McFarland et al., Phys. Rev. B 80, 161310(R) (2009)

11:39AM J24.00003 Magnetic resonance characterization of silicon nanowires¹, MARCO FANCIULLI, Department of Material Science, University of Milano-Bicocca, Italy and MDM Laboratory, IMM-CNR, Agrate Brianza, Italy, MATTEO BELLI, ANTONIO VELLEI, MDM Laboratory, IMM-CNR, Agrate Brianza, Italy, CARMEN CANEVALI, DAVIDE ROTTA, STEFANO PALEARI, MARTINA BASINI, Department of Material Science, University of Milano-Bicocca, Italy — Silicon nanowires (SiNWs) have been extensively investigated in the last decades. The interest in these nanostructures stems from both fundamental and applied research motivations. The functional properties of one- and zero-dimensional silicon structures are significantly different, at least below a certain critical dimension, from those well known in the bulk. The key and peculiar functional properties of SiNWs find applications in nanoelectronics, classical and quantum information processing and storage, optoelectronics, photovoltaics, thermoelectric, battery technology, nano-biotechnology, and neuroelectronics. We report our work on the characterization by continuous wave (CW) and pulse electron spin resonance (CW, FT-EPR) and electrically detected magnetic resonance (EDMR) measurements of silicon nanowires (SiNWs) produced by different top-down processes. SiNWs were fabricated starting from SOI wafers using standard e-beam lithography and anisotropic wet etching or by metal-assisted chemical etching. Further oxidation was used to reduce the wire cross section. Different EDMR implementations were used to address the electronic wave function of donors (P, As) and to characterize point defects at the SiNWs/SiO₂ interface.

¹The support of Fondazione Cariplo, ELIOS Project is acknowledged.

11:51AM J24.00004 Ab initio study of confinement effects and hyperfine structure in chalcogen doped Silicon nanostructures¹, ALBERTO DEBERNARDI, CNR-IMM, MDM laboratory Agrate Brianza, GUIDO PETRETTO, ANDREA MASSE, MARCO FANCIULLI, CNR-IMM, MDM laboratory Agrate Brianza, University Milano-Bicocca — In recent years, increasing interest has been focused on Si nanostructures as building blocks for ultra-scaled electronic devices where quantum mechanic effects are relevant. We have investigated the atomic and electronic structures of a single chalcogen donor in H passivated Si nanostructures of different size by means of the plane-wave pseudopotential techniques we used in Ref. [1] to study Se doped Si (001) nanowires (NW). Our results showed an increase in the gap with diminishing diameter of Si NW. We studied the size dependence of electronic properties and hyperfine constant of single substitutive chalcogen impurity in Si-NWs (001) and (111) oriented, and Si-dots and their dependence on the distance from the NW axis or the centre of the dot. We show that the hyperfine parameters are strongly dependent on the impurity position: we proved that surface effects can lead to strong differences in the hyperfine parameters depending on the chalcogen location inside the nanowire, suggesting a way to determine experimentally the position of the defect on the basis of electron paramagnetic resonance spectra. Preliminary results on chalcogen doped Ge nanowires complete the work. [1] G. Petretto, A. Debernardi, and M. Fanciulli, Nano Letters, Vol. 11, 4509 (2011).

¹We acknowledge Fondazione CARIPLO for financial support and CASPUR for computational resources partially provided within the CISNA project

12:03PM J24.00005 Segregation and diffusion of boron dopants in the Si/SiO₂ interface, YOUNG JUN OH, HYEON-KYUN NOH, GEUN-MYUNG KIM, K.J. CHANG, Department of Physics, Korea Advanced Institute of Science and Technology — Boron dopants in metal-oxide-semiconductor field-effect transistors exhibit very peculiar behavior such as transient enhanced diffusion, clustering, and segregation. Especially, B segregation to the Si/SiO₂ interface significantly affects the dopant distribution and thereby the device performance. However, there is a lack of studies on the mechanism for B segregation and diffusion in the Si/SiO₂ interface. In this work, we perform first-principles density-functional calculations to understand how B dopants diffuse and segregate to SiO₂. We generate two Si/SiO₂ interface structures, in which crystalline alpha-quartz and amorphous SiO₂ are placed on Si. Among various B configurations, we find that an interstitial B is energetically more favorable in the oxide, compared with a substitutional B and a self-interstitial-B complex in Si. We examine the effect of point defects such as a floating bond and an oxygen vacancy in SiO₂ on B segregation and also investigate B diffusion pathways across the Si/SiO₂ interface.

12:15PM J24.00006 Hybrid functional calculations for native defects and dangling bonds in α -Al₂O₃¹, MINSEOK CHOI, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — Al₂O₃ is a promising material for use as a gate dielectric in III-V-based MOS devices, including in GaN-based transistors. Recent developments indicate that despite the relatively high structural quality, the presence of charge traps and fixed-charge centers near the interface between the oxide and nitride still poses serious problems for device performance. Native defects and dangling bonds in the Al₂O₃ dielectric or in the vicinity of the interface are the most likely causes. To aid in the identification of these centers, we perform density functional calculations with a hybrid functional for point defects and dangling bonds in α -Al₂O₃. We determine the position of the defect transition levels in the gap of the oxide, and analyze the level positions with respect to the nitride band edges. Our results show that O vacancies and Al dangling-bonds can produce charge traps and Al interstitials act as fixed charges in GaN-based *n*-MOSFETs.

¹This work was supported by the ONR DEFINE MURI program

12:27PM J24.00007 Role of oxygen-related defects in hafnia¹, MANISH JAIN, Department of Physics, University of California, Berkeley and Lawrence Berkeley National Laboratory, JAMES R. CHELIKOWSKY, University of Texas, Austin, STEVEN G. LOUIE, Department of Physics, University of California, Berkeley and Lawrence Berkeley National Laboratory — Hafnia has recently received much attention because of its potential application as high-k dielectric material replacing silica in microelectronic devices. Point defects in hafnia - in particular oxygen vacancies and interstitials - can play an important role as traps or sources of fixed charge. In this study, we perform electronic structure calculations on oxygen-related defects in monoclinic hafnia using a combined density functional theory (DFT) and GW formalism. We have previously shown that upon including quasiparticle defect levels and the appropriate electrostatic corrections within a supercell calculation, this formalism corrects for the error in calculating formation energy and charge transition levels using standard DFT. In this study, we calculate the formation energy of these defects as a function of the Fermi level and the chemical potential of oxygen to determine which of these defects are most stable.

¹This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231 and DE-SC0001878. Computational resources have been provided by NSF through TeraGrid resources at NICS.

12:39PM J24.00008 Vibrational spectroscopy of cast Si used to fabricate solar cells: microscopic properties of nitrogen and oxygen impurities¹, HAOXIANG ZHANG, MICHAEL STAVOLA, Lehigh University, MIKE SEACRIST, MEMC Electronic Materials — Cast Si with grain sizes from a few mm to a few cm is commonly used for the fabrication of solar cells. Nitrogen impurities are introduced into cast Si by the SiNx coating of the crucible used for casting. Much is known about N and O centers in single-crystal Si used in microelectronics [1]. We have used vibrational spectroscopy to probe the concentration and defect configurations of nitrogen centers in cast Si used to fabricate solar cells. The interaction of N with O impurities that are present has also been investigated. The dominant N center in cast Si is a N-N interstitial pair. N-O complexes are also formed. Which defect complexes are present depends on the impurity content of the multi-crystalline Si sample, which can vary widely, and its thermal history. [1] H. Ch. Alt and H. E. Wagner, J. Appl. Phys. **106**, 103511 (2009) and the references contained therein..

¹Supported by the Silicon Solar Research Center SiSoC Members through NCSU Subaward No. 2008-0519-02 and NSF Grant DMR 0802278

12:51PM J24.00009 The chemical trends of a new defect cluster: DDX centers, JIE MA, SU-HUAI WEI, national renewable energy laboratory — DX center is a major “killer” defect limiting n-type doping in group II-VI and III-V semiconductors. It converts a shallow donor to deep one, which is a major reason for the saturation of free-electron carriers in the doping process. Several structure models of isolated DX centers have been proposed in the literatures, such as the broken-bond model (BB-DX), and the α and β cation-cation bond model (CCB-DX). All these DX centers can be stabilized with hydrostatic pressure or reduced dimensionality and size. In group III-V and II-VI semiconductors, it has been common believe that cation-site induced DX centers are easier to form than anion-site induced ones. Because DX centers trap an extra electron, therefore, another defect in the system must donate the electron and form a positive charged defect. We show, using GaAs as an example, that in heavily doped semiconductor, the negative charged DX center and positive charged donor can couple strongly through the Coulomb interaction, forming the dominant DDX center. The DDX centers are still deep level defects. However, unlike the DX center, the DDX centers have different chemical trends, i.e., anion-site DDX center is easier to form than cation-site DDX centers. A simple model is proposed to explain the new trends.

1:03PM J24.00010 Valence state manipulation of single Fe impurities in GaAs, PAUL KOENRAAD, JUANITA BOCQUEL, Eindhoven University of Technology, VICTORIA KORTAN, MICHAEL FLATTE, University of Iowa, RICHARD CAMPION, BRYAN GALLAGHER, University of Nottingham — Cross-sectional STM was used to characterize Fe doped GaAs. We show that, by controlling the tip-induced band bending, Fe atoms can be brought from their isoelectronic state (Fe^{3+})-3d5 state into their (Fe^{2+})-3d6 ionized acceptor state. This STM-induced valence manipulation that involves the (de)population of the d-shell of the Fe atom differs from our previous experiments on Mn-acceptors and Si-donors where we changed its charge state by adding or removing a valence band hole or a conduction band electron respectively that is bound by the impurity. In addition for specific tunneling conditions a peculiar contrast is observed under which Fe atoms appear as dark anisotropic features.

1:15PM J24.00011 Local Environment Effects on Single Zn and Mn Acceptors in Gallium Arsenide, NANCY SANTAGATA, DONGHUN LEE, JAY GUPTA, The Ohio State University — The ability to precisely control the properties of single dopants in semiconductors is of interest not only for the improvement of current technologies but also for the development of next generation devices. Recent work in our group has exploited the single atom precision afforded by a scanning tunneling microscope to explore how the properties of dopants in gallium arsenide depend on their local environment. Specifically, we have shown that Zn dopants located within the same layer and occupying identical binding sites exhibit dissimilarities that are dependent upon the proximity to neighboring subsurface Zn acceptors.(1) Further, we demonstrated control of the ionization state of single Mn acceptors by both defect- and tip-induced band bending.(2) Finally, we achieved tunable control over the binding energy of Mn acceptors by varying the proximity to charged As vacancies.(3) This talk will review these findings and elaborate on the application of these techniques to characterize defects in wide bandgap materials, where the origin of properties like ferromagnetism are not yet well understood. 1. Appl. Phys. Lett. 99, 053124 (2011). 2. Nano Lett. 11, 2004 (2011). 3. Science 330, 6012 (2010).

1:27PM J24.00012 Recombination dynamics of excitons bound to nitrogen isoelectronic centers in GaAs, PHILIPPE ST-JEAN, GABRIEL ÉTHIER-MAJCHER, École Polytechnique de Montréal, JOHN F. KLEM, Sandia National Laboratories, SÉBASTIEN FRANCOEUR, École Polytechnique de Montréal — Using time-resolved photoluminescence, we have studied the radiative recombination dynamics of excitons bound to single nitrogen dyads in GaAs. For in-plane dyads of C_{2v} symmetry considered in this work, the lifetime of all four allowed optical transitions, polarized either along or perpendicular to the dyad, decreases with temperature. Over the temperature range studied, the lifetimes of transitions of same polarization remain highly similar, but they are sensitively longer for transitions polarized along the dyad. These results indicate that 1) the spatial orientation of the exciton wavefunction is an important factor in the recombination dynamic, 2) the transfer dynamics between bright states appears negligible, and 3) the transfer to or from dark states is not significant for temperature over 5 K. These findings enhance the understandings of isoelectronic centers which are promising candidates for the implementation of atomic size memories based on a single charge or spin.

1:39PM J24.00013 First-principles study of InX (X=P,Sb) semiconductors, OSCAR D. RESTREPO, ROHAN MISHRA, WOLFGANG WINDL, The Ohio State University — III-V semiconductors are gaining increasing interest for applications due to the possibility of engineering their electronic properties by choosing and combining different elements. Additional design parameters can come from confinement effects which have led to intensified research on nanowires for electronic applications. Among the lesser studied III-V semiconductors with large technological potential are indium-based compounds, where InSb with an extremely small band gap in the infrared range is the staple material for infrared detector devices and InP (with a larger band gap of 1.42 eV) is considered as a promising material for nanowire-based applications. For these materials, many basic questions that have been answered for more-mainstream semiconductors are still unanswered, these include effective masses, optical properties, and the influence of defects on their properties. In order to address some of these questions, we have performed an exhaustive exploration of the defect energetics of InP using first-principles calculations. We also report a detailed comparison of calculated effective masses and optical properties of InSb with experiments. We have used both GGA and HSE06 to treat exchange-correlations. This work was supported by NSF MRSEC DMR-0820414.

1:51PM J24.00014 Simple intrinsic defects in GaP and InP, PETER A. SCHULTZ, Sandia National Laboratories, Albuquerque, NM — To faithfully simulate evolution of defect chemistry and electrical response in irradiated semiconductor devices requires accurate defect reaction energies and energy levels. In III-Vs, good data is scarce, theory hampered by band gap and supercell problems. I apply density functional theory (DFT) to intrinsic defects in GaP and InP, predicting stable charge states, ground state configurations, defect energy levels, and identifying mobile species. The SeqQuest calculations incorporate rigorous charge boundary conditions removing supercell artifacts, demonstrated converged to the infinite limit. Computed defect levels are not limited by a band gap problem, despite Kohn-Sham gaps much smaller than the experimental gap. As in GaAs, [P.A. Schultz and O.A. von Lilienfeld, Modeling Simul. Mater. Sci. Eng. 17, 084007 (2009)], defects in GaP and InP exhibit great complexity—multitudes of charge states, bistabilities, and negative U systems—but show similarities to each other (and to GaAs). Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

2:03PM J24.00015 Defects in GaSb and InAs/GaSb superlattices¹, JIANWEI WANG, YONG ZHANG, Electrical and Computer Engineering, University of North Carolina at Charlotte — Unintentionally doped GaSb is known to be p-type. One possible explanation for the p-type conductivity is due to the existence of Ga on Sb anti-site defects that behave as acceptors. Such an acceptor-like defect state could potentially impact the performance of an IR detector based on a type II superlattice InAs/GaSb. We use pseudopotential density functional theory to investigate this defect state in both bulk GaSb and the superlattice. We calculate the defect levels with and without spin-orbit interaction and with the p-d band separation and bandgaps corrected. Although the defect might be acceptor-like, its energy level does not necessarily follow the GaSb band edge that is shifted in the superlattice due to quantum confinement.

¹Work supported by ARO-MURI

Tuesday, February 28, 2012 11:15AM - 2:15PM —

Session J25 DCOMP GSCCM DMP: Focus Session: Simulation of Matter at Extreme Conditions: Shock Compression and Other High-Strain-Rate Phenomena 257A

11:15AM J25.00001 Single two-zone elastic-plastic shock waves in solids, VASILY ZHAKHOVSKY, MIKALAI BUDZEVICH, University of South Florida, NAIL INOGAMOV, Landau Institute for Theoretical Physics, Russian Academy of Sciences, IVAN OLEYNIK, University of South Florida, CARTER WHITE, Naval Research Laboratory — A new regime of shock wave propagation in solids, corresponding to a single two-zone elastic-plastic shock-wave, was discovered using a novel moving window molecular dynamics technique. Both leading low-pressure elastic and trailing high-pressure plastic fronts move with the same speed and have a fixed separation that can extend to several microns. The material in the elastic zone is in a metastable state, having a pressure that substantially exceeds the critical shock strength characteristic of the onset of the well-known split-elastic-plastic, two-wave regime. The single two-zone elastic-plastic shock wave is a quite general phenomenon observed in our simulations for a broad class of crystalline materials, including aluminum, nickel, diamond, and Lennard-Jones crystals. It is the existence of the two-zone, elastic-plastic regime that allows for a consistent explanation of the anomalously high elastic wave amplitudes observed in recent experiments.

11:27AM J25.00002 The Role of Shock Induced Defect Structure in Spall Failure, JUSTIN WILKERSON, K.T. RAMESH, The Johns Hopkins University — Spall failure is a complex multiscale, multirate process. On the macroscale the process involves a period of shock compression followed by dynamic tension set up by the stress wave interactions. During the shock compression, the material undergoes a myriad of shock stress magnitude and pulse duration dependent microscopic processes that may include dislocation multiplication, nucleation, trapping, pile-up, annihilation, recovery, cell evolution, as well as vacancy generation and clustering. In addition to shock hardening the material, this new shock induced defect structure seeds the material with potential void nucleation sites that may be activated during the proceeding period of dynamic tensile loading. Upon nucleation, the voids undergo dynamic growth to coalescence, constrained by inertia and viscoplastic resistance to deformation. A multiscale predictive framework is developed to analyze the role of these time-dependent processes in the experimentally observed spall strength dependence on initial microstructure, preheated temperature, tensile loading rate, pulse duration, and shock stress magnitude.

11:39AM J25.00003 Physics of hyper-velocity impacts of micrometer and sub-micrometer sized particles, ANNA MOCKER, IRS, University of Stuttgart, Germany, KLAUS HORNUNG, Universitaet der Bundeswehr Muenchen, Germany, ZOLTAN STERNOVSKY, KEITH DRAKE, SASCHA KEMPF, CCLDAS, University of Colorado at Boulder, EBERHARD GRÜN, MPI-K, Heidelberg, Germany, FIEGE FIEGE, University of Heidelberg, Germany, RALF SRAMA, IRS, University of Stuttgart, Germany — The phenomena occurring during hypervelocity microparticle impact are manifold and the basis for the variety of applications. The processes of interest are particle fragmentation, impact ionization, impact flashes, and TOF mass spectrometry. To relate the parameters of individual particle impacts with the resulting measured values, a comprehensive program of impact experiments under well known experimental conditions for a wide variety of impact parameters is needed. For this, dust particles are accelerated to hypervelocity speeds with an electrostatic accelerator and the resulting plasma cloud is analyzed with suitable instruments. A detailed investigation using latest analyzing techniques like high-speed cameras and sensitive high-resolution spectrometers promises new instrument concepts and insights into short timescale high-pressure states of matter. Linear TOF mass spectroscopy provides the opportunity to measure the dynamic and thermodynamic properties of the impact ions. Together with a deeper theoretical understanding of the impact process and the subsequent expansion and other experimental approaches, this method can be a powerful tool to investigate the state of the hot compressed matter due to the related residual ion species.

11:51AM J25.00004 Shock Ejecta Entrainment in Gas¹, MICHAEL FURNISH, Sandia National Laboratories — In a continuation of earlier work, paired metal shock ejecta experiments, with and without helium fill, are used to measure shock ejecta motion in gas. The vacuum ejecta experiments use Asay foils and PDV to characterize ejecta properties, and the gas ejecta experiments use PDV. FFT analysis of the PDV signals gives a qualitative indication of the presence of such ejecta and of its motion; this can be “calibrated” via the Asay foil data. For modest amounts of ejecta (allowing enough light to reach the free surface and return to the probe to give a strong free surface velocity signal), the FFT amplitudes are roughly proportional to the ejecta areal density, where the proportionality constant depends on the shape and size distribution of the ejecta particles. We assume these are consistent for the two samples in each experiment pair, although limitations to this assumption (e.g. ejecta disruption by the gas) are discussed. An additional caveat is that PDV only measures the motion of ejecta with particle sizes exceeding the 1550 nm light wavelength. Experiments to assess optimal generators of shock ejecta detectable by PDV are also presented. Indium was found to work well in the pressure regime studied.

¹Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

12:03PM J25.00005 Why nano-projectiles work differently than macro-impactors- role of plastic flow¹, E.M. BRINGA, CONICET and Instituto de Ciencias Basicas, Universidad Nacional de Cuyo, Mendoza, 5500 Argentina, CHRISTIAN ANDERS, GEROLF ZIEGENHAIN, Fachbereich Physik und Forschungszentrum OPTIMAS, Universitat Kaiserslautern, Germany, GILES GRAHAM, Mineralogy Department, The Natural History Museum, London SW7 5BD, United Kingdom, J. FREDDY HANSEN, Lawrence Livermore National Laboratory, Livermore CA 94550, USA, NIGEL PARK, AWE, Plc Aldermaston, Reading, UK, NICK TESLICH, Lawrence Livermore National Laboratory, Livermore CA 94550, USA, HERBERT URBASSEK, Fachbereich Physik und Forschungszentrum OPTIMAS, Universitat Kaiserslautern, Germany — Hypervelocity impacts provide a way to take localized regions of a target to extreme pressure and temperature conditions. Resulting crater features can be challenging for hydrocode simulations and test the validity of constitutive models. We will present atomistic simulation data on crater formation due to hypervelocity impact of nanoprojectiles of up to 55 nm diameter and with targets containing up to ten billion atoms, and compare them to available experimental data on micron-, mm-, and cm-sized projectiles. We show that previous scaling laws do not hold in the nano-regime and outline the reasons: within our simulations we observe that the cratering mechanism changes, going from the smallest to the largest simulated scales, from an evaporative regime to a regime where melt and plastic flow dominate, as it is expected in larger micro-scale experiments. The importance of strain-rate dependence of strength and of dislocation production and motion under these extreme conditions will be discussed.

¹E.B. thanks support from PICT2009-0092

12:15PM J25.00006 Elastic-plastic response and polymorphic phase transition in shock-compressed diamond, YOU LIN, ROMAIN PERRIOT, VASILY ZHAKHOVSKY, Department of Physics, University of South Florida, XIANG GU, Department of Applied Physics, Aalto University, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, Department of Physics, University of South Florida — Shock wave propagation in diamond along the $\langle 110 \rangle$ crystallographic direction was simulated by molecular dynamics (MD) using the reactive empirical bond order (REBO) potential. In addition to known regimes of shock wave propagation, such as single elastic, split elastic-plastic, and single plastic shock wave, two new regimes were observed: 1) a split elastic-elastic shock wave associated with a polymorphic phase transition; 2) a single two-zone elastic-plastic shock wave with the leading elastic zone followed by the plastic zone. In the case of the split elastic-elastic shock wave, the onset of phase transition occurs at a pressure below the Hugoniot elastic limit (HEL); therefore, the solid-solid transformation takes place in the uniaxially compressed material in the absence of plasticity. Within the single two-zone elastic-plastic shock wave, the material in the elastic zone is in a metastable state at a pressure exceeding the HEL. The metastable elastic state decays into the plastic state within the plastic zone, both elastic and plastic fronts moving with the same speed.

12:27PM J25.00007 ABSTRACT WITHDRAWN —

12:39PM J25.00008 The Shock Response of Granular and Consolidated Ta₂O₅¹, TRACY VOGLER, SETH ROOT, WILLIAM REINHART, Sandia National Laboratories, GREGG FENTON, DENNIS GRADY, Applied Research Associates — The dynamic behavior of granular and nearly fully dense tantalum pentoxide (Ta₂O₅) has been explored through planar impact experiments. The experiments span from the compaction regime to the ultra-high pressure range utilizing gas guns and the Z machine. These data provide a valuable data set for the extension of the P- λ model to the high-pressure regime. A thermodynamic approach due to Rice and Walsh is employed in the model to treat highly distended materials that can display anomalous compressibility. When the model is calibrated to the gas gun and Z data, we test its applicability against the data of Miller et al. from laser experiment on low-density aerogels. Even in these very different conditions, the model does a credible job of predicting the material behavior, suggesting that the approach may be useful as a general modeling tool for the high-pressure regime.

¹Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

12:51PM J25.00009 Optical emission from $\text{Gd}_3\text{Ga}_5\text{O}_{12}$ single crystals shock compressed from 40 to 300 GPa, XIANMING ZHOU, National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, China, WILLIAMS NELLIS, Physics Department, Harvard University, JIABO LI, JUN LI, XUN LIU, XIUXIA CAO, WANGUANG ZHAO, QIANG WU, National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, China, TSUTOMU MASHIMO, Shock Wave and Condensed Matter Research Center, Kumamoto University, CAEP, PR CHINA TEAM, HARVARD UNIVERSITY COLLABORATION, KUMAMOTO UNIVERSITY COLLABORATION — The question of the shock pressure at which a strong material reaches thermal equilibrium is an important one that depends on strength and has never been answered for any strong material. To answer the range of shock pressures in which shock dissipation is dominated by entropy (damage and disorder) or by shock heating (T), we have performed time-resolved optical emission and transmission measurements on strong GGG single crystals under wide-range uniaxial compression from ~ 40 GPa to ~ 300 GPa with a sixteen-wavelength pyrometer. Temperatures T and emissivities ϵ were derived from gray-body fits up to 300 GPa. These data: (i) determine shock pressures at which GGG reaches thermal equilibrium and melting, (ii) essentially confirm previously calculated shock temperatures of GGG, (iii) demonstrate the complete transition from heterogeneous shock heating at lower pressures (small ϵ) to thermally-equilibrated bulk heating (large ϵ) at higher pressure (never before been done in strong materials), and (iv) characterize GGG as an anvil for use in studying metallic fluid hydrogen.

1:03PM J25.00010 Laser-driven focusing shock waves in a thin liquid layer¹, DAVID VEYSSET, THOMAS PEZERIL, GAGAN SAINI, STEVEN KOOI, ALEX MAZNEV, KEITH NELSON, Massachusetts Institute of Technology — Direct real-time visualization of converging shock waves in a few micron thick liquid layer is demonstrated in an all-optical experiment. The set-up includes an axicon that focuses an intense picosecond excitation pulse into a ring-shaped pattern in a water layer. Optical excitation induces a shock wave that propagates in the plane of the sample and converges toward the center resulting in cylindrical focusing of the shock front. Streak-camera images with a quasi-cw probe beam yield real-time records of the entire shock propagation. Talbot imaging and interferometry with a femtosecond probe pulse are used to obtain full field images at variable delays. Shock pressure values calculated from the velocity of the shock front demonstrate the effect of shock focusing and agree with density profiles obtained by quantitative analysis of interferometric images. The configuration of the experiment provides ample access for optical diagnostics of the shocked material and can be combined with a wide range of spectroscopic probes.

¹This work was supported by the U.S. Army Research Office through the Institute for Soldier Nanotechnologies, Grant DAAD19-02-D-0002.

1:15PM J25.00011 From fingering to fracture in a complex fluid, BAUDOUIN SAINTYVES, CEA-Saclay — We present a novel experiment – a specific Hele-Shaw cell with mobile sides which can be pulled at a prescribed velocity - with which both liquids and solids can be loaded with the same boundary conditions, beyond the small deformation regime. With such a system, one can examine quantitatively the response of a viscoelastic material when the loading rate is varied. In the case of viscous Newtonian liquids, an air bubble is shown to destabilize in a Saffman-Taylor manner, forming a finger which elongates in the direction in which the mobile sides are pulled. In contrast, in a Maxwell liquid, we observe a different kind of instability, which gives rise to more complex patterns. This instability leading to local stress concentrations, it is immediately followed by fracture. The displacement field is evaluated in each case by using tracers and image correlations.

1:27PM J25.00012 Nonlinear Elasticity as a Guide for Exploring High Pressure/Shear Stability, T.W. WRIGHT, Johns Hopkins University — Recent constitutive representation theorems for nonlinear anisotropic elasticity, Wright [2011], show the characteristics of elastic response for materials in any point group. All anisotropic representations consist of a sum of six terms, and each term consists of a scalar function of anisotropic invariants times a “tensor generator,” which has the same invariance under group transformations as the stress itself. Knowledge of these representations shows promise as a guide for exploring material stability under extreme loading conditions. Although much is known both experimentally and theoretically about material stability under high pressure, far less is known about the effect of large shear stress superimposed on high pressure. Stress has six independent components, so study of the effects of pressure alone leaves the other five dimensions unexplored. Rather than random DFT calculations in the five dimensional deviatoric space, the known structure of the six term representations suggests that systematic study of just one additional dimension at a time could be accomplished by following changes in just one additional term in the representation at a time. These ideas will be illustrated in the context of a program designed to explore the effect of shear on amorphization in B4C, a ceramic often used for ballistic protection. *T.W. Wright, Bootstrap elasticity: From linear to nonlinear constitutive representations, accepted for publication, J. Elasticity.*

1:39PM J25.00013 Multi million-to-Billion Atom Molecular Dynamics Simulations of Cavitation-Induced Damage on a Silica Slab, ADARSH SHEKHAR, KEN-ICHI NOMURA, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, Collaboratory for Advanced Computing and Simulations, University of Southern California — Cavitation bubble collapse causes severe damage to materials. For example, cavitation erosion is a major threat to the safety of nuclear power plants. The cavitation bubbles may also be utilized for preventing stress corrosion cracking with water jet peening technology. We have performed multi million-to-billion atoms molecular dynamics simulations to investigate the shock-induced cavitation damage mechanism on an amorphous silica slab in water. The system consists of a 60nm thick silica slab immersed in water in an MD box of dimension $285 \times 200 \times 200$ nm³. A nanobubble is created by removing water molecules within a sphere of radius 100 nm. To apply a planar shock, we assign a uniform particle velocity v_p on the entire system towards a planar momentum mirror. We have performed the simulation with two kinds of bubbles, an empty bubble and a bubble filled with inert gas. The simulation results reveal nanojet formation during bubble collapse causing damage on the silica surface; however, the damage was significantly reduced in the case of the filled bubble. We will discuss the effect of the presence of inter gas inside the nanobubble on the pressure distribution, the extent of damage, and collapse behavior corresponding the shock front.

1:51PM J25.00014 Akrology; the physics of the extreme behaviour of metals and energetics, NEIL BOURNE, AWE — Structures designed for extreme environments must be designed not only for the magnitude of the load that they will experience, but also the time for which that load acts upon them. At the core of the problem lies the loading impulse experienced by materials and the operating deformation mechanisms that are excited. Our experience of materials' physics, gathered by investigating response to mechanical loads, has suggested a series of descriptive constructs within which we build our picture of behaviour. At the highest loadings and the shortest loading times this perception is coloured by experience gathered from historical considerations. This paper suggests a framework by which to interpret data collected on the response of metals and explosives. It suggests that strength is a quantity that decays over time and that fundamentally approaches zero in the limit of infinite time. Controlling this decay is the business of engineering to design structures that will survive in the environments our times of interest define.

2:03PM J25.00015 Equation of State of a Solid: Potts-Percolation Model, MIRON KAUFMAN, Cleveland State University, H.T. DIEP, Universite de Cergy-Pontoise, France — We include stress and strain in a Potts-percolation model of a solid, see J. Phys.: Condens. Matter 20, 075222 (2008) and Phys Rev E80, 031116 (2009). Neighboring atoms are connected by a bond of Lennard-Jones energy. If the energy is larger than a threshold the bond is more likely to fail, while if the energy is lower than the threshold the bond is more likely to be alive. We compute the equation of state: stress as function of strain and temperature by using renormalization group and Monte Carlo simulations. The phase diagram and the equation of state are determined. When the Potts heat capacity is divergent the continuous transition is replaced by a weak first-order transition through the van der Waals loop mechanism. When the Potts transition is first order the stress exhibits a large discontinuity as function of the strain.

Tuesday, February 28, 2012 11:15AM - 2:15PM —
Session J26 DCOMP: Focus Session: What is Computational Physics? 257B

11:15AM J26.00001 Aneesur Rahman Prize for Computational Physics Lecture: Photonic Crystals and Genetic Algorithms: Adventures of a Computational Physicist¹, KAI MING HO², Department of Physics and Astronomy and Ames Laboratory, Iowa State University — I will review some of our work in the computation of photonic crystals, focusing on our discovery of the photonic band gap in diamond structures. I will also describe our conception of the cut-and-paste genetic algorithm in materials discovery structure search and discuss applications of the algorithm from early studies of atomic clusters geometries to more recent applications for structures of surfaces, interfaces, nanowires, and bulk crystals.

¹Support from the U. S. Department of Energy Basic Energy Sciences Office is gratefully acknowledged.

²Ho 31310 APS Aneesur Rahman Prize Winner

11:51AM J26.00002 Computational Science as a Data and Compute Intensive Environment: How do we Prepare the Future for it?, NORA SABELLI, SRI International — Much has been said about the data- and compute-driven transformations that science is undergoing. Much has also been said about the impacts this transformation will have in society, impacts that are not limited to science professionals. But not much has been said about the transformations that will have to take place for this impact on society to be positive. This talk will ask if we know enough about what the multiple institutions that educate society's members should be doing to serve the new needs, and discuss some challenging questions that could inform future action.

12:27PM J26.00003 New Approaches for Microscopic Hydrodynamics for the Study of Fluid-Structure Interactions Subject to Thermal Fluctuations¹, PAUL ATZBERGER, UC Santa Barbara — Many problems in fluid mechanics involve the interaction of a hydrodynamic flow with an elastic structure. Recent advances in biology and engineering further motivate such studies at small length and time scales. At such scales traditional continuum mechanics descriptions must be augmented to take into account microscopic phenomena, such as spontaneous thermal fluctuations. This presents a variety of challenges both in formulating appropriate physical models and in computational simulation. In the context of fluid-structure interactions, additional challenges arise from the often subtle interplay between elastic mechanics, hydrodynamic coupling, and thermal fluctuations. In this talk, we present a set of new approaches which address central mathematical, physical, and computational issues for how to incorporate in the description of such fluid-structure interactions thermal fluctuations. We also address important numerical issues in the approximation of the resulting stochastic partial differential equations. We also discuss results for specific illustrative applications including studies of polymeric fluids, vesicles, gels, and lipid bilayer membranes.

¹NSF CAREER Award : NSF-DMS-0956210

12:39PM J26.00004 Extending the Flux Operator with the Husimi Projection, DOUGLAS MASON, MARIO BORUNDA, ERIC HELLER, Harvard University — A common tool among physics in the transport community is the probability flux operator, but connecting this operator to measurement has not received much attention. We have extended the definition of flux by using coherent states, rendering it both measurable and infinitely more useful. For instance, we can use our extended definition to study closed systems and the classical dynamics of individual quantum states, and then connect these dynamics to resonant states interacting with an environment. This analytical technique, based on semi-classics, brings new tools to bear on wavefunction analysis and visualization

12:51PM J26.00005 Finite Element Modeling of Open Domain Quantum Scattering¹, A.V. ILYASHENKO, A.G. GIANFRANCESCO, C.R. BOUCHER, L.R. RAM-MOHAN, Worcester Polytechnic Institute — We study quantum scattering in the open domain in 2D using the finite element method. We solve the Schrödinger equation in a circular region using an arbitrary triangular mesh with a plane wave source and an arbitrary (finite) scattering potential. We employ perfectly matched layers (PML) around the region of interest to simplify the derivative Cauchy BCs to Dirichlet BCs. With PML, fewer resources are needed to account for the open domain without going to the asymptotic region as is usually done, while obtaining the “near-field” evanescent solutions when they are present. The scattering total cross-section, the differential cross-section, and the phase shifts can be determined by performing a partial wave analysis on the computed solution. Examples of this technique and results on multi-component, spin dependent scattering for spintronics will be presented.

¹This work was supported by the NSF under grant #ECS-0725427 and by AFRL/DARPA under grant #FA8650-10-1-7046.

1:03PM J26.00006 Solution of a Schroedinger equation containing a general non local potential, JOSEPH POWER, GEORGE RAWITSCHER¹, University of Connecticut — The non locality is given by an integral kernel $K(r,r')$ that is general. We solve the corresponding Lippmann-Schwinger integral equation a) by expanding the wave function into a Fourier series (Galerkin method), and b) by a spectral method involving Chebyshev polynomials (CP). We apply them to the case of the much used Perey-Buck kernel [1], and find that, by using 50 sine functions, method a) requires an hour of computing time, while method b) using 50 CP's takes less than one second and is precise to $1:10^5$. Previously the spectral method could be applied only to a kernel of rank 1, representing for example the knock-on exchange process [2], but with our new procedure we will be able to compare relatively easily the effect of several types of non localities [3].

[1] F. G. Perey and B. Buck, Nucl. Phys. **A 32**, 353 (1962).

[2] G.H.,Rawitscher, S.Y. Kang, and I. Koltracht, J. Chem. Phys., **118**,9149-9157, (2003).

[3] M. I. Jaghoub, M. F. Hassan and G. H. Rawitscher, Phys. Rev. **C 84**,034618(2011).

¹George Rawitscher (member of the APS) is sponsoring Joseph Power, a graduate student at UConn.

1:15PM J26.00007 Accurate and fast numerical solution of Poisson's equation for arbitrary, space-filling convex Voronoi polyhedra: near-field corrections revisited¹, AFTAB ALAM, Ames Laboratory, Ames IA, BRIAN G. WILSON, LLNL, Livermore California, DUANE D. JOHNSON, Ames Laboratory, Ames IA — We present an accurate and rapid solution of Poisson's equation for space-filling, arbitrarily-shaped, convex Voronoi polyhedra (VP); the method is $O(N)$, where N is the number of distinct VP representing the system. In effect, we resolve the longstanding problem of fast but accurate numerical solution of the near-field corrections (NFC), contributions to each VP potential from nearby VP – typically involving multipole-type conditionally-convergent sums, or fast Fourier transforms. Our method avoids all ill-convergent sums, is simple, accurate, efficient, and works generally, i.e., for periodic solids, molecules, or systems with disorder or imperfections. We demonstrate the method's practicality by numerical calculations compared to exactly solvable models.

¹Research sponsored by the seed funding with Ames Laboratory, which is operated for DOE by Iowa State University under contract DE-AC02-07CH11358.

1:27PM J26.00008 Sonoluminescence and Vacuum Radiation , JUSTIN MELUNIS, EDUARDO FLORES, Rowan University — Sonoluminescence is the generation of light from sound. Our goal is to understand why a bubble trapped in water could generate light from sound. In our work we investigate the contribution of the dynamical Casimir effect to this phenomenon. In previous work researchers have approached this problem as a semi static Casimir effect and have not been able to show a significant contribution of the Casimir effect to sonoluminescence. In our approach, we treat the surface of the bubble as a highly reflecting surface, thus, the electric field of the zero-point modes at the surface is zero. Thus, when the bubble collapses the zero-point modes inside and outside are disturbed. Since the dynamics of zero-point mode fields obey Maxwell equations we can simulate their dynamics using programs like Mathematica. We study the radiation of the excited zero-point mode field.

1:39PM J26.00009 Second harmonic generation in three-dimensional metamaterials based on homogeneous centrosymmetric spheres , JINYING XU, Beijing Computational Science Research Center — The theory of second harmonic generation in three-dimensional metamaterials consisting of arbitrary distributions of spheres made of centrosymmetric materials is developed by means of the multiple scattering method. The electromagnetic field at both the fundamental frequency and second harmonic, as well as the scattering cross section, are calculated in a series of particular cases such as a single metallic sphere, two metallic spheres, chains of metallic spheres, and other periodic distributions of the metallic spheres. It is shown that the linear and nonlinear optical response of all ensembles of metallic spheres is strongly influenced by the excitation of surface plasmon-polariton resonances. The physical origin for such a phenomenon has also been analyzed. A new class of SHG devices made of such materials is anticipated.

1:51PM J26.00010 Characterizing the frequency response curve of large rooms in the short and long time regimes¹ , ANNA KLALES, SUZANNE PITTMAN, MATTHEW BARR, MARIO BORUNDA, ERIC HELLER, Harvard University — Room acoustics can be modeled by real Gaussian statistics, corresponding to randomized ray trajectories and characterized for instance by the reverberation time T60 (free field to decay by 60 decibels) which is independent of position or source point in a room. In his 1954 paper, Manfred Schroeder found universal statistical features of the steady state frequency response curve of large rooms, based upon the assumption of Gaussian probability distributions of the pressure. For example, he found the standard deviation from the mean level is 11 decibels for any concert hall, regardless of the shape of the room or its T60, within reasonable limits. Using semi-classical and numerical methods, we find non-universal (room dependent) corrections to Schroeder's universal results for the statistics of the frequency response curve. Along with corrections to the steady-state frequency response, we present the behavior of the frequency response curve for short to intermediate times.

¹This research was supported by an NSF graduate research fellowship

2:03PM J26.00011 ABSTRACT WITHDRAWN —

Tuesday, February 28, 2012 11:15AM - 2:15PM —
Session J27 FIP GERA: Invited Session: International Energy Perspectives 258AB

11:15AM J27.00001 Energy production and use in China , MARK LEVINE, Lawrence Berkeley National Laboratory
— No abstract available.

11:51AM J27.00002 Economics of energy Alternatives , CARMINE DIFIGLIO, US Department of Energy — No abstract available.

12:27PM J27.00003 Future Trends and Issues in Nuclear Power , RICHARD LESTER, Massachusetts Institute of Technology — No abstract available.

1:03PM J27.00004 Science for Sustainable Energy: Recommendations of the 2010 BESAC Report , ALEXIS MALOZEMOFF, AMSC, 64 Jackson Rd, Devens MA 01434 — In August 2010, DOE's Basic Energy Sciences Advisory Committee issued a major report on Science for Energy Technology. The report identified opportunities for science to help overcome roadblocks to progress in emerging clean energy technologies and thus to have much needed near-term impact on our energy infrastructure. The report covered diverse areas including solar electricity from photovoltaics, advanced nuclear energy, carbon sequestration, electrochemical energy storage, power grid technologies including power electronics and superconductors, solid state lighting, biofuels, building efficiency, fuel cells and wind power. In addition, mechanisms were suggested to facilitate progress, in particular, by strengthening the link between basic research and industry. The talk will review the highlights of this report.

1:39PM J27.00005 Fuel from Sunlight: Prospects and Approaches , ELLEN STECHEL, Sandia National laboratory
— No abstract available.

Tuesday, February 28, 2012 11:15AM - 2:15PM —
Session J28 FIAP DCOMP: Focus Session: Frontiers in Computational Thermodynamics of Materials 258C

11:15AM J28.00001 The role of Wang-Landau sampling in materials development¹ , DAVID LANDAU, Center for Simulation Physics, University of Georgia — An understanding of the thermodynamic behavior of materials as well as the prediction of the properties of "materials by design" often depends upon knowledge of the free energy of the system under study. Computer simulations offer a powerful tool for such investigations, but traditional methods often suffer from long time scales and metastable states due to the roughness of the free energy landscape. Wang-Landau sampling² is a powerful alternative to traditional Monte Carlo algorithms which can alleviate many such problems. We will review the Wang-Landau algorithm and discuss various implementations as well as possible application to materials development.

¹Supported by the National Science Foundation.

²F. Wang and D. P. Landau, Phys. Rev. Lett. 86, 2050 (2001); F. Wang and D. P. Landau, Phys. Rev. E 64, 05610 (2001).

11:51AM J28.00002 Dissolving the Periodic Table in Zirconia: Data Mining for Insight, BRYCE MEREDIG, CHRIS WOLVERTON, Northwestern University — A standard approach to understanding physical phenomena in materials is to manually search for clear trends or correlations in data (i.e., descriptors) governing those materials. Pettifor maps are a classic example of such empirically constructed models. But what if a data set is too large and/or chemically diverse to explain by straightforward human inspection? We present such a case by calculating from first principles the solubility thermodynamics of 70 dopant cations in cubic zirconia. This data set, spanning three charge states and most non-synthetic metals in the periodic table, defies simple “manual” explanation. Instead, we employ data mining algorithms and statistical methods to cluster the dopants into distinct classes, and then to build intuitive models for each class’ thermodynamics in zirconia. Thus, we show that formal data mining techniques are a powerful means of elucidating meaningful property relationships in complex data sets.

12:03PM J28.00003 High-throughput discovering half-metals from materials magnetic properties database, JUNKAI XUE, SHIDONG WANG, KESONG YANG, Department of Mechanical Engineering and Materials Science, Duke University, CHAITANYA DAS PEMMARAJU, STEFANO SANVITOS, School of Physics and CRANN, Trinity College, Dublin-2, Ireland, STEFANO CURTAROLO, Department of Mechanical Engineering and Materials Science, Duke University — Half-metal materials have been found by investigating their magnetism data, such as band gap and spin polarization around the Fermi level. An efficient algorithm has been implemented to create a database to aid discovering materials magnetism properties. With this tool, a series of new half-metals has been obtained. We present this magnetism data as well as how the online database is used.

12:15PM J28.00004 First Principles Modeling of the Temperature Dependent Ternary Phase Diagram for the Cu-Pd-S System, WILLIAM HUHN, MICHAEL WIDOM, Carnegie Mellon University — A method for the prediction of temperature dependent phase diagrams using first principles calculations combined with thermodynamics principles will be discussed. Our method allows us to model the phase diagram without any empirical fitting parameters. Due to the importance of sulfidation when dealing with hydrogen separation using copper palladium membranes, we have chosen as our test case the Cu-Pd-S ternary phase diagram which has been experimentally determined. By applying thermodynamic principles and a simple solid solution model, temperature-dependent features of the Cu-Pd-S system can be explained, specifically solubility ranges for substitutions in select crystalline phases. We have also performed electronic density of states calculations to determine the physical origin of the favorability of select substitutions at T=0K. Work is currently underway to use this method to create phase diagrams where no known experimental results exist, specifically the P-Pd-S system.

12:27PM J28.00005 Wang-Landau Without Binning, G. BROWN, Oak Ridge National Laboratory / Florida State, D. NICHOLSON, KH. ODBADRAKH, M. EISENBACH, A. RUSANU, Oak Ridge National Laboratory — Results are presented for Wang-Landau calculations on a Heisenberg model of BCC Fe that describe the density of states as function defined for all accessible energies instead of a function tabulated at discrete values of the energy. The density of states function described here is an analytic result valid near the ground state supplemented by a polynomial expansion. The probability density of Wang-Landau random walkers is sampled for a fixed density of states, and that probability density can be used to improve the estimated density of states. Methods for evaluating the convergence of the density of states are discussed along with the diffusion behavior of the random walkers. This work was performed at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725, and sponsored by the Laboratory Directed Research and Development Program (ORNL), by the Mathematical, Information, and Computational Sciences Division; Office of Advanced Scientific Computing Research (US DOE), and by the Division of Materials Sciences and Engineering; Office of Basic Energy Sciences (US DOE). Computer resources provided by Florida State University.

12:39PM J28.00006 Thermodynamic Stability of Actinide-Dioxide Solid Solutions and Surface Interactions with Water¹, MARK ASTA, Department of Materials Science and Engineering, University of California, Berkeley — Fluorite-structured actinide dioxides are the most common forms of fuel used in nuclear energy production worldwide. This talk will provide an overview of insights into the energetics of these compounds derived through the combination of density-functional-theory-based computational studies (including Hubbard-U corrections) and calorimetric measurements. The talk will focus on two main topics: the mixing energetics of cation solid solutions, and the energetics of water adsorption on the surfaces of these compounds. For the first topic, we present results for ThO₂ and UO₂ based solid solutions, highlighting the roles of elastic energy arising from cation size mismatch, electrostatic interactions, and charge-transfer reactions, in governing the sign and magnitude of the mixing energetics. For water adsorption, we contrast results for surface and adsorption energies on two fluorite-structured compounds, ThO₂ and CeO₂, that are relevant for understanding the behavior of water on actinide oxide surfaces more generally. Through a comparison between calorimetric measurements and computational results we assess the level of accuracy achieved in the computational modeling, and suggest areas where further experimental studies would be particularly useful.

¹This work was supported as part of the Materials Science of Actinides, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Basic Energy Sciences under award number DE-SC0001089.

1:15PM J28.00007 Structure and stability of Al₂Fe and Al₅Fe₂, MICHAEL WIDOM, Carnegie Mellon University, MAREK MIHALKOVIC, Slovakian Academy of Sciences — We employ first principles total energy and phonon calculations to address the structure and stability of Al₂Fe and Al₅Fe₂. The observed structure of Al₂Fe, which is reported as stable in the assessed Al-Fe phase diagram, is distinguished by an unusually low triclinic symmetry. The initial crystallographic structure determination additionally featured an unusual hole large enough to accommodate an additional atom. Our calculations indicate the hole must be filled, but predict the triclinic structure is unstable relative to a simpler tetragonal structure based on the prototype Mo Si₂. This tetragonal structure is interesting because it is predicted to be nonmagnetic, electrically insulating and high density, while the triclinic structure is magnetic, metallic and low density. We reconcile this seeming contradiction by demonstrating a high vibrational entropy that explains why the triclinic structure is stable at high temperatures. Finally, we note that orthorhombic Al₅Fe₂ is also destabilized by the tetragonal structure but may be stabilized at high temperatures, again by vibrational entropy and partial occupancy associated with the diffusion of Al atoms along channels.

1:27PM J28.00008 Equation of state of paramagnetic CrN from ab initio disordered local moments molecular dynamics, IGOR ABRIKOSOV, PETER STENETEG, BJÖRN ALLING, IFM, Linköping University, Sweden — A first-principles method is suggested for the calculation of thermodynamic properties of magnetic materials in their high temperature paramagnetic phase [1]. It is based on ab-initio molecular dynamics and simultaneous redistributions of the disordered but finite local magnetic moments. We apply this disordered local moments molecular dynamics (DLM-MD) method to the case of CrN and simulate its equation of state. In particular the debated [F. Rivadulla et al., Nat Mater 8, 974 (2009); B. Alling et al., Nat Mater 9, 283 (2010)] bulk modulus is calculated in the paramagnetic cubic phase and is shown to be very similar to that of the antiferromagnetic orthorhombic CrN phase for all considered temperatures.

[1] P. Steneteg, B. Alling, I. A. Abrikosov, arXiv:1110.1331v1 [cond-mat.mtrl-sci]

1:39PM J28.00009 Lattice dynamics of anharmonic solids from first principles, OLLE HELLMAN, IGOR ABRIKOSOV, SERGEI SIMAK, IFM, Linköping University, Sweden — An accurate and easily extendable method to deal with lattice dynamics of solids is offered. It is based on first-principles molecular dynamics simulations and provides a consistent way to extract the best possible harmonic—or higher order—potential energy surface at finite temperatures. It is designed to work even for strongly anharmonic systems where the traditional quasi-harmonic approximation fails. The accuracy and convergence of the method are controlled in a straightforward way. Excellent agreement of the calculated phonon dispersion relations at finite temperature with experimental results for bcc Li and bcc Zr is demonstrated. In addition to that the bcc-hcp phase diagram for Zr is calculated with high accuracy. arXiv:1103.5590v3 [cond-mat.mtrl-sci]

1:51PM J28.00010 Unified cluster expansion method applied to the configurational thermodynamics of cubic $\text{Ti}_{1-x}\text{Al}_x\text{N}$, BJÖRN ALLING, IFM, Linköping University, ANDREI RUBAN, MSE, Royal Institute of Technology, Sweden, AYAT KARIMI, IPMC, École Polytechnique Fédérale de Lausanne, Switzerland, LARS HULTMAN, IGOR ABRIKOSOV, IFM, Linköping University — We study the thermodynamics of cubic $\text{Ti}_{1-x}\text{Al}_x\text{N}$ using a unified cluster expansion approach for the alloy problem [1]. The purely configurational part of the alloy Hamiltonian is expanded in terms of concentration and volume-dependent effective cluster interactions. By separate expansions of the chemical fixed lattice, and local lattice relaxation terms of the ordering energies, we demonstrate how the screened generalized perturbation method can be fruitfully combined with a concentration-dependent Connolly-Williams cluster expansion method, getting the best out of both two schemes that are traditionally used separately. Utilizing the obtained Hamiltonian in Monte Carlo simulations we access the free energy of $\text{Ti}_{1-x}\text{Al}_x\text{N}$ alloys and construct the isostructural phase diagram. The results show striking similarities with the previously obtained mean-field results: The metastable c-TiAlN is subject to coherent spinodal decomposition over a large part of the concentration range, e.g., from $x \approx 0.33$ at 2000 K.

[1] B. Alling, A. V. Ruban, A. Karimi, L. Hultman, and I. A. Abrikosov, PHYSICAL REVIEW B 83, 104203 (2011)

2:03PM J28.00011 Atomistic modeling of thermodynamic equilibrium of plutonium, TONGSIK LEE, STEVE VALONE, Los Alamos National Laboratory, MIKE BASKES, Los Alamos National Laboratory and University of California, San Diego, SHAO-PING CHEN, Los Alamos National Laboratory, ANDREW LAWSON, Retired — Plutonium metal has complex thermodynamic properties. Among its six allotropes at ambient pressure, the fcc delta-phase exhibits a wide range of anomalous behavior: extraordinarily high elastic anisotropy, largest atomic volume despite the close-packed structure, negative thermal expansion, strong elastic softening at elevated temperature, and extreme sensitivity to dilute alloying. An accurate description of these thermodynamic properties goes far beyond the current capability of first-principle calculations. An elaborate modeling strategy at the atomic level is hence an urgent need. We propose a novel atomistic scheme to model elemental plutonium, in particular, to reproduce the anomalous characteristics of the delta-phase. A modified embedded atom method potential is fitted to two energy-volume curves that represent the distinct electronic states of plutonium in order to embody the mechanism of the two-state model of Weiss, in line with the insight originally proposed by Lawson et al. [Philos. Mag. 86, 2713 (2006)]. By the use of various techniques in Monte Carlo simulations, we are able to provide a unified perspective of diverse phenomenological aspects among thermal expansion, elasticity, and phase stability.

Tuesday, February 28, 2012 11:15AM - 2:15PM –

Session J29 GQI: Focus Session: Quantum Information for Quantum Foundations - Informational Principles and Fundamental Structures 259A

11:15AM J29.00001 Information Causality as a physical principle, VALERIO SCARANI, Centre for Quantum Technologies and Department of Physics, National University of Singapore — It is known that the physical principle of “no-signaling” alone does not single out quantum correlations, and that the post-quantum no-signaling correlations share many of the features that are supposed to define quantum physics (intrinsic randomness, no-cloning, violation of Bell’s inequalities...). This talk focuses on the principle of Information Causality (IC), which generalizes no-signaling and has been proved to come close to singling out quantum correlations. I shall review the successes of IC and also the difficulties that the subsequent research is meeting. In particular, I shall emphasize how a generalization of the initial bipartite scenario to a multipartite one is a most urgent necessary step.

11:51AM J29.00002 Tensor network states for quantum foundations, JACOB BIAMONTE, CQT Singapore, ISI Foundation Torino — Penrose developed a graphical language to reason about networks of connected tensors and applied these techniques to quantum theory. Here we present the development of a framework and tool set based on Penrose tensor networks that enables one to address certain questions of a foundational nature in quantum theory. A quantum tensor theory is one in which a fixed collection of tensors with clearly defined composition laws defines a physical theory. We show that each element of a universal collection of such tensors gives rise to a physical operation, allowed by the rules of quantum mechanics. Although each of these (possibly) atemporal operations is indeed physical, certain sequences of them could represent processes that violate the rules of quantum theory. The question is to determine when this is the case and we arrive at some perplexing conclusions.

12:03PM J29.00003 On the Feynman Problem¹, GIACOMO D'ARIANO, Università di Pavia — Foundations of Quantum Field Theory can be connected to foundations of Quantum Theory if we can derive the former in terms of the latter with two additional postulates of locality and topological homogeneity of interactions between quantum systems, in the hypothesis that a quantum field is ultimately made of a numerable set of quantum systems that are unitarily interacting. But, in order to do that we need to be able to simulate quantum field by a quantum computer. In the paper “Simulating Physics with Computers” (Int. J. Th. Phys, 21 467 (1982)) Richard Feynman raised the problem whether it is possible to simulate Fermi fields by a quantum computer—in short if we can “qubit-ize” a Fermi field, keeping the field interaction local on qubits. In this talk I will show how this problem is solved for any space-dimension, upon introducing a new general Jordan-Wigner map between field and qubits, and by adding witnessing auxiliary qubits. I will also derive the unique vacuum for the Fermi fields and for the auxiliary fields. The solution of the Feynman problem allows us to simulate quantum fields by a quantum cellular automata, also providing a kind of Planck-scale version of quantum field theory. Computer simulations will be projected at the end of the talk

¹Founded by Coquit FP7 project, Italian PRIN and INFN.

12:15PM J29.00004 Origin of Feynman’s Rules of Quantum Theory and Complementarity, PHILIP GOYAL, SUNY Albany — Complex numbers are an intrinsic part of the mathematical formalism of quantum theory, and are perhaps its most mysterious feature. If one considers how to combine experimental arrangements to generate new experimental arrangements, a set of five simple symmetries involving two binary operators naturally arises. Recently, I have shown that these symmetries, together with the probabilistic nature of measurement outcomes and the principle of complementarity (formalized in a novel way as the Principle of Information Duality) naturally lead to Feynman’s rules of quantum theory (including their complex nature) [1]. In this paper, I present recent development of this work showing that the assumption of complementarity can be dropped, and, instead, a fundamental theorem from number theory—Frobenius’ theorem—can be applied to show that the only formalism compatible with the experimental symmetries are real and complex quantum theory. I shall conclude with a discussion of physical principles which can be used to rule out real quantum theory.

[1] Origin of Complex Quantum Amplitudes and Feynman’s Rules, P. Goyal, K. Knuth, J. Skilling, Phys. Rev. A 81, 022109 (2010)

12:27PM J29.00005 Partially Ordered Sets of Quantum Measurements and the Dirac Equation

, KEVIN H. KNUTH, SUNY Albany — Events can be ordered according to whether one event influences another. This results in a partially ordered set (poset) of events often referred to as a causal set. In this framework, an observer can be represented by a chain of events. Quantification of events and pairs of events, referred to as intervals, can be performed by projecting them onto an observer chain, or even a pair of observer chains, which in specific situations leads to a Minkowski metric replete with Lorentz transformations (Bahreyni & Knuth, 2011. APS B21.00007). In this work, we unify this picture with the Process Calculus, which coincides with the Feynman rules of quantum mechanics (Goyal, Knuth, Skilling, 2010, arXiv:0907.0909; Goyal & Knuth, Symmetry 2011, 3(2), 171), by considering quantum measurements to be events. This is performed by quantifying pairs of events, which represent transitions, with a pair of numbers, or a quantum amplitude. In the 1+1D case this results in the Feynman checkerboard model of the Dirac equation (Feynman & Hibbs, 1965). We further demonstrate that in the case of 3+1 dimensions, we recover Bialnycki-Birula's (1994, Phys. Rev. D, 49(12), 6920) body-centered cubic cellular automata model of the Dirac equation studied more recently by Earle (2011, arXiv:1102.1200v1).

12:39PM J29.00006 An Observer-Based Foundation of Geometry

, NEWSHAW BAHREYNI, Department of Physics, University at Albany, Albany NY 12222, KEVIN H. KNUTH, Department of Physics, University at Albany, Albany NY 12222, Department of Informatics, University at Albany, Albany NY 12222 — The fact that some events influence other events enables one to define a partially ordered set (poset) of events, often referred to as a causal set. A chain of events, called observer chain, can be quantified by labeling its events numerically. Other events in a poset may be quantified with respect to an observer chain/chains by projecting them onto the chain, resulting in a pair of numbers. Similarly, pairs of events, called intervals, can be quantified with four numbers. Under certain conditions, this leads to the Minkowski metric, Lorentz transformations and the mathematics of special relativity (Bahreyni & Knuth, APS March Meeting 2011). We exploit the same techniques to demonstrate that geometric concepts can be *derived* from order-theoretic concepts. We show how chains in a poset can be used to define points and line segments. Subsequent quantification results in the Pythagorean Theorem and the inner product as well as other geometric concepts and measures. Thus the geometry of space, which is assumed to be fundamental, emerges as a result of quantifying a partially ordered set. More importantly, this proposed foundation of geometry is entirely observer-based, which may provide a natural way toward integration with quantum mechanics.

12:51PM J29.00007 Quantum state space as a maximal consistent set¹

, GELO NOEL TABIA, University of Waterloo, Perimeter Institute for Theoretical Physics, and Institute for Quantum Computing — Measurement statistics in quantum theory are obtained from the Born rule and the uniqueness of the probability measure it assigns through quantum states is guaranteed by Gleason's theorem. Thus, a possible systematic way of exploring the geometry of quantum state space expresses quantum states in terms of outcome probabilities of a symmetric informationally complete measurement. This specific choice for representing quantum states is motivated by how the associated probability space provides a natural venue for characterizing the set of quantum states as a geometric construct called a maximal consistent set. We define the conditions for consistency and maximality of a set, provide some examples of maximal consistent sets and attempt to deduce the steps for building up a maximal consistent set of probability distributions equivalent to Hilbert space. In particular, we demonstrate how the reconstruction procedure works for qutrits and observe how it reveals an elegant underlying symmetry among five SIC-POVMs and a complete set of mutually unbiased bases, known in finite affine geometry as the Hesse configuration.

¹This work was supported in part by the U. S. Office of Naval Research (Grant No. N00014-09-1-0247).

1:03PM J29.00008 SIC-POVMs and Lie Algebras¹

, HOAN DANG, Perimeter Institute for Theoretical Physics and University of Waterloo, MARCUS APPLEBY, CHRISTOPHER FUCHS, Perimeter Institute for Theoretical Physics — A symmetric informationally complete positive operator valued measure (SIC-POVM) is usually thought of as a highly symmetric structure in quantum state space. However Appleby, Flammia and Fuchs (J. Math. Phys. 52, 022202, 2011) have shown that the existence of a SIC-POVM in dimension d is equivalent to a proposition concerning the Lie Algebra $\mathfrak{gl}(d, \mathbb{C})$. Related to this they show that there is, associated to each SIC-POVM, a rich and intricate geometric structure in the adjoint representation space of $\mathfrak{gl}(d, \mathbb{C})$. In this talk we present a deeper exploration of this structure.

¹This work was supported in part by the U. S. Office of Naval Research (Grant No. N00014-09-1-0247) and by the Natural Sciences and Engineering Research Council of Canada.

1:15PM J29.00009 The Galois Group of Symmetric Measurements

, MARCUS APPLEBY, Perimeter Institute, 31 Caroline St N, Waterloo, Ontario, Canada, HULYA YADSAN-APPLEBY, University College, Gower St, London WC1E 6BT, UK, GERHARD ZAUNER, None — The problem of proving (or disproving) the existence of symmetric informationally complete positive operator valued measures (SICs) has been the focus of much effort in the quantum information community during the last 12 years. In this talk we describe the Galois invariances of Weyl-Heisenberg covariant SICs (the class which has been most intensively studied). It is a striking fact that the published exact solutions (in dimensions 2–16, 19, 24, 35 and 48) are all expressible in terms of radicals, implying that the associated Galois groups must be solvable. Building on the work of Scott and Grassl (J. Math. Phys. 51, 042203 (2010)) we investigate the Galois group in more detail. We show that there is an intriguing interplay between the Galois and Clifford group symmetries. We also show that there are a number of interesting regularities in the Galois group structure for the cases we have examined. We conclude with some speculations about the bearing this may have on the SIC existence problem.

1:27PM J29.00010 Quantum Nonlocal Boxes Exhibit Stronger Distillability

, JIBRAN RASHID, PETER HOYER, University of Calgary — Given the apparent limited distillability of nonlocal boxes (NLBs), we initiate a study of the distillation of correlations for NLBs that output quantum states rather than classical bits. We propose a new non-adaptive protocol for nonlocality distillation which asymptotically distills correlated quantum nonlocal boxes to the value 3.098, whereas in contrast, the optimal non-adaptive parity protocol for classical NLBs asymptotically distills to the value 3.0. The protocol is also proven to be an optimal non-adaptive protocol for 1, 2 and 3 copies by formulating nonlocality distillation as a semi-definite programming optimization problem. Even if we restrict our attention to non-adaptive protocols, qNLBs offer improved distillation over NLBs. A generalization of our SDP approach that allows for adaptive protocols may reveal a similar improvement in general. This may imply distillability for nonlocal correlations that are currently not known to be distillable. As a consequence of the work on nonlocality distillation we provide numerical evidence that correlations with non-trivial marginals which are not known to satisfy the macroscopic locality principle may be distillable even when corresponding correlations with trivial marginals are not.

1:39PM J29.00011 ABSTRACT WITHDRAWN —

1:51PM J29.00012 ABSTRACT WITHDRAWN —

2:03PM J29.00013 The necessity of entanglement and the equivalency of Bell's theorem with the second law of thermodynamics¹, IAN DURHAM, Saint Anselm College — We demonstrate that both Wigner's form of Bell's inequalities as well as a form of the second law of thermodynamics, as manifest in Carathéodory's principle, can be derived from the same assumptions. The results suggest that Bell's theorem is merely a well-disguised statement of the second law. It also suggests that entanglement is necessary for quantum theory to be in full accord with the second law.

¹Work partially supported by a grant from FQXi.

Tuesday, February 28, 2012 11:15AM - 2:15PM – Session J30 GQI: Open Quantum Systems and Decoherence 259B

11:15AM J30.00001 Heisenberg scaling of time-limited quantum metrology with realistic decoherence, MAXIME HARDY, WILLIAM A. COISH, Department of Physics, McGill University, Montreal, Quebec, Canada H3A 2T8 — The prospect of using entanglement to improve various metrology tasks is one of the most promising avenues for a near-term real-world benefit from genuine quantum phenomena [1]. However, in the standard scenario, history-independent Markovian dephasing removes the quantum advantage [2]. We revisit the problem of quantum metrology using the model of trapped ions subject to non-Markovian phase damping decoherence caused by Gaussian noise with finite correlation length and time (a slight generalization of the model used in Ref. [3]). Assuming a fixed available measurement time shorter than the noise correlation time (the non-Markovian limit) and a noise source that is local in space, we recover Heisenberg scaling ($\sim 1/N$). This allows one to measure an "instantaneous" frequency to a higher precision than the time-averaged noise amplitude and moreover to a higher precision than classically allowed. Interestingly, for this protocol we show that the optimal number of measurements to be performed within the measurement time is three.

[1] V. Giovannetti, S. Lloyd, and L. Maccone Nature Photonics 5, 222 (2011)

[2] S. F. Huelga et al. Phys. Rev. Lett. 79, 3865 (1997)

[3] T. Monz et al. Phys. Rev. Lett. 106, 130506 (2011)

11:27AM J30.00002 ABSTRACT WITHDRAWN –

11:39AM J30.00003 Entanglement and diffusive behavior of a driven Floquet system coupled to noise¹, BENJAMIN M. FREGOSO, JUSTIN WILSON, VICTOR GALITSKI, JQI, UMD — Attempting to improve the persistence of quantum effects in systems interacting with a bath, we consider a periodically-driven quantum system and focus on its quantum dynamics in the Floquet space. As a toy model, we first consider a harmonic oscillator interacting with a bath and investigate the diffusive behavior in the statistics of observables in the presence of a periodic driving force and analyze the system within the Floquet theory. We then extend this analysis to look at the entanglement of two oscillators interacting with a bath, and investigate whether a periodic driving force can improve the persistence of entanglement between the two systems. We discuss possible experimental realization of our exactly-solvable model with trapped ions. We discuss a Lie-algebraic contraction scheme to map the oscillator properties to spin the systems in an environment. Extensions of our theory to more complicated driven quantum systems will also be discussed. This research is supported by JQI-PFC.

¹This research is supported by JQI-PFC.

11:51AM J30.00004 A Lie-algebraic approach to decoherence in a quantum spin system¹, JUSTIN WILSON, BENJAMIN FREGOSO, VICTOR GALITSKI, Joint Quantum Institute, University of Maryland, College Park — Quantum spin systems interacting with environment lose quantum coherence and information due to the debilitating effects of the noise. Quantitative description of decoherence even in the simplest spin-1/2 systems is technically complicated and the conventional approach (e.g., calculating T_1 and T_2) involves a number of strong approximations. In order to go beyond this approximation scheme and identify its regime of validity, we use the Lie-algebraic contraction, which reduces the $su(2)$ algebra into the solvable oscillator algebra to connect the two dynamical systems. We take advantage of the general exact solution to the latter and build a regular expansion in the contraction parameter to describe dissipative quantum dynamics of the spin. This procedure allows for a controlled non-perturbative treatment of the non-Markovian effects. New interesting effects include deviations from pure diffusion due to bath spectrum and non-Markovian effects in both systems. Our approach could shed light on the spin decoherence problem and noise characterization in experiments relevant for quantum computing.

¹This research is supported by JQI-PFC

12:03PM J30.00005 Quantum simulator of an open quantum system using superconducting qubits: exciton transport in photosynthetic complexes, SARAH MOSTAME, PATRICK REBENTROST, ALEXANDER EISFELD, Harvard University, ANDREW J. KERMAN, Lincoln Laboratory - Massachusetts Institute of Technology, DIMITRIS I. TSOMOKOS, University of London, ALAN ASPURU-GUZIK, Harvard University — In the initial stage of photosynthesis, light-harvested energy is transferred with remarkably high efficiency to a reaction center, with the vibrational environment assisting the transport mechanism. It is of great interest to mimic this process with present-day technologies. Here we propose an analog quantum simulator of open system dynamics, where noise engineering of the environment has a central role. In particular, we propose the use of superconducting qubits for the simulation of exciton transport in the Fenna-Matthew-Olson protein, a prototypical photosynthetic complex. Our method allows for a single-molecule implementation and the investigation of energy transfer pathways as well as non-Markovian and spatiotemporal noise-correlation effects.

12:15PM J30.00006 Quantum signatures of chaos in quantum tomography¹, VAIBHAV MADHOK, CARLOS RIOFRIO, IVAN DEUTSCH, University of New Mexico — We study the connection between quantum chaos and information gain in the time series of a measurement record used for quantum tomography. The record is obtained as a sequence of expectation values of a Hermitian operator evolving under repeated application of the Floquet operator of the quantum kicked top on a large ensemble of identical systems. We find an increase in information gain and hence higher fidelities in the process when the Floquet maps employed increase in chaoticity. We make predictions for the information gain using random matrix theory in the fully chaotic regime and show a remarkable agreement between the two. Finally we discuss how this approach can be used in general as a benchmark for information gain in an experimental implementation based on nonlinear dynamics of atomic spins measured weakly by a the Faraday rotation of a laser probe.

¹CQUIC (Center for Quantum Information and Control)

12:27PM J30.00007 Non-Markovian behavior of small and large complex quantum systems, CARLOS PINEDA, Instituto de Fisica, Universidad Nacional Autonoma de Mexico, Mexico D.F. 01000, Mexico, MARKO ZNIDARIC, Physics Department, Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia, IGNACIO GARCÍA-MATA, Instituto de Investigaciones Fisicas de Mar del Plata (IFIMAR-CONICET), Funes 3350, 7600 Mar del Plata, Argentina — The channel induced by a complex system interacting strongly with a qubit is calculated exactly under the assumption of randomness of its eigenvectors. The resulting channel is represented as an isotropic time dependent oscillation of the Bloch ball, leading to non-Markovian behavior, even in the limit of infinite environments. Two contributions are identified: one due to the density of states and the other due to correlations in the spectrum. Prototype examples, one for chaotic and the other for regular dynamics are explored.

12:39PM J30.00008 Quantum correlation of an optically controlled open quantum system¹, CHING-KIT CHAN, L.J. SHAM, Department of Physics, Center for Advanced Nanoscience, University of California San Diego — A precise time-dependent optical control of an open quantum system relies on an accurate account of the quantum interference among the system, the photon control and the dissipative environment. In the spirit of the Keldysh non-equilibrium Green's function approach, we develop a diagrammatic technique to precisely calculate this quantum correlation for a fast multimode coherent photon control against slow relaxation, valid for both Markovian and non-Markovian systems. We demonstrate how this novel formalism can lead to a better accuracy than existing approximations of the master equation. We also describe extensions to cases with controls by photon state other than the coherent Glauber state.

¹This research was supported by the U.S. Army Research Office MURI award W911NF0910406.

12:51PM J30.00009 Effects of counter rotating terms on quantum discord and entanglement between two atoms in a dissipative cavity, FERDI ALTINTAS, RESUL ERYIGIT, Abant Izzet Baysal University — We have investigated the role of counter-rotating interaction terms in the Rabi Hamiltonian on the creation and dynamics of entanglement and quantum discord between two identical atoms interacting with a lossy single mode cavity field for a system initially in different product states. For some initial states, the counter-rotating terms are found to lead to steady states in the long time limit which can have high quantum discord, but have no entanglement. The effect of cavity decay rate on these steady states quantum discord has been also investigated, surprisingly the increase in cavity decay rate is found to enhance the steady state quantum discord. Moreover, for certain initial states the effect of counter rotating terms are found to be detrimental to the quantum correlations when counter rotating terms in interaction Hamiltonian are taken into account.

1:03PM J30.00010 Pointer state engineering in open quantum systems¹, LORENZA VIOLA, KAVEH KHODJASTEH, Dartmouth College, VIATCHESLAV DOBROVITSKI, Ames Laboratory — Pointer states have a long history in fundamental quantum theory and a practical relevance as long-lasting high-fidelity states in open quantum systems. For generic dissipative dynamics, however, pointer states need not exist or, when they do, need not coincide with states of interest. I will show how open-loop control procedures may be used to engineer dissipation in such a way that any desired initial pure state can be guaranteed to survive with high minimum fidelity over time and retrieved on demand. Quantitative fidelity bounds and constructive control protocols will be presented, and validated through simulation in paradigmatic single- and two- qubit dissipative scenarios. I will also argue that the state selectivity observed in recent dynamical decoupling experiments can be naturally understood within the pointer state engineering framework.

¹Supported by the NSF through Award No. PHY-0903727 and by the DOE-Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

1:15PM J30.00011 Crossover from adiabatic to antiadiabatic quantum pumping with dissipation¹, GIUSEPPE ERNESTO SANTORO, FRANCO PELLEGRINI, SISSA and CNR/IOM, CARLOTTA NEGRI, FABIO PISTOLESI, Laboratoire d'Ondes et Matière d'Aquitaine, CNRS and Université de Bordeaux, NICOLA MANINI, ETSF and Dipartimento di Fisica, Università degli Studi di Milano, ERIO TOSATTI, SISSA and CNR/IOM — Quantum pumping, in its different forms, is attracting attention from different fields, from fundamental quantum mechanics, to nanotechnology, to superconductivity. We investigate the crossover of quantum pumping from the adiabatic to the anti-adiabatic regime in the presence of dissipation, and find general and explicit analytical expressions for the pumped current in a minimal model describing a system with the topology of a ring forced by a periodic modulation of frequency ω . The solution allows following in a transparent way the evolution of pumped DC current from much smaller to much larger ω values than the other relevant energy scale, the energy splitting introduced by the modulation. We find and characterize a temperature-dependent optimal value of the frequency for which the pumped current is maximal.

¹Research supported by the Italian CNR through ESF Eurocore/FANAS/AFRI, by the Italian Ministry of University and Research, through PRIN 20087NX9Y7, and by the French ANR, contract QNM ANR10-BLAN-0404-03.

1:27PM J30.00012 Open Quantum Walks and Dissipative Quantum Computing, FRANCESCO PETRUCCIONE, University of KwaZulu-Natal — Open Quantum Walks (OQWs) have been recently introduced as quantum Markov chains on graphs [S. Attal, F. Petruccione, C. Sabot, and I. Sinayskiy, E-print: <http://hal.archives-ouvertes.fr/hal-00581553/fr/>]. The formulation of the OQWs is exclusively based upon the non-unitary dynamics induced by the environment. It will be shown that OQWs are a very useful tool for the formulation of dissipative quantum computing and quantum state preparation. In particular, it will be shown how to implement single qubit gates and the CNOT gate as OQWs on fully connected graphs. Also, OQWs make possible the dissipative quantum state preparation of arbitrary single qubit states and of all two-qubit Bell states. Finally, it will be shown how to reformulate efficiently a discrete time version of dissipative quantum computing in the language of OQWs.

1:39PM J30.00013 Non-Markovian dynamics of a solid-state charge qubit measured by a quantum point contact, CHUNG-CHIN JIAN, PO-WEN CHEN, HSI-SHENG GOAN, Department of Physics, National Taiwan University, NTU TEAM — We study a system of a charge qubit consisting of an electron in two coupled quantum dots (CQD's) detected by a quantum point contact (QPC). We derive perturbatively the non-Markovian quantum master equation for the CQD's system and calculate the transport current through the QPC (considered as a reservoir) to second order in the system-reservoir interaction. The non-Markovianity of the whole system comes from the energy-dependent tunneling amplitudes and energy-dependent densities of states of the QPC, which are modeled as a spectral density with a Lorentzian shape. In the non-Markovian case, the decay coefficients in the derived master equation and transport current are time-dependent and involve the real and imaginary parts of the contributions from the QPC reservoir correlation functions. In the wide-band limit (WBL), the various Markovian master equations in different parameter regimes are recovered, and the contributions of the imaginary parts are found to vanish. However, in the non-Markovian regime, the contributions of the imaginary parts significantly influence the dynamics of the charge qubit and thus the transport current. Especially, the non-Markovian transient currents through QPC differ significantly from the WBL Markovian counterparts and thus may serve as a witness for the non-Markovian behavior in the QPC-qubit system.

1:51PM J30.00014 Hierarchical equations of motion: A fundamental theory for quantum open systems¹, YIJING YAN, Hong Kong University of Science and Technology — As a powerful alternative to the influence functional path integral formalism, HEOM has been exploited in the study of various systems. In this talk, I will present some recent advancement on the HEOM-based nonlinear/nonequilibrium response theory and efficient implementation methods. Numerical demonstrations include coherent two-dimensional spectroscopy signals of light-harvesting model systems, and transport current noise spectrums through Anderson model quantum dots, operated in high-order co-tunneling regime.

¹Supported partially by the Hong Kong UGC (AoE/P-04/08-2) and China NNSF (No.21033008).

2:03PM J30.00015 Fidelity of the ground state in adiabatic quantum computation, QIANG DENG, DMITRI AVERIN, Department of Physics and Astronomy, Stony Brook University, MOHAMMAD AMIN, PETER SMITH, D-Wave Systems Inc., Canada — The energy gap between the ground and excited states of a qubit register performing an adiabatic quantum computation (AQC) algorithm is expected to provide additional stability against decoherence by environmental noise. However, the precise quantitative magnitude of this effect is still an open question. In this work, we show that fidelity of the ground state provides the ultimate quantitative measure of the AQC stability against decoherence. Even if the qubit register is not driven out of the ground state by the time evolution of the algorithm, the ground state is deformed by the qubit-environment interaction. The extent of this deformation can be characterized by the same noise correlators that determine the relaxation rates in the gate-model QC. We derive finite-temperature expression for the ground-state fidelity and calculate it numerically for the 16-qubit instances of adiabatic quantum optimization.

Tuesday, February 28, 2012 11:15AM - 2:15PM –
Session J31 DMP: Focus Session: Topological Insulators: Synthesis and Characterization -
Transport 260

11:15AM J31.00001 Transport in Topological Insulator Thin Films, VALLA FATEMI, HADAR STEINBERG, JEAN-BAPTISTE LALOE, FERHAT KATMIS, LUCAS ORONA, JAGADEESH MOODERA, PABLO JARILLO-HERRERO, MIT — We report on electronic transport measurements on Bi₂Se₃ thin-film devices and show that an ambipolar modulation can be achieved via the electric field effect by using a top-gate with a high- κ dielectric insulator. By analyzing the evolution of the weak anti-localization magnetoconductance behavior with respect to gate voltage and temperature, we find that we are able to modulate the effective number of channels, demonstrating that the coherent coupling between the surface and the bulk is tunable. Moreover, we investigate the formation and behavior of tunable p-n junctions on thin-film devices with multiple local top-gates.

11:27AM J31.00002 Bi₂Se₃ and Bismuth: A comparison of transport in topological and trivial materials¹, ANTHONY RICARDELLA, Penn State University, MICHEL VAN MAASAKKERS, Eindhoven University of Technology, DUMING ZHANG, JOON SUE LEE, NITIN SAMARTH, Penn State University — The simple surface state structure of Bi₂Se₃ has made it one of the most promising materials for harnessing transport through topologically protected surface states. Identifying unambiguous signatures of transport through these states is difficult however due to residual bulk conductivity and the formation of 2D electron gases near the surface due to band bending. As in bulk bismuth these non-topological states are subject to strong-spin orbit coupling. Very thin films of bismuth are predicted to be 2D topological insulators and thus are interesting themselves for a topological to non-topological transition as a function of thickness. Analysis of signatures such as weak anti-localization and linear magnetoresistance are compared between high quality MBE grown films of these materials to determine what can and cannot be ascribed to transport through protected surface states.

¹Supported by DARPA and NSF-MRSEC.

11:39AM J31.00003 Low-temperature magnetoresistance in electrically gated Bi₂Se₃ thin films, J.S. LEE, A.M. DASILVA, A. RICARDELLA, D.M. ZHANG, J.K. JAIN, NITIN SAMARTH, Dept. of Physics, Penn State University, University Park PA 16802 — Although transport in samples of 3D topological insulators often has a large contribution from bulk conduction, the surface transport can be studied by electrical gating of topological insulator thin films. We have measured thin films of Bi₂Se₃ grown by molecular beam epitaxy and subsequently photolithographically patterned with a high- κ gate dielectric (HfO₂) using atomic layer deposition. Gate voltage-dependent Hall effect and magnetoresistance were measured over a temperature range $0.5\text{K} \leq T \leq 20\text{K}$ in both perpendicular and parallel magnetic fields up to 6 T. Applying a negative gate voltage forms a depletion layer at the top of the thin film and decouples the surface from bulk carriers. We use the weak antilocalization effect at low magnetic field to study the transport contribution of surface and bulk channels. We also discuss scattering mechanisms contributing to surface and bulk conduction. Supported by ONR and NSF-MRSEC.

11:51AM J31.00004 Thickness Independent Surface Transport of Bi₂Se₃ on Al₂O₃(0001) Substrates, NAMRATA BANSAL, Rutgers University, YONG SEUNG KIM, 3Graphene Research Institute, Sejong University, South Korea, MATTHEW BRAHLEK, ELIAV EDREY, SEONGSHIK OH, Rutgers University — The key requirement for exploiting the newly emerging three-dimensional (3D) topological insulators (TI) as a novel platform for coherent spin-polarized electronics is TI thin films with dominant surface transport properties. So far, while researchers have been able to observe the existence of surface states locally *in situ*, verification over a wide thickness range outside the growth chamber has not yet been reported. Here, we report large signature of surface transport in TI Bi₂Se₃ thin films. The Bi₂Se₃ films used for this study were grown on c-axis Al₂O₃ substrates with MBE. Hall-effect measurements in the standard Van der Pauw geometry provided clear evidence of two conducting channels for 4QL-2750QL thick samples, with the transport properties for one of the channel being thickness independent and the other varying with thickness. This thickness independent carrier density of $\sim 1.5 \times 10^{13} \text{ cm}^{-2}$ has been observed over the entire thickness range down to 2 QL, clearly suggesting that this is due to surface states. Furthermore, another surface transport property directly related to the topological protection mechanism, the weak-antilocalization (WAL) effect, exhibited similar thickness- and bulk-independent characteristics.

12:03PM J31.00005 Electronic transport in MBE-grown Bi₂Se₃ topological insulator thin film field effect devices, TAI-LUNG WU, JIFA TIAN, HELIN CAO, YI XUAN, Department of Physics and Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47907, XINYU LIU, JACK FURDYNA, Department of Physics, University of Notre Dame, Notre Dame, IN 46556, YONG P. CHEN, Department of Physics and Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47907, QMD TEAM — Topological insulators (TI), such as Bi₂Se₃ and Bi₂Te₃, have attracted a lot of attention due to their exotic electronic properties. Bi₂Se₃ TI films grown by molecular beam epitaxy (MBE) are promising for studying the nature of topologically protected surface states due to their large size, high quality, the capability to tune the thickness and interface with various semiconductor substrates. In this study, thin films of Bi₂Se₃ have been grown on GaAs (001) semi-insulating substrates in a III-V/II-VI dual chamber MBE system. To study the electronic properties, micrometer scale Hall-bar devices with high- κ dielectric (Al₂O₃) top gates have been fabricated. Systematical measurements of temperature dependent and electrical field modulated magnetotransport are performed to exam the conduction contributed by the surface states.

12:15PM J31.00006 Weak anti-localization behavior in Bi₂(SeTe)₃ grown on GaAs (001) substrate, JOSEPH HAGMANN, JACEK FURDYNA, MALGORZATA DOBROWOLSKA, XINYU LIU, University of Notre Dame — A series of Bi₂(SeTe)₃ thin films were grown by molecular beam epitaxy on GaAs(001) substrates in order to obtain ternary Te-Bi-Se-Bi-Te alloys with large bulk resistivities. X-Ray diffraction data reveals many reflections from only the {003}-type lattice planes, indicative of highly directed c-axis growth of these films despite the very different crystal symmetries of the film and the substrate along the film growth direction. The X-ray data reveal that a wide spectrum of mixed Bi₂(SeTe)₃ alloys can be obtained by this method [1]. Our studies show that the alloy films are highly uniform, and the crystallinity is comparable to that of films grown on substrates with hexagonal surface structure. In this work, we have carried out comprehensive magneto-transport measurements on a series of Bi₂(SeTe)₃ thin films. We find that the conductivities of the films are strongly affected by alloy composition, and that insulating samples can be obtained at Se concentrations of ~30%. Moreover, we observe weak anti-localization behavior in all samples, which is also composition-dependent. In order to understand diffusive transport in these topological insulator alloys, both disorder and electron-electron interaction effects are considered in our analysis. [1] X. Liu et al, J. Vac. Sci. Tech. B (submitted).

12:27PM J31.00007 Transport in topological insulator films¹, JIAN WANG, International Center for Quantum Materials, Peking University, Beijing 100871, ASHLEY DASILVA, MEENAKSHI SINGH, JOON SUE LEE, JAINENDRA JAIN, NITIN SAMARTH, MOSES H.W. CHAN, The Center for Nanoscale Science and Department of Physics, The Pennsylvania State University, University Park, PA 16802, USA, CUI-ZU CHANG, KE HE, XU-CUN MA, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, QI-KUN XUE, Department of Physics, Tsinghua University, Beijing 100084, China, HANDONG LI, MAOHAI XIE, Physics Department, The University of Hongkong, Pokfulam Road, Hongkong, China — The prediction and the subsequent confirmation of topological insulators is one of the most exciting discoveries in condensed matter physics. In the transport study of topological insulator films, we demonstrate that an excellent agreement between theory and experiment is achieved when both disorder and interaction are taken into account. In addition, measurements under an in-plane magnetic field, along and perpendicular to the bias current show opposite magnetoconductance. Furthermore, Bi₂Se₃ topological insulator thin films contacted by superconducting (In, Al and W) electrodes show an abrupt resistance upturn when the electrodes become superconducting. Concomitant with the upturn in resistance, there is a significant weakening of the superconductivity of the electrodes.

¹This work was financially supported by the Penn State MRSEC under NSF grant DMR-0820404, the National Natural Science Foundation of China (No. 11174007), and NBRP of China (No. 2012CB921300).

12:39PM J31.00008 Magneto-transport study of the topological insulator Bi₂Te₃¹, PRAMOD KUMAR, ARUNA RAMANAYAKA, RAMESH MANI, Georgia State University — Topological insulators are electronic materials that have a bulk band gap like an ordinary insulator, but have protected surface or edge states. Many materials have been realized as topological insulators, including the HgTe/CdTe superlattice, Bi_{1-x}Sb_x, Bi₂Se₃, Sb₂Te₃ and Bi₂Te₃. Topological insulators are interesting not only because of their fundamental importance but also their great potential for future applications. Here, we examine the magneto-transport properties of exfoliated Bi₂Te₃ specimens prepared from Bi₂Te₃ single crystals using the scotch tape method. Indium and silver paint contacts were applied to the exfoliated specimens and magneto-transport was examined at liquid helium temperatures at moderate magnetic fields. The results of these experiments will be described here within the context of the ongoing interest in topological insulators.

¹ARO: W911NF-07-01-0158, DOE: DE-SC0001762

12:51PM J31.00009 Theoretical study of carrier transport and screening in topological insulator Bi₂Se₃¹, SHAFFIQUE ADAM, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD, E.H. HWANG, Condensed Matter Theory Center, University of Maryland, College Park, MD, M.D. STILES, CNST, NIST, Gaithersburg, S. DAS SARMA, CMTc, UMD, College Park — This theoretical work is motivated by two recent experiments on Bi₂Se₃ examining the charge inhomogeneity [1-2] close to the topologically protected crossing point of surface bands in these bulk topological insulators. Reminiscent of graphene close to charge neutrality [3-4], the energy landscape becomes highly inhomogeneous, forming a sea of electron and hole puddles, which determine the properties at low carrier density. Here, we show that the induced carrier density fluctuations are of order 1 % of the impurity density, providing a small-parameter with which we can perform a controlled perturbation theory. Analytic results are obtained for the minimum conductivity and puddle auto-correlation length. We also find that the band asymmetry between electron and holes states is a necessary ingredient to understand the aforementioned experiments. **References:** [1] H. Beidenkopf et al, "Spatial fluctuations of helical Dirac fermions on the surface of topological insulators," Nat. Phys. online publ., (2011) [2] D. Kim et al., "Minimum conductivity and charge inhomogeneity in Bi₂Se₃," arXiv:1105.1410. [3] S. Adam et al., "A self-consistent theory for graphene transport," PNAS **104**, 18392 (2007). [4] S. Das Sarma et al., "Electronic transport in 2D graphene," Rev. Mod. Phys. **83**, 407 (2011).

¹This work is supported in part by LPS-NSA-CMTC.

1:03PM J31.00010 Minimum conductivity and charge inhomogeneity in Bi₂Se₃ in the topological regime¹, DOHUN KIM, SUNGJAE CHO, NICHOLAS BUTCH, PAUL SYERS, KEVIN KIRSCHENBAUM, JOHNPIERRE PAGLIONE, MICHAEL FUHRER, University of Maryland — Using electrolytic and dielectric dual gating method, we report charge transport measurements of mechanically exfoliated Bi₂Se₃ in the topological insulator (TI) regime. We show that the surfaces of thin, low-doped Bi₂Se₃ crystals are strongly electrostatically coupled, and a gate electrode can be used to completely remove bulk charge carriers and bring both surfaces through the Dirac point nearly simultaneously with well-defined ambipolar electronic conduction of gapless surface states. In particular, we focus on linear carrier density dependent conductivity away from the Dirac point and a charge-inhomogeneous minimum conductivity region similar to that observed in graphene. An extension of the theory of charge disorder in graphene to Bi₂Se₃ explains well the mobility at high carrier density and the doping level at zero gate voltage. We show that the observed minimum conductivity is governed by induced carrier density that is self-consistently determined by the screened, charged impurity potential, as experimentally observed in recent STM study on surfaces of TIs.

¹The authors acknowledge support from Center for Nanophysics and Advanced Materials (CNAM).

1:15PM J31.00011 Gate-tunable electronic transport in topological insulator Bi₂Te₃ thin films synthesized by metal-organic chemical vapor deposition, HELIN CAO, Physics department, Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47907, RAMA VENKATASUBRAMANIAN, JONATHAN PIERCE, Center for Solid State Energetics, RTI International, Research Triangle Park, NC 27709, TAI-LUNG WU, JIFA TIAN, ISAAC CHILDRES, Physics department, Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47907, YONG CHEN, Physics department, Birck Nanotechnology Center, School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN 47907 — Topological insulator is a new state of matter with a nominally insulating gap in the bulk and non-trivial metallic states on the surface. One of the proto-type topological insulator materials, Bi₂Te₃, can be synthesized in the form of high quality, wafer scale thin films by metal-organic chemical vapor deposition (MOCVD). Here we present an experimental study of Bi₂Te₃ thin films with thickness ranging from a few nm's to 1 μm synthesized by MOCVD on semi-insulating GaAs (001) substrates. Hall bar shaped devices using atomic layer deposition (ALD) high-k Al₂O₃ or HfO₂ as gate dielectric have been fabricated. We have measured the magneto-transport (including both R_{xx}, 4-terminal longitudinal resistance, and R_{xy}, the Hall resistance) at various temperatures and gate voltages to probe the possible transport signatures of the topological surface states. We have also studied gate-tunable weak anti-localization in R_{xx}(B) for ultra-thin films.

1:27PM J31.00012 Ambipolar field effect in the ternary topological insulator $(\text{Bi}_x\text{Sb}_{1-x})_2\text{Te}_3$ by composition tuning, YULIN CHEN, DESHENG KONG, JUDY CHA, QIANFAN ZHANG, JAMES ANALYTIS, KEJI LAI, ZHONGKAI LIU, SEUNG-SAE HONG, KRISTIE KOSKI, Stanford University, SUNG-KWAN MO, ZAHID HUSSAIN, Lawrence Berkeley National Lab, IAN FISHER, ZHI-XUN SHEN, YI CUI, Stanford University, STANFORD UNIVERSITY COLLABORATION, LAWRENCE BERKELEY NATIONAL LAB COLLABORATION — Topological insulators exhibit a bulk energy gap and spin-polarized surface states that lead to unique electronic properties, with potential applications in spintronics and quantum information processing. However, transport measurements have typically been dominated by residual bulk charge carriers originating from crystal defects or environmental doping, and these mask the contribution of surface carriers to charge transport in these materials. Our recent work demonstrates that the ternary sesquichalcogenide $(\text{Bi}_x\text{Sb}_{1-x})_2\text{Te}_3$ is a tunable topological insulator system. By tuning the ratio of bismuth to antimony, we are able to reduce the bulk carrier density by over two orders of magnitude, while maintaining the topological insulator properties. As a result, we observe a clear ambipolar gating effect in $(\text{Bi}_x\text{Sb}_{1-x})_2\text{Te}_3$ nanoplate field-effect transistor devices, similar to that observed in graphene field-effect transistor devices. The manipulation of carrier type and density in topological insulator nanostructures demonstrated here paves the way for the implementation of topological insulators in nanoelectronics and spintronics.

1:39PM J31.00013 Signature of Topological Insulators in Conductance Measurements, SEOKMIN HONG, VINH DIEP, SUPRIYO DATTA, Purdue University — Following the discovery of spin-polarized states at the surface of three-dimensional topological insulators (TI) like Bi_2Te_3 and Bi_2Se_3 , there are intense interests in possible electrical measurements demonstrating unique signatures of these unusual states. A recent interesting proposal suggests that a signature of TI material should be a change in the conductance measured between a normal contact and a magnetic contact when the magnetization of the latter is reversed. However, the generalized Onsager relation suggests that no such change is expected in two-terminal setups and a multi-terminal set up is needed to observe the proposed effect. We present numerical results using a Non-Equilibrium Green Function (NEGF) based model capable of covering both ballistic and diffusive transport regimes seamlessly. Simple expressions based on a semi-classical picture describe some of the results quite well. Finally, we estimate the magnitude of signal expected in realistic samples that have recently been studied experimentally and have shown evidence of surface conduction.

1:51PM J31.00014 Coupling between 3-D topological insulator and superconductor¹, VLADIMIR ORLYANCHIK, MARTIN STEHNO, CHRISTOPHER NUGROHO, DALE VAN HARLINGEN, University of Illinois at Urbana-Champaign, NAMRATA BANSAL, MATTHEW BRAHLEK, SEONGSHIK OH, Rutgers, The State University of New Jersey — Topological insulators are band insulators in the bulk with gapless topologically protected surface states. Recently it has been predicted that 3-D topological insulators (TI) can host zero energy modes called Majorana fermions. Many theoretical proposals for observation of the zero energy excitations involve coupling between the surface states of TI and s-wave superconductors (SC). A prerequisite for such experiments is a highly tunable surface which is decoupled from the residual bulk carriers and well established coupling between TI and superconductor. Here we present transport measurements performed in high quality MBE grown thin films of Bi_2Se_3 . Along with presenting evidence for significant contribution of the surface states to the electrical transport, we discuss the dependence of TI-SC coupling on temperature, gate voltage and thickness of TI films.

¹Supported by Microsoft Station-Q program

2:03PM J31.00015 Aging effect on carrier density and mobility of thin film Bi_2Se_3 and Bi_2Te_3 grown on Al_2O_3 , NIKESH KOIRALA, MATTHEW BRAHLEK, Rutgers University-Department of Physics and Astronomy, NAMRATA BANSAL, Rutgers University- Department of Electrical and Computer Engineering, SEONSHIK OH, Rutgers University-Department of Physics and Astronomy — Topological Insulators (TI) are materials with topologically protected metallic surface states and insulating bulk states. Bi_2Se_3 and Bi_2Te_3 are viable TI material as they possess bulk band gap as well as continuous surface band. However, there is bulk conduction as well in these materials due to Fermi surface lying in the bulk conduction band. Natural n-type doping due to ambient oxygen and water vapor and/or creation of Se/Te vacancies create bulk contamination, leading to change in carrier density and mobility. We report transport measurement data on epitaxially grown thin films of these materials which show the dependence of charge carrier density and mobility on environmental exposure time of these samples. In addition, we will present our data on samples capped with various materials.

Tuesday, February 28, 2012 11:15AM - 2:15PM –

Session J32 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides - Domain Structures and Switching 261

11:15AM J32.00001 Superdomains and Flux Closure Patterns in Ferroelectrics¹, MARTY GREGG, Queens University Belfast — Microstructural complexity has been a recognized feature of ferroelectric materials since the earliest optical microscopy studies on BaTiO_3 over 60 years ago,^{2,3} in which rich patterns of domain states were observed. Arlt and Sasko⁴ famously highlighted the existence of bands of domain structures forming herringbone patterns and, in so doing, helped to establish the notion that domain architectures exist over a number of different length scales: hierarchies naturally develop in which coarse-scale “superdomains” are themselves composed of sets of finer-scale “subdomains.” What was not widely recognised, was that these “superdomains” could act as functional entities in their own right, with net polarisation and spontaneous strain being the vector sum of these quantities from constituent “subdomains”. In this talk, we will explore the dominant role that superdomain functionality can have on the behaviour of ferroelectrics, at least at the meso and nanoscales. Observations made on single crystal thin film sheets and nanodots of BaTiO_3 (machined using a Focused Ion Beam Microscope) will be presented and several key points will be made: (i) that boundaries between superdomains generally adhere to the same constraints as those seen in subdomains (for example, that the divergence in the net superdomain polarisation across boundaries is zero); (ii) that superdomains demonstrate the same scaling laws (Landau-Kittel scaling) as were originally developed for simple subdomains; (iii) that ferroelectric switching can be entirely mediated by superdomains rather than subdomains; (iv) that flux closure objects, which extend beyond the nanoscale, require the existence of superdomains. The dynamics of flux closure formation, due to depolarising fields, has also been mapped and will be presented.

¹The EPSRC is acknowledged for financial support.

²P. W. Forsbergh, Phys. Rev. 76, 1187 (1949).

³W. Merz, Phys. Rev. 95, 690 (1954).

⁴G. Arlt and P. Sasko, J. Appl. Phys. 51, 4956 (1980).

11:51AM J32.00002 Superdomain dynamics in single-crystal BaTiO₃ lamellae, RAYMOND MCQUAID, LEO MCGILLY, Queens University Belfast, PANKAJ SHARMA, ALEXEI GRUVERMAN, University of Nebraska, Lincoln, MARTY GREGG, Queens University Belfast — In the 1950's early studies pioneered by Merz established that 180° domain reversal in bulk BaTiO₃ could be described by a 3-stage switching process [see H. L. Stadler, *Ferroelectrics* 137, 1992]. This involved formation of a reversed domain nucleus, forward growth of a needle shaped domain towards the opposite electrode followed finally by sideways expansion. In a recent study [R. G. P. McQuaid, *Nat. Comms.* 2, 2011] we used Piezoresponse Force Microscopy (PFM) to monitor the switched domain states that developed in single-crystal BaTiO₃ slices machined (by Focused Ion Beam) to thin film thicknesses and incorporated into a coplanar geometry. We found that switched states are constrained to exist within a rigid framework of ordered ferroelastic stripe domains. Surprisingly, we see that switching occurs solely by the movement of a complex 180°-type boundary which separates 'bundles' of these domain stripes. We see that it is at the collective 'superdomain' level, rather than for individual domains, where the classic Merz nucleation and growth modes are observed. We use PFM imaging to track the realtime boundary position during switching and attempt model fits to understand its field driven dynamics.

12:03PM J32.00003 Theoretical study of ferroelectric switching of Pt/BaTiO₃ Slabs, KURT FREDRICKSON, ALEX DEMKOV, The University of Texas at Austin — BaTiO₃(BTO) is a well known ferroelectric perovskite, which is tetragonal at room temperature. The energy barrier for polarization switching is small at 9.7 meV; however, its energy barrier clamped between two metal electrodes is an open question. It has been shown (Junquera & Ghosez, *Nature* 422, 506 (2003)) that the ferroelectric behavior is highly thickness dependent. We examine thin slabs of BTO sandwiched between electrodes of Pt and calculate the polarization barriers using density functional theory to see whether the barrier should be surmountable. We have found that the energy barrier/unit cell reaches the bulk value at only 10 unit cells of BTO. We also examine the polarization of the relaxed slabs and compare them to bulk BTO, and find that the center of the slab exhibits bulk rumpling at 20 unit cells of BTO.

12:15PM J32.00004 Probing Nanoscale Ferroelectric Domain Switching Mechanisms with Scanning Probe Microscopy¹, VASUDEVA RAO ARAVIND, Clarion University of Pennsylvania, SENLI GUO, AMIT KUMAR, STEPHEN JESSE, SERGEI KALININ, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, VENKATRAMAN GOPALAN, Pennsylvania State University, University Park, PA, CLARION UNIVERSITY COLLABORATION, CENTER FOR NANOPHASE MATERIALS SCIENCES COLLABORATION, PENNSYLVANIA STATE UNIVERSITY COLLABORATION — Ferroelectric domains and domain walls have been a focus topic for research, owing to their applications in memory devices, ultrasonic imaging devices, etc. Recently, ferroelectric domain walls have been demonstrated to exhibit a rich panoply of nanoscale switching behaviors (V. R. Aravind *et al*, *Physical Review B* 82, 024111 (2010)). In this presentation, we report our study of domain reversal and polarization relaxation behavior of ferroelectric domain walls under localized electric field provided by a scanning probe microscope tip. Our studies show the relaxation behaviors differs at different distances from a 180 degree domain wall, throwing light on the microscopic mechanisms of polarization reversal.

¹We acknowledge the financial support from National Science Foundation, NSF-ROA 0908718.

12:27PM J32.00005 In situ TEM studies of interaction between ferroelastic and ferroelastic domains during ferroelectric switching, PENG GAO, CHRISTOPHER NELSON, JACOB JOKISAARI, Department of Materials Science and Engineering, University of Michigan, SEUNG-HYUB BAEK, CHUNG WUNG BARK, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of WisconsinMadison, XIAOQING PAN, Department of Materials Science and Engineering, University of Michigan — Dynamic interaction between ferroelastic (90 degree) and ferroelectric (180 degree) domains in lead zirconate titanate during ferroelectric switching was investigated by in situ TEM. It was found that 90 degree domain walls were immobile under applied bias and act as obstacles to 180 degree domain wall motion. Pinning of the incident 180 degree domain wall occurs directly at the leading 90 degree domain wall and results in a charged head-to-head polarization vector configuration and thereby a large surface energy. This causes the roughening of the domain wall which was atomically sharp before switching. Subsequent switching occurs through the nucleation of a new domain on the opposite 90 degree domain wall and ultimately results in 180 degree switching across the film with the 90 degree domain wall still present. Although they were immobile, the 90 degree domains could sometimes be erased by an external electrical field parallel to the normal axis polarization and would return when the field was removed. This suggests that a pre-pulse opposite to the desired writing direction which momentarily erases these domains may improve switching efficiency.

12:39PM J32.00006 Vortex polarization, strain induced phase transitions and dielectric response in ultra-thin PbTiO₃ nanowires from first principles¹, GHANSHYAM PILANIA, R. RAMPRASAD, University of Connecticut — Nature of ferroelectricity in nanostructures and the resulting dielectric response are of both fundamental and applied interest. Here, using density functional theory (DFT) based computations, we investigate polarization configurations as a function of axial strain in ultra-thin PbTiO₃ [001] nanowires. Our computations involved relaxed and axially strained free-standing nanowires with varying sidewall terminations and diameters. While stress-free nanowires with their sidewalls terminated by PbO surfaces displayed purely rectilinear axial polarization at all sizes, the TiO₂-terminated nanowires, at a critical diameter of 16 Å, display a non-rectilinear vortex polarization transverse to the nanowire axis. We discuss the origins of such behavior. We also predict the existence of novel stress-induced phase transitions between the mutually exclusive vortex and the axial polarization states in both the PbO- and TiO₂-terminated nanowires. Normal mode vibrational frequency analysis of these nanowires further confirms these results. Furthermore, by employing density functional perturbation theory in combination with effective medium dielectric theory we calculate dielectric permittivity of the ferroelectric nanowires and compare it with the corresponding bulk results.

¹This research is based upon work supported by the Office of Naval Research. Computational support was provided through a National Science Foundation Teragrid Resource Allocation.

12:51PM J32.00007 Domain Wall Nucleation and Propagation within Ferroelectric Nanowires in High Strength Electric Fields¹, KEVIN MCCASH, University of South Florida, ARVIND SRIKANTH, University of Illinois at Urbana-Champaign, INNA PONOMAREVA, University of South Florida — Ferroelectric nanowires have attracted a lot of attention recently, thanks to their ability to develop electric polarization at the nanoscale [1]. Such a unique feature could potentially lead to the use of such nanowires in nanoscale, ultra fast, high-density memory elements. Here we take advantage of accurate first-principles-based simulations to study ultra fast polarization reversal in ultra thin ferroelectric nanowires made of PbTi_{0.6}Zr_{0.4}O₃ alloy. Our computational experiments reveal that polarization reversal in such nanowires is both qualitatively and quantitatively different from their bulk counterparts and exhibits unique features that could find potential use in nanoscale ferroelectric memory elements. [1] P.M. Rørvik, T. Grande, and M.-A. Einarsrud (2011), One-Dimensional Nanostructures of Ferroelectric Perovskites. *Advanced Materials*, 23: 4007-4034

¹The present work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under award DE-SC0005245

1:03PM J32.00008 Terahertz Frequency Dynamics of Ferroelectric Nanowires¹ , RYAN HERCHIG,

University of South Florida, KIMBERLY SCHULTZ, Carthage College, KEVIN MCCASH, INNA PONOMAREVA, University of South Florida — A thorough understanding of ferroelectric nanostructures is imperative considering their utility in creating nanoscale devices for the technology of the future. One such ferroelectric nanostructure which may prove useful in the design of nanosensors is the nanowire. We report our study on ferroelectric nanowires of $\text{Pb}(\text{Zr}_{0.4}\text{Ti}_{0.6})\text{O}_3$ alloy done using classic molecular dynamics with first-principle-based effective Hamiltonian[1] and Evans-Hoover thermostat. We found that 1) the polarization of such nanowires can be reversed and 2) that the nanowires temperature can be controlled by the application of a terahertz electric field pulse. The dependence of these properties on the frequency, width, and amplitude of the pulse is explored and discussed in addition to a possible energy dissipation mechanism. [1] L. Bellaiche *et al*, Phys. Rev. Lett. 8, 5427 (2000).

¹The present work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under award DE-SC0005245 (computational studies) and by the Army Research Office under contract 57787-EL.c

1:15PM J32.00009 Origin of 90° Domain Wall Pinning in $\text{Pb}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{O}_3$ Heteroepitaxial Thin

Films , DONG SU, Center for Functional Nanomaterials, Brookhaven National Lab, QINGPING MENG, MMYUNG-GEUN HAN, CMPMS, Brookhaven National Lab, CARLOS VAZ, YARON SEGAL, MATTHEW MARSHALL, FRED WALKER, Department of Applied Physics and CRISP, Yale University, MONICA SAWICKI, CHRISTINE BROADBRIDGE, Department of Physics, Southern Connecticut State University, CHARLES AHN, Department of Applied Physics and CRISP, Yale University — Researchers have studied the effect of ferroelectric fields in controlling the spin state via electric fields in multiferroic composite structures. For instance, in a bilayer system composed of a ferroelectric perovskite ($\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$) and a colossal magnetoresistive (CMR) manganite ($\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3$, LSMO), the spin state in the CMR film can be controlled by switching the ferroelectric polarization state, thereby generating a large magnetoelectric coupling. For this system, the domain's structure and switchability is critically important to the device's performance. We describe transmission-electron-microscopy study of the ferroelectric domains in an epitaxial $\text{Pb}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{O}_3$ (PZT) film grown on $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3/\text{SrTiO}_3$ (001). We directly observe the pinning of 90° domain walls by pairs of misfit dislocations with Burgers vectors $\mathbf{a}[100]$ and $\mathbf{a}[001]$. Model calculations based on the elastic theory confirm our finding that, in addition to the depolarization field surrounding the dislocation, the strain field of misfit dislocation-pairs plays the primary role in the formation and pinning of a domains.

1:27PM J32.00010 Dynamics of Nanowalls In Ferroelectric Ultrathin Films¹ , QINGTENG ZHANG,

RYAN HERCHIG, INNA PONOMAREVA, Department of Physics, University of South Florida — Nanoscale ferroelectric films can exhibit nanostripes that are nanoscopic regions of “up” and “down” polarizations, hence forming domain walls which separate nanodomains with different polarization directions. The dynamical properties of domain walls are of technological importance since they are at the heart of ultradense ferroelectric memory technology and may play an important role in nanoscale ferroelectric sensors, actuators, and others. Here [1] we take advantage of accurate first-principle-based simulations to reveal the intrinsic dynamics of nanodomains in ultra-thin $\text{PbTi}_{0.6}\text{Zr}_{0.4}\text{O}_3$ films with thickness ranging from 2 to 20 nm. We first demonstrate that the nanodomain walls oscillate under driving AC-field of sub-switching amplitude. Secondly, we reveal that nanowalls can exhibit two types of intrinsic dynamics (resonance and relaxation) at the same frequencies. Thirdly, we prove that at nanoscale the dynamics is determined by the domain size which manifests itself via a unique size-driven transition from relaxational to resonance dynamics.

[1] Q. Zhang et al, Phys. Rev. Lett. 107, 177601 (2011).

¹The present work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under award DE-SC0005245 (computational studies).

1:39PM J32.00011 Nanoscale Ferroelectric Switching in Thin Films by in-situ TEM for Magnetoelectric Applications , CHRISTOPHER NELSON, PENG GAO, JACOB JOKISAARI, University of Michigan, COLIN HEIKES, CAROLINA ADAMO, ALEXANDER MELVILLE, Cornell University, SEUNG-HYUB BAEK, CHAD FOLKMAN, University of Wisconsin-Madison, BENJAMIN WINCHESTER, YIJIA GU, Penn State University, YUANMING LIU, University of Washington, KUI ZHANG, University of Michigan, ENGE WANG, School of Physics, Peking University, China, JIANGYU LI, University of Washington, LONG-QING CHEN, Penn State University, CHANG-BEOM EOM, University of Wisconsin-Madison, DARRELL SCHLOM, Cornell University; Kavli Institute at Cornell for Nanoscale Science, Ithaca, XIAOQING PAN, University of Michigan

— The ferroelectric switching along the low-dimensional axis of nanoscale multiferroic BiFeO_3 thin films is studied in this work using in-situ transmission electron microscopy. With this technique, the atomic scale polarization distribution and the controlling influence of defects on growth kinetics are observed. Despite the inhomogeneous external field applied by a surface probe, nucleation sites are determined by the built-in fields formed within carrier depletion regions at the electrode interfaces. Homogenous full-film switching is often impeded by the pinning of domain growth by such features as point defect assemblies and from independent switching in the near-interface region. This inhomogeneity along the normal film axis has significant implications for the interpretation of surface probe ferroelectric switching measurements and for magnetoelectric applications which require ferroelastic switching at the interface.

1:51PM J32.00012 Domain dynamics during ferroelectric switching , XIAOQING PAN, PENG GAO, CHRISTOPHER NELSON, JACOB JOKISAARI, Department of Materials Science and Engineering University of Michigan, Ann Arbor, Michigan 48109, SEUNG-HYUB BAEK, CHUNG-WUNG BARK, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin, Madison, Wisconsin 53706, DARRELL SCHLOM, Department of Materials Science and Engineering Cornell University, Ithaca, NY 14853

— Ferroelectric materials are characterized by a spontaneous polarization that can be reoriented by an applied electric field. The ability to form and manipulate domains at the nanometer scale is key to device applications such as nonvolatile memories. The ferroelectric switching is mediated by defects and interfaces. Thus, it is critical to understand how the domain forms, grows, and interacts with defects. Here we show the nanoscale switching of a tetragonal $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$ thin film under an applied electric field using *in situ* transmission electron microscopy. We found that the intrinsic electric fields formed at ferroelectric/electrode interfaces determine the nucleation sites and growth rates of domains and the orientation and mobility of domain walls, while dislocations exert a weak pinning force on domain wall motion. We also show that localized 180° polarization switching initially form domain walls along unstable planes. After removal of the external field, they tend to relax to low energy orientations. In sufficiently small domains this process results in complete backswitching. Our results suggest that even thermodynamically favored domains are still subject to retention loss, which must be mitigated by overcoming a critical domain size.

2:03PM J32.00013 Modeling Micron Size Multi-domain Ferroelectric Switching using a Massively Parallel Time Domain Phase-Field Model , KHALID ASHRAF, SAYEEF SALAHUDDIN, UC Berkeley, LABORATORY OF EMERGING AD EXPLORATORY DEVICES TEAM

— For the study of devices incorporating multi-domain ferroelectric materials, it is necessary to extend the current capabilities of the phase field model up to the micron scale where experiments are typically performed. Also arbitrary electrical and mechanical boundary conditions need to be incorporated relatively easily. In this work, we report a time domain implementation of the 3D phase field model that can simulate multi-domain ferroelectric switching. This massively parallel implementation enables us to study the switching properties of micron size devices with $\sim 10^9$ degrees of freedom. We used a mixed finite difference and finite element grid, for calculating the nonlocal electrostatic and elastic interactions respectively. All the local and non-local interactions are shown to scale linearly up to thousands of processors. The model can take into account arbitrary electrical and mechanical boundary conditions suitable for the study of devices with arbitrary structures. Using this model, we report the simulation results of ferroelectric switching in devices incorporating the multi-ferroic material BiFeO_3 . We explain the domain growth mechanism observed in multiple experiments reported recently on various surfaces of BiFeO_3 .

Tuesday, February 28, 2012 11:15AM - 2:03PM – Session J34 DCP: Focus Session: Impact of Ultrafast Lasers III: Biophysics 107A

11:15AM J34.00001 Probing Electronic Excitations in Molecules by Coherent Multidimensional UV and X Ray Spectroscopy, SHAUL MUKAMEL, University of California, Irvine — Two-dimensional ultraviolet (2DUV) spectra of protein backbone (far UV) and side chains (near UV) provide new insights into the protein structures, dynamics and functions. Simulated chirality-induced 2DUV spectra reveal characteristic patterns of protein secondary structures and allow monitoring the aggregation mechanism of amyloid fibrils and predicting the aggregation propensity of peptides. Time-domain experiments that employ sequences of attosecond x-ray pulses in order to probe electronic and nuclear dynamics in molecules are made possible by newly developed bright coherent ultrafast sources of soft and hard x-rays. By creating multiple core holes at selected atoms and controlled times it should be possible to study the dynamics and correlations of valence electrons as they respond to these perturbations. The stimulated x-ray Raman spectrum of *trans*-N-methylacetamide and Cysteine at the Nitrogen, Sulfur and the Oxygen K-edges in response to two soft x-ray pulses is calculated by treating the core excitations at the Hartree-Fock static-exchange level (STEX) level. The signal is interpreted in terms of the dynamics of valence electronic wave packets prepared and detected in the vicinity of (either the nitrogen or the oxygen) atom. The evolving electronic charge density and as electronic coherences are visualized using a basis set of time-dependent natural orbitals. Effects of orbital relaxation upon core excitations are resolved. A two-dimensional extension of the technique that involves a sequence of three resonant Raman pulses will be presented. Extensions to multidimensional spectroscopy with photoelectron detection are proposed.

11:51AM J34.00002 Conformation of self-assembled porphyrin dimers in liposome vesicles by phase-modulation 2D fluorescence spectroscopy, ALEJANDRO PERDOMO-ORTIZ, Department of Chemistry and Chemical Biology, Harvard University, GEOFFREY A. LOTT, JAMES K. UTTERBACK, Department of Physics, Oregon Center for Optics, University of Oregon, JULIA R. WIDOM, Department of Chemistry, Oregon Center for Optics, Institute of Molecular Biology, University of Oregon, ALÁN ASPURU-GUZIĆ, Department of Chemistry and Chemical Biology, Harvard University, ANDREW H. MARCUS, Department of Chemistry, Oregon Center for Optics, Institute of Molecular Biology, University of Oregon — By applying a phase-modulation fluorescence approach to 2D electronic spectroscopy (PM-2D FS), we studied the conformation-dependent exciton coupling of a porphyrin dimer embedded in a phospholipid bilayer membrane. Our measurements specify the relative angle and separation between interacting electronic transition dipole moments and thus provide a detailed characterization of dimer conformation. PM-2D FS produces 2D spectra with distinct optical features, similar to those obtained using 2D photon-echo spectroscopy. Specifically, we studied magnesium meso tetraphenylporphyrin dimers, which form in the amphiphilic regions of 1,2-distearoyl-sn-glycero-3-phosphocholine liposomes. Comparison between experimental and simulated spectra show that although a wide range of dimer conformations can be inferred by either the linear absorption spectrum or the 2D spectrum alone, consideration of both types of spectra constrain the possible structures to a “T-shaped” geometry. These experiments establish the PM-2D FS method as an effective approach to elucidate chromophore dimer conformation.

12:03PM J34.00003 2-Dimensional Fluorescence Spectroscopy: Determining the Temperature-Dependent Conformations of Porphyrin Dimers and Nucleic Acids¹, JULIA WIDOM, University of Oregon, ALEJANDRO PERDOMO-ORTIZ, ALAN ASPURU-GUZIĆ, Harvard University, ANDREW MARCUS, University of Oregon — I will describe spectroscopic studies on a covalently-linked zinc tetraphenylporphyrin dimer embedded in a phospholipid bilayer membrane. Using phase-modulation 2-Dimensional Fluorescence Spectroscopy (2D FS, a fluorescence-detected version of 2D electronic spectroscopy) along with linear absorption and fluorescence spectroscopy, it was found that the dimer adopts two predominant conformations in the membrane, and that the relative populations of these two states change as a function of temperature. Simultaneously fitting the linear absorption spectrum and the 2D FS spectra at four different excitation wavelengths revealed a wealth of information about these two states, including their relative populations, relative fluorescence quantum yields, the strength of the exciton coupling present in each state, and the approximate angles between the electronic transition dipole moments of the two porphyrins. Ongoing analysis focuses on elucidating the relaxation and energy transfer dynamics of this system through the population time dependence of the 2D spectra. Finally, I will present preliminary results from experiments in which 2D FS was performed with ultraviolet excitation to study the conformations of DNA constructs labeled with a fluorescent analogue of guanine.

¹This work was funded by the National Science Foundation and the Oregon Nanoscience and Microtechnologies Institute.

12:15PM J34.00004 Probing photosynthetic structure and function using multidimensional spectroscopy, JENNIFER OGILVIE, University of Michigan — No abstract available.

12:51PM J34.00005 Exploring Relaxation Processes in Components of DNA with UV Non-linear Spectroscopy, ANDREW MORAN, BRANTLEY WEST, JORDAN WOMICK, University of North Carolina — Underlying photoinduced relaxation in DNA is a complex world of solute-solvent interactions and fluctuations in the geometries of macromolecules. Electronic excitations are rapidly deactivated by nuclear motions through conical intersections, thereby suppressing the formation of lesions (e.g., thymine dimers) known to inhibit cellular function. At the instant following internal conversion, the bases are left in “hot” quantum states, wherein a subset of vibrational modes possess a highly non-equilibrium distribution of excitation quanta. The transfer of this energy to the surrounding also involves intriguing fundamental physics. We examine these processes in small components of DNA by conducting femtosecond laser spectroscopies at cryogenic temperatures. Our experiments utilize several recent advances in nonlinear optics. Parametric processes in argon gas are used to generate 25fs pulse durations at 265nm. These short pulses are employed in a variety of measurements (e.g., transient grating, 2D photon echo, fluorescence down-conversion) with the goal of understanding relaxation mechanisms. Our data suggest that excited state deactivation in DNA is quite sensitive to the exchange of vibrational energy between the bases and segments of the backbone.

1:03PM J34.00006 Early optical response of fluorescent molecules studied by synthetic optically delayed pulses¹, ARKAPRABHA KONAR, JAY SHAH, TAPAS GOSWAMI, VADIM LOZOVY, MARCOS DANTUS, Michigan State University — The early optical response of fluorescent molecules in solution is probed by pairs of collinear pulse replicas. Two approaches are followed. First approach mimics an interferometer, replicating interference as a function of time delay between the pulses. For the second approach, each pulse spans the entire laser bandwidth, sharing no common frequencies with the second pulse, thus no interference is observed between the pulses. In both cases, the pair of pulses is delayed with attosecond resolution to study IR 144. Both fluorescence at right angles or the stimulated emission along the output beam as a function of time delay is monitored. At high intensities when approximately 10% of the dye molecules are excited, the second pulse can stimulate emission from molecules excited by the first pulse, thereby giving rise to interference fringes every 2.66 fs. When the pulse replicas are generated by multiple independent comb shaping, it is evident that the interference fringes for stimulated emission bear an out of phase relationship with those observed from fluorescence and have a maxima at time zero. This is masked with conventional pulse replicas that interfere.

¹Department of Energy

1:15PM J34.00007 Quantum mechanical light harvesting mechanisms in photosynthesis, GREGORY SCHOLES, University of Toronto — More than 10 million billion photons of light strike a leaf each second. Incredibly, almost every red-coloured photon is captured by chlorophyll pigments and initiates steps to plant growth. Last year we reported that marine algae use quantum mechanics in order to optimize photosynthesis [1], a process essential to its survival. These and other insights from the natural world promise to revolutionize our ability to harness the power of the sun. In a recent review [2] we described the principles learned from studies of various natural antenna complexes and suggested how to utilize that knowledge to shape future technologies. We forecast the need to develop ways to direct and regulate excitation energy flow using molecular organizations that facilitate feedback and control—not easy given that the energy is only stored for a billionth of a second. In this presentation I will describe new results that explain the observation and meaning of quantum-coherent energy transfer.

[1] Elisabetta Collini, Cathy Y. Wong, Krystyna E. Wilk, Paul M. G. Curmi, Paul Brumer, and Gregory D. Scholes, “Coherently wired light-harvesting in photosynthetic marine algae at ambient temperature” *Nature* 463, 644-648 (2010).

[2] Gregory D. Scholes, Graham R. Fleming, Alexandra Olaya-Castro and Rienk van Grondelle, “Lessons from nature about solar light harvesting” *Nature Chem.* 3, 763-774 (2011).

1:51PM J34.00008 Temperature dependence of proton transfer kinetics in the green fluorescent protein¹, BRIDGET SALNA, ABDELKRIM BENABBAS, PAUL CHAMPION, J. TIMOTHY SAGE, Northeastern University, JASPER VAN THOR, ANN FITZPATRICK, Imperial College London — In green fluorescent protein (GFP), near UV photoexcitation leads to proton transfer from the chromophore phenolic oxygen along a proton “wire” consisting of an internal water molecule, Ser205 and Glu222. Using transient absorption kinetics, the complete cycle, including the picosecond excited-state proton transfer, the nanosecond radiative emission, and the slower ground state proton back-transfer reactions have been studied holistically as a function of temperature. This experiment was performed for both the hydrogenated and deuterated forms of GFP. We have extracted the Arrhenius prefactors and activation energy barriers for both the forward and back proton transfer kinetics. A large kinetic isotope effect for the ground state proton back-transfer has been observed at high temperatures suggesting that tunneling plays an important role. At lower temperatures the data suggest a cross-over to a different pathway for the back-transfer reaction. To investigate this hypothesis we studied the E222D mutant of GFP, which substitutes aspartate for glutamate on the proton wire. The H/D kinetics of this mutant explicitly test for the source of proton donors and indicate that proton transfer proceeds along the same pathway in the native protein at room temperature.

¹This work is supported by NSF CHE-1026369.

Tuesday, February 28, 2012 11:15AM - 2:03PM — Session J35 DCP: Liquids 107B

11:15AM J35.00001 Ion shape effect on dynamics of ionic liquids, HONGJUN LIU, EDWARD MAGINN, University of Notre Dame — Ionic liquids (ILs) are a group of salts composing of an organic cation and organic or inorganic anion with melting points below 100 °C and have many suitable properties, such as negligible vapor pressure, low flammability, high ionic conductivity and high thermal stability for various applications. Moreover, a great number of ILs with a variety of physical and chemical properties can be synthesized from a combination of different cations (most differently substituted imidazolium, pyridinium, and quaternary ammonium or phosphonium ions) and anions. One can judiciously select from a multitude of ILs to suit a specific application, where the concept of designer solvent comes from. To expedite the development process of target ILs, it is crucial to understand the relationship between ion shape and dynamics of ILs. We studied a wide range of ILs with different ion shape pairings and found the planar-planar paired ILs have a better dynamics as a whole.

11:27AM J35.00002 Thermodynamic Phase Diagram of Hydrogen in Nano-porous Silica, ELI VAN CLEVE, SERGEI KUCHEYEV, Lawrence Livermore National Laboratory — One of the major challenges faced by inertial confinement fusion (ICF) is spherical uniformity of fuel capsules. Most current ignition target designs call for spherically uniform layers of deuterium-tritium (DT) mix in a solid phase. Smooth solid DT layers of high-quality single crystals are necessary, requiring stringent layering protocols. Liquid DT confined in a low-density nano-porous scaffold layer is a possible alternative target, having greatly relaxed layering requirements. Hydrogen in vycor, which has a high density and a relatively uniform pore size distribution, has previously been studied. The porous materials used for this study are silica aerogels. These have ultralow densities and broad pore size distributions. We discuss the thermodynamic phase diagram of hydrogen and deuterium condensed in silica aerogels studied using relaxation calorimetry. We find that crystallization temperatures of both isotopes are suppressed inside the aerogel; however, the freezing takes place over a relatively wide range of temperatures and non-trivially depends on the hydrogen filling fraction. We discuss the correlation of freezing temperatures with the pore size distribution. This work was performed under the auspices of the U.S. DOE my LLNL under Contract DE-AC52-07NA27344.

11:39AM J35.00003 ABSTRACT WITHDRAWN —

11:51AM J35.00004 Quasi-free Electron Energy in Near Critical Point He, YEVGENIY LUSHTAK, SAMANTHA DANNENBERG, CHERICE EVANS, Department of Chemistry, Queens College – CUNY, Flushing, NY and Chemistry Department, the Graduate Center – CUNY, Manhattan, NY, GARY FINDLEY, Chemistry Department, University of Louisiana at Monroe, Monroe, LA — We present the quasi-free electron energy $V_0(\rho)$, where ρ is the density, in He from low density to the density of the gas/He-I/He-II triple point, at various noncritical temperatures and on an isotherm near the critical isotherm. These data, which were obtained using field enhanced photoemission, represent the first extended density overview of $V_0(\rho)$ for He, especially near the critical point. A novel critical point effect is observed and is accurately fitted to the local Wigner-Seitz model, thereby showing that this model, which was developed for attractive systems, can also be applied to repulsive systems.

The experimental measurements reported here were performed at the University of Wisconsin Synchrotron Radiation Center (NSF DMR-0537588). This work was supported by grants from the Petroleum Research Fund (45728-B6) and from the National Science Foundation (NSF CHE-0956719).

12:03PM J35.00005 COSMO-3D: Introducing Steric Effects into COSMO Solvation Models¹, ERIN MCGARRITY, Delft Technical University, JAN VAN DER EERDEN², Condensed Matter and Interfaces-Debye Institute for Nanomaterials Science, Utrecht University, Netherlands, GERARD KROOSHOF, DSM Research, Netherlands — We will present a modified COSMO-based thermodynamical model which can be used for the prediction of solvation in liquid mixtures. The method provides values for the surface-segment interactions and molecular contact areas as functions of the relative positions of all the segment pairings of the constituent molecules in a mixture. These expressions are obtained by placing the complete molecules into contact at each segment pair to determine if the molecules overlap, and using a probing particle to determine the total area of contact. The former expression can be used to discard terms from the COSMO-based segment sums which correspond to overlapping molecular configurations. The areas are used to determine the average contact energies based on Onsager's theory for dielectric screening. Our method allows us to remove three parameters from the original model without any loss of accuracy. We will show the results of our model as applied to binary mixture vapor-liquid equilibrium predictions.

¹This work is funded by the Netherlands Institute for Sustainable Process Technology (PH-00-02A).

²Current Address: Radboud University Nijmegen, Donders Institute for Brain, Cognition and Behaviour, Netherlands

12:15PM J35.00006 Charge induced hydrophobic/hydrophilic metallic surfaces, LUANA PEDROZA, ADRIEN POISSIER, MARIVI FERNANDEZ-SERRA, Stony Brook University — Understanding the interaction of water-metal systems in an atomic level is of fundamental importance in many areas, such as catalysis and materials science. We here present a detailed first-principles molecular dynamics study of bulk water molecules confined within Pd(111) surfaces. We show that there is a charge transfer between the substrate and the water inducing an asymmetry in the order of water molecules at Pd surfaces. Our results show that the hydrophobic/hydrophilic character of a metallic surface depend on its charge, which can be controlled by an applied voltage. We also propose a methodology to obtain the dipole moment of each water molecule and show how they are affected by the substrate induced polarization effects.

12:27PM J35.00007 Pulling adsorbed polymers at an angle: A low temperature theory, GERASIM ILIEV, University of Toronto/York University, STUART WHITTINGTON, University of Toronto — We consider several partially-directed walk models in two- and three-dimensions to study the problem of a homopolymer interacting with a surface while subject to a force at the terminal monomer. The force is applied with a component parallel to the surface as well as a component perpendicular to the surface. Depending on the relative values of the force in each direction, the force can either enhance the adsorption transition or lead to desorption in an adsorbed polymer. For each model, we determine the associated generating function and extract the phase diagram, identifying states where the polymer is thermally desorbed, adsorbed, and under the influence of the force. We note the different regimes that appear in the problem and provide a low temperature approximation to describe them. The approximation is exact at $T=0$ and models the exact results extremely well for small values of T . This work is an extension of a model considered by S. Whittington and E. Orlandini.

12:39PM J35.00008 Low-Energy Electron Induced Reactions in Condensed Methanol, MICHAEL BOYER, Clark University, MAVIS BOAMAH, KRISTAL CHAMBERLAIN, CHANMAYE MYAE SOE, Wellesley College, ANDREW BASS, LEON SANCHE, Université de Sherbrooke, CHRISTOPHER ARUMAINAYAGAM, Wellesley College — We investigate the dynamics of low-energy electron-induced reactions in condensed thin films of methanol (CH_3OH) through electron stimulated desorption (ESD) and post-irradiation temperature programmed desorption (TPD) experiments. ESD experiments indicate that the anions which desorb from the methanol thin film during electron irradiation are predominantly formed through the dissociation of temporary negative ions formed by electron capture by methanol molecules, a process known as dissociative electron attachment (DEA). However, based on investigation of reaction products remaining in the methanol thin film post-irradiation through TPD experiments, DEA is not the obvious primary mechanism by which methoxymethanol ($\text{CH}_3\text{OCH}_2\text{OH}$) and ethylene glycol ($\text{HOCH}_2\text{CH}_2\text{OH}$) are formed. Evidence indicates formation of these molecules may be driven by both DEA and electron impact excitation.

12:51PM J35.00009 The Widom line and noise power spectral analysis of a supercritical fluid¹, SUNGHO HAN, CLARE YU, Department of Physics and Astronomy, University of California, Irvine — In a typical pressure-temperature phase diagram for a fluid, there is a first order phase transition line between the liquid and the vapor phases that terminates at a critical point. Beyond this critical point lies the supercritical regime where one can go continuously between the liquid and vapor phases. In the supercritical region, there is a line of specific heat maxima, called the Widom line, which is often regarded as an extension of the liquid-vapor coexistence line. Using molecular dynamics simulations of a Lennard-Jones fluid, we find that the noise power spectrum of the density fluctuations on the Widom line of the liquid-vapor transition can be divided into 3 frequency regions. The intermediate frequency region with $1/f$ noise appears as the temperature approaches the Widom temperature from above or below. Furthermore, we find that the power spectra of both the density and potential energy fluctuations at low frequency have a maximum on the Widom line, suggesting that the noise power can provide an alternative signature of the Widom line.

¹This work was supported by DOE grant DE-FG02-04ER46107

1:03PM J35.00010 Disappearance of Widom Line for Liquid-Liquid Phase Transition with Horizontal Coexistence Line, JIAYUAN LUO, Boston University, LIMEI XU, Peking University, SERGEY BULDYREV, Yeshiva University, AUSTEN ANGELL, Arizona State University, GENE STANLEY, Boston University — The study of spherically symmetric two-scale Jagla model with both repulsive and attractive ramps has been very successful in demonstrating the anomalous behavior of liquids (especially water) and its relation with respect to the existence of a liquid-liquid (LL) critical point. However, the co-existence line of Jagla model shows a positive slope, which is opposite to what has been found in the simulations of water. To more convincingly link the result of the study on Jagla model with that of water, we applied discrete molecular dynamics to Gibson and Wilding's modified Jagla model and found that by shrinking both the attractive and repulsive ramps, the slope of the coexistence line can be reduced to zero. However, at these values of the parameters, the LL critical point becomes completely unstable with respect to crystal and glass. We further studied the Widom line, defined as extreme of response functions and also continuation of the coexistence line into one phase region, and found Widom line disappeared in the case of zero slope of the coexistence line, due to the equal enthalpy of low-density liquid (LDL) and high-density liquid (HDL).

1:15PM J35.00011 Effects of pressure on transitions between disordered phases in supercooled liquid Si¹, ALEX ANTONELLI, KARL GARCEZ, Universidade Estadual de Campinas — In the last 20 years, there has been an increasing interest in liquid-liquid transitions. Substances that exhibit negative melting slopes are considered to undergo such transitions. In this work, we study the pressure effects on the transitions between the disordered phases in supercooled liquid Si through Monte Carlo simulations and efficient methods to compute free energies. Our calculations, using a realistic interatomic potential for Si, indicate that at zero pressure the liquid-liquid phase transition, between the high density liquid and the low density liquid, occurs at a temperature 325 K below melting. We found that the liquid-liquid transition temperature decreases with increasing pressure, following the liquid-solid coexistence curve. As pressure increases, the liquid-liquid coexistence curve approaches the region where the glass transition between the low density liquid and the low density amorphous takes place. Above 5 GPa, our calculations show that the liquid-liquid transition is suppressed by the glassy dynamics of the system. We also found that above 5 GPa, the glass transition temperature is lower than that at lower pressures, suggesting that under these conditions the glass transition occurs between the high density liquid and the high density amorphous.

¹Supported by FAPESP, CNPq and FAEPEX-UNICAMP.

1:27PM J35.00012 Thermodynamics of Supercooled Water, VINCENT HOLTEN, CHRISTOPHER BERTRAND, MIKHAIL ANISIMOV, JAN SENGERS, Department of Chemical and Biomolecular Engineering and Institute for Physical Science and Technology, University of Maryland, College Park, MD 20742 — We present the currently available experimental information for the thermodynamic properties of supercooled ordinary and heavy water and the possibility of modeling these thermodynamic properties on a theoretical basis. Part of the interest into the thermodynamic behavior of supercooled water is caused by an anomalous temperature dependence of the heat capacity, the compressibility and the thermal expansivity. We show that by assuming the existence of a virtual liquid-liquid critical point in supercooled water, the theory of critical phenomena can give an accurate account of the experimental thermodynamic-property data up to a pressure of 150 MPa. In addition, we show that a semi-empirical extension of the theoretical model can account for all currently available experimental data in the supercooled region, up to 400 MPa. Critical-point thermodynamics describes the available thermodynamic data on supercooled water within experimental accuracy, thus establishing a benchmark for any further developments in this area.

1:39PM J35.00013 Diffusivity crossover and liquid-liquid transition in solutions of hard spheres in Jagla particles, DARIO CORRADINI, Center for Polymer Studies and Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, Massachusetts 02215, USA, PAOLA GALLO, Dipartimento di Fisica, Universita' Roma Tre, Via della Vasca Navale 84, I-00146 Roma, Italy, SERGEY V. BULDYREV, Department of Physics, Yeshiva University, 500 West 185th Street, New York, New York 10033, USA, H. EUGENE STANLEY, Center for Polymer Studies and Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, Massachusetts 02215, USA — We study by discrete molecular dynamics simulations the relation between the thermodynamics and the diffusive behavior in solutions of hard spheres in Jagla particles, close to their liquid-liquid critical point. For comparison, we also show the same properties in the bulk Jagla particles system. The hard spheres and the Jagla model are used as spherically symmetric potentials for small hydrophobic solutes in water. We find that the fragile to strong dynamic transition observed when studying the diffusive behavior is always coupled to the low density to high density liquid transition. Above the liquid-liquid critical pressure the diffusivity crossover happens exactly at the Widom line of the systems, where the thermodynamic response functions show maxima. Below the liquid-liquid critical pressure, the diffusivity crossover corresponds to the crossing of the limit of mechanical stability lines and it shows hysteresis when going from high to low temperatures or vice versa. These findings prove that the strong connection between dynamics and thermodynamics found for bulk Jagla particles persists in hydrophobic solutions for concentrations from low to moderate.

1:51PM J35.00014 Small-to-Large Polaron Transition in Water, SHAHRIAR SHADKHOV, ROBIJN BRUINSMA, Department of Physics and Astronomy, University of California, Los Angeles — Heavier charged particles, such as protons, dissolved in water form a hydration shell, which partially shields the charge and significantly increases their effective mass. On the other hand, electrons do not form a hydration shells in water. Leggett's path-integral formalism can be combined with Feynman's polaron theory to construct a theory for the effective mass of a charged particle in water in terms of the charge structure factor, $S(\mathbf{q}, \omega)$ of water, or alternatively, the frequency and wavefunction dependent dielectric function of water. Measurements of $S(\mathbf{q}, \omega)$ for density fluctuations indicate that water has a soft mode with a wave number in the range of an inverse Angstrom. By combining these experiments with analytical and numerical models of the dielectric function of water, we discuss the small-to-large polaron transition in water.

Tuesday, February 28, 2012 11:15AM - 2:15PM – Session J36 DCP: Focus Session: New Energy III 107C

11:15AM J36.00001 Tailoring Surface Chemical Properties Using Electronic Structure Theory, JENS NORSKOV, Stanford University — Electronic structure methods based on density functional theory have reached a level of sophistication where they can be used to describe complete catalytic reactions on transition metal surfaces. This opens the possibility that computational methods can be used to tailor surfaces with desired chemical properties. Recent progress in this direction for transition metal catalysts will be discussed. A series of concepts will be introduced to describe and understand trends in reactivity from one metal surface to the next. It is shown how these concepts can be used to identify the factors determining the catalytic activity of a given transition metal surface, and how this can form the basis for screening of a large number of metals and alloys for catalytic properties.

11:51AM J36.00002 Ab initio reaction pathways for dissociative adsorption of dioxygen on Al (111)¹, FLORIAN LIBISCH, CHEN HUANG, PEILIN LIAO, MICHELE PAVONE, EMILY CARTER, Dep. of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ — We investigate the interaction of dioxygen with a clean aluminum (111) surface. The theoretical description of this fundamental process is challenging due to the discrete, abrupt charge transfer (CT) from the metal surface to the molecule. Indeed, experimental investigations suggest a sizeable activation barrier not accounted for by a conventional DFT description, due to exchange-correlation functional errors. We adopt a different approach, embedding a small (12 atoms) aluminum cluster in a DFT-derived potential simulating the remainder of the Al surface. The interaction between this embedded cluster and an approaching O₂ molecule is treated using high-level correlated wave function methods (CASSCF, CASPT2) that allow for a correct description of the CT process involved. We map out the potential energy surface (PES) as a function of dioxygen bond length, orientation, and position. In agreement with experiment, we find an activation barrier of ~500 meV, which corresponds primarily to the cost to induce CT. Additionally, the PES is consistent with oxygen abstraction as the dominant process in the case of incident perpendicular orientation, confirming the mechanism proposed to explain the surprisingly large fraction of single oxygen atoms found in STM measurements.

¹We gratefully acknowledge support from the Max Kade foundation NY, the Office of Naval research, as well as the Princeton university and the DoD supercomputer centers.

12:03PM J36.00003 Alkane and CO₂ Activation by Modified Oxide Catalysts, HORIA METIU, University of California, Santa Barbara — I will present computational and experimental results concerning the effect of cation or anion doping on the catalytic activity of oxides. We are mainly interested in the activation of alkanes or of CO₂ and their conversion to useful products.

12:39PM J36.00004 First-principles calculations of Fischer-Tropsch processes catalyzed by nitrogenase enzymes¹, JOEL VARLEY, LARS GRABOW², JENS NORSKOV³, Stanford University — The nitrogenase enzyme system of the bacteria *Azotobacter vinelandii*, which is used in nature to catalyze ammonia synthesis, has been found recently to catalyze the efficient conversion of carbon monoxide (CO) into hydrocarbons under ambient temperature and pressure [1]. These findings indicate that nitrogenase enzymes could inspire more efficient catalysts for electrochemical CO and CO₂ reduction to liquid fuels. The nitrogenase variants, in which vanadium substitutes the molybdenum in the active site of the enzyme, show distinct features in their reaction pathways to hydrocarbon production. To compare and contrast the catalytic properties of these nitrogenase enzymes, we perform first-principles calculations to map out the reaction pathways for both nitrogen fixation and for the reduction of CO to higher-order hydrocarbons. We discuss the trends and differences between the two enzymes and detail the relevant chemical species and rate-limiting steps involved in the reactions. By utilizing this information, we predict the electrochemical conditions necessary for the catalytic reduction of CO into fuels by the nitrogenase active sites, analogous to a Fischer-Tropsch process requiring less extreme conditions.

[1] Y. Hu, C.C. Lee, M.W. Ribbe, Science **333**, 753 (2011)

¹This work was supported by the Global Climate and Energy Project (GCEP) at Stanford University.

²University of Houston

³SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory

12:51PM J36.00005 Low-temperature dehydrogenation catalysis of isophorone ($C_9H_{14}O$) on Pd(111), XINGUO REN, WEI LIU, ADITYA SAVARA, WIEBKE LUDWIG, KARL-HEINZ DOSTERT, SWETLANA SCHAUERMANN, ALEXANDRE TKATCHENKO, HANS-JOACHIM FREUND, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, Germany — Selective hydrogenation and dehydrogenation of hydrocarbons is one of the most extensively used processes in catalysis. In particular, it is important to design catalysis which can occur at or below room temperature. Here, we investigate the adsorption and dehydrogenation of a model organic/metal catalyst: isophorone ($C_9H_{14}O$) on the Pd(111) surface. Density-functional theory (DFT) calculations including van der Waals (vdW) interactions are carried out to elucidate the adsorbate geometry and reaction dynamics. The vdW interactions dramatically modify the potential-energy surface and enhance the binding energy by about 1 eV. The combination of our theoretical results with the analysis of infrared (IR) spectra and temperature-programmed desorption (TPD) experiments leads us to propose a dehydrogenation pathway from the weakly chemisorbed reactant ($C_9H_{14}O$) to the strongly chemisorbed product ($C_9H_{10}O$), which occurs after four C-H bond cleavages. The obtained low dehydrogenation temperature (130-150 K) from PBE+vdW barriers, including zero-point energy vibrations, is consistent with the TPD analysis.

1:03PM J36.00006 Interfacial binding in catalytic and photovoltaic materials, and the energetics of elementary surface processes during catalytic fuels production and utilization¹, CHARLES T. CAMPBELL², University of Washington — The fundamental understanding of reactivity trends in organic and inorganic chemistry has led to spectacular scientific advances over the past 50 years in synthetic chemistry. At the basis of this understanding is knowledge of the strengths of the relevant chemical bonds being broken and formed. In this regard, surface chemistry is several decades behind. Yet surface chemical reactivity dictates our choices of materials for energy technology, including catalysts for clean fuels production and utilization, fuel cell electrodes, photocatalysts and photovoltaics. This past decade has seen important advances in our ability to measure surface chemical bond energies and to use them to make predictions of relevance to energy technology. We will review those advances here, with a focus on: (1) the interfacial bonding strength between the metal and the support material in metal nanoparticle catalysts, with emphasis on the roles of particle size and the support in catalyst reactivity and stability, (2) the interfacial reactions that occur between the metal electrode and the semiconducting polymer in organic photovoltaic (OPV) devices, and the heats of those reactions, and (3) the adsorption energies of small molecules on Pt(111), with emphasis on intermediates in catalytic steam reforming, oxidation and dehydrogenation, which reveal a strong correlation between the strength with which adsorbates bond to the Pt(111) surface and their bond energy to the H atom in gas-phase molecules. These measurements provide important benchmarks for comparisons with new computational methods designed to improved energy accuracy beyond standard periodic DFT.

¹Supported by NSF and DOE-OBES-Chemical Sciences Division.

²Department of Chemistry Box 351700, Seattle, WA 98195-1700

1:39PM J36.00007 Ab initio modeling of EXAFS spectra of nanoparticles, SAMUEL CHILL, The University of Texas, AARON YEVIK, ANATOLY FRENKEL, Yeshiva University, GRAEME HENKELMAN, The University of Texas — The structure of nanoparticles in the 1-3 nm range is often investigated using extended x-ray adsorption fine structure (EXAFS). Structural information for nanoparticles is typically determined from the fits to EXAFS data using the bulk structure for theoretical calculations. The average coordination numbers, interatomic distances, and their mean squared disorder can be found. The applicability of this procedure is less obvious when the particles are strongly disordered, i.e., when there are significant structural differences between the nanoparticles and the corresponding bulk structure. We use molecular dynamics (MD) simulations of 2 nm nanoparticles to construct EXAFS spectra ab initio, with the atom-by-atom approach, averaged over the time of the MD run. We obtain that the analysis of this data done by conventional procedures reveals significant differences between the actual (time- and configuration- average) structure of the simulated nanoparticles and what was determined from data analysis using a bulk reference. We demonstrate that EXAFS spectra calculated for a variety of theoretical models of nanoparticles can be directly compared to the experiment and thus used to determine the best-fit structure.

1:51PM J36.00008 Predicting the Catalytic Reactions using Random Phase Approximation, J. YAN, SUNCAT Center for Interface Science and Catalysis, SLAC, Stanford University, T. OLSEN, J.J. MORTENSEN, K.W. JACOBSEN, K.S. THYGESEN, Center for Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark, F. ABILD-PEDERSEN, J.K. NORSKOV, SUNCAT Center for Interface Science and Catalysis, SLAC, Stanford University — Density functional theory has become the workhorse for simulations of catalytic reactions and computational design of novel catalysis. The generally applied semi-local exchange-correlation functionals have successfully predicted catalytic reaction trends over a variety of surfaces. However, in order to achieve quantitative predictions of reaction rates for molecule-surface systems, in particular where there is weak Van der Waals interactions or strong correlation, it is of vital importance to include non-local correlation effects. The use of random phase approximation (RPA) to construct the correlation energy, combined with the exact, self-interaction free exchange energy, offers a non-empirical way for accurately describe the adsorption energies [1] and dispersion forces [2]. We have recently implemented RPA in the GPAW code [3-4], an electronic structure package using projector augmented wave method and real space grids. In this talk I will present our initial results comparing RPA and generalized gradient functionals for the activation energies and reaction energies for transition metal or metal oxide surfaces.

[1] L. Schimka, et.al, Nature Mat. 9, 741 (2010) [2] T. Olsen, et.al, Phys. Rev. Lett. 107, 156401 (2011) [3] J. Yan, et.al, Phys. Rev. B 83, 245122 (2011). [4] J. Yan, et.al, Phys. Rev. Lett. 106, 146803 (2011)

2:03PM J36.00009 In situ XAS of Pt monolayer model fuel cell catalysts: balance of nanostructure and bimetallic interactions¹, DANIEL FRIEBEL, SLAC National Accelerator Laboratory, VENKAT VISWANATHAN, SUNCAT Center for Interface Science and Catalysis, ASK LARSEN, CAMD, Technical University of Denmark, DANIEL J. MILLER, HIROHITO OGASAWARA, SLAC National Accelerator Laboratory, TOYLI ANNIYEV, None, CHRISTOPHER P. O'GRADY, JENS NØRSKOV, SUNCAT Center for Interface Science and Catalysis, ANDERS NILSSON, SLAC National Accelerator Laboratory — The mechanism of the electrochemical oxygen reduction reaction (ORR) has been well understood based on DFT calculations, but there has been a lack of supporting experimental data, due to the difficulties of probing the electrocatalyst surface in situ. Our new approach using Pt monolayer model catalysts provides true surface sensitivity for - originally bulk sensitive - x-ray absorption spectroscopy (XAS) and, owing to the high resolution of the Bragg analyzer at SSRL beamline 6-2, allows for in situ detection of chemisorbed O and OH, whose stability can be used as a descriptor in predicting the activity of new ORR catalyst materials. Our ability to control the growth mode in the Pt/Rh(111) model system allows us to generate Pt nanostructures with highly different O affinities from identical starting materials.

¹This work was funded by the Department of Energy, Office of Basic Energy Sciences.

**Tuesday, February 28, 2012 11:15AM - 12:39PM –
Session J37 SPS: SPS Undergraduate Research IV 108**

11:15AM J37.00001 Life as a Hiltern¹, COURTNEY LEMON, California State Polytechnic University, Pomona — The Mather Policy Intern Program, conducted through the Society of Physics Students, is an innovative internship encouraging physics students to get involved in science policy. Funded by the John and Jane Mather Foundation for Science and the Arts and the American Institute of Physics, Mather Interns spend a summer at the Capitol, working as congressional interns for a representative or committee. As the first female student inducted into the Mather Policy Intern program, the author presents Life as a Hiltern, detailing her summer working with Representative Rush Holt, the only physicist currently serving in the U.S. House of Representatives.

¹Thank you to the John and Jane Mather Foundation for Science and the Arts for funding this project.

11:27AM J37.00002 Zinc Oxide Coated Carbon Nanotubes for Energy Harvesting Applications¹, AUSTIN MOHNEY, Lock Haven University, DAVID STOLLBERG, Georgia Institute of Technology — Small scale electrical devices depend on bulky batteries that require recharging or replacement. In biomedical monitoring, where sensors could be implanted inside the body, maintenance of batteries presents a problem. It would be beneficial if small scale devices could generate their own power and alleviate their dependence on batteries. Piezoelectric nanogenerators have proven themselves as a viable means for ambient energy harvesting. Piezoelectric materials, such as zinc oxide (ZnO), produce a voltage difference when subjected to mechanical strain. Manipulation of this voltage can allow for the storage of energy to power small scale devices. The objective of this research is to manufacture a piezo-generator that can transduce mechanical vibrations into electrical energy. Carbon nanotubes, selected for their strong, flexible, and conductive properties, are used as a structural backbone for a ZnO piezoelectric coating and a Ag electrode coating. A Schottky diode interface is used to rectify the current output of the device. The devices yielded an average current output of .79 microAmps. SEM imaging was used to characterize the fabrication process. A Keithley 2700 digital multimeter was used to characterize the current output of the devices.

¹Georgia Tech Research Institute & NSF SURF Program at Georgia Tech.

11:39AM J37.00003 Influence of carbon nanotubes diameter on thermal conductivity of polyester based nanocomposites, ROMEO DE COSS-MARTÍNEZ, GRACIELA INÉS QUIÑONES-WEISS, JAZMÍN ANELY DOPORTO-VALLADARES, Facultad de Ingeniería de la Universidad Autónoma de Yucatán, CARIDAD GUADALUPE VALES-PINZÓN, Department of Applied Physics, Cinvestav-Mérida, MIGUEL ÁNGEL ZAMBRANO-ARJONA, JOSÉ ÁNGEL MENDEZ-GAMBOA, RUBÉN ARTURO MEDINA-ESQUIVEL, Facultad de Ingeniería de la Universidad Autónoma de Yucatán, JUAN JOSÉ ALVARADO-GIL, Department of Applied Physics, Cinvestav-Mérida — Carbon nanotubes (CNTs) are considered good candidates to improve the physical properties of polymeric materials. It is well known that CNTs have one of the highest thermal conductivities in nature. However, it has been found that thermal resistance between polymer matrix and CNTs, at nanometric scale, could imply a disadvantage to obtain high thermal conductivity nanocomposites. In this work, the effect of CNTs diameter on the effective thermal conductivity of composites based on polyester resin is studied. In particular, the effects of CNT's diameter and volume fraction are analyzed. The thermal conductivity of the nanocomposites is obtained determining the thermal diffusivity by photothermal radiometry and from the values of their specific heat capacity.

11:51AM J37.00004 Electrical characterization of field effect transistors made from C-nanotubes covered with poly(3-hexylthiophene)¹, LUIS POMALES, NICHOLAS PINTO, University of Puerto Rico - Humacao, MITCHELL LERNER, ALAN JOHNSON JR., University of Pennsylvania — Organic transistors were fabricated using a thin film of regio-regular poly(3-hexylthiophene-2,5-diyl) spun from a 0.5 wt% solution in CHCl₃ on doped Si/SiO₂ substrates with and without CNT's. The performance of devices with percolating networks of CVD grown single-wall carbon nanotubes (SWNT's) between the source (S) and drain (D) electrodes and without SWNT's are compared. Nanotubes are used as a way to shorten the effective mean distance between the S/D terminals while retaining the wide spacing macroscopic shadow mask technique for S/D fabrication. We found that devices made with SWNT's do not exhibit S/D current saturation but have a charge mobility of 1.2×10^{-2} cm²/V-s and an on/off ratio of 9, while the device without SWNT's show clear saturation with a charge mobility of 8.6×10^{-4} cm²/V-s and an on/off ratio of 870. The devices made with nanotubes possess a larger off state current although they show a ~14X increase in the mobility which can thus be increased without using sophisticated lift-off techniques to shorten the S/D distance.

¹NSF

12:03PM J37.00005 Physical Manipulation of the Na/K Pump¹, DAVID EVE, Massachusetts College of Liberal Arts, CLAUSELL MATHIS, WEI CHEN, University of South Florida — It has been demonstrated that a well-designed oscillating electric field can synchronize and modulate the functions of the Na⁺/K⁺ ATPase pump, a ubiquitous active transporter in the cell membrane. Current work aims to improve this technique in order to synchronize the individual steps in the pumping cycle, allowing all of the individual pumps to run simultaneously. Using frog skeletal muscle fibers and the double Vaseline-gap voltage clamp technique, we are working to design wave pulses, which will isolate the voltage dependent steps of the active ion transport. This will improve the signal-to-noise ratio and provide insight into the protein conformation changes that occur during active transport.

¹This work was supported by NSF REU program (award No DMR-1004873)

12:15PM J37.00006 Characterization of the GaN-MgO Transistor Interface: More Power and Efficiency¹, JOSE SANCHEZ, University of Puerto Rico at Mayaguez, DIVINE KUMAH, FRED WALKER, Yale University — In this age of high-energy consumption, the development of more efficient and more reliable devices is indispensable. Gallium nitride (GaN)-based devices are an option in achieving this goal. GaN's wide bandgap of 3.4 eV allows the device to handle large amount of current before leakage makes its energy consumption inefficient. The characteristics of GaN, in conjunction with those of Magnesium oxide (MgO), would allow for improvement of different electronic applications such as mobile phone communication technology. In this work, the fabrication of the GaN/MgO device was done by Molecular Beam Epitaxy. This device was grown under a variety of parameters where the growth temperature, growth chamber pressure, and the rate of material deposition were changed. To determine the optimal growth parameters, current-voltage and capacitance-voltage measurements were conducted on to evaluate the effects of these growth conditions. Atomic Force Microscopy was also used in characterizing the crystallinity and morphology of the samples. A conclusion of the research is that by improving the roughness of the substrate, the breakdown voltage of the MgO layer and the overall performance of the device can be improve, yielding a device with very low energy loss in the current transmission process.

¹The research was conducted under the Leadership Alliance, The Summer Undergraduate Research Fellowship (SURF) Program at Yale University, and the Center for Research on Interface Structure and Phenomena (CRISP) REU programs.

12:27PM J37.00007 Generating more electricity from water¹, DANIEL MOSER, GUOPING ZHANG, Indiana State University: Department of Chemistry and Physics — The Kelvin water drop generator is an ingenious method of using naturally occurring water to induce charge separation in water droplets by allowing them to fall through cross-wired conductors. While being a simple and clean source of energy, the generator has never been considered practical due to its low current output. The goal of this experiment was to discover what conditions were required to obtain maximum voltage. Manipulating where a water stream breaks into droplets inside the conductor, we were able to take advantage of the conductor's geometry and electric field to induce the largest charge separation inside the water droplets. We also explored methods on how to reduce charge cancellation during the operation of the apparatus.

¹Department of Energy Grant #DE-FG02-06ER46304.

Tuesday, February 28, 2012 11:15AM - 1:51PM –
Session J39 DCMP: Exciton, Polariton, and Electron Dynamics in two-dimensional semiconductor structures 109B

11:15AM J39.00001 Valence-band Mixing in Strain-based Traps for Indirect Excitons in Coupled Quantum Wells¹, JEFFREY WUENSCHHELL, NICHOLAS SINCLAIR, DAVID SNOKE, University of Pittsburgh, LOREN PFEIFFER, KEN WEST, Princeton University — Excitons in a coupled quantum well system under an applied bias are spatially separated, with electrons and holes in opposite wells. The pair can interact via the Coulomb interaction, but recombination is suppressed. Indirect excitons exhibit a long (up to tens of microseconds), tunable lifetime and are of interest to those studying high density excitonic phase transitions in equilibrium. Recent experiments have revealed sharply temperature- and density-dependent transitions in the luminescence pattern of strain-trapped indirect excitons [1]. Localized strain shifts the valence and conduction bands, creating a trap for the case of hydrostatic stretching [2]. Two factors differentiate this technique from electrostatic traps, the splitting between the light- and heavy-hole exciton states varies with stress and the presence of shear strain modifies the symmetry of the ground state. Due to strong dependence of the radiative lifetime on the tunneling rate, the indirect heavy- and light-hole excitons have drastically different recombination rates; meaning that mixing sharply alters the luminescence pattern. We will discuss the modeling of the structure of the single-particle potential and the role that interband mixing plays in the appearance of high density phase transitions.

¹This work was supported by the US Department of Energy, DoE Grant DE-FG02-99ER457080.

11:27AM J39.00002 Dark excitons and Bose-Einstein condensation in strain-trapped excitons in coupled quantum wells¹, NICHOLAS SINCLAIR, JEFF WUENSCHHELL, University of Pittsburgh, KENNETH WEST, LOREN PFEIFFER, Princeton University, DAVID SNOKE, University of Pittsburgh — It is possible to make excitons in coupled quantum wells with very long lifetime compared to their thermalization, allowing us to study equilibrium behavior. Using a localized stress to create traps for excitons in coupled quantum wells, we have demonstrated that at low temperature, high density, and large stress, the spatial pattern of photoluminescence (PL) from interwell excitons transitions to one with a dimmed center. This pattern emerges despite the center remaining the region of highest exciton density. This darkening is related to a strain-induced interaction between the light hole and heavy hole states. However, while this explanation provides a mechanism to explain many of the features, a few important predictions of this theory are not borne out by experiments. An alternate explanation is possible, utilizing an increasing population of dark ($J=2$) excitons and a separation of the dark and bright species. It has been proposed that a Bose-Einstein Condensate in this system would occur in a dark state, and this transition is consistent with the onset criteria of the pattern formation and explains how a slight bright/dark energy difference could lead to spatial separation of the species. Experiments employing a magnetic field to turn 'dark' excitons slightly 'bright' should allow the disambiguation of the role of dark excitons in this system. I will review this pattern formation and discuss data from experiments employing a magnetic field.

¹This work was supported by the DOE grant DE-FG02-99ER45780.

11:39AM J39.00003 Trapping Long-Lifetime Superfluid Polaritons Using a Laser-Generated Barrier¹, B. NELSEN, M. STEGER, G. LIU, D. SNOKE, University of Pittsburgh, K. WEST, L. PFEIFFER, Princeton University — We present results with new microcavity structures that have polaritons that live as long as 100 ps, about two orders of magnitude longer than in previous structures. We show that an exciton reservoir can be used to create a potential barrier for a superfluid polariton gas. In these experiments, we use a non-resonant laser to create a superfluid polariton gas at the same location as a population of excitons. The excitonic component of the polariton can coherently scatter with the excitons. Since the excitons have mass four orders of magnitude larger than the polaritons, they form essentially a static barrier for the polaritons. By resolving the polaritons both in real space and momentum space, we determine that the polaritons roll down the potential barrier created by the excitons. These results are consistent with numerical solutions of the Gross-Pitaevskii equation for the measured parameters of this system. The potential to use the exciton reservoir as a barrier/trap will allow exciting new ways to study macroscopic coherence phenomena such as Josephson oscillations and superfluid vortices.

¹This material is based upon work supported by the National Science Foundation under Grant No. 0706331.

11:51AM J39.00004 All Optical Switching Using Exciton-Polariton Renormalization in Microcavities¹, M. STEGER, B. NELSEN, C. GAUTHAM, D. SNOKE, University of Pittsburgh, L. PFEIFFER, K. WEST, Princeton University — We report on a method of all-optical switching based on resonantly pumped exciton-polariton microcavities. Depending on geometry, each optical transistor could be used to make an AND or an AND NOT gate. Optical switching in these samples may be limited by the lifetime of the polaritons, allowing for near THz frequency switching. These gates could be used for fast signal processing or optical computing. Where optical computing calls for signals and gates to be at the same wavelength, we can use a gate beam at an angle, since the dispersion relation of polaritons allows for the absorption of a gate higher in energy than the $k=0$ state. High exciton and free carrier densities lead to a renormalization of the lower polariton (LP) and increase its energy. If the $k=0$ LP becomes resonant with the signal beam, then the gate may be used to turn on transmission (or consequently turn off reflectivity) of that signal. We will present achievable on/off ratios and switching speeds as well as discuss modulating an intense signal with a weaker gate.

¹This was supported by the National Science Foundation Grants DMR-0706331 and ECCS-0801869.

12:03PM J39.00005 Two-Dimensional Mott-Hubbard Electrons in an Artificial Honeycomb Lattice¹, V. PELLEGRINI, M. GIBERTINI, B. KARMAKAR, NEST-CNR, and Scuola Normale Superiore, Pisa, S. YUAN, Radboud University Nijmegen, Netherlands, M. POLINI, NEST-CNR, and Scuola Normale Superiore, Pisa, G. VIGNALE, University of Missouri, Columbia, USA, M. KATSNELSON, Radboud University Nijmegen, Netherlands, A. PINCZUK, Columbia University, USA, L.N. PFEIFFER, K.W. WEST, Princeton University, USA, A. SINGHA, Bose Institute, Kolkata, India. — Artificial crystal lattices can be used to tune repulsive Coulomb interactions between electrons. We trapped electrons, confined as a two-dimensional gas in a gallium arsenide quantum well, in a nanofabricated lattice with honeycomb geometry [1,2]. In our most recent studies [3] we probed the excitation spectrum of electrons in the honeycomb lattice with lattice spacing ranging down to 90nm in a magnetic field identifying collective modes that emerged from the Coulomb interaction in the artificial lattice, as predicted by the Mott-Hubbard model. These observations allow us to determine the Hubbard gap and suggest the existence of a Coulomb-driven ground state [3]. The proposed research promises to further expand current realms of study of quantum simulators. While the experiments are challenging, studies of electrons confined to artificial lattices should provide key perspectives on strong electron correlation in condensed matter science.

- [1] M. Gibertini et al. Phys. Rev. B **79**, 241406 (2009)
- [2] G. De Simoni et al. Appl. Phys. Lett. **97**, 132113 (2010)
- [3] A. Singha et al. Science **332**, 1176 (2011)

¹Supported by CNR and NSF

12:15PM J39.00006 Cooperative carrier dynamics in InGaAs/GaAs quantum wells in high magnetic fields, JI-HEE KIM, TIM NOE, Dept. of Electrical & Computer Engineering, Rice University, YONGRUI WANG, ALEKSANDER K. WOJCIK, Dept. of Physics and Astronomy, Texas A&M University, STEPHEN A. MCGILL, National High Magnetic Field Laboratory, ALEXEY A. BELYANIN, Dept. of Physics and Astronomy, Texas A&M University, JUNICHIRO KONO, Dept. of Electrical & Computer Engineering, Rice University — Ultrafast spectroscopy in strong magnetic fields provides a powerful means for studying quantum coherence in many-body systems. A high magnetic field leads to tunable energy quantization, which in turn results in a substantial enhancement of densities of states and suppression of scattering. Here, we study superfluorescence (SF), i.e., cooperative spontaneous emission of ultradense electron-hole plasmas in InGaAs quantum wells in a perpendicular magnetic field up to 17.5 T. We observe SF both through time-resolved photoluminescence and differential transmission (DT) measurements. We create an ultradense electron-hole plasma with an intense femtosecond laser pulse, and after a certain delay, an ultrashort burst of coherent radiation emerges. At the same time, an abrupt decrease in population from full inversion to zero was observed through DT measurements. Furthermore, the DT signals strongly depended on the probe energy, showing an anomalous negative DT signal (i.e., induced absorption) under certain circumstances.

12:27PM J39.00007 High-Order Sideband Generation in Quantum Wells Driven by Intense THz Radiation: Electron-Hole Recollisions¹, BENJAMIN ZAKS, Department of Physics and the Institute for Terahertz Science and Technology, University of California at Santa Barbara, REN-BAO LIU, Department of Physics and the Centre of Optical Sciences, The Chinese University of Hong Kong, MARK SHERWIN, Department of Physics and the Institute for Terahertz Science and Technology, University of California at Santa Barbara — Non-linear mixing of optical beams with intense terahertz beams has been observed in semiconductor heterostructures both as changes to the absorption spectrum and as sideband generation. Sidebands are generated when a material has a non-linear dielectric response that mixes the electric field of the two beams and produces radiation at the optical frequency plus or minus multiples of the THz frequency. Perturbatively generated sidebands have been observed up to fourth order when the optical beam resonantly excites excitons in GaAs quantum wells. We present here our observation of high-order sideband generation (HSG) from excitons in InGaAs QWs. Sidebands of up to 18th order are observed. From the THz intensity dependence and THz polarization dependence (linear-circular) of the sideband generation, we show that the observed phenomenon is non-perturbative. We note that the exciton system driven by an intense THz field is analogous to an atomic system driven by intense optical fields, as is the case for high-order harmonic generation (HHG). The recollision model used to describe HHG in atoms is then extended to describe HSG in excitons. Experimental results indicate that the recollision model is a valid description of the nature of HSG in excitons.

¹Supported by NSF grant DMR-1006603

12:39PM J39.00008 Intersubband electrons coupled to zone-folded coherent acoustic phonons in a GaN/AlN superlattice, CYNTHIA AKU-LEH, KLAUS REIMANN, MICHAEL WOERNER, Max-Born Institut, Max-Born Strasse 2A, 12489 Berlin, Germany, EVA MONROY, CEA Grenoble, rue des martyrs 17, 38054 Grenoble, France, DANIEL HOFSTETTER, University of Neuchâtel, 1 Rue Abraham Louis Breguet, 2000 Neuchâtel, Switzerland — We present spectrally-resolved resonant pump-probe measurements on a strongly polar GaN/AlN superlattice. The transmitted and reference probe spectra are detected at the same read out rate. Analysis of the normalized probe spectra reveals electronic contributions as well as the first three folded longitudinal acoustic phonons, matching calculated frequency values predicted by the elastic continuum model. The observed modes couple strongly to intersubband electrons and modulate the spectral width and position of the intersubband absorption. We conclude that this electron-phonon coupling takes place via piezoelectric effects and a phonon-induced modulation of the subband effective mass.

12:51PM J39.00009 Intersubband polariton bleaching observed in ultrafast mid-infrared spectroscopy, SIMONE ZANOTTO, RICCARDO DEGL'INNOCENTI, JI-HUA XU, Scuola Normale Superiore and CNR-NANO, GIORGIO BIASIOL, Laboratorio TASC and CNR-IOM, LUCIA SORBA, ALESSANDRO TREDICUCCI, Scuola Normale Superiore and CNR-NANO — Strong coupling between intersubband transition in quantum wells and microcavity field leads to the concept of intersubband (ISB) polaritons. Their linear properties have been explored for several years, mainly focusing on optical spectra and electroluminescence. Among the implemented microcavity geometries, the one based on a photonic crystal (Zanotto et. al., Appl. Phys. Lett. 2010) is particularly interesting as it allows simultaneous access to both polariton branches at anticrossing. Here we report on the nonlinear response of ISB polaritons, investigating their bleaching, an effect already studied in the excitonic framework. When ISB polaritons are probed by an intense mid-infrared laser pulse, the typical double-peaked transmission spectrum is converted in a single-peaked one. By tuning the intensity of the femtosecond pulse that covers both polariton branches, the whole range between weak and strong coupling regimes has been swept. This study reveals that there is a threshold for pumping above which polariton states are destroyed, and restricts the pump intensity range that can be employed in an optically-pumped ISB polariton laser. Moreover, as a consequence of nonlinear optical properties, saturable absorbers and optically bistable devices could be implemented.

1:03PM J39.00010 Pump-probe experiment in LaMnO₃/SrTiO₃ superlattices and thin film, PUREVDORJ MUNKHBAATAR, Department of Physics, Chonbuk National University, Republic of Korea, B. TSERMAA, Department of Geophysics, National university of Mongolia, Mongolia, J.S. KIM, Department of Physics, Chonbuk National University, Republic of Korea, W.S. CHOI, S.S.A. SEO, H.N. LEE, Oak Ridge National Laboratory, K. MYUNG-WHUN, Department of Physics, Chonbuk National University, Republic of Korea — We present the time dependent transmittance of LaMnO₃ thin film and [(LaMnO₃)_n/(SrTiO₃)₈]₂₀ (n=2 and 8) superlattices grown on SrTiO₃ substrate. We used the laser pulse pump-probe technique. We observed two phonon oscillation in the LaMnO₃ film at 8 THz and at 15 THz. In the superlattices, 8 THz mode seemed obliterated. The phonon oscillation damping time constant was also different. In LaMnO₃ thin film, we could observe the oscillation until ~ 1.5 ps. In the superlattices, the damping time constant was smaller: ~ 0.7 ps for n=8 superlattice and ~ 0.3 ps for n=2 superlattice. We will discuss number of phonon mode and the damping time constant in terms of the sample geometry and the electronic structure.

1:15PM J39.00011 Excitonics of Hybrid Nanostructures Arranged with Mixed Dimensionality, PEDRO LUDWIG HERNANDEZ MARTINEZ, Bilkent University, Nanyang Technological University, ALEXANDER O. GOVOROV, Ohio University, HILMI VOLKAN DEMIR, Bilkent University, Nanyang Technological University — We present a complete study of the Förster-type nonradiative energy transfer in hybrid nanostructures composed of nanoparticles, nanowires and quantum wells, and investigate the effects of quantum confinement in different dimensions. We systematically consider all possible combinations in terms of dimensionality for exciton-exciton interactions in these hybrid architectures, and analyze the resulting energy transfer rates for item-to-item excitonic coupling as a function of dimensionality. We derive a full set of analytical expressions and show that the exciton transfer strongly depends on the dimensionality and geometry of the hybrid system. Arrangements of such nanostructures with mixed dimensionality ranging from the low dimensionality to the high offer important high-efficiency applications in photovoltaics [1,2], while in the reciprocal case (from the high dimensionality to the low) in light generation [3] and LEDs [4]. [1] J. Sambur, et al., Science 330, 63 (2010). [2] M. D. Kelzenberg, et al., Nature Materials 9, 239–244 (2010). [3] R. Yan, et al., Nature Photonics 3, 569–576 (2009). [4] H.V. Demir, et al., Nano Today (2011) doi:10.1016/j.nantod.2011.10.006

1:27PM J39.00012 Many-particle effects in the photoluminescent response of silicon quantum-dot solids, JOSEPH B. MILLER, AUSTIN R. VAN SICKLE, North Dakota State University, REBECCA R. ANTHONY, UWE R. KORTHSHAGEN, University of Minnesota, DANIEL M. KROLL, ERIK K. HOBBIE, North Dakota State University — Monodisperse colloidal suspensions of ligand-coated silicon nanocrystals (SiNCs), synthesized through a nonthermal low-pressure plasma reaction, are prepared through density-gradient ultracentrifugation in mixed organic solvents. The SiNC fractions are then self-assembled into close-packed quantum-dot “solids” and clusters, and photoluminescent properties of the resulting ordered ensembles are characterized through optical spectroscopy. We find striking manifestations of particle-particle interactions in the measured optical response, and we model these effects using Monte Carlo simulations of the photobleaching kinetics in dense SiNC packings.

1:39PM J39.00013 Spectral dependence of the Aharonov Bohm effect in the magneto-photoluminescence of layered ZnTe-ZnSe structures, BIDISHA ROY, Queens College of CUNY, The Graduate Center of CUNY, HAOJIE JI, SIDDHARTH DHOMKAR, Queens College of CUNY, The Graduate Center of CUNY, LE PENG, City College of CUNY, The Graduate Center of CUNY, RICHARD MOUG, City College of CUNY, UTTAM MANNA, Columbia University, MARIA TAMARGO, City College of CUNY, FRED CADIEU, Queens College of CUNY, IGOR KUSKOVSKY, Queens College of CUNY, The Graduate Center of CUNY — Aharonov-Bohm (AB) oscillations in the magneto-photoluminescence (PL) intensity of multilayered ZnTe/ZnSe structures grown via migration enhanced epitaxy (MEE) using three submonolayer deposition cycles of Zn-Te-Zn sandwiched between ZnSe barriers confirmed the presence of type-II ZnTe-based QDs. These co-exist with isoelectronic centers (ICs) as evident from the PL spectra. The spectral dependence of the transition magnetic field and the magnitude of the AB oscillation in intensity are investigated. A qualitative probing of distribution in the ensemble of QDs and ICs was done. The transition magnetic field changed from a lower value at the lower energy side of the PL emission to a higher value at the higher energy side which confirmed the lateral QD size distribution. AB oscillations at spectral positions dominated by emission from ICs were also observed suggesting that the presence of QDs also affects the ICs although the magnitude of the oscillation in the AB peak decreases at such spectral positions.

Tuesday, February 28, 2012 11:15AM - 2:15PM — Session J40 DBIO: Multi-cellular Processes and Development 156A

11:15AM J40.00001 A Quantitative Analysis of Axonal Growth and Connectivity in Cortical Neurons, JAMES WHITE, Physics and Astronomy and Biomedical Engineering, Tufts University, ELISE SPEDDEN, SAWYER BERNATH, Physics and Astronomy, Tufts University, DAVID KAPLAN, Biomedical Engineering and Chemical Engineering, Tufts University, TIMOTHY ATHERTON, CRISTIAN STAI, Physics and Astronomy, Tufts University — Developing neurons extend processes (axons and dendrites), which are led by a distally positioned growth cone. The growth cone both secretes and senses signaling molecules, that may either attract or repel nearby growing processes. While knowledge on the qualitative effects of several secreted growth factors on axon development (e.g. axon length and number of neurons developing processes) are known, a more detailed mathematical model describing the process of axonal guidance remains to be developed. Towards this end, we have collected time-lapse microscopy data of the axonal development of cortical neurons. Image analysis provides information on the rate of growth, arc length, and curvature of the processes as a function of time and the spatial positioning of the neurons. These results will be discussed in relation to theoretical studies that model axon growth in response to varying gradients of attractive forces, representative of the effect that signaling molecules may have on axon guidance.

11:27AM J40.00002 Collective cell migration in a periodic potential, THOMAS ANGELINI, JOLIE BREAUX, STEVEN ZEHNDER, University of Florida — The strength of cell-substrate adhesion can be modulated by the elasticity of substrate material. Thus, a cell culture surface with periodically varying elasticity is analogous to a periodic potential for cell adhesion. Rich collective dynamics emerge in systems of adatoms on crystal lattice surfaces due to the mismatch between the preferred spacing of adatoms and the periodic potential associated with the crystal lattice. Here we explore a biological analog of atoms in a periodic potential; we study the collective dynamics of cells on a substrate with periodically patterned elasticity. Preliminary results will be presented.

11:39AM J40.00003 Collective Cell Migration on Deformable Substrates, ADRIAN PEGORARO, Harvard University, ALLEN EHRLICHER, Harvard, MING GUO, Harvard University, THOMAS ANGELINI, University of Florida, DAVID WEITZ, Harvard University — In many biological processes, such as wound healing, tumor migration, or embryo development, cell migration is influenced by collective dynamics and coupling between cells. While cell-cell contact is one form of mechanical coupling, long-range interactions mediated by a deformable substrate lead to both spatial and temporal correlations during cell migration that extend over many cell lengths. While it is known that interactions between nearby but not contacted single cells are modified by substrate stiffness, it is not yet clear how changes to the substrate properties affect collective cell migration. This is especially important in the understanding of cancer cell migration since the mechanical properties of these cells change during disease progression; as such we expect that the influence of the substrate to change over time. To investigate this further, we study collective cell migration on deformable substrates of different stiffness to test whether changes in short range interactions between cells are correlated with changes in collective cell migration. Furthermore, we mix cells from different cancer stages and study their migration patterns to test whether correlations exist between different cell types during migration.

11:51AM J40.00004 Impact of jamming on collective cell migration, KENECHUKWU DAVID NNETU, MELANIE KNORR, STEVE PAWLIZAK, THOMAS FUHS, MAREIKE ZINK, JOSEF A. KÄS, Institut für Experimentelle Physik I, Universität Leipzig, D-04103, Leipzig, Germany — Multi-cellular migration plays an important role in physiological processes such as embryogenesis, cancer metastasis and tissue repair. During migration, single cells undergo cycles of extension, adhesion and retraction resulting in morphological changes. In a confluent monolayer, there are inter-cellular interactions and crowding, however, the impact of these interactions on the dynamics and elasticity of the monolayer at the multi-cellular and single cell level is not well understood. Here we study the dynamics of a confluent epithelial monolayer by simultaneously measuring cell motion at the multi-cellular and single cell level for various cell densities and tensile elasticity. At the multi-cellular level, the system exhibited spatial kinetic transitions from isotropic to anisotropic migration on long times and the velocity of the monolayer decreased with increasing cell density. Moreover, the dynamics was spatially and temporally heterogeneous. Interestingly, the dynamics was also heterogeneous in wound-healing assays and the correlation length was fitted by compressed exponential. On the single cell scale, we observed transient caging effects with increasing cage rearrangement times as the system age due to an increase in density. Also, the density dependent elastic modulus of the monolayer scaled as a weak power law. Together, these findings suggest that caging effects at the single cell level initiates a slow and heterogeneous dynamics at the multi-cellular level which is similar to the glassy dynamics of deformable colloidal systems.

12:03PM J40.00005 Self-rheology of cell monolayers, ROMARIC VINCENT, XAVIER SERRA-PICAMAL, VITO CONTE, ESTER ANON, XAVIER TREPAT, Institute for Bioengineering of Catalonia, University of Barcelona — Collective migration of cell sheets is a central feature of fundamental biological processes including morphogenesis, tissue regeneration, and cancer invasion. The dynamics of such processes are heavily determined by the rheology of the sheet and of the constituent cells. Such material properties have been extensively measured using a broad variety of rheological techniques, but none of these techniques has probed the ultraslow time scales that are central to collective cell migration, and exceed thousands of seconds. Here we present a novel approach we call 'Self rheology' that probes cell rheology using the pulses of strain rate that cells spontaneously generate. Using this approach, we show that stress and strain rate are in quadrature, thus indicating that the dominant stresses that govern collective cell migration are elastic. The monolayer's Young modulus is found to be an order of magnitude lower than the stiffness of single cells determined through active micro-rheology techniques at shorter time scales. This elastic behavior is followed by a fluidization regime at higher strains, which we interpret in terms of cell rearrangements. "Self-rheology" provides a new approach to study the dynamics of collective cellular processes at ultraslow time scales.

12:15PM J40.00006 Collective mechanics of undifferentiated cells drives ventral furrow formation in *Drosophila* embryo¹, ANA HOCEVAR, PRIMOZ ZIHERL, Jozef Stefan Institute, Ljubljana, Slovenia, MATTEO RAUZI, European Molecular Biology Laboratory, Heidelberg, Germany, MARIA LEPTIN, Universitaet zu Koeln, Koeln, Germany — We propose a 2D mechanical model of ventral furrow formation in *Drosophila* embryo that is based on undifferentiated epithelial cells of identical mechanical properties whose energy resides at their cortex. Depending on the relative tensions of the apical, basal, and lateral sides, the minimal-energy states of the embryo cross-section include circular and buckled furrow shapes. We discuss the possible shape transformation from a circular to an invaginated shape consistent with experimental observations, arguing that generic collective mechanics may contribute to the robustness of tissue shape changes in embryonic development. A small increase of the area of the mesoderm cells is sufficient to pin down the invagination. This agrees with experimental data which show that just before the outset of gastrulation, the apical, basal, and lateral sides of the mesoderm cells indeed are larger than in the rest of the embryo.

¹We thank the EMBL Advanced Light Microscopy Facility and Carl Zeiss for continuous support of the EMBL ALMF. This work was supported by the Slovenian Research Agency through Grant No. P1-0055 and by NSF Grant No. DMR05-47230.

12:27PM J40.00007 Collective Cell Mechanics in 3D Scaffolds, JOLIE BREAUX, STEVEN ZEHNDER, University of Florida, LUCAS OSTERBUR, JENNIFER LEWIS, University of Illinois, Urbana-Champaign, THOMAS ANGELINI, University of Florida — Mechanical cell behavior is influential in tissue health and dynamic cellular processes such as wound healing, and angiogenesis. Traction force microscopy (TFM) is often used to measure cell generated forces while mechanical testing methods such as atomic force microscopy (AFM) are employed to determine materials properties of cells. Extant cell mechanics methods including TFM and AFM are optimal for cells cultured on flat, 2D surfaces. However, the development of new cell mechanics techniques in 3D systems is essential to elucidate the behavior of tissues. In this presentation we introduce results from live-cell time-lapse measurements of mechanical cell behavior in highly ordered 3-D scaffolds. Preliminary data will be presented.

12:39PM J40.00008 Biomechanics of the endothelium substrate influences leukocyte transmigration¹, KIMBERLY STROKA, HELIM ARANDA-ESPINOZA, Fischell Department of Bioengineering, University of Maryland — The effects of shear flow and cytokines on leukocyte transmigration are well understood. However, the effects of substrate stiffness on transmigration remain unexplored. We have developed an in vitro model that allows us to study leukocyte transmigration as a function of varying physiological substrate stiffness. Interestingly, leukocyte transmigration increased with increasing substrate stiffness below the endothelium. Intercellular adhesion molecule-1 expression, stiffness, cytoskeletal arrangement, morphology, and cell-substrate adhesion could not account for the dependence of transmigration on substrate stiffness. We also explored the role of cell contraction and observed that (1) neutrophil transmigration caused large hole formation in monolayers on stiff substrates. (2) Neutrophil transmigration on soft substrates was increased by decreasing cell-cell adhesion. (3) Inhibition of myosin light chain kinase normalized the effects of substrate stiffness by reducing cell contraction on stiff substrates. These results demonstrate that neutrophil transmigration is regulated by MLCK-mediated generation of gaps at cell borders through substrate stiffness-dependent endothelial cell contraction.

¹Authors acknowledge support from NSF CMMI-0643783

12:51PM J40.00009 Growth variability in a tissue governed by stress dependent growth, KAREN ALIM, Harvard, AREZKI BOUDAUD, INRA, CNRS, ENS, Université de Lyon — Cell wall mechanics lie at the heart of plant cell growth and tissue morphogenesis. Conversely, mechanical forces generated at tissue level can feedback on cellular dynamics. Differential growth of neighboring cells is one eminent origin of mechanical forces and stresses in tissues where cells adhere to each other. How can stresses arising from differential growth orchestrate large scale tissue growth? We show that cell growth coupled to the cell's main stress can reduce or increase tissue growth variability. Employing a cell-based two dimensional tissue model we investigate the dynamics of a tissue with stress depending growth dynamics. We find that the exact cell division rule strongly affects not only the tissue geometry and topology but also its growth dynamics. Our results should enable to infer underlying growth dynamics from live tissue statistics.

1:03PM J40.00010 Emergent mechanical behavior in a minimal model for embryonic tissues, LISA MANNING, Department of Physics, Syracuse University, MARCOS LANIO, JARED TALBOT, EVA-MARIA SCHOETZ, Lewis-Sigler Institute for Integrative Genomics, Princeton University — We develop a minimal model for the mechanical properties of embryonic tissues that contains only three parameters and yet accurately reproduces many structural and dynamical features in zebrafish embryonic tissue explants. We verify model predictions for tissue surface tensiometer experiments and fusion assays, and contrast our model with existing models that are either difficult to constrain experimentally or insufficient to explain our experimental observations. The model tracks one degree of freedom per cell and introduces several types of interactions between cells to capture intracellular degrees of freedom, such as single cell viscoelasticity, adhesion, and active force generation. A key observation is that the motion of cells past one another, which must be generated by cells actively exerting tension on contacts, is best described by a special type of structured noise (both multiplicative and colored), instead of the white noise typically used in Brownian dynamics simulations. With such a noise term we can reproduce the glassy, viscoelastic dynamics in the bulk and explain how this new type of active "droplet" with very short-range interactions manages to have no "vapor pressure." We discuss how this well-calibrated model can be used to study morphogenesis and pattern formation in developing tissues.

1:15PM J40.00011 Spatially limited growth of an epithelium, MAXIME DEFORET, OLIVIER COCHET, AXEL BUGUIN, PASCAL SILBERZAN, Physico-Chimie Curie - UMR 168 - CNRS - Institut Curie, BIOLOGY INSPIRED PHYSICS AT MESO-SCALES TEAM — We present a study dealing with the growth of an epithelium on a spatially limited adhesive substrate. Adhesive patterns (typical size: 50 μ m to 500 μ m) are created by micro-fabrication techniques: A protein repellent polymeric gel homogeneously grafted on a coverslip is selectively ablated by plasma treatment through a thin layer of photoresist. The technique achieves a high resolution of patterning (around 2 μ m). After seeding cells (MDCK) on circular adhesive patterns, we let the monolayer grow for 30 hours after reaching the confluence. We use physical descriptors to describe migration and compaction. Two days after the confluence, we observe and characterize by confocal microscopy, the appearance of a tridimensionnal assembly of cells in the peripheral zone of the adhesive pattern (a "rim"). Moreover using other patterns, the existence of a tissue line tension and internal pressure is investigated.

1:27PM J40.00012 Information propagation and nutrient flow in *Physarum polycephalum* ,

GABRIEL AMSELEM, FRANCOIS PEAUDECEERF, KAREN ALIM, School of Engineering and Applied Sciences, Harvard University, JACQUES DUMAIS, ANNE PRINGLE, Department of Organismic and Evolutionary Biology, Harvard University, MICHAEL BRENNER, School of Engineering and Applied Sciences, Harvard University — Basal organisms such as slime mold and fungi grow as extended networks that can reach several square meters in size. Despite lacking a central coordination center, these organisms are able to globally reshape their morphology in response to local cues, such as the presence of a patch of nutrient. How are local signals integrated in these organisms, and how do they lead to an overall response? To answer this question, we focus on the flow of nutrients in the slime mold *Physarum polycephalum*. This slime mold exhibits internal flow oscillations, as well as periodic contractions of its veins. Using plastic masks, we constrain network growth to simple geometries. This allows for an experimental characterization of the relationship between the contractions and the flow. We next describe the change in the overall oscillation pattern when a food source is presented locally to the slime mold, and its implication on the internal flow. Internal flows are both inferred from the contraction pattern and experimentally measured using fluorescent markers.

1:39PM J40.00013 Scaling of Traction Stresses with Size of Cohesive Cell Colonies¹ , AARON F.

MERTZ, Yale University, SHILADITYA BANERJEE, Syracuse University, YONGLU CHE, Yale University, M. CHRISTINA MARCHETTI, Syracuse University, VALERIE HORSLEY, ERIC R. DUFRESNE, Yale University — We explore the mechanical properties of colonies of cohesive cells adherent on soft substrates. Specifically, we image the spatial distribution of traction stresses exerted by colonies of primary mouse keratinocytes on fibronectin-coated silicone gels. These cells have strong cell-cell adhesions mediated by E-cadherin. We observe that the work performed by a colony on its substrate is concentrated at the colony's periphery. The total work is strongly correlated to the geometrical size of the colony but not to number of cells. In other words, the mechanical output of a large single cell mimics that of a cohesive colony with the same overall size. We compare our findings to a recent theoretical model that treats the cohesive colony as an active gel.

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1:51PM J40.00014 Elasticity of adherent active cells on a compliant substrate¹ , SHILADITYA BANER-

JEE, Department of Physics, Syracuse University, AARON F. MERTZ, ERIC R. DUFRESNE², Department of Physics, Yale University, M. CRISTINA MARCHETTI, Department of Physics and Syracuse Biomaterials Institute, Syracuse University — We present a continuum mechanical model of rigidity sensing by living cells adhering to a compliant substrate. The cell or cell colony is modeled as an elastic active gel, adapting recently developed continuum theories of active viscoelastic fluids. The coupling to the substrate enters as a boundary condition that relates the cell's deformation field to local stress gradients. In the presence of activity, the substrate induces spatially inhomogeneous contractile stresses and deformations, with a power law dependence of the total traction forces on cell or colony size. This is in agreement with recent experiments on keratinocyte colonies adhered to fibronectin coated surfaces. In the presence of actomyosin activity, the substrate also enhances the cell polarization, breaking the cell's front-rear symmetry. Maximal polarization is observed when the substrate stiffness matches that of the cell, in agreement with experiments on stem cells.

¹This work was supported by NSF grants to MCM (DMR-0806511 and DMR-1004789) and ERD (DBI-0619674) and NSF graduate fellowship to AFM.

²Additional Affiliations: Department of Mechanical Engineering and Materials Science, Department of Chemical and Environmental Engineering, Department of Cell Biology, Yale University.

2:03PM J40.00015 Wave transmission through cell-cell coupling , CHENLU WANG, MEGHAN DRISCOLL, SAGAR

CHOWDHURY, S.K. GUPTA, WOLFGANG LOSERT, University of Maryland-College Park — We previously found that waves of high boundary curvature travel from the front to the back of individual *D. discoideum* cells. We investigated the behavior of curvature waves in small groups of adherent cells, in particular, we investigated the transmission of the waves through cell-cell coupling. We analyzed the motion of individual cells in short streams of varying length, which are cells that follow one other. Furthermore, we developed a technique that uses holographic optical tweezers to grip cells indirectly and push them into one another, thereby forming artificial cell-cell contacts. Using that technique, we observed the affect of waves in coupled cells. We also compared the shape dynamics of groups of cells to the shape dynamics of cells within those groups. We extended these methods to suspended cells, which exhibit different wave dynamics.

Tuesday, February 28, 2012 11:15AM - 2:15PM –

Session J41 DFD: Vortex Dynamics, Turbulence and Geophysical Flows 156B

11:15AM J41.00001 Two point correlations between velocity sums and differences in turbu-

lence , NICHOLAS ROTILE, GREG VOTH, SUSANTHA WIJESINGHE, Wesleyan University — In turbulent flows, the universality of small scales has been a subject of ongoing investigation. Recent work has explored the degree to which small scales are independent of large scales by measuring correlations between velocity differences over a distance r (whose variance is dominated by scales near r) and velocity sums over the same distance (whose variance is dominated by large scales). Some correlations between velocity differences and sums are required by the Navier-Stokes equations (Hosokawa, Prog. Theor. Phys. Lett., 118:169, 2007.) This talk will focus on experimental measurements of correlations between velocity sums and velocity differences in a turbulent flow between oscillating grids. We find that these correlations provide an accurate way to measure the energy dissipation rate that complements existing methods based on the third order structure functions. The correlations which are required by Navier-Stokes dynamics do not appear to violate the assumption of independence between the large and small scales, however there are other correlations in our measurements that show clear dependence of the small scales on the large scales.

11:27AM J41.00002 Variance of scalar fluctuations using backwards relative dispersion in turbulent channel flows , CHIRANTH SRINIVASAN, DIMITRIOS PAPAVALASSIOU, The University of Oklahoma — Temperature fluctuations at a location in a turbulent flow field are brought about by the arrival of particle pairs with different scalar concentrations. Studying backwards relative dispersion can be an alternative way to describe the local variance in scalar fluctuation. This work uses a numerical approach that couples a direct numerical simulation with the tracking of scalar markers to obtain scalar statistics in an infinitely long turbulent channel flow. Focusing on the anisotropic direction perpendicular to the channel walls, the two-particle correlation coefficients are used to determine a Lagrangian material time scale as a function of distance from the wall. Introducing a model that follows Durbin's theory [1], the variance of the temperature fluctuation is calculated by assuming that particle pairs that arrive at a particular location carry with them the mean temperature acquired at the location they were at a previous time. This earlier location is determined by utilizing the Lagrangian backwards timescale. Results obtained from this model are tested at two different Reynolds numbers (at $Re_\tau = 150$ and 300) and for each Re case at several different Prandtl numbers (from 0.1 to 1,000). **References** [1] Durbin, P.A., J. Fluid Mech., 100, 279-302, 1980

11:39AM J41.00003 Measuring anisotropy as a function of scale in turbulence using 3D particle tracking, SUSANTHA WIJESINGHE, GREG VOTH, Department of Physics, Wesleyan University, Middletown, CT 06459 — We report the first full 3D experimental measurements of anisotropy as a function of scale in turbulence. From 3D particle tracks obtained with stereoscopic high speed video, we measure the Eulerian structure functions and decompose them into irreducible representation of $SO(3)$ rotation group. This method allows us to quantify the anisotropy in different sectors, specified by j and m of the spherical harmonics $Y_{jm}(\theta, \phi)$, at all scales in the flow. We study a turbulent flow between two oscillating grids in an octagonal tank filled with 1100 l of water with $Re_\lambda = 265$. An image compression system processes high-speed video from four cameras in real-time allowing us to acquire huge data sets required for full 3D measurement of anisotropy as a function of scale. Careful selection of a sample of measurements with isotropic orientations is necessary to ensure that anisotropy of the measurement system does not affect the measured anisotropy of the flow. Increasing j sectors show faster decay of anisotropy as scale decreases, consistent with the idea that the small scales should become isotropic at very high Reynolds number. However, conditioning the measured anisotropy on the instantaneous velocity reveals that characterization of anisotropy in an inhom

11:51AM J41.00004 Rotation rate of rods in turbulent flow, SHIMA PARSA, GREG VOTH, Wesleyan University — We present the first time resolved experimental measurements of the motion of small rod-like particles in turbulent flow. The orientation and position of rods are measured using Lagrangian particle tracking with images from multiple high speed cameras in a flow between two oscillating grids. We work at low particle density so rod-rod interaction can be ignored. The probability distribution of the rotation rate of the rods has extended tails indicating the presence of rare events with large rotation rate. Rods rotation rate is determined by the velocity gradients of the flow, so measurements of the rotation rate provide indirect access to statistics of the velocity gradient of the flow as well as the energy dissipation rate. However, tracer rods preferentially sample the flow since their orientation becomes correlated with the local axes of the velocity gradient tensor. The result is that the typical rotation rate of rods is much smaller than it would be if they were randomly oriented.

12:03PM J41.00005 Statistics of Macroturbulence from Flow Equations¹, BRAD MARSTON, THOMAS IADECOLA, WANMING QI, Brown University — Probability distribution functions of stochastically-driven and frictionally-damped fluids are governed by a linear framework that resembles quantum many-body theory. Besides the Fokker-Planck approach, there is a closely related Hopf functional method²; in both formalisms, zero modes of linear operators describe the stationary non-equilibrium statistics. To access the statistics, we generalize the flow equation approach³ (also known as the method of continuous unitary transformations⁴) to find the zero mode. We test the approach using a prototypical model of geophysical and astrophysical flows on a rotating sphere that spontaneously organizes into a coherent jet. Good agreement is found with low-order equal-time statistics accumulated by direct numerical simulation, the traditional method. Different choices for the generators of the continuous transformations, and for closure approximations of the operator algebra, are discussed.

¹Supported in part by NSF DMR-0605619.

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12:15PM J41.00006 Motion of a Thread in Compressible Turbulence, RORY CERBUS, WALTER GOLDBURG, Department of Physics and Astronomy, University of Pittsburgh — Particles that float on a turbulent tank of water form a system that is compressible in the two dimensions on which they move. Here we study, with an overhead camera, the snake-like motion of a $10 \mu\text{m}$ thread that floats on the surface. The thread, of length much greater than the integral scale L_I of the underlying turbulence, cannot respond to the small-scale turbulent motions at the surface; its Young's modulus is too large. As a result, the mean curvature of the thread is of the order $1/L_I$. Measured properties include velocity structure functions of the thread $S_n(r)$ (including the third moment), the local curvature along the thread (a random variable), and "Richardson diffusion" of pairs of points along the thread separated by distances r . Supported by NSF Grant DMR 0604477 and the Okinawa Institute of Science Technology.

12:27PM J41.00007 Statistical Equilibria of Turbulence on Surfaces of Different Symmetry¹, WANMING QI, BRAD MARSTON, Brown University — We test the validity of statistical descriptions of freely decaying 2D turbulence by performing direct numerical simulations (DNS) of the Euler equation with hyperviscosity on a square torus and on a sphere. DNS shows, at long times, a dipolar coherent structure in the vorticity field on the torus but a quadrupole on the sphere². A truncated Miller-Robert-Sommeria theory³ can explain the difference. The theory conserves up to the second-order Casimir, while also respecting conservation laws that reflect the symmetry of the domain. We further show that it is equivalent to the phenomenological minimum-entropy principle by generalizing the work by Naso et al.⁴ to the sphere. To explain finer structures of the coherent states seen in DNS, especially the phenomenon of confinement, we investigate the perturbative inclusion of the higher Casimir constraints.

¹Supported in part by NSF DMR-0605619.

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⁴A. Naso, P. H. Chavanis, and B. Dubrulle, Eur. Phys. J. B **77**, 284 (2010).

12:39PM J41.00008 Design and Evolution of Shaped Vortices, DUSTIN KLECKNER, WILLIAM T.M. IRVINE, University of Chicago — We present a novel method for generating vortex lines of arbitrary shapes. We then image their dynamics using a high speed scanning technique which provides three-dimensional information at up to 500 volumes per second. We create a variety of configurations and study the effect of geometry on their evolution.

12:51PM J41.00009 Insights into vortex merger using the core growth model, FANGXU JING, Georgia Institute of Technology, EVA KANSO, PAUL NEWTON, University of Southern California — We revisit the two vortex merger problem (both symmetric and asymmetric) for the Navier-Stokes equations using the core growth model for vorticity evolution coupled with the passive particle field and an appropriately chosen time-dependent rotating reference frame. Using the combined tools of analyzing the topology of the streamline patterns along with careful tracking of passive fields, we highlight the key features of the stages of evolution of vortex merger, pinpointing deficiencies in the low-dimensional model with respect to similar experimental/numerical studies. The model, however, reveals a far richer and delicate sequence of topological bifurcations than has previously been discussed in the literature for this problem, and at the same time points the way towards a method of improving the model.

1:03PM J41.00010 Entrainment of solid particles by energetic flow events, MANOUSOS VALYRAKIS, Virginia Tech — The focus of this research study is to investigate the utility and applicability of a recently proposed criterion for the prediction of incipient entrainment of sediment particles. Recently introduced theoretical frameworks and stochastic approaches are presented. At near incipient flow conditions the magnitude of energetic flow events follows a power law distribution, over a wide range of frequencies, similar to many other geophysical phenomena. This implies that highly energetic flow structures, which have a good potential of impinging on an exposed particle and displacing it downstream, occur less frequently. This is in agreement with the intermittent and episodic character of particle entrainment observed from mobile particle flume experiments at low flow stages. Further, analysis of synchronous time series of particle entrainment and local instantaneous flow upstream of it, allows for extraction and characterization of the scales and magnitudes that are relevant to the displacement of individual particles. In addition to having a sound theoretical basis, the modeling approach is shown to perform well in accurately defining the condition of incipient motion and various levels of probability of particle entrainment.

1:15PM J41.00011 Modeling and dynamics of sand bed vortex ripples, JUSTIN KAO, ABIGAIL KOSS, TAYLOR PERRON, Massachusetts Institute of Technology — Vortex ripples arise through the instability of a flat sand bed under oscillatory water flow, for example due to wave action at a beach or continental shelf. Fully developed vortex ripples display complex interactions through the mutual influence of fluid flow and bed topography on each other, via sediment transport. We discuss a mechanistic model of ripple dynamics in which the hydrodynamic influence is linearized, and show that this reduced model nonetheless captures many of the ripple dynamics observed in experiments. Cross-sectional profiles of experimentally generated ripples constrain the modeled sediment flux and provide support for our approximations.

1:27PM J41.00012 The statistics of wind driven ocean currents, YOSEF YOSEF, GOLAN BEL, Dept. of Solar Energy and Environmental Physics, Ben-Gurion University of the Negev — Ocean currents play an important role in the climate system, yet the properties and origin of their statistics is not fully understood. Using the Ekman layer model we show that the statistical properties of the depth integrated surface currents are associated with the temporal correlations of the wind driving the surface currents—when the temporal correlations of the wind are long the probability distribution of the current magnitude is proportional to that of the wind stress. When the temporal correlations of the wind are short the current approaches zero where each component of the current follows a Gaussian distribution such the current magnitude follows the Rayleigh distribution. Using two idealized cases we show that in between these two limits the second (and higher) moment of the current magnitude reaches a maximal value. The results are validated using an oceanic general circulation model.

1:39PM J41.00013 Modulation of Atlantic tropical cyclones by El Nino - Southern Oscillation, CONSTANTIN ANDRONACHE, Boston College — North Atlantic tropical cyclones (TC) usually form in the northern hemisphere summer and fall with a maximum of activity in September. El Nino–Southern Oscillation (ENSO) has been shown to impact seasonal levels of Atlantic basin TC activity. ENSO is the strongest year to year climate fluctuation on Earth. It originates in the tropical Pacific through coupled ocean-atmosphere interactions mediated by surface wind stress and sea surface temperature (SST) variations. Understanding the effects of ENSO on the seasonal variations of TC activity has important practical consequences for seasonal forecast of hurricanes in North Atlantic. In this study we use the NOAA Extended Reconstructed Sea Surface Temperature, the TC counts in North Atlantic, and the NCEP/NCAR reanalysis data to investigate the relationship between significant ENSO events and TC activity during the hurricane season. Model calculations show that forecasted ENSO SSTA can be used as predictors of TC in North Atlantic region. Such results are illustrated in the context of current efforts to understand climate predictability relevant to North Atlantic tropical storms.

1:51PM J41.00014 Fingers and Toes in Miscible Viscous Flows, RADHA RAMACHANDRAN, IRMGARD BISCHOF-BERGER, SIDNEY NAGEL, University of Chicago — The displacement of a more viscous fluid by a less viscous one in a porous medium produces complex fingering patterns. To study this phenomenon a Hele-Shaw geometry is used in which the gap-averaged equations for flow between two parallel plates has the same form as Darcy's law for flow in porous media. Our experiments use a radial Hele-Shaw cell as well as a two dimensional porous medium of densely packed granular beads between two circular glass plates, to study viscous fingering in miscible fluids. For immiscible fluids it is known that the most-unstable wavelength for interface growth depends on surface tension, viscosity difference, velocity and plate spacing. In contrast, we find that for *miscible fluids* the large-scale structure (i.e., the ratio of finger length to overall size of the pattern) is set entirely by the viscosity ratio rather than the viscosity difference of the two fluids. We further investigate the role played by other dimensionless parameters in determining the fine structure and evolution of these fingering patterns in the two geometries.

2:03PM J41.00015 Thermal plumes in locally heated vertical soap films, NICOLAS ADAMI, STÉPHANE DORBOLO, HERVÉ CAPS, Université de Liège, GRASP TEAM — A vertical soap film is maintained by injection of a soap solution from the top. The film is then locally heated. Thermal plumes may be observed to rise in the film, depending on the magnitude of the heating and injected flows. The nearly-2D nature of the system allows to visualize the motion of the plumes using an infrared camera. A model is proposed to describe the growth, emergence, and stationarity of the plumes in the film by taking into account both magnitudes of the heating ΔT and injected flow Q . Oscillatory behaviors of both the full-grown plumes size and direction with respect to the vertical direction may also be observed. Particular soap film thickness dynamics shows to be the origin of those phenomena.

Tuesday, February 28, 2012 11:15AM - 1:51PM –

Session J42 DBIO GSNP: Focus Session: Stochastic Population Dynamics I - Cyclic competition and population stability 156C

11:15AM J42.00001 Cyclic competition of four or more species: Results from mean field theory and stochastic simulations¹, R.K.P. ZIA, Physics Department, Virginia Tech, Blacksburg, VA 24061 — Population dynamics is a venerable subject, dating back two centuries to Malthus, Verhulst, Lotka, Volterra, and many others. Nonetheless, new and interesting phenomena are continually being discovered. For example, the recent discovery of "Survival of the Weakest" in cyclic competition between 3 species with no spatial structure (Berr, Reichenbach, Schottenloher, and Frey, Phys. Rev. Lett. 102, 048102 (2009)) attracted considerable attention, e.g., <http://www.sciencedaily.com/releases/2009/02/090213115127.htm>. Considering a similar system with 4 or more species, we find a more intuitively understandable principle which appears to underpin all systems with cyclically competing species. We will present several interesting aspects of the 4 species system – from non-linear dynamical phenomena in a deterministic mean-field approach to remarkable extinction probabilities in the stochastic evolution of a finite system. Some insights into the deterministic dynamics, gained from generalizing this system to one with any number of species with arbitrary pairwise interactions, will also be discussed.

¹Supported in part by NSF-DMR-0904999 and 1005417.

11:51AM J42.00002 Varieties of extinction scenarios when four species compete cyclically¹, S.O. CASE, C.H. DUNEY, M. PLEIMLING, R.K.P. ZIA, Virginia Tech — We study a stochastic system with N individuals, consisting of four species competing cyclically: $A + B \rightarrow A + A, \dots, D + A \rightarrow D + D$. Randomly choosing a pair and letting them react, N is conserved but the fractions of each species evolve non-trivially. At late times, the system ends in a static, absorbing state — typically, coexisting species AC or BD . The master equation is shown and solved exactly for $N = 4$, providing a little insight into the problem. For large N , we rely on simulations by Monte Carlo techniques (with a faster dynamics where a reaction occurs at every step). Generally, the results are in good agreement with predictions from mean field theory, after appropriate rescaling of Monte Carlo time. The theory fails, however, to describe extinction or predict their probabilities. Nevertheless, it can hint at many remarkable behavior associated with extinction, which we discover when studying systems with extremely disparate rates.

¹Supported in part by NSF-DMR-0705152, 0904999, 1005417.

12:03PM J42.00003 The effects of mobility on the one-dimensional four-species cyclic predator-prey model¹, DAVID KONRAD, MICHEL PLEIMLING, Virginia Tech — The dynamics of a one-dimensional lattice composed of four species cyclically dominating each other is very much dependent on the rates of mobility in the system. We realize mobility as the exchange of two particles located at two nearest neighbor sites with some species dependent rate s . Allowing for only one particle per site, the different species interact cyclically, with species dependent consumption rate k , such that $k + s \leq 1$. When varying the exchange rates, we see vastly different behavior when compared to the three-species model. The patterns of domain growth and decay still show an overall power law behavior, however the fundamental trend of domain growth does not follow the three-species case. We also look at the space-time diagrams to see precisely how the domains form, grow, and decay.

¹Supported in part by the US National Science Foundation through Grant DMR-0904999.

12:15PM J42.00004 Boundary conflicts and cluster coarsening: Waves of life and death in the cyclic competition of four species¹, AHMED ROMAN, MICHEL PLEIMLING, Virginia Tech — In the cyclic competition among four species on a two-dimensional lattice, the partner particles, which swap positions on the lattice with some probability, produce clusters with a length that grows algebraically as $t^{1/z}$ where z is the dynamical exponent. Further investigation of the dynamics at the boundary of the clusters is realized by placing one partner particle pair in the upper half of the system and the other pair in the lower half. Using this technique, results about the fluctuations of the interface are obtained. We also observe wave fronts in the case of non-symmetric reaction rates where extinction of a partner particle pair takes place.

¹Supported in part by the US National Science Foundation through Grant DMR-0904999.

12:27PM J42.00005 Discriminating the effects of spatial extent and population size in cyclic competition among species, DAVID LAMOUROUX, STEPHAN EULE, THEO GEISEL, JAN NAGLER, Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — Quantifying and understanding the stability and biodiversity of ecosystems is a major task in biological physics as well as in theoretical ecology. From the perspective of game theory, this is highly relevant for questions pertaining to the emergence of cooperation or the coexistence of cyclically competing species. The latter has been recently proposed as a paradigm for biodiversity and it has been shown that the mobility of individuals can support the stability of biodiversity by the formation of spirals. In this contribution, we present a population model for species under cyclic competition that extends earlier lattice models to allow the single cells to accommodate more than one individual by introducing a per cell carrying capacity. We confirm that the emergence of spirals induce a transition from an unstable to a stable regime. This transition however does not appear to be sharp and we find a broad intermediate regime that exhibits an ambiguous behavior. The separation of the two regimes by the usual scaling analysis is thus hampered. The newly introduced carrying capacity offers an alternative way of characterizing the transition. We thus overcome the original limitations by separately analyzing the effect of spatial extent and population size.

12:39PM J42.00006 Stochastic extinction dynamics of HIV-1¹, IRA SCHWARTZ², US Naval Research Laboratory, ERIC FORGOSTON³, Montclair State University, LEOR WEINBERGER⁴, Gladstone Institute of Virology and Immunology and University of California, San Francisco — We consider an HIV-1 within host model in which T cells are infected by the virus. Due to small numbers of molecules, stochastic effects play an important role in the dynamical outcomes in that two states are observed experimentally: a replication state in which the virus is active, or a dormant state leading to latency in which the virus becomes active after a delay. The two states are conjectured to be governed by the Tat gene protein transcription process, which does not possess two stable attractors. Rather, the active state is stable, while the dormant state is unstable. Therefore the dormant state can only be achieved through the dynamics of stochastic fluctuations in which noise organizes a path to dormancy. Here we use optimal path theory applied to a Tat gene stochastic model to show how random fluctuations generate the dormant state by deriving a path which optimizes the probability of achieving the dormant state. We explicitly show how the probability of achieving dormancy scales with the transition rate parameters.

¹We acknowledge support from the Office of Naval Research and the National Institutes of Health

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12:51PM J42.00007 Experimental observation of critical slowing down before population collapse, LEI DAI, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA., DAAN VORSELEN, Department of Physics and Astronomy, VU University, Amsterdam, The Netherlands., CARMEL DUDLEY, ONUR ORNEK, KIRILL KOROLEV, JEFF GORE, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA. — Tipping points marking population collapse and other critical transitions in natural systems (*e.g.* ecosystems, the climate) can be described by a fold bifurcation in the dynamics of the system. Theory predicts that the approach of bifurcations will result in an increasingly slow recovery from small perturbations, a phenomenon called critical slowing down. Here we demonstrate the direct observation of critical slowing down before population collapse using replicate laboratory populations of the budding yeast *Saccharomyces cerevisiae*. We mapped the bifurcation diagram experimentally and found a significant increase in both the size and timescale of the fluctuations of population density near a fold bifurcation, in agreement with the theory. We further confirmed the utility of theoretically predicted warning signals by observing them in two different slowly deteriorating environments. To extend the application of warning signals to spatially extended populations, we proposed and identified several indicators based on the emergence of spatial patterns. Our results suggest that generic temporal and spatial indicators of critical slowing down can be useful in predicting tipping points in population dynamics.

1:03PM J42.00008 Extinction of Bacterial Populations: A Change of Paradigm?¹, INGO LOHMAR, BARUCH MEERSON, Racah Institute of Physics, The Hebrew University, Jerusalem — It is now well-established that individual bacteria of many types switch stochastically between two phenotypes: fast-growing “normals” susceptible to antibiotics, and slowly-growing “persisters” hardly affected by the drug. In the competition of species during exponential growth, persisters are a burden, but they may become beneficial when introducing “stress” phases like drug treatment. We suggest to shift the focus to the *persistence* of an established population. Due to fluctuations, the population will (after a long time) eventually go extinct; persisters act as a life insurance against this. We study a simple stochastic model of these processes. Using a WKB approximation, we find the most likely path to extinction and quantify the extinction risk under both favorable and adverse conditions. Analytical results are obtained both in the biologically relevant regime when the switching is rare compared with the birth and death processes, and in the opposite regime of frequent switching. We explain how persisters strongly reduce the extinction risk and show that rare switches are most beneficial to this end. [I. Lohmar and B. Meerson, *Phys. Rev. E* **84** 051901 (2011)]

¹This work was supported by the Minerva foundation (IL), by the Israel Science Foundation (Grant No. 408/08), and by the U.S.-Israel Binational Science Foundation (Grant No. 2008075).

1:15PM J42.00009 Invasion, Coexistence, and Extinction Driven by Preemptive Competition and Sex Ratio¹, FERENC MOLNAR, Dept. of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, THOMAS CARACO, Dept. of Biological Sciences, University at Albany, GYORGY KORNISS, Dept. of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute — We investigate competitive invasion in a simple population dynamics model, where females can differ genetically in the sex ratio of their offspring, and males can differ in mortality. Analyzing of the mean-field dynamics, we obtain conditions for ecological stability of a given sex-ratio allele for any mortality rate parameters. We also found that stable coexistence of the two alleles is possible, but only males can differ; one female phenotype is present. Our results show that the success of invasion is determined by the female birth sex ratio. A lower female ratio never excludes a larger female sex ratio; in case of coexistence, the surviving female phenotype always has the greater female sex ratio. Finally, we identified an interesting invasion-to-extinction scenario: successful invasion followed by extinction occurs when the invader initially propagates with the resident allele, but after excluding the resident, cannot survive on its own.

¹Supported in part by NSF Grants Nos. DEB-0918392 and DEB-0918413.

1:27PM J42.00010 Vaccine enhanced extinction in stochastic epidemic models¹, LORA BILLINGS, Montclair State University, LUIS MIER-Y-TERAN, Johns Hopkins Bloomberg School of Public Health, IRA SCHWARTZ, U.S. Naval Research Laboratory — We address the problem of developing new and improved stochastic control methods that enhance extinction in disease models. In finite populations, extinction occurs when fluctuations owing to random transitions act as an effective force that drives one or more components or species to vanish. Using large deviation theory, we identify the location of the optimal path to extinction in epidemic models with stochastic vaccine controls. These models not only capture internal noise from random transitions, but also external fluctuations, such as stochastic vaccination scheduling. We quantify the effectiveness of the randomly applied vaccine over all possible distributions by using the location of the optimal path, and we identify the most efficient control algorithms. We also discuss how mean extinction times scale with epidemiological and social parameters.

¹Supported by by National Institute of General Medical Sciences Award No. R01GM090204.

1:39PM J42.00011 Fast stochastic algorithm for simulating evolutionary population dynamics¹, LEV TSIMRING, JEFF HASTY, WILLIAM MATHER, University of California, San Diego — Evolution and co-evolution of ecological communities are stochastic processes often characterized by vastly different rates of reproduction and mutation and a coexistence of very large and very small sub-populations of co-evolving species. This creates serious difficulties for accurate statistical modeling of evolutionary dynamics. In this talk, we introduce a new exact algorithm for fast fully stochastic simulations of birth/death/mutation processes. It produces a significant speedup compared to the direct stochastic simulation algorithm in a typical case when the total population size is large and the mutation rates are much smaller than birth/death rates. We illustrate the performance of the algorithm on several representative examples: evolution on a smooth fitness landscape, NK model, and stochastic predator-prey system.

¹Supported by NIH

Tuesday, February 28, 2012 11:15AM - 2:15PM – Session J43 GSNP DFD: Invited Session: Stochastic Geometry and Conformal Invariance in Non-Equilibrium and Disordered Systems 157AB

11:15AM J43.00001 Stochastic geometry of turbulence, GREGORY FALKOVICH, Weizmann Institute of Science — Geometric statistics open the window into the most fundamental aspect of turbulence flows, their symmetries, both broken and emerging. On one hand, the study of the stochastic geometry of multi-point configurations reveals the statistical conservation laws which are responsible for the breakdown of scale invariance in direct turbulence cascades. On the other hand, the numerical and experimental studies of inverse cascade reveal that some families of isolines can be mapped to a Brownian walk (i.e. belong to the so-called SLE class) and are thus not only scale invariant but conformally invariant. That means that some aspects of turbulence statistics can be probably described by a conformal field theory. The talk is a review of broken and emerging symmetries in turbulence statistics.

11:51AM J43.00002 Stochastic geometry in disordered systems, applications to quantum Hall transitions, ILYA GRUZBERG, The University of Chicago — A spectacular success in the study of random fractal clusters and their boundaries in statistical mechanics systems at or near criticality using Schramm-Loewner Evolutions (SLE) naturally calls for extensions in various directions. Can this success be repeated for disordered and/or non-equilibrium systems? Naively, when one thinks about disordered systems and their average correlation functions one of the very basic assumptions of SLE, the so called domain Markov property, is lost. Also, in some lattice models of Anderson transitions (the network models) there are no natural clusters to consider. Nevertheless, in this talk I will argue that one can apply the so called conformal restriction, a notion of stochastic conformal geometry closely related to SLE, to study the integer quantum Hall transition and its variants. I will focus on the Chalker-Coddington network model and will demonstrate that its average transport properties can be mapped to a classical problem where the basic objects are geometric shapes (loosely speaking, the current paths) that obey an important restriction property. At the transition point this allows to use the theory of conformal restriction to derive exact expressions for point contact conductances in the presence of various non-trivial boundary conditions.

12:27PM J43.00003 Efficient SLE algorithms and numerical pitfalls of the method¹, TOM KENNEDY, Departments of Mathematics and Physics, University of Arizona — We consider a physical experiment or a numerical simulation of a physical phenomena that produces a random family of two-dimensional curves. We would like to know if there is a conformal invariance underlying this stochastic geometry. The Schramm-Loewner evolution (SLE) is a conformally invariant stochastic process which depends on a single parameter κ . For different values of κ it is known to describe the scaling limit of many conformally invariant 2d systems, e.g. percolation, the Ising model, self-avoiding walks and many more. So it is a natural candidate for describing the stochastic geometry of other physical systems. The classical Loewner equation provides a correspondence between curves in the plane and “driving functions,” and SLE is obtained by taking the driving function to be a Brownian motion. Given a collection of random curves in the plane one would like to determine if the curves come from an SLE process for some value of κ . One method is to compute the driving processes of the curves and test if they are a Brownian motion. We discuss algorithms for doing this efficiently and some of the pitfalls in this approach.

¹research supported by NSF grant DMS-0758649

1:03PM J43.00004 Search for Conformal Invariance in Two-dimensional Compressible Turbulence, - STEFANUS, University of Pittsburgh — We present a viable way of experimentally testing for conformal invariance at the surface of a turbulent fluid. The theory being tested here is related to the behavior of random curves on a plane and is associated with the work of Loewner, Schramm and others. It is usually referred to as Schramm-Loewner evolution (SLE). The scalar random variables that are put to this test are the vorticity and the divergence of the surface flow. Both of these variables display certain characteristics of Brownian motion, but the divergence field does not exhibit the Gaussian behavior required by SLE.

1:39PM J43.00005 Schramm-Loewner (SLE) analysis of quasi two-dimensional turbulent flows, SIMON THALABARD, SPEC/IRAMI/CEA Saclay — Quasi two-dimensional turbulence can be observed in several cases: for example, in the laboratory using liquid soap films, or as the result of a strong imposed rotation as obtained in three-dimensional large direct numerical simulations. We study and contrast SLE properties of such flows, in the former case in the inverse cascade of energy to large scale, and in the latter in the direct cascade of energy to small scales in the presence of a fully-helical forcing. We thus examine the geometric properties of these quasi 2D regimes in the context of stochastic geometry, as was done for the 2D inverse cascade by Bernard et al. (2006). We show that in both cases the data is compatible with self-similarity and with SLE behaviors, whose different diffusivities can be heuristically determined.

Tuesday, February 28, 2012 11:15AM - 2:15PM –

Session J44 DPOLY: Focus Session: Dynamics of Polymers: Phenomena Due to Confinement

I 157C

11:15AM J44.00001 A closer look at the two-layer model, DONGDONG PENG, Boston University — Previously we have measured the viscosity of short-chain, unentangled polystyrene films coated on silicon covered with a 100 nm thick oxide layer. We found that a two-layer model, portraying the films as being made of a 3 nm thick mobile layer sitting on top of a bulk-like inner layer, was able to describe our data very well. More recently, we extended similar measurements to entangled films with a higher molecular weight of 212 kg/mol. We found that the same two-layer model was able to describe the viscosity measurements, but would imply an unphysically large stretching of the polymer chains in the films or else the near-surface chains would have to be oblate spheroids with an aspect ratio of about 4. In this talk, I will discuss new results we obtain from films with higher molecular weights of up to 2316 kg/mol and also films that are deposited on a different kind of substrate, namely hydrogen terminated silicon. Implications of these results on the two-layer model will be discussed.

11:27AM J44.00002 Inter- and intra-chain Proximity in PS and PMMA free-standing thin films Studied by Fluorescence NRET, JIE XU, GI XUE, Nanjing University — The reduction in glass transition temperature (T_g) for free-standing thin polymer film has attracted a long term discussion. We found that the inter- and intra-chain coupling/constraint restricts the molecular motion of polymer chains and thus results in the deviation in glass transition dynamics. To observe inter-chain proximity and control the inter-chain interaction, we attached carbazoyl probe (donor) and anthryl probe (acceptor) to some side groups of different chains respectively. Meanwhile, we also attached both donor and acceptor to one chain to characterize the intra-chain constraint. A close proximity of the donor to the acceptor results in a higher NRET efficiency. So the NRET results can provide information about chain proximity and packing density in polymer thin film. With decreasing film thickness h , the density of the films was reduced. The magnitude of the reduction in packing density for PS free-standing films was much larger than that in PMMA, resulted a larger reduction in T_g for PS film.

11:39AM J44.00003 Surface Dynamics of Partially Tethered Polymer Films, MARK FOSTER, JIN KUK LEE, Dept. of Polymer Science, The University of Akron, BULENT AKGUN, NIST Center for Neutron Research, ZHANG JIANG, SURESH NARAYANAN, X-ray Science Division, Argonne National Laboratory, SUSHIL SATIJA, NIST Center for Neutron Research — The surface dynamics of thin polystyrene (PS) melt films can be tailored by tethering some of the chains to a supporting substrate. The relaxation of surface height fluctuations for these films depends on the density of grafting, molecular weight of tethered chains, and extent to which tethered chains extend into the layer. The surface dynamics of “partially tethered” thin films have been studied using X-ray photon correlation spectroscopy (XPCS). PS chains have been grafted to substrates with low grafting densities untethered deuterated PS (dPS) chains spun cast on the tethered chains, and the films annealed to create layers containing both tethered and untethered chains. The degree to which the tethered PS extends into the untethered dPS chains has been measured by neutron reflectivity.

11:51AM J44.00004 Structural characterization of irreversibly adsorbed polymer layers at the polymer/solid interface - In-situ grazing incidence angle x-ray scattering studies¹, NAISHENG JIANG, FEN CHEN, XIAMENG CHEN, ZEXI HAN, CHEN LIANG, PETER GIN, Department of Materials Science and Engineering, Stony Brook University, MITSUNORI ASADA, Kurashiki Research Center, Kuraray Co., Ltd., Japan, MAYA ENDOH, TAD KOGA, Department of Materials Science and Engineering, Stony Brook University — In recent years, great attention has been paid to irreversibly adsorbed polymer layers formed on solid substrates since they can modify various properties of polymeric materials confined at the nanometer scale. In this talk, by the combined use of in-situ grazing incidence small angle x-ray scattering and x-ray reflectivity techniques, we aim to characterize the detailed structures of the adsorbed layers composed of different homopolymers (polystyrene, polybutadiene, poly (ethylene oxide), and poly (methyl methacrylate)) prepared on silicon substrates. We will highlight the generality/differences in the structures, leading to a better understanding of the formation process of the adsorbed layers at the impenetrable solid interfaces.

¹We acknowledge the financial support from NSF Grant No. CMMI-084626.

12:03PM J44.00005 Relaxation of Polyisoprene in Nanoscale Confinement , SUNG A. KIM, PRAVEEN AGARWAL, LYNDEN ARCHER, Cornell University — This talk introduces a simple model of confined polymers in polymer nanoparticle composites. Most studies about confined polymer dynamics have been investigated from the system of polymers in porous media or the polymer thin film structure. This new class of polymer nanoparticle hybrid materials, termed Nanoscale Ionic Materials (NIMs), is synthesized in bulk scale with convenient controllability of diverse properties to create the confined polymers in nanoscale. cis-Polyisoprene (PI), type A polymer whose dipole moments are parallel along the chain backbone, are synthesized by anionic polymerization and then tethered to spherical silica nanoparticles. Broadband Dielectric Spectroscopy measures responses to the applied electric field which are normal mode relaxation indicative of whole chain relaxation, and also segmental relaxation. We show that relaxations of PI are slower when simultaneously confined and tethered. We also show that molecular weight and grafting density have a profound effect on dynamics of the twice-confined PI chains.

12:15PM J44.00006 Molecular simulations of confined polymer glasses , ROBERT RIGGLEMAN, AMIT SHAVIT, University of Pennsylvania — For many technological applications ranging from semiconductor manufacturing to membranes for separations and flexible displays, the properties of glass-forming materials confined on the nanoscale are of critical importance. For example, common semiconductor manufacturing techniques rely on the mechanical integrity of amorphous polymer nanostructures. Experiments over the past several years have demonstrated that many of the properties of polymer glasses (e.g., the glass transition temperature, T_g , and the elastic constants) can change significantly and in unintuitive ways when confined to dimensions below approximately 100 nm. These confinement effects depend strongly on the detailed polymer chemistry. In this talk, I will describe our recent work using molecular simulations to study the effects of nanoscale confinement on both the dynamic and mechanical properties of a series of coarse-grained polymer models. Our coarse-grained models systematically explore the effects of polymer chemistry by gradually changing the polymer backbone stiffness and analyzing changes in various properties in free-standing thin films. We find that the confinement effects can vary drastically depending on the properties measured, and in some cases we observe significant ordering of our polymer chains

12:27PM J44.00007 Structure and Dynamics of Polymer / Single Wall Carbon Nanotube Nanocomposites , NIGEL CLARKE, ARGYRIOS KARATRANTOS, University of Sheffield, KAREN WINEY, RUSSELL COMPOSTO, University of Pennsylvania — We simulate the static¹ and dynamic² properties of monodisperse polymers in the presence of a SWCNT using molecular dynamics. The SWCNT has a large aspect ratio and radius smaller than the polymer radius of gyration. We find that although the local chain structure is significantly affected, the overall configuration, as characterized by the radius of gyration, is not perturbed by either the interaction strength between the polymer and the SWCNT or by variations in the SWCNT radius. In contrast, for the dynamics of entangled polymers, we find a significant heterogeneity, with the center of mass polymer diffusion being affected by the strength of the enthalpic interaction between monomers and the SWCNT, as well as the SWCNT radii. In addition, we find that the polymer chain diffusivity perpendicular to the SWCNT is smaller than that parallel to the SWCNT in the case of entangled polymers.

¹Karatrantos A., Composto R.J., Winey K.I., Clarke N., Macromolecules, accepted.

²Karatrantos A., Composto R.J., Winey K.I., Clarke N., in preparation.

12:39PM J44.00008 Polymer Conformations in SWCNT/Polystyrene Nanocomposites using SANS¹ , WEI-SHAO TUNG, University of Pennsylvania, NIGEL CLARKE, University of Sheffield, RUSSELL J. COMPOSTO, KAREN I. WINEY, University of Pennsylvania — Polymer conformations are a critical factor that affects the performance of polymer nanocomposites. Using small angle neutron scattering, we probe chain conformations and confinement of polymers in SWCNT/polystyrene nanocomposites. We established the contrast matching criteria by measuring nanocomposites with different dPS:PS ratios (79:21 to 63:37) for two different SWCNT loadings and found the best ratio of dPS:PS (72.5:27.5) which gives us a similar scattering strength as SWCNT. Therefore, the scattering signal from SWCNT are screened and contribute little to the total scattering intensity. By making contrast matched samples, we are able to focus on the scattering intensity from polymer chains and determine R_g by fitting the intensity data. We found that the R_g of the polymer chain increases weakly with 1 wt% (< 5%) nanotube and then strongly (>25%) with 3 wt% nanotube, while the chain conformation still follows Gaussian statistics.

¹National Science Foundation NSF/EPSRC Materials World Network DMR-0908449

12:51PM J44.00009 Structures and Dynamics of Polymers Adsorbed on Supported Cationic Lipid Membrane , CHEN-MING CHANG, YUK-GYN LAU, JIH-CHIANG TSAI, WEN-TAU JUAN, Institute of Physics, Academia Sinica, Taipei, Taiwan — The structures and dynamics of polymers adsorbed on various surfaces have received attentions not only as a subject concerning fundamental polymer physics, but also for their important roles in many industrial and biological processes. In this talk, I will discuss our recent work utilizing single-molecule imaging to study the conformation and dynamics of fluorescent dye labeled λ -DNA molecules adsorbed on supported cationic lipid membrane. High-magnification snapshots of individual molecules, combined with statistical analyses on their apparent size and anisotropy as well as dynamic analyses on their diffusions, reveal interesting details that could have been overlooked in measurements based on ensemble averaging and theories based on polymers in 2D.

1:03PM J44.00010 Structure and Dynamics in Hyperbranched Nanohybrids , K. CHRISOPOULOU, S. FOTIADOU, S.H. ANASTASIADIS, Foundation for Research and Technology-Hellas and Univ. of Crete, Greece, B. FRICK, ILL, France — The structure and dynamics of a hyperbranched polyester-amide (Hybrane[®] 1200, $M_n=1200$, $T_g=45^\circ\text{C}$) polymer and its nanocomposites with natural montmorillonite (Na^+ -MMT) are investigated to offer a detailed picture of its behavior in bulk and under confinement and reveal its potential use for various applications. The static properties were studied utilizing X-ray diffraction (XRD), while the dynamics using energy-resolved elastic and quasi-elastic neutron scattering (QENS). XRD reveals that the polymer chains reside within the galleries of the Na^+ -MMT producing an intercalated nanocomposite. The elastically scattered intensity for the polymer exhibits two distinct relaxation steps, which are attributed to the methyl group rotation and to the segmental motion. The intensity for the nanocomposite shows the first step broader than the respective of the pure polymer indicating restricted local motion whereas it indicates frozen dynamics under confinement at temperatures higher than the bulk polymer glass transition temperature, T_g . The QENS spectra measured at temperatures covering the regimes below and above T_g are in agreement with the elastic measurements. Sponsored by the Greek GSRT ($\Sigma\text{YNEPTA}\Sigma\text{IA}$; 09 $\Sigma\text{YN} - 42 - 580$) and by the EU (CP-IP 246095-2).

1:15PM J44.00011 Large Amplitude Shear Deformations of Nano-Filled Elastomers: Evidence of Glassy Dynamics in the Vicinity of the Fillers , DIDIER LONG, PAUL SOTTA, CNRS/Rhodia, SAMY MERABIA, CNRS/Universite Lyon I, AURELIE PAPON, ESPCI, FRANCOIS LEQUEUX, HELENE MONTES, CNRS/ESPCI, LAURENT GUY, Rhodia — Adding fillers in elastomers is known to increase the elastic modulus and the wear resistance of elastomers, but also to increase non-linear dissipation, a phenomenon known as the Payne effect. Indeed, when submitted to deformations of the order of a few per cents or more, the elastic modulus can decrease down to values much smaller than the initial one. On the other hand, when submitted to large amplitude oscillatory shear, frequency analysis shows that the contribution of higher harmonics to the response is quite small. This might appear somehow as a paradox since the non-linear behavior of filled elastomers can be strongly marked. We proposed a possible physical origin of these various features. We do it by comparing experimental results performed on model elastomers to the prediction of a model proposed recently, based on the presence of glassy bridges linking neighboring particles. The non-linear response is a consequence of a shift towards shorter time scales (as compared to the non-perturbed distribution) of the relaxation time distribution when a large amplitude periodic solicitation is applied. The non-harmonic response is the consequence of the fluctuation during one cycle of the distribution of relaxation times and is thus a much smaller effect.

1:27PM J44.00012 Polymer Diffusion Slows Down in Nanocomposites Containing Hard Nanospheres¹, RUSSELL COMPOSTO, SANGAH GAM, KAREN WINEY, University of Pennsylvania, NIGEL CLARKE, University of Sheffield, JEFFREY METH, E.I. DuPont de Nemours & Co. — Here, we present two experimental studies of tracer diffusion in polymer nanocomposites (PNCs). Tracer diffusion of deuterated polystyrene (dPS) in a PS matrix containing phenyl-grafted silica (13nm and 29nm) represents a PNC with a weak polymer/particle interaction [1]. However, tracer diffusion of deuterated poly(methyl methacrylate) (dPMMA) in a PMMA matrix containing hydroxyl-terminated silica (13 nm and 28nm) represents a PNC with a strongly attractive polymer/particle interaction. In the former case, the normalized diffusion coefficients fall on a master curve when plotted against the confinement parameter, namely the interparticle separation normalized by the probe size. However in the latter case, the reduced diffusion coefficients in the PMMA matrix with 13nm nanoparticles are less than those with 29nm nanoparticles, suggesting that enthalpic interactions play a role in slowing down diffusion. These experimental studies indicate that a successful model of polymer dynamics must include contributions due to constraints imposed by the nanoparticles as well as interactions between polymer and nanoparticles.

[1] Gam, S., et. al., *Macromolecules* **44**, 3494-3501, 2011.

¹NSF Materials World Network

1:39PM J44.00013 Time and Temperature Dependent Surface Stiffness of Poly(alpha-methylstyrene)(PAMS) through Particle Embedment¹, TASKIN KARIM, GREGORY MCKENNA, Texas Tech University — In the present work, we have used the particle embedment technique with sub-micron particles to study the time dependence surface modulus of poly(alpha-methylstyrene)(PAMS) at different temperature ranging from room temperature to $1.1T_g$ of PAMS. The surface was found softer at room temperature and at $1.02T_g$ compared to the bulk film while at $1.1T_g$ the surface was found stiffer compared to the macroscopic modulus measured for the same PAMS. The embedment of the particle is determined from atomic force microscope measurements and the modulus was determined using the elastic analysis of Johnson, Kendall and Roberts (JKR) with surface energy estimates of the work of adhesion as the driving force for embedment. REFERENCES 1. K. L. Johnson, K. Kendall and A. D. Roberts, *P. Royal Society of London A*, **324**,301-313 (1971). 2. J. H. Teichroeb and J. A. Forrest, *Physical Review Letter*, **91**,016104 (2003).

¹ NASA under grant NNX07AD44A and NSF under grant CMMI-0928453

1:51PM J44.00014 The Calorimetric Glass Transition of Polystyrene Ultrathin Films¹, SIYANG GAO, YUNG P. KOH, SINDEE SIMON, Texas Tech University — Although the glass transition behavior of polystyrene ultrathin films has been widely studied, calorimetric measurements are limited due to difficulties in sample preparation. Here we report the use of a rapid scanning calorimeter based on a membrane sensor to measure the rate-dependent glass transition temperature (T_g) for single ultrathin films. Both microtomed and spin-coated films are investigated. Preliminary results suggest that the magnitude of the T_g depression is similar to that observed for freely-standing films. The T_g depression also depends on the cooling rate such that at the highest rates used (1000 K/s), the depression is only a few degrees. The kinetics of dewetting are followed, with T_g values increasing as a function of time and finally reverting to the bulk values after several hours at 160 °C.

¹National Science Foundation DMR-1006972

2:03PM J44.00015 Dynamics of anchored polymer chains in a tunable micelle confinement system, HENGXI YANG, CHELSEA CHEN, GA RAM JUN, PETER GREEN, University of Michigan — We investigated the dynamics of the polyisoprene (PI) component confined within micelles in the blends of polystyrene-*b*-polyisoprene (PS-*b*-PI) diblock copolymers and polystyrene (PS) homopolymers, using broadband dielectric spectroscopy (BDS). In these blend, the diameter of the PS-*b*-PI micelle cores, composed of the PI component, increased with increasing molecular weight of the PS host, P , and reached a plateau at high P regime. The BDS results show that the dynamics of the PI component were fastest within the smallest micelle cores. Additionally, the relaxation intensities were weakest within smallest micelle cores. The local glass transition temperature (T_g) of the PI component was 201 K when its core diameter is ~29 nm, while the T_g dropped to 193 K with a core diameter of ~21 nm. Although faster dynamics with confinement has been previously observed in several systems, few have examined confinement at length scales much greater than that of the typical cooperative rearranging region, which is normally a few nanometers. Therefore, our study may shed new light on understanding the dynamical behavior of confinement, especially in domains formed in microphase separated block copolymer structures.

Tuesday, February 28, 2012 11:15AM - 12:39PM –
Session J45 DPOLY: Padden Award Symposium 159

11:15AM J45.00001 Field-Theoretic Studies of Nanostructured Triblock Polyelectrolyte Gels, DEBRA AUDUS, GLENN FREDRICKSON, University of California, Santa Barbara — Recently, experimentalists have developed nanostructured, reversible gels formed from triblock polyelectrolytes (Hunt et al. 2011, Lemmers et al. 2010, 2011). These gels have fascinating and tunable properties that reflect a heterogeneous morphology with domains on the order of tens of nanometers. The complex coacervate domains, aggregated oppositely charged end-blocks, are embedded in a continuous aqueous matrix and are bridged by uncharged, hydrophilic polymer mid-blocks. We report on simulation studies that employ statistical field theory models of triblock polyelectrolytes, and we explore the equilibrium self-assembly of these remarkable systems. As the charge complexation responsible for the formation of coacervate domains is driven by electrostatic correlations, we have found it necessary to pursue full “field-theoretic simulations” of the models, as opposed to the familiar self-consistent field theory approach. Our investigations have focused on morphological trends with mid- and end-block lengths, polymer concentration, salt concentration and charge density.

11:27AM J45.00002 Effect of Confinement on Proton Transport in Nanostructured Block Copolymer/Ionic Liquid Membranes, MEGAN L. HOARFROST, University of California, Berkeley, MADHU S. TYAGI, NIST Center for Neutron Research, RACHEL A. SEGALMAN, JEFFREY A. REIMER, University of California, Berkeley — Nanostructured membranes containing structural and proton-conducting domains are of great interest for a wide range of applications requiring high conductivity coupled with high thermal stability. Understanding the effect of nanodomain confinement on proton-conducting properties in such materials is essential for designing new, improved membranes. This relationship has been investigated for a lamellae-forming mixture of poly(styrene-*b*-2-vinylpyridine) (PS-*b*-P2VP) with ionic liquid composed of imidazole and bis(trifluoromethane)sulfonimide (HTFSI), where the ionic liquid selectively resides in the P2VP domains of the block copolymer. Quasi-elastic neutron scattering and NMR diffusion measurements reveal high levels of a fast proton hopping transport mechanism, which we hypothesize is due to changes in the hydrogen bond structure of the ionic liquid under confinement. This, in combination with unique ion aggregation behavior, leads to a lower activation energy for macroscopic ion transport compared to that in a mixture of ionic liquid with P2VP homopolymer. These results portend the rational design of nanostructured membranes having improved mechanical properties and conductivity.

11:39AM J45.00003 Controlling Au Nanorod Dispersion in Thin Film Polymer Blends¹, MICHAEL J.A. HORE, RUSSELL J. COMPOSTO, Dept. of Materials Science and Engineering, University of Pennsylvania — Dispersion of Au nanorods (Au NRs) in polymer thin films is studied using a combination of experimental and theoretical techniques. Here, we incorporate small volume fractions of polystyrene-functionalized Au NRs ($\phi_{rod} \approx 0.05$) into polystyrene (PS) thin films. By controlling the ratio of the brush length (N) to that of the matrix polymers (P), we can selectively obtain dispersed or aggregated Au NR structures in the PS-Au(N):PS(P) films. A dispersion map of these structures allows one to choose N and P to obtain either uniformly dispersed Au NRs or aggregates of closely packed, side-by-side aligned Au NRs. Furthermore, by blending poly(2,6-dimethyl-p-phenylene oxide) (PPO) into the PS films, we demonstrate that the Au nanorod morphology can be further tuned by reducing depletion-attraction forces and promoting miscibility of the Au NRs. These predictable structures ultimately give rise to tunable optical absorption in the films resulting from surface plasmon resonance coupling between the Au NRs. Finally, self-consistent field theoretic (SCFT) calculations for both the PS-Au(N):PS(P) and PS-Au(N):PS(P):PPO systems provide insight into the PS brush structure, and allow us to interpret morphology and optical property results in terms of wet and dry PS brush states.

¹Supported by NSF Polymer (DMR09-07493), MRSEC (DMR05-20020), and IGERT (DGE-0221664).

11:51AM J45.00004 Influence of Charge and Network Inhomogeneities on the Swollen-Collapsed Transition in Polyelectrolyte Nanogels, PRATEEK JHA, JOS ZWANIKKEN, Northwestern University, FRANÇOIS DETCHEVERRY, LPMCN, Université de Lyon, JUAN DE PABLO, University of Wisconsin-Madison, MONICA OLVERA DE LA CRUZ, Northwestern University — Polyelectrolyte nanogels are sub-microscopic networks of solvent-permeated polyelectrolyte chains that undergo large reversible volume changes for a range of environmental stimuli. This volume phase transition behavior finds use in targeted drug delivery, optical switching in photonic crystals, and many other applications that require controlled tunability. Although the strength of electrostatic interactions have a strong influence on the nanogel response, these interactions are not well captured by the classical mean-field theories of macroscopic gels. We develop a simplified Poisson-Boltzmann model of spherical gels, that highlights the importance of charge inhomogeneities and the associated Coulomb interactions in determining the response of gels. Our analysis reveals that nanometer-sized gels, collapsed gels, and gels in media with low salinity or high dielectric constant, have large regions of excess charge, and show clear deviations from the classical Donnan picture of polyelectrolyte gels. The detailed swelling-collapse behavior is obtained using the theoretically-informed coarse-grained simulations, which includes the effects of network imperfections and thermal fluctuations. The simulations capture the universal features of volume phase transition in nanogels.

12:03PM J45.00005 Enhanced electron mobility of n-channel polymer thin film transistors by use of low-k polymer dielectric buffer layer, FELIX SUNJOO KIM, SAMSON JENEKHE, University of Washington — Understanding the factors that govern charge transport in polymer thin film transistors is of interest in developing high-performance polymer transistors and circuits. Engineering the dielectric properties of the gate insulator of a field-effect transistor represents one of the promising approaches to improving the performance of the devices. We show that insertion of a low-k polymer dielectric layer between a silicon dioxide gate dielectric and poly(benzobisimidazobenzophenanthroline) (BBL) semiconductor of n-channel organic transistors increases the field-effect electron mobility by two orders of magnitude. The enhanced electron mobility was accompanied by increased on/off current ratio, superior multicycling stability with negligible hysteresis, and enhanced durability in air. Systematic studies of a series of polymer dielectrics showed that the electron mobility increased exponentially with decreasing dielectric constant, which can be understood in terms of the reduced energetic expense of charge carrier/dipole interaction.

12:15PM J45.00006 Imaging three dimensional bicontinuous networks in bulk heterojunction solar cells, JAMES T. ROGERS, LOUIS A. PEREZ, ALAN J. HEEGER, UC Santa Barbara, HIROSHI JINNAI, Kyushu University, GUILLERMO C. BAZAN, EDWARD J. KRAMER, UC Santa Barbara — Highly efficient, solution processable, organic photovoltaics typically consist of a two component donor-acceptor type heterojunction structure comprised of a low bandgap conjugated polymer donor blended with a fullerene acceptor. Efficient charge extraction from these blends demands that donor and acceptor components form nanoscale phase separated percolating pathways to their respective electrodes. Although the existence of this bicontinuous interpenetrating network, termed a bulk heterojunction (BHJ), is hypothesized to be requisite for efficient device operation, attempts to characterize BHJ structures using conventional transmission electron tomography (TEM) techniques have failed. Energy filtered TEM (EF-TEM) is demonstrated to overcome the inadequacies of conventional TEM, enabling three-dimensional (3D) imaging of high efficiency BHJ structures with nanometer resolution. Considered in combination with x-ray scattering measurements, the 3D chemical maps derived from EF-TEM are used to offer a plausible mechanism of BHJ formation in devices reaching 7.1% efficiency.

12:27PM J45.00007 Single molecule dynamics of self-associating polymers, CHARLES SING, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — Recent progress has been made experimentally in understanding the importance of reversible interactions in polymer systems, with systems such as stimuli-responsive gels demonstrating tunable properties. We extend these ideas to single molecules, since this type of behavior is especially important in biological polymers where molecular interactions can be both reversible and long-lived. We have developed simulation models where a Bell-like association model is incorporated into a Brownian Dynamics simulation, so that we represent a self-associating polymer in a coarse-grained fashion. We find that there are exciting implications of these binding properties on the dynamics of polymers both in and out of equilibrium. The introduction of this extra time scale to a dynamic polymer system manifests itself in drastic changes in polymer properties under dynamic loading; in particular, self-associating polymers in shear flow demonstrate large non-monotonic effects and single-molecule pulling scenarios demonstrate pulling behaviors reminiscent of biological molecules. This thus represents a physical model that has intriguing implications in both biological and synthetic polymer systems.

Tuesday, February 28, 2012 11:15AM - 2:15PM –
Session J46 DPOLY: Invited Session: Electrostatic Interactions in Polymeric and Biological Systems 160ABC

11:15AM J46.00001 Ion Specific Effects at Interfaces, YAN LEVIN, Instituto de Física, Universidade Federal do Rio Grande do Sul — Availability of highly reactive halogen ions at the surface of aerosols has tremendous implications for the atmospheric chemistry. Yet neither simulations, experiments, nor existing theories are able to provide a fully consistent description of the electrolyte-air interface. In this talk a new theory will be presented which allows us to explicitly calculate the ionic density profiles, the surface tension, and the electrostatic potential difference across the solution-air interface [1,2]. The theory takes into account both ionic hydration and polarizability [3]. The theoretical predictions are compared to experiments and are found to be in excellent agreement. Finally, the implications of the present theory for stability of lyotropic colloidal suspensions will be considered [4], shedding new light on one of the oldest puzzles of physical chemistry — the Hofmeister effect.

[1] Y. Levin, A.P. dos Santos, and A. Diehl, Phys. Rev. Lett. **103**, 257802 (2009).

[2] A. P. dos Santos, A. Diehl, and Y. Levin, Langmuir **26**, 10778 (2010)

[3] Y. Levin, Phys. Rev. Lett. **102**, 147803 (2009)

[4] A. P. dos Santos and Yan Levin, Phys. Rev. Lett. **106**, 167801 (2011)

11:51AM J46.00002 Solvation of ions in bulk and at interfaces: What can density functional theory teach us?¹, CHRISTOPHER MUNDY, Pacific Northwest National Laboratory — Insights from molecular simulation have influenced both experiment and theory regarding the understanding of the specific ion effect. Although there seems to be a consensus that large polarizable anions exist at the air-water interface, the understanding of the precise molecular interactions that give rise to surface adsorption remain elusive. I will present our work on the adsorption of iodide at the air-water interface using density functional theory (DFT) based interaction potentials. I will discuss similarities and differences of the results obtained using different descriptions of molecular interaction. Last, we are able to reconcile the results obtained with molecular simulation using standard empirical potentials with the dielectric continuum theory of Levin and co-workers.

In collaboration with Marcel Baer, Pacific Northwest National Laboratory; Douglas Tobias, Abe Stern, University of California, Irvine, CA; and Yan Levin, Instituto de Física, UFRGS, Porto Alegre, RS, 91501-970, Brazil.

¹This work was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences. Pacific Northwest National Laboratory is operated by Battelle for the US Department of Energy.

12:27PM J46.00003 Simulation of single molecule stretching experiments on denatured ssDNA¹, MARK STEVENS, Sandia National Laboratories — We have performed simulations of stretching denatured ssDNA using a bead-spring model to compare with recent single molecule experiments. Each bead represents a singly charged base or monomer in the ssDNA. The salt and counterions are explicitly treated. An equal and opposite force is applied to the two terminal beads, and the force-extension curves are calculated at a range of forces. In denatured ssDNA, the bases of ssDNA are blocked from pairing making the flexible polyelectrolyte model applicable. The recent single molecule stretching experiments² on denatured ssDNA have studied the effect of added salt treating both 1:1 and 2:1 salts. These experiments found force-extensions curves exhibit two regimes: at low forces, the extension $R \sim f^\gamma$, where $\gamma = 0.60 - 0.69$ and a high force regime where $R \sim \log f$. The force-extension curves can be scaled to produce overlap for the salt dependence. The force at the crossover between the two regimes f_c scales as $c_s^{1/2}$ for 1:1 salt, but as I^3 for 2:1 salt, where I is the ionic strength. The simulation data reproduce the experimental overlap for both salt cases. The two regimes including the logarithmic behavior at large forces are present in the simulation results. The simulation results imply that the behavior is due to a competition between electrostatics, entropy and the applied force and that other molecular interactions can be neglected. Thus, the standard theoretical methods are not missing an important term in the free energy, although approximation level may be an issue. We will present simulation data on the conformations as a function of applied force and discuss the implications for analytic theory.

¹This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation.

²McIntosh and O.A. Saleh, *Macromolecules* **44**, 2328 (2011).

1:03PM J46.00004 Charge-regularization effects on polyelectrolytes, MURUGAPPAN MUTHUKUMAR, University of Massachusetts — When electrically charged macromolecules are dispersed in polar solvents, their effective net charge is generally different from their chemical charges, due to competition between counterion adsorption and the translational entropy of dissociated counterions. The effective charge changes significantly as the experimental conditions change such as variations in solvent quality, temperature, and the concentration of added small electrolytes. This charge-regularization effect leads to major difficulties in interpreting experimental data on polyelectrolyte solutions and challenges in understanding the various polyelectrolyte phenomena. Even the most fundamental issue of experimental determination of molar mass of charged macromolecules by light scattering method has been difficult so far due to this feature. We will present a theory of charge-regularization of flexible polyelectrolytes in solutions and discuss the consequences of charge-regularization on (a) experimental determination of molar mass of polyelectrolytes using scattering techniques, (b) coil-globule transition, (c) macrophase separation in polyelectrolyte solutions, (c) phase behavior in coacervate formation, and (d) volume phase transitions in polyelectrolyte gels.

1:39PM J46.00005 Effect of electrostatic interactions on lubrication in polymeric and biological systems¹, JAN-MICHAEL CARRILLO, Institute of Materials Science and Department of Physics, University of Connecticut — Many connective tissues, such as cartilage demonstrate excellent lubrication and wear characteristics. Cartilages in mammalian joints can withstand pressures of the order of ten atmospheres and have remarkably low friction coefficient in the range of 0.001-0.03. The surface of the cartilage is covered with bottle-brush-like polyelectrolyte layer consisting of glycoproteins. This brush layer, which faces a similar layer on the opposing cartilage, is sheared as two surfaces slide passing each other during joint motion. We have performed molecular dynamics simulations of charged and neutral bottle-brush macromolecules tethered to substrates to understand the role of the electrostatic and hydrodynamic coupling between brush layers on the lubricating properties in biological and polymeric systems. Glycoprotein layers were modeled as two opposing layers of highly charged bottle-brush macromolecules composed of Lennard-Jones particles grafted to a substrate. Simulations have shown that charged bottle-brush systems have lower friction under shear and weaker dependence of the disjoining pressure on substrate separation than neutral bottle-brush systems. This was explained by formation of lubricating layer with excess of counterions located in the middle between brush-bearing surfaces. In overlapping brush layers the disjoining pressure between brush-bearing surfaces is controlled by the bottle-brush bending rigidity. Under shear, the main deformation mode of the charged bottle-brush layers is associated with the bottle-brush backbone deformation resulting in backbone deformation ratio and shear viscosity being universal functions of the Weissenberg number. In the case of neutral bottle-brush systems there is coupling between backbone and side chain deformation. This violates universality in backbone deformation ratio and manifests itself in shear viscosity dependence on the shear rate. The shear viscosity as a function of the shear rate for the neutral bottle-brush systems has two plateaus and two shear thinning regimes.

¹NSF # DMR-1004576

Tuesday, February 28, 2012 11:15AM - 2:15PM —
Session J48 DPOLY: Focus Session: Gelation and Glass Transition in Colloids and Soft Matter Systems II 161

11:15AM J48.00001 Kinetic arrest and activated relaxation in dense suspensions of attractive nonspherical colloids, RUI ZHANG, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — The coupled translation-rotation activated dynamics in dense suspensions of uniaxial short-range attractive homogeneous (hDC) and Janus (JDC) colloids are studied using the microscopic nonlinear Langevin equation theory based on the concept of a dynamic free energy surface. For larger aspect ratios, three activated regimes, repulsive glass (RG), attractive glass (AG) and gel (G), are predicted where translation and rotation are always strongly coupled. Physical clustering in the JDC system suppresses the re-entrant RG-fluid(F) process. For hDCs of small enough aspect ratio, multiple kinetic arrest transitions, novel re-entrant phenomena, and a dynamical quadruple point emerge associated with F, G, RG, AG, and plastic glass (PG) states. Colloid translational and rotational motions are strongly coupled in the gel, but decoupled (slower translation) in the other activated regimes due to the presence of two distinct hopping processes. Both translation and rotation activated relaxation rates are non-monotonic functions of attraction strength at high volume fractions. Translation-rotation decoupling universally weakens as attraction strength grows, and exhibits a different volume fraction dependence at low, intermediate, and high attraction strengths.

11:27AM J48.00002 Rearrangements, Vibrations and Microscopic Glassy Dynamics and Structure in Quasi-2D Dense Colloidal Gels¹, MATTHEW LOHR, ARJUN YODH, University of Pennsylvania — In this work, we investigate the microscopic dynamics of quasi-2D dense attractive colloidal systems. We confine bidisperse polystyrene spheres between glass coverslips in a suspension of water and 2,6-lutidine; as we increase the temperature of the sample into a critical regime, lutidine wets the colloids, creating a strong attractive interaction ($> 4\text{ kT}$). We specifically study suspensions in the “dense gel” regime, i.e., at a volume fraction high enough that the attractive particles form a spanning cluster, yet just low enough that there exists some structural heterogeneity larger than the individual particle size. We track the particle locations via bright-field video microscopy and analyze the dynamics of both lower-volume-fraction gel states and higher-volume-fraction glassy states. Specifically, we make correlations between local structure, rearrangement-prone regions, and low-frequency vibrational modes. In doing so, we not only characterize the structural and dynamical differences and similarities between colloidal gels and glasses, but we also gain further insight into the origins of dynamic heterogeneity in glassy systems.

¹This work was supported by the National Science Foundation through DMR-0804881, the PENN MRSEC DMR11-20901, and NASA NNX08AO0G.

11:39AM J48.00003 Dynamical Phases and Rheology of Rod-Sphere Nanoparticle Mixtures, RYAN JADRIC, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — Colloidal mixtures involving sticky nonspherical particles that form glasses and gels are relatively unexplored compared to their single component analogs. We develop and apply a microscopic statistical dynamical approach (mode coupling and nonlinear Langevin equation theories) at the center-of-mass level for dense isotropic mixtures of spheres and rods as a function of (short range) attraction strength, aspect ratio, and composition. Based on the mixture structural pair correlations as input, up to seven dynamical phases (transiently localized states with activated dynamics) are predicted corresponding to fluid, repulsive glass, attractive glass, gel, a mixed coexisting glass-gel state, and several partially localized states. The dynamical complexity increases with aspect ratio, and reflects a rich competition between repulsive force caging, physical bond formation and rod interpenetration. Removal of the nanosphere attraction destroys the double gel state but otherwise has minor consequences. The elastic shear modulus and absolute yield stress are also studied, and order of magnitude changes are found along various trajectories in the dynamical phase diagram. Rods are found to generically impart greater bulk rigidity than spheres.

11:51AM J48.00004 Phonons and Rearrangements in Disordered Colloidal Glasses¹, ARJUN YODH, University of Pennsylvania — I will describe experiments which explore the behaviors of disordered particle suspensions at high packing fraction (e.g., see references [1-5]). Recent systems studied include two-dimensional glasses composed of temperature-sensitive microgel particles, and colloidal glasses in binary fluid which permit interaction potential to be switched from attractive to repulsive. Displacement correlation matrix techniques are employed to derive phonon modes and phonon density of states, and video microscopy is employed to study particle rearrangements. Connections between phonons and stress-induced rearrangements will be described, and detailed observations of the properties of cooperative rearrangement events in attractive versus repulsive glasses will be presented.

[1] Chen, K., Manning, M.L., Yunker, P.J., Ellenbroek, W.G., Zhang, Z., Liu, A.J., and Yodh, A.G., *Phys Rev Lett* 107, 108301 (2011).

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[3] Chen, K., Ellenbroek, W.G., Zhang, Z.X., Chen, D.T.N., Yunker, P.J., Henkes, S., Brito, C., Dauchot, O., van Saarloos, W., Liu, A.J., and Yodh, A.G., *Phys Rev Lett* 105, 025501 (2010).

[4] Yunker, P., Zhang, Z.X., and Yodh, A.G., *Phys Rev Lett* 104, 015701 (2010).

[5] Yunker, P., Zhang, Z.X., Aptowicz, K.B., and Yodh, A.G., *Phys Rev Lett* 103, 11, 115701 (2009).

¹This work is supported by the NSF (DMR-0804881, MRSEC DMR-1120901) and NASA (08AO0G).

12:27PM J48.00005 Characterization of local shear zones that govern the deformation of colloidal glasses, KATHARINE JENSEN, Department of Physics, Harvard University, Cambridge, MA, NOBUTOMO NAKAMURA, Department of Mechanical Science and Bioengineering, Osaka University, Osaka, Japan, DAVID WEITZ, Department of Physics and School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, FRANS SPAEPEN, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA — Colloidal glass provides a unique experimental system with which to study the structure, defects, and dynamics of a generic amorphous material. We report experiments on 1.55- μm -diameter, hard-sphere silica colloidal glasses under conditions of uniform shear. We use confocal microscopy to follow the 3D, real-time trajectories of roughly 100,000 particles during homogeneous deformation and explore the roles of both glass density and applied strain rate. In this way, we probe the elastic, anelastic, and plastic response of the system, with particular focus on identifying specific mechanisms of deformation. In plastic deformation, we directly observe “shear defects” or “shear transformation zones” (STZs) as clusters of particles that behave as Eshelby inclusions, undergoing highly localized plastic strain. These clusters can be identified as regions that are best fits to the Eshelby strain field throughout the sample. We correlate the development of these regions with local density-related properties, including the Voronoi volume and the free volume of both individual particles and connected clusters of particles.

12:39PM J48.00006 Elasticity and microstructure of colloidal gels undergoing strain-induced yielding, LILIAN HSIAO, RICHMOND NEWMAN, SHARON GLOTZER, MICHAEL SOLOMON, University of Michigan — The mechanism of yielding in colloidal gels, particularly for high strain-rate deformations that are typical of materials applications, is not fully understood. Here, we examine the oscillatory response and stress relaxation of a colloidal gel formed by short-range depletion interactions to find a correlation between the macroscopic rheological behavior and their microstructural features. We use confocal laser scanning microscopy to directly observe the strain-dependent evolution of 3D gel structure within a shearing device. The gels are made up of monodisperse poly(methyl methacrylate) spheres of different sizes and volume fractions dispersed in refractive index matched solvents. We impose simple shear flows of various strains on the gel and observe the 3D structural change after deformation. This is done using a UV light-activated photopolymer, which allows particle configurations to be locked in place rapidly ($< 0.6\text{ s}$) after yielding. We characterize the transition from a dense network to interconnected clusters using the contact number distribution. Our results show that rigid, stress-bearing clusters play an important part in contributing to the gel elasticity at large strains.

12:51PM J48.00007 Complex oscillatory yielding in model hard sphere glasses, GEORGE PETEKIDIS, NICK KOUMAKIS, FORTH & Univ. of Crete, Greece, FORTH TEAM — The yielding behaviour of hard sphere glasses under large amplitude oscillatory shear has been studied by experimental rheology and Brownian Dynamics simulations. Here we focus on varying the frequency of oscillation probing the interplay between Brownian motion and shear-induced diffusion. Stress, structure and dynamics are followed by rheology and BD simulations. Two frequency regimes are revealed: At low frequencies Brownian motion is dominant, assisting particles to escape their cage during a single step yielding process, identified by a peak of G'' at around the $G' = G''$ crossover. At high frequencies shear induced particle collisions causes cage breaking with the maximum energy dissipation marked by the G'' peak taking place beyond the $G' = G''$ crossover. Intermediate frequencies present a complex yielding behaviour influenced by both mechanisms that leads to a double peak in G'' that has not been reported before in HS glasses. The nonlinear response is quantified by the higher harmonics present in the stress signal. While at low frequencies the strength of higher harmonics reaches a constant value at high strains, in the intermediate and high frequency regime a non-monotonic behaviour is detected with characteristic large amplitude strains exhibiting apparent harmonic response.

1:03PM J48.00008 Interactions of Dislocations with Twin Boundaries in Hard-Sphere Colloidal Crystals, MARIA PERSSON GULDA, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, United States, ERIC MAIRE, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, United States and MATEIS, INSA-Lyon, Villeurbanne, France, DAVID WEITZ, Department of Physics, Harvard University, Cambridge, MA, United States, FRANS SPAEPEN, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, United States — The interaction of dislocations with twin or grain boundaries is a key factor in understanding the strength and strain hardening of crystals. Confocal tracking of particles in a colloidal crystal allows a detailed look at the mechanisms of such interactions at the particle scale, analogously to what happens on the atomic scale in conventional crystals. The grain boundaries are prepared by sedimentation onto templates in the [110] $\Sigma 3$ orientation. A complex set of interactions is observed: additional twinning, the emission of a pair of partial dislocations, and the formation of kinks in the original twin boundary.

1:15PM J48.00009 Gel formation and aging in weakly attractive nanocolloid suspensions, JAMES HARDEN, Department of Physics, University of Ottawa, HONGYU GUO, Department of Physics, University of California, San Diego, SUBRAMANIAN RAMAKRISHNAN, Department of Chemical and Biomedical Engineering, Florida State University, ROBERT LEHENY, Department of Physics and Astronomy, Johns Hopkins University — We present combined x-ray photon correlation spectroscopy (XPCS) and rheometry studies of the evolution of concentrated suspensions of nanometer-scale colloids undergoing thermo-reversible gelation and aging. After a quench through the gel point, suspensions display a protracted latency period in which they remain fluid followed by a gelation regime in which the shear modulus grows rapidly. The XPCS intermediate scattering function displays two features, a plateau value that provides information about constrained local dynamics and a terminal decay related to relaxation of residual stress. From the wave-vector dependence of the plateau value, a localization length can be extracted. At intermediate colloidal volume fractions ($\phi \simeq 0.20$), the relationship between the localization length and the shear modulus agrees quantitatively with a prediction based on a simplified mode coupling theory, while deviations from the predicted scaling at a higher volume fraction ($\phi \simeq 0.43$) are observed near the gel point. While some features of slow strain from stress relaxation correlate with the evolving rheology, others appear decoupled from the macroscopic behavior.

1:27PM J48.00010 Phase-Change Dynamics in Attractive, Polydisperse Colloidal Suspensions¹, JOHN MERGO, Cornell University, School of Applied and Engineering Physics, ITAI COHEN, Cornell University, Department of Physics, ANTHONY DINS-MORE, University of Massachusetts Amherst, Department of Physics — Understanding the single-particle dynamics of phase changes in polydisperse suspensions is important for predicting the structures that arise in these systems. In this talk, we discuss the results of experiments on the melting and freezing of polydisperse colloidal particles. In these experiments, micron-sized colloidal particles are sedimented in water onto a glass coverslip to form a quasi two-dimensional gas. The particles experience an attractive interaction due to a size-tunable depletant added to the mixture. This allows both melting and freezing to be probed in the same experiment. Optical images with single-particle resolution are recorded and each particle is tracked through the duration of the experiment. Interestingly, we find that the increase in polydispersity may stabilize the fluid phase, which has previously been shown to be metastable in experiments on monodisperse particles. In particular, we explore the stability, structure, and dynamics of this fluid phase and how the structures in this phase solidify over time.

¹This work was supported in part through NSF DGE-0654193, NSF DGE-0903653, and with additional support through NSF DMR-0907195.

1:39PM J48.00011 The role of picosecond dynamics in relaxation of molecular glasses¹, MARCUS CICERONE, QIN ZHONG, FENG DING, JACK DOUGLAS, MADHUSUDAN TYAGI, DAVID SIMMONS, National Institute of Standards and Technology — The importance of the relative amplitude of elemental relaxation processes, specifically of the fast β relaxation process ($\langle u^2 \rangle$), to long-time relaxation processes have been emphasized in a number of theoretical models. In this talk I will focus on transport properties and their relationship to $\langle u^2 \rangle$ in supercooled liquids and glasses. In these studies we use antiplasticization to systematically tune molecular packing. These results provide insights into the role that localization and the concomitant emergence of an excess density of states plays in relaxation of and transport in molecular glasses.

¹This work was funded under NIH/NIBIB Grant R01 EB006398-01A1

1:51PM J48.00012 AC Impedance Study of the Structural Transformation of Graphite Suspensions¹, JIANJIAN WANG, GANG CHEN, Massachusetts Institute of Technology — Recently graphite suspensions have been demonstrated to possess very high thermal conductivity enhancements with high stability. However, the thermal conductivity is quite sensitive to the internal structures of the suspensions or the different states of the particulates in the liquids. At low graphite loadings, the graphite particulates can only form evenly distributed isolated clusters in the host material. As the graphite loading increases, the clusters will start merging together to form a 3D percolation network and the graphite suspension becomes gel-like. For the first time, we have observed a sharp kink behavior in the thermal conductivity of suspensions at the percolation threshold. Combined microstructural and AC impedance spectroscopy studies suggest that this kink arises from the change in the bonding strength between graphite flakes as the suspensions go through a transition from isolated clusters to percolated structures. Our studies shed light on the heat conduction mechanisms of nanofluids, suspensions and composites.

¹This work is supported by AFOSR.

2:03PM J48.00013 Large colloidal crystals grown by centrifugation onto a template, DANIEL PENNACHIO, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, KATHARINE JENSEN, Department of Physics, Harvard University, Cambridge, MA, DAVID WEITZ, Department of Physics, Harvard University, Cambridge, MA; School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, FRANS SPAEPEN, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA — Colloidal crystals are commonly formed by sedimenting a colloidal solution at 1g onto a patterned template. Slow sedimentation was previously believed to be a requisite for growing large, perfect crystals without crossover to an amorphous sediment. By increasing the relative gravitational force applied to a monodisperse sample of hard-sphere, 1.55 μm diameter silica colloids, we examined the effect of increased sedimentation velocity on the growth of face-centered cubic crystals on a (100) template. We varied relative centrifugal force up to 3000g, time of centrifugation, lattice parameter, and crystal thickness to assess their effect on crystal quality. Single crystals up to 52 μm thick were grown for all centrifugation speeds. Crystal defects were predominantly stacking faults (bounded by partial dislocations), most of which formed after the critical thickness was reached. The critical thickness, which is a function of the lattice mismatch between crystal and template, was measured directly by varying the crystal thickness. Final stacking fault and vacancy concentrations were independent of centrifugal force and time. We also examined samples centrifuged onto other templates to elucidate the critical role of the template design in directing crystal versus glass formation.

Tuesday, February 28, 2012 11:15AM - 2:15PM –
Session J49 DPOLY: Focus Session: Crystallization in Single-, Multicomponent, and Hybrid Systems | 162A

11:15AM J49.00001 Orientation of conjugated polymers: epitaxy versus mechanical rubbing¹, MARTIN BRINKMANN, Institut Charles Sadron, CNRS- University of Strasbourg, France — Orientation of conjugated polymers like regioregular poly(3-alkylthiophene)s (P3AT) is of high importance as it can be used to exploit their high intrinsic charge transport anisotropy in the elaboration of devices e.g. OFETs and OLEDs. Orientation has been achieved by two different approaches: i) epitaxy and ii) mechanical rubbing. Herein we describe and compare these two orientation methods. On the one hand side, a large palet of structures, nanomorphologies and orientations can be achieved by controlled epitaxial crystallization of polymers like P3HT, PBTTT or polyfluorenes. Not only can epitaxy afford highly oriented and crystalline films of P3ATs, but also highly oriented fibers with a characteristic shish-kebab morphology. The application of Electron Diffraction analysis (rotation-tilt) on highly oriented polymer layers is an original and powerful method to unravel the crystal packing of conjugated polymers. On the other hand side, mechanical rubbing of conjugated polymers, especially P3HT can also lead to highly oriented films without the use of an orienting substrate. The mechanism of thin film orientation has been analyzed in detail using Transmission Electron Microscopy, Grazing-Incidence X-ray diffraction and optical spectroscopy. It is demonstrated that the molecular weight Mw of the polymer impacts the maximum orientation achieved by rubbing. The Mw-dependence of orientation is explained in terms of chain folding and entanglements that prevent the reorientation and reorganization of the pi-stacked chains, especially for Mw ≥ 50kDa. Electron diffraction and HR-TEM show that epitaxially rubbed films differ in terms of *intra-lamellar* order within layers of pi-stacked chains. Whereas the epitaxially rubbed P3HT films show a semi-crystalline structure with crystalline domains bearing 3D order, the rubbed P3HT films exhibit rather a 2D nematic-like order.

¹Financial support by ANR (PNANO) and Region Alsace is gratefully acknowledged.

11:51AM J49.00002 Solution Assembly of Hybrid Poly (3-hexyl thiophene) and Cadmium Selenide Nanowires, FELICIA BOKEL, EMILY PENTZER, TODD EMRICK, RYAN HAYWARD, University of Massachusetts Amherst — Optimizing morphology of self-assembled systems containing both electron carrying (n-type) and hole carrying (p-type) materials holds promise for the fabrication of improved devices, such as solar cells. In this talk, two routes to formation of hybrid p-n composite fibrils consisting of crystalline p-type poly(3-hexyl thiophene) (P3HT) nanowires with n-type cadmium selenide (CdSe) quantum dots and nanorods into well-defined structures will be discussed. The first method involves co-crystallization of freely soluble P3HT and P3HT-functionalized CdSe nanorods to form crystalline hybrid nanowires upon addition of a marginal solvent. Transmission electron microscopy reveals that nanorods preferentially orient parallel to and flank the sides of fibrils. In a second route to forming hybrid materials, chain-end functionalized P3HT is crystallized into fibrillar nanowires. Introduction of nanoparticles promotes binding at the fibril edge, forming parallel composite pathways or “superhighways.” These assembly approaches represent efficient means to organization of conjugated polymers and semiconducting nanostructures, thus offering new opportunities for optoelectronic device design.

12:03PM J49.00003 Correlating crystallization and ionic conductivity of PEO/graphene oxide nanocomposite, SHAN CHENG, DERRICK SMITH, GRACE HSUAN, CHRISTOPHER LI, Drexel University — Polyethylene oxide (PEO) is one of the best candidates for solid state electrolyte due to its chemical stability and strong ability to form complex with lithium salts. Crystallization behavior of PEO directly affects the lithium ion transport, and in turn the ionic conductivity of the electrolyte. By adding two dimensional graphene oxide nanosheets into PEO matrix, mechanical property of the latter is significantly strengthened, while the crystallization behavior of PEO is also altered by the graphene oxide sheets. The crystallization of PEO/graphene oxide nanocomposites was studied by differential scanning calorimetry (DSC) and the orientations of graphene oxide and PEO crystal were studied by small angle X-ray scattering and wide angle X-ray diffraction. PEO/graphene oxide nanocomposite doped with lithium salt was further fabricated and characterized by electrochemical impedance spectroscopy. Anisotropic ionic conductivity was observed for the nanocomposite electrolyte due to the orientation of graphene oxide and directional growth of PEO crystals.

12:15PM J49.00004 Nucleation and Crystallization in nucleated Polymers, CHRISTOPH SCHICK, EVGENY ZHURAVLEV, ANDREAS WURM, University of Rostock — Crystallization is commonly considered as nucleation followed by a growth process. Here we apply the recently developed technique, differential fast scanning calorimetry (DFSC), for a unique, new look at the crystal growth of poly(epsilon-caprolactone) (PCL) and PCL carbon nanotube composites from 185 K, below the glass transition temperature, to 330 K, close to the equilibrium melting temperature. The DFSC allows temperature control of the sample and determination of its heat capacity during temperature treatments by employing cooling and heating rates from 50 to 50,000 K/s. First, the crystal nucleation and overall crystallization half times were determined simultaneously in the range of temperatures where crystallization of PCL occurs. After attempting to analyze the experiments with the classical nucleation and growth model a new methodology is described, which addresses the specific problems of crystallization of flexible linear macromolecules. The structures seem to range from having practically unmeasurable latent heats of ordering (nuclei) to being clearly-recognizable, ordered species with rather sharp disordering endotherms at temperatures from the glass transition to equilibrium melting (increasingly perfect and larger crystals). The mechanisms and kinetics of growth (if any) involve a detailed understanding of the interaction with the surrounding rigid amorphous fraction (RAF) in dependence of crystal size and perfection. E. Zhuravlev, J.W.P. Schmelzer, B. Wunderlich and C. Schick, Kinetics of nucleation and crystallization in poly(epsilon-caprolactone) (PCL), Polymer 52 (2011) 1983-1997.

12:27PM J49.00005 Spherulite Growth in Polymer-Nanoparticle Blends¹, GORAN UNGAR, Seoul National University and University of Sheffield, EUNWOO LEE, Seoul National University, RUIBIN ZHANG, University of Sheffield, JYONGSIK JANG, Seoul National University, SEOUL NATIONAL UNIVERSITY, WCU C2E2 TEAM, UNIVERSITY OF SHEFFIELD TEAM — Blends of polymers with inorganic nanoparticles (NP) were studied by polarized optical and fluorescence microscopy. Silica nanoparticles with a range of diameters from 7 to 100 nm were used. Neat NPs as well as NPs surface-functionalized with a range of groups from strongly to weakly interacting, were blended with poly(ethylene oxide). A purpose-built T-jump microscopy cell was used allowing rapid temperature equilibration at high supercoolings. Lautitzen-Hoffman type analysis revealed that, although the NPs slow down the standard growth rate G_0 in the order PEO - Me-treated SiO₂ - untreated SiO₂ - COOH-treated SiO₂ - NH₂-treated SiO₂, the surface free energy σ decreases in the same order. This suggests that the NPs reduce macromolecular mobility, but at the same time help reduce the secondary nucleation barrier to some extent. Other polymers and NP types, including quantum dots, were also studied. The work also examines the spatial distribution of NPs in the spherulitic polymer nanocomposites.

¹Supported by WCU program through the National Research Foundation of Korea (R31-10013).

12:39PM J49.00006 Synthesis and morphology of hydroxyapatite/polyethylene oxide nanocomposites with block copolymer compatibilized interfaces, JI HOON LEE, MEISHA SHOFNER, Georgia Institute of Technology — In order to exploit the promise of polymer nanocomposites, special consideration should be given to component interfaces during synthesis and processing. Previous results from this group have shown that nanoparticles clustered into larger structures consistent with their native shape when the polymer matrix crystallinity was high. Therefore in this research, the nanoparticles are disguised from a highly-crystalline polymer matrix by cloaking them with a matrix-compatible block copolymer. Specifically, spherical and needle-shaped hydroxyapatite nanoparticles were synthesized using a block copolymer templating method. The block copolymer used, polyethylene oxide-b-poly(methacrylic acid), remained on the nanoparticle surface following synthesis with the polyethylene oxide block exposed. These nanoparticles were subsequently added to a polyethylene oxide matrix using solution processing. Characterization of the nanocomposites indicated that the copolymer coating prevented the nanoparticles from assembling into ordered clusters and that the matrix crystallinity was decreased at a nanoparticle spacing of approximately 100 nm.

12:51PM J49.00007 Confined crystallization in compatibilized Polyamide 6/High Density Polyethylene blends, SIMONA CECCIA, ALEXANDRA ARGOUD, LISE TROUILLET-FONTI, DIDIER R. LONG, PAUL SOTTA, CNRS/Rhodia UMR5268, St.Fons (France) — Blending polymers can be considered the easiest way to obtain new materials with tuned properties thanks to the possibility to control blend morphologies. The blend characteristics depend on the properties of each component, on composition and on morphologies developed during polymers processing. In case of semi-crystalline blended polymers, mechanical performances are closely related to the crystalline morphology. Therefore, it is essential that crystallinity is maintained after blending in order to keep or enhance the properties. This may be a challenge when the blends exhibit multiphase morphologies with sub-micrometer domain sizes. In this work, we study the crystallization behavior of compatibilized Polyamide 6/High Density Polyethylene (PA6/PE) blends by means of the Differential Scanning Calorimetry technique. Blends with various morphologies (dispersed, stretched dispersed, fibrillar and co-continuous) are obtained by reactive extrusion and varying blend composition and processing parameters. Blend composition and morphology turn out to greatly affect the bulk crystallization temperatures of both PA6 and PE. When the polymer is confined in domains of a few micrometers the crystallization temperature peak shifts to lower temperatures. Thus, the smaller the domain size the lower the crystallization temperature in case of dispersed morphologies. Moreover, in multi-scale morphologies showing polymer droplets in the nanometer range, fractionated crystallization (multiple crystallization peaks) is observed.

1:03PM J49.00008 Crystallization and Microphase Separation in Chiral Block Copolymers, RONG-MING HO, Department of Chemical Engineering, National Tsing Hua University, Taiwan — Block copolymers composed of chiral entities, denoted as chiral block copolymers (BCP*s), were designed to fabricate helical architectures from self-assembly. A helical phase (denoted H*) was discovered in the self-assembly of poly(styrene)-*b*-poly(L-lactide) (PS-PLLA) BCPs*. To examine the phase behavior of the PS-PLLA, self-assembled superstructures resulting from the competition between crystallization and microphase separation of the PS-PLLA in solution were examined. A kinetically controlled process by changing non-solvent addition rate was utilized to control the BCP* self-assembly. Single-crystal lozenge lamellae were obtained by the slow self-assembly (i.e., slow non-solvent addition rate) of PS-PLLA whereas amorphous helical ribbon superstructures were obtained from the fast self-assembly (i.e., fast non-solvent addition rate). As a result, the formation of helical architectures from the self-assembly of the PS-PLLA reflects the impact of chirality on microphase separation, but the chiral effect might be overwhelmed by crystallization. Consequently, various crystalline PS-PLLA nanostructures in bulk were obtained by controlling the crystallization temperature of PLLA ($T_{c, PLLA}$) at which crystalline helices and crystalline cylinders occur while $T_{c, PLLA} < T_{g, PS}$ (the glass transition temperature of PS) and $T_{c, PLLA} \geq T_{g, PS}$, respectively. Anisotropic arrangement of the PLLA crystallites grown within the microdomains was identified. The formation of this exclusive crystalline growth is attributed to the spatial confinement effect for crystallization. While $T_{c, PLLA} < T_{g, PS}$, winding crystals with specific crystallographic orientation within the helical microdomains can be found. By contrast, while $T_{c, PLLA} \geq T_{g, PS}$, the preferential growth may modulate the curvature of microdomains by shifting the molecular chains to access the fast path for crystalline growth due to the increase in chain mobility. As a result, a spring-like behavior of the helical nanostructure can be driven by crystallization so as to dictate the transformation of helices and to result in crystalline cylinders.

1:39PM J49.00009 Chain conformation and crystallization in PEO / layered silicate nanocomposites, SPIROS H. ANASTASIADIS, K. CHRISOPOULOU, S. BOLLAS, Foundation for Research and Technology-Hellas and Univ. of Crete, Heraklion Crete, Greece, K.S. ANDRIKOPOULOS, S. FOTIADOU, Aristotle University of Thessaloniki, Greece, G.A. VOYIATZIS, Institute of Chemical Engineering & High Temperature Chemical Processes, Patras, Greece — The polymer chain conformation under confinement and the polymer morphology are investigated in hydrophilic PEO/Na⁺-montmorillonite nanohybrids synthesized by melt and/or solution intercalation. Intercalated hybrids with mono- and bi-layers of PEO chains are obtained for all compositions covering the complete range from pure polymer to pure clay. For low polymer concentrations, where all the polymer chains are intercalated, PEO is purely amorphous. As PEO concentration increases further, the polymer chains adsorbed on the outer surface of the clay particles remain amorphous as well. It is only when there is large amount of excess polymer outside the completely filled galleries that the bulk polymer crystallinity is abruptly recovered. The conformation of the confined or adsorbed polymer chains, as probed by Raman and FTIR spectroscopies, is found more disordered than the PEO melt even at higher temperatures; this is evident by the dramatic increase of the gauche conformations of the C-C bond along the chain backbone. Sponsored by the Greek GSRT (ΣΥΝΕΡΓΑΣΙΑ; 09ΣΥΝ – 42 – 580) and by the EU (CP-IP 246095-2).

1:51PM J49.00010 Lamellar Orientation Inversion under Dynamic Interplay between Simultaneous Crystallization and Phase Separation, CHARLES HAN, ICCAS, WEICHAO SHI, None, ICCAS TEAM — Crystallization dynamics and lamellar orientation may be affected under the dynamic interplay between crystallization and phase separation for a two component system. If phase separation is really weak, lamellae grow in the radial direction within spherulites. However, when strong phase separation intervenes, the lamellae growth could be oriented in the tangential direction in a concentric alternating concentration ring pattern. This lamellar orientation inversion is reflected by a birefringence inversion under optical microscopy and will be illustrated by a study of the PEO/PMMA system.

2:03PM J49.00011 Phase separation of DMDBS from iPP, and controlled crystalline orientation, K. SREENIVAS, NCL, Pune, India, GURUSWAMY KUMARASWAMY, NCL, R.S. BASARGEKAR, Reliance Industries Limited — We report an unexpected dependence of DMDBS phase separation temperature on the molecular weight of the matrix isotactic polypropylene (iPP). DMDBS crystallizes out at lower temperatures for iPP with decreasing molecular weight (and correspondingly lower tacticity). This molecular weight dependence is unique to iPP, and is not observed for either syndiotactic PP or for random ethylene-PP copolymers. We show that thermodynamic Flory-type arguments are unable to rationalize the observed results. We also report results on extrusion film casting of iPP containing DMDBS and show that flow-alignment of DMDBS networks template the orientation of PP crystals. The modulus and yield strength increase on addition of DMDBS, relative to the neat iPP. Tensile modulus and yield stress of drawn films increase with the degree of orientation, and we are able to achieve a substantial increase even at relatively low draw ratios.

Tuesday, February 28, 2012 11:15AM - 2:03PM –
Session J50 DPOLY DBIO: Focus Session: Translocation through Nanopores - Novel Devices and Computational Approaches 162B

11:15AM J50.00001 Integrated Nanopore Detectors in a Standard Complementary Metal-Oxide-Semiconductor Process¹, ASHFAQUE UDDIN, CHIN-HSUAN CHEN, SUKRU YEMENICIOGLU, KAVEH MILANINIA, ELLIE CORIGLIANO, Dept. of Electrical and Computer Engineering, UCSB, MADOO VARMA, Integrated Biosystems Lab, Intel Corporation, LUKE THEOGARAJAN, Dept. of Electrical and Computer Engineering, UCSB — High-bandwidth and low-noise nanopore sensor and detection electronics are crucial in achieving single-DNA base resolution. A potential way to accomplish this goal is to integrate solid-state nanopores within a CMOS platform, in close proximity to the biasing electrodes and custom-designed amplifier electronics. Here we report the development of solid-state nanopore devices in a commercial CMOS potentiostat chip implemented in On-Semiconductor's 0.5 micron technology. By using post-CMOS micromachining, a free-standing oxide membrane and electrodes are fabricated utilizing the N+ polysilicon/oxide/N+ polysilicon capacitor structure available in the aforementioned process. Nanopores with sub-5 nm diameter are drilled in the membrane using a Transmission Electron Microscope. The integrity of pores is validated by measuring current-voltage and noise characteristics. DNA translocation experiments are also performed utilizing these on-chip pores. In addition, electrical tests performed on the CMOS potentiostat circuitry show that the post-CMOS micromachining process does not have any detrimental effect on the CMOS circuitry.

¹This work was supported by Intel Corporation and NSF CAREER Award

11:27AM J50.00002 Graphene Gating of Solid State Nanopores for DNA Translocation, KIMBERLY VENTA, MATTHEW PUSTER, MARIJA DRNDIC, University of Pennsylvania — We report on ionic current measurements through gated solid state nanopores. Devices consist of Si_3N_4 membranes covered with a graphene sheet connected off-membrane to a gold contact pad. The graphene is insulated from solution with a TiO_2 layer deposited by atomic layer deposition, and the gold is exposed by an SF_6 etch. An electron-beam sculpted nanopore below 10 nm in diameter is drilled through the silicon nitride, graphene, and titania. Applying a voltage to the graphene modulates the ionic current through the pore. We measured the current-voltage characteristics for different gate potentials for our devices. We characterized the leakage current from the graphene as well as the ionic current noise in these pores to complement our current-voltage measurements. These results can lead to measurements of the influence on DNA translocation of a potential at the pore and set the groundwork for characterization of graphene-based sensing of DNA at a nanopore.

11:39AM J50.00003 Nanochannel Device with Embedded Nanopore: a New Approach for Single-Molecule DNA Analysis and Manipulation, YUNING ZHANG, WALTER REISNER, McGill University — Nanopore and nanochannel based devices are robust methods for biomolecular sensing and single DNA manipulation. Nanopore-based DNA sensing has attractive features that make it a leading candidate as a single-molecule DNA sequencing technology. Nanochannel based extension of DNA, combined with enzymatic or denaturation-based barcoding schemes, is already a powerful approach for genome analysis. We believe that there is revolutionary potential in devices that combine nanochannels with nanopore detectors. In particular, due to the fast translocation of a DNA molecule through a standard nanopore configuration, there is an unfavorable trade-off between signal and sequence resolution. With a combined nanochannel-nanopore device, based on embedding a nanopore inside a nanochannel, we can in principle gain independent control over both DNA translocation speed and sensing signal, solving the key draw-back of the standard nanopore configuration. We will discuss our recent progress on device fabrication and characterization. In particular, we demonstrate that we can detect - using fluorescent microscopy - successful translocation of DNA from the nanochannel out through the nanopore, a possible method to 'select' a given barcode for further analysis. In particular, we show that in equilibrium DNA will not escape through an embedded sub-persistence length nanopore, suggesting that the embedded pore could be used as a nanoscale window through which to interrogate a nanochannel extended DNA molecule.

11:51AM J50.00004 fd Virus as a Model Stiff Polymer for Translocation Experiments with Solid-State Nanopores¹, ANGUS MCMULLEN, XU LIU, MIRNA MIHOVILOVIC, DEREK STEIN, JAY TANG, Brown University — We report preliminary experimental results of the translocation of the filamentous virus fd through a solid-state nanopore. fd virus is suitable for translocation and detection in a voltage-biased nanopore because it is highly charged, 880 nm long, and 6.6 nm in diameter. Importantly, fd has a persistence length of $\sim 2 \mu\text{m}$, a forty-fold increase over dsDNA, making fd a model stiff polymer for testing theories of polymer translocation dynamics. fd cannot coil in solution, therefore the dispersion of fd translocation times can test a model by Lu et al. that ascribes DNA translocation velocity fluctuations to the distribution of initial conformations of the DNA coil. That picture is in contrast with an alternative model by Li et al., which attributes the spread of DNA translocation times to thermal velocity fluctuations. The physics of fd capture by a nanopore also differs significantly from DNA since the ends of the virus cannot diffusively search for the pore independently of the middle. As a result, the rate of fd capture from solution may not increase monotonically with the applied voltage across the pore; it is possible for fd to become kinetically trapped against the nanopore membrane by the electric field. We will compare the distribution of translocation times of fd virus to distributions for DNA and discuss the influence of the virus's orientation and interactions with the nanopore on the translocation speed and the measured current blockage. We will also examine the dependence of capture rate on the applied voltage.

¹Supported by NSF Grant No. CBET0846505 and IMNI at Brown Univ.

12:03PM J50.00005 Studies of DNA Translocation Dynamics Using Asymmetrical Nanopores¹, XU LIU, KARRI DIPETRILLO, JASON CHAN, DEREK STEIN, Brown University — Despite extensive studies of DNA translocations through voltage-biased solid-state nanopores, the influence of the DNA coil on the translocation dynamics remains poorly understood. We investigated this issue experimentally by controlling the separation between the DNA coil and the nanopore. We studied lambda DNA translocations through devices comprising a 400 nm-high, 2500 nm-wide, disc-shaped cavity bounded from above by a 20 nm-thin silicon nitride membrane with a 10 nm wide nanopore in the center, and from below by at 400 nm-thick silicon nitride membrane with a 300 nm-wide opening in the center. The asymmetric nanopore-cavity structure introduced an 800 nm gap between the initial DNA coil and the nanopore when a molecule translocated from below, but no gap when it translocated from above. Translocation times were longer and the integrated charge deficit was larger for molecules translocating from below. These results are explained by the viscous drag on the DNA outside the pore, whose importance relative to the drag inside the pore we quantify. We outline a consistent model of DNA translocation speeds that depends on the initial configuration of the DNA coil, similar to the velocity fluctuation model of Lu et al.

¹ This material is based upon work supported by the National Science Foundation under Grant No. CBET0846505.

12:15PM J50.00006 First-passage-time analysis of DNA translocation in solid-state nanopores¹, DANIEL LING, East Greenwich High School, Rhode Island, XINSHENG LING, Brown University — We report a DNA translocation experiment using solid-state nanopores and 48 kb lambda DNA samples. As reported previously, the DNA translocation dynamics in such standard solid-state nanopore experiments appear to be complex and multiple folded translocation pathways are observable. We use the translocation events with little or no detectable folded structures to construct a distribution function for the DNA translocation times. We find that the translocation time distribution can be fitted using the first-passage-time probability density function derived by Schrodinger for 1-D Brownian motion with a drift. The voltage dependence of the extracted DNA drift velocity shows excellent agreement with the Stokes' law at high voltages. Deviation from the Stokes' law is found at low voltages, but can be attributed to a systematic error in how different types of folded DNA translocations are sorted.

¹The measurements were carried out by D.L. in the lab of Prof. Derek Stein at Brown University with the supervision of Jason Chan, and assistance by Karri DiPetrillo and Xu Liu.

12:27PM J50.00007 Some aspects of polymer translocation dynamics through nanopore: comparison of recent the theories with simulation results¹, ANIKET BHATTACHARYA², University of Central Florida — Translocation of a flexible polymer chain through a narrow pore has still remained an active field of research. Earlier theoretical studies of Sung and Park,³ Muthukumar,⁴ Chuang, Kantor and Kardar, Kantor and Kardar⁵ for a flexible chain have been complemented by more recent theories of Sakaue⁶ where tension propagation (TP) along the chain backbone at the *cis* side resulting in a nonuniform stretching of the chain has been proposed to be a key input for theoretical studies. Recently these elements of the TP theory has been incorporated in to a Brownian dynamics (BDTP) scheme and numerical studies of the equations of motion are in excellent agreement with prior simulation studies.⁷ A driven translocating chain is essentially *out-of-equilibrium*⁸ which results in *cis-trans* asymmetries both in conformations and in dynamics. Therefore, results from theoretical studies should capture these features. In this talk first I will first present results from Langevin dynamics simulation citing several cases where how this *cis-trans* asymmetry affects the chain conformations and the translocation dynamics. Then I will discuss relevance of these results in the context of existing theories.

¹Partially supported by NSF-CHEM.

²Work done in collaboration with Prof. Kurt Binder, Prof. Wokyung Sung, Prof. Tapio Ala-Nissila and Timo Ikonen.

³W. Sung and P. J. Park, Phys. Rev. Lett. **77**, 783 (1996).

⁴M. Muthukumar, J. Chem. Phys. **111**, 10371 (1999).

⁵J. Chuang, Y. Kantor and M. Kardar, Phys. Rev. E **65**, 011802 (2001); Y. Kantor and M. Kardar, *ibid.* **69**, 021806 (2004).

⁶T. Sakaue, Phys. Rev. E **76**, 021803 (2007); *ibid.* **81**, 041808 (2010).

⁷T. Ikonen, A. Bhattacharya, T. Ala-Nissila and W. Sung (submitted).

⁸A. Bhattacharya and Kurt Binder, Phys. Rev. E. **81**, 041804 (2010); A. Bhattacharya *et al.*, Eur. Phys. J. E **29**, 423 (2009).

1:03PM J50.00008 DNA translocation measurements in solid-state nanopores fabricated using helium-ion microscope, LIPING LIU, Southeast University (Nanjing, China) and Brown University, WANG MIAO, Brown University, CHUONG HUYNH, Zeiss America, QUANJUN LIU, Southeast University, Nanjing, China, XINSHENG LING, Brown University — We report high-quality DNA translocation measurements in solid-state nanopores drilled in free-standing SiN membranes by using a helium-ion beam in a Zeiss helium-ion microscope (HIM). We show that the HIM nanopores have similar performance as the TEM-drilled pores.

1:15PM J50.00009 Dynamics of Simultaneous, Single Ion Transport through Two Single-Walled Carbon Nanotubes: Observation of a Three-State System, STEVEN SHIMIZU, WONJOON CHOI, CHANG YOUNG LEE, MOON-HO HAM, MICHAEL STRANO, Massachusetts Institute of Technology — The ability to actively manipulate and transport single molecules in solution has the potential to revolutionize chemical synthesis and catalysis. In previous work, we developed a nanopore platform using the interior of a single-walled carbon nanotube (diameter = 1.5 nm) for the Coulter detection of single cations of Li⁺, K⁺, and Na⁺. We demonstrate that as a result of their fabrication, such systems have electrostatic barriers present at their ends that are generally asymmetric, allowing for the trapping of ions. We show that above this threshold bias, traversing the nanopore end is not rate-limiting and that the pore-blocking behavior of two parallel nanotubes follows an idealized Markov process with the electrical potential. Such nanopores may allow for high-throughput linear processing of molecules as new catalysts and separation devices.

1:27PM J50.00010 Polymer Translocation through a Nanopore Modulated by a Sticky Site, HENDRICK W. DE HAAN, GARY W. SLATER, Department of Physics, University of Ottawa — We examine the translocation of a long polymer that has one “sticky site” where a single monomer experiences an attraction to the pore. Using a quasistatic model for the translocation dynamics and employing numerically exact methods to generate results, high precision values for the translocation times are obtained across a wide range of driving forces and sticky site well depths. It is found that the interplay between the sticky site well depth, the driving force, and entropic effects can lead to unexpected results such as a non-monotonic variation of the critical well depth with the driving force and abnormally long translocation times due to the generation of a metastable state at a critical driving force. The dynamics are also found to be strongly dependent on the location of the sticky site: a site near the head of the polymer increases the probability of successful translocation while a site in the middle acts merely as a “speedbump.” Treating the sticky site as a perturbation to an otherwise diffusive process (low driving forces) or driven process (high driving forces) yields good agreement with the numerical results.

1:39PM J50.00011 Translocation dynamics of a semi-flexible chain through a nano-pore¹, RAMESH ADHIKARI, ANDY W.C. LAU, Florida Atlantic University, ANIKET BHATTACHARYA, University of Central Florida — We study translocation dynamics of a semi-flexible chain through a nano-pore in two dimensions (2D) using Langevin dynamics simulation. Specifically, we show how the mean first passage time (MFPT) and the probability distribution of the MFPT are both influenced by the bending rigidity of the chain. Furthermore, we monitor the chain conformations both at the *cis* and the *trans* sides and relate these results with recent theories and experiments for a translocating chain through a nano-pore.

¹Partially supported by NSF-CHEM (AB); Supported by NSF-DMR-0701610 (RA and AL),

1:51PM J50.00012 Characterization of Idealized Helical Repeat Proteins in Silicon Nitride Nanopores¹, JIALI LI, BRADLEY LEDDEN, University of Arkansas, DAVID TALAGA, Montclair State University, AITZIBER CORTAJARENA, LYNNE REGAN, Yale University — In this work, we report the measurement of consensus tetratricopeptide repeat (CTPR) proteins with single silicon nitride nanopores. The CTPR proteins were measured in KCl solution at pH below and above its isoelectric point (pI), as well as with and without denaturing agent, Guanidine HCl. When a CTPR protein molecule transits through a nanopore driven by an applied voltage, it partially blocks the ions (K⁺ and Cl⁻) flow in the nanopore and generates a characteristic electric current blockage signal. The current blockage signal reveals information about the size, conformation, and primary sequence of the CTPR protein molecule. Previous translocation studies carried out with DNA have established that higher bias voltages result in shorter duration current blockages indicating that DNA translocates faster at a stronger electric field. However, our CTPR translocation studies show that longer duration current blockades were observed at higher bias voltages. We discuss how the inhomogeneous distribution of the primary charge sequence of the CTPR proteins predicts translocation barriers that are proportional to the bias voltage. Larger barriers at higher bias voltages will result in longer translocation times, consistent with our experimental results.

¹We acknowledge the funding support provided by NHGRI/NIH R21HG003290, NSF/MRSEC 080054, ABI-111/710, and NIH R01GM071684.

Tuesday, February 28, 2012 11:15AM - 2:03PM —
Session J51 DCMP DFD: Liquid Crystals: Smectic, Ferroelectric, Nanocomposites and DNA
Boston Conference Center 154

11:15AM J51.00001 Two-Dimensional Microfluidics: Hydrodynamic Interactions in Ultra-Thin Smectic Liquid Crystal Films¹, ZOOM NGUYEN, AARON GOLDFAIN, CHEOL PARK, JOE MACLENNAN, MATT GLASER, NOEL CLARK, Physics, University of Colorado at Boulder, LCMRC TEAM — Hydrodynamics is important in nature and has a wide range of applications in science and industry. Most studies of fluid dynamics have been carried out in 3D systems, but there is an increasing interest in the hydrodynamics in confined geometries. Smectics can form ultra-thin, stable fluid films of uniform but readily variable thickness, a structure which enables the quantitative study of 2D hydrodynamics. Hydrodynamic interactions in 2D extend much further across the fluid than in 3D, and all the dynamics is confined to a well-defined plane, facilitating clean, high-contrast and high-resolution experiments. Here, we explore the hydrodynamic interactions of disk-like smectic islands with other islands and with a straight film boundary acting as a 1D wall. High speed video microscopy confirms that the translational diffusion of an island is anisotropic in the vicinity of another island or the wall, and this anisotropy persists even at large separations many times the island radius.

¹This work was supported by NASA Grant NAG-NNX07AE48G, and by NSF MRSEC Grant DMR-0820579

11:27AM J51.00002 Two-Dimensional Microfluidics: hydrodynamics of drops and interfaces in flowing smectic liquid crystal channels¹, ZHIYUAN QI, ZOOM NGUYEN, CHEOL PARK, JOE MACLENNAN, MATT MACLENNAN, NOEL CLARK, Physics, University of Colorado at Boulder, LC TEAM — The quantization of film thickness in freely suspended fluid smectic liquid crystal film enables the study of the hydrodynamics of drops and interfaces in 2D. We report microfluidic experiments, in which we observe the hydrodynamics of 2D drops flowing in channels. Using high-speed video microscopy, we track the shape of 2D drops and interfaces, visualizing the deterministic lateral displacement-based separation and pinched flow separation phenomena previously observed only in 3D. Finally, we demonstrate techniques for 2D drop generation and sorting, which will be used for 2D microfluidic applications.

¹Work supported by NSF MRSEC Grant DMR- 0820579 and NASA Grant NAG No. NNX07AE48G

11:39AM J51.00003 Smectic liquid crystal cells with a “dirty” substrate, QUAN ZHANG, LEO RADZIHOVSKY, Department of Physics, University of Colorado, Boulder, CO 80309 — I will describe our recent studies of smectic liquid crystal cells with a “dirty” substrate. Acting as quenched disorder, such substrate heterogeneity destabilizes long-range smectic order on the surface and in the bulk for arbitrarily weak randomness. We analyze the statistics of the corresponding distortions, their decay into the bulk, topological defects and the role of nonlinear smectic elasticity. We will discuss our predictions in the context of recent experiments on ferroelectric smectic-C liquid crystals.

11:51AM J51.00004 Structural Reorganization of 4 - Cyano - 4' - octyloxybiphenyl (8OCB) revealed by Fast Scanning Calorimetry¹, DONGSHAN ZHOU, JING JIANG, ZHIJIE HUANG, WEI JIANG, GI XUE, Nanjing University, DONGSHAN ZHOU TEAM — 4-Cyano-4'-octyloxybiphenyl (8OCB) is a liquid crystal with a few crystalline polymorphic modifications, of which the square plate form is the most elusive. Square plate form was reported to be only solution grown at low temperature and transformed to metastable parallelepiped form immediately even at -20 OC. With the chip calorimeter, we got the smectic glass of 8OCB when it was quenched from the melt with cooling rate of 20, 000 K/s. In the subsequent reheating with rates ranged from 2,000 K/s to 7,000 K/s, we could find two melting peaks located at 310K and 320K, respectively. Under faster heating, the peak at 310K became dominating, while the peak at 320K weakening. At heating rate of 8000 K/s, there was only melting peak of 310K. If further increased the heating rate, the melting peak at 310K would become smaller again because the crystal growth was suppressed until basically invisible at heating rate of about 20,000 K/s. This work shows that the square plate form is the dominating form when grown from the smectic glass, but it starts transforming to the parallelepiped form at heating slower than 8000 K/s. At heating slower than 1000 K/s, the transformation is completed and there is no chance to capture the square plate form.

¹This work is financially supported by the National Basic Research Program of China (973 Program, 2012CB821500) and National Natural Science Foundation of China (No: 20874045, 21027006).

12:03PM J51.00005 A Biaxial Banana Liquid Crystal Phase with Short-range Layer Ordering¹, YONGQIANG SHEN, TAO GONG, DONG CHEN, RENFAN SHAO, CHENHUI ZHU, MATTHEW GLASER, JOSEPH MACLENNAN, DAVID WALBA, NOEL CLARK, Liquid Crystal Materials Research Center, University of Colorado at Boulder — W623, a single-tail, bent-core molecule with a polar termination on one end and a siloxane-terminated tail on the other, exhibits a ferroelectric, orthorhombic, fluid smectic liquid crystal phase, the SmAP_F. Powder x-ray diffraction (XRD) measurements reveal an exotic structural transition on cooling from the SmAP_F to a SmX phase, in which resolution-limited fluid smectic layering reflections give way to four much broader peaks, indicating short-range layer ordering. This behavior points to the kind of internal frustration that gives rise to our recently discovered helical nanofilament phases. We have performed two-dimensional XRD on aligned samples and discovered that one of the four peaks is from the in-plane order. Freeze-fracture transmission electron microscope (FFTEM) measurements confirm that there is two-dimensional short-range order in the SmX phase, with one periodicity in the layer plane and another normal to the layers. The in-plane periodicity can be measured directly from the packing of fibrils to be about 8 nm, consistent with the in-plane x-ray reflection peak. We will present depolarized transmission light microscopy, high-resolution XRD, and FFTEM studies of pure W623, and of mixtures of W623 with the calamitic liquid crystal 8CB.

¹This work is supported by NSF MRSEC Grant DMR-0820579 and by NSF Grant DMR-1008300.

12:15PM J51.00006 A Bent – Shape Leaning Smectic Liquid Crystal Material, CUIYU ZHANG, NICK DIORIO, Kent State University, S. RADHIKA, B.K. SADASHIVA, Raman Research Institute, ANTAL JAKLI, Kent State University — Liquid crystals of bent-shape molecules theoretically can form four types of fluid smectic layer structures: (a) A polar smectic phase (called SmAP) where both molecular plane and the line connecting the end of average molecules (director) are perpendicular to the layer normal; (b) A double tilted chiral polar structure; (c) A single tilted phase (SmCP) where only the molecular plane is tilted with respect to the layer normal. The fourth possibility, where the director is tilted with respect to the layer normal, the “leaning” SmLP phase, has never been verified experimentally. Here we present the first bent-core material that forms a SmLP structure, thus proving the reality of all theoretically predicted bent-core smectic phases.

12:27PM J51.00007 Effective Conductivity due to Continuous Polarization Reorientation in Fluid Ferroelectrics¹, JOSEPH MACLENNAN, YONGQIANG SHEN, TAO GONG, RENFAN SHAO, EVA KORBLOVA, DAVID WALBA, NOEL CLARK, Liquid Crystal Materials Research Center, University of Colorado at Boulder — In crystal ferroelectrics, the macroscopic polarization density $\mathbf{P}$ is stabilized to a set of discrete orientations by the underlying lattice, and ferroelectricity characterized by field-induced switching of $\mathbf{P}$ between these stable states. Fluid ferroelectrics exhibit $\mathbf{P}$ with no energy barriers to its reorientation. As a result, $\mathbf{P}$ can respond to applied electric field in a continuous fashion. We show here that, due to the reorientation of $\mathbf{P}$, an otherwise insulating fluid ferroelectric behaves electrically as a resistive medium, with conductivity in the semiconducting range. Measurements of cell dynamics are reported for the SmAP_F material W623, a bent-core liquid crystal (LC) with large macroscopic polarization that we find to exhibit nearly ideal field-induced block polarization reorientation. We have investigated theoretically the dynamic behavior of block polarization in the SmAP_F phase, finding that a reorienting LC polarization block behaves electrically as a resistor. Experimental studies of W623 confirm this behavior, revealing the low resistance of the block-reorienting LC and the corresponding characteristic flat-topped step in the current response.

¹This work is supported by NSF MRSEC Grant DMR-0820579 and by NSF Grant DMR-1008300.

12:39PM J51.00008 Microscopic origins of first-order SmA-SmC phase behavior and electro optics in de Vries smectic liquid crystals¹, Z. KOST-SMITH, M.A. GLASER, P.D. BEALE, N.A. CLARK, Dept. of Physics, University of Colorado — Many de Vries liquid crystals exhibit a first-order SmA-SmC phase transition. The original de Vries hollow cone model, in which molecules in the SmA phase are tilted with respect to the layer normal but are uniformly distributed in azimuthal orientation, ϕ , has been used successfully to model many properties of de Vries materials, but the microscopic origins of first-order behavior remain obscure. We describe a microscopic mechanism for first-order behavior in de Vries smectics based on the hollow cone model, embodied in a generalized planar spin model where effective interactions between tilted molecules in the smectic layer planes are represented by a nearest-neighbor pair potential, $u(\phi_{ij})$, with a minimum of variable width around $\phi_{ij} = \phi_i - \phi_j = 0$. Using mean-field theory and Monte Carlo simulation, we find that the SmA-SmC transition is second order for a relatively broad minimum in the potential, and becomes first-order as the minimum narrows. This reflects the expected behavior due to excluded volume interactions in a tilted smectic, in which increasing cone angle leads to a more steeply varying effective azimuthal potential. This model naturally explains the observed first-order behavior in the framework of a hollow cone model.

¹This work was supported by NSF MRSEC Grant DMR-0820579 and NSF Grant DMR-1008300

12:51PM J51.00009 Morphology and Dynamics of Liquid Crystalline Molecules Confined in Nano-pores, MALGORZATA JASIURKOWSKA, WILHELM KOSSACK, ROXANA ENE, CIPRIAN IACOB, WYCLIFFE KIPNUSU, PERIKLIS PAPADOPOULOS, JOSHUA SANGORO, University of Leipzig, Germany, MARIA MASSALSKA-ARODZ, Polish Academy of Sciences, Krakow, Poland, FRIEDRICH KREMER, University of Leipzig, Germany, UNIVERSITY OF LEIPZIG, GERMANY TEAM, POLISH ACADEMY OF SCIENCES, KRAKOW, POLAND COLLABORATION — Broadband dielectric and Infrared spectroscopy are combined to study the molecular dynamics of the liquid crystalline compounds belong isothiocyanatobiphenyl homologous series (abbreviated as nBT) confined in pores of mean diameters from 4 nm to 10.5 nm. In bulk, the studied substances show only one liquid crystalline phase: the SmE phase with orthorhombic arrangement within the molecular layers. In contrast to well-known bulk dielectric properties of nBTs, confinement leads to modification of the molecular dynamics. Two relaxation processes are detected. The slower process corresponds to molecular reorientation around short axis and it is faster in pores than in bulk. The second process is attributed to a librational motion of the molecules close to the walls. Both processes exhibit an Arrhenius-type temperature dependence. Detailed analysis of the temperature dependent infrared spectra indicates the different impact of confinement on the rigid and flexible molecular units of nBTs. Transition Moment Orientational Analysis is employed to explore the orientational order of molecules in pores.

1:03PM J51.00010 Temperature Dependence of Smectic Liquid Crystals Mixed With Magnetic Nanoparticles¹, JEFFERSON W. TAYLOR, University of Maryland - College Park, LYNN K. KURIHARA, Naval Research Laboratories, LUZ J. MARTINEZ-MIRANDA, University of Maryland - College Park — We investigate the properties of bulk liquid crystal mixed with a magnetic nanoparticle (CoFe) as a function of temperature. We compare our results to those of a heat capacity measurement of Cordoyiannis et al.² and compare the way the smectic as a function of temperature the way the nematic behaves. We study how the liquid crystal reorganizes in the presence of the functionalized nanoparticles as a function of temperature and compare it to how it behaves at room temperature.³ The X-rays give rise to three or four peaks whose evolution in temperature varies depending on their origin. In particular the second peak does not seem to vary much with temperature, and can be associated with the first several molecular layers attached to the nanoparticles.

¹This work was supported by NSF-DMR-0906344.

²George Cordoyiannis, Lynn K. Kurihara, Luz J. Martinez-Miranda, Christ Glorieux, and Jan Thoen, Phys. Rev. E **79**, 011702 (2009)

³L. J. Martínez-Miranda, and Lynn Kurihara, J. Appl. Phys, **105**, p. 084305 (2009).

1:15PM J51.00011 The Role of ZnO Particle Size, Shape and Concentration on Liquid Crystal Order and Current-Voltage Properties for Potential Photovoltaic Applications¹, LUZ J. MARTINEZ-MIRANDA, JANELLE BRANCH², ROBERT THOMPSON, JEFFERSON W. TAYLOR, LOURDES SALAMANCA-RIBA, University of Maryland - College Park — We investigate the role order plays in the transfer of charges in ZnO nanoparticle - octylcyanobiphenyl (8CB) liquid crystal system for photovoltaic applications as well as the role the nominally 7x5x5nm³ or 20x5x5nm³ ZnO nanoparticles play in improving that order. Our results for the 5nm nanoparticles show an improvement in the alignment of the liquid crystal with increasing weight percentage of ZnO nanoparticles¹. Our results for the 7x5x5 nm³ sample show that the current is larger than the current obtained for the 5 nm samples. We find that order is improved for concentrations close to 35% wt ZnO for both the 7x5x5 nm³ and 20x5x5 nm³. We have analyzed the X-ray scans for both the 7x5x5 and the 20x5x5 nm³ samples. The signal corresponding to the liquid crystal aligned parallel to the substrate is much smaller than the peak corresponding to the liquid crystal aligned approximately at 70° with respect to the substrate for the 7x5x5 nm³ sample whereas this same peak is comparable or more intense for the 20x5x5 nm³ sample. 1. L. J. Martínez-Miranda, Kaitlin M. Traister, Iriselies Meléndez-Rodríguez, and Lourdes Salamanca-Riba, Appl. Phys. Letts, **97**, 223301 (2010).

¹This work was supported by NSF-DMR- MRSEC-0520471, and its REU program, and in part by NSF-DMR-0906433.

²REU student from Florida Institute of Technology

1:27PM J51.00012 ZnO Nanowire Arrays with Liquid Crystals for Photovoltaic Applications¹

, LOURDES SALAMANCA-RIBA, JOSHUA TAILLON, LUZ MARTINEZ-MIRANDA, Materials Science and Engineering Department, University of Maryland, College Park, MD — Liquid crystals are small monodisperse molecules with high mobilities and are easy and cheap to process. In addition, some of their phases exhibit molecular orientation that can provide a path for the electrons, or holes, to move from one electrode to the other. We have added a smectic A liquid crystal (8CB) to ZnO nanowire arrays of different diameters and have observed a photovoltaic effect as a function of the concentration of ZnO in the liquid crystal. The nanowire arrays are covered with 8CB liquid crystal for hole conduction. We have observed an increase in the light absorption of the PV cells as a function of wavelength of the light for the ZnO nanowire cells. We present a detailed study of the structure of the system.

¹Supported by NSF under MRSEC DMR 0520471.

1:39PM J51.00013 Ligation of Complementary Oligomers in Liquid Crystals of nanoDNA¹

GREGORY SMITH, DAVID WALBA, NOEL CLARK, LCMRC, CU Boulder, WEIXIAN XI, TAO GONG, CHRISTOPHER BOWMAN, Chemical Engineering, CU Boulder, TOMMASO FRACCIA, GIULIANO ZANCHETTA, TOMMASO BELLINI, University of Milan, LIQUID CRYSTAL MATERIALS RESEARCH CENTER, UNIVERSITY OF COLORADO, BOULDER COLLABORATION, DEPARTMENT OF CHEMICAL AND BIOLOGICAL ENGINEERING, UNIVERSITY OF COLORADO, BOULDER COLLABORATION, DIPARTIMENTO DI CHIMICA, BIOCHIMICA E BIOTECNOLOGIE, UNIVERSITY OF MILAN, MILAN COLLABORATION — The chromonic stacking mode of short oligomeric DNA upon forming liquid crystalline phases presents an intriguing possibility for liquid crystal autocatalysis, the promotion, by LC ordering, of chemical synthesis that stabilizes LC ordering. In such a scenario the concentration and physical organization of ligation reactants and the fluidity of the liquid crystal phase promotes the appropriate chemical ligation of oligomers. Because it is a mode of elongation free of other catalysts, this offers a tantalizing means of oligonucleotide self-elongation that might have implications in prebiotic life. We present here work toward elucidating possible catalytic enhancement by liquid crystalline phase formation. Ligation approaches based on water soluble carbodiimide base activation and photopolymerization will be presented.

¹This work was supported by NSF MRSEC Grant DMR-0820579.

1:51PM J51.00014 Liquid Crystal Ordering of Random DNA Oligomers

, TOMMASO BELLINI, GIULIANO ZANCHETTA, TOMMASO FRACCIA, ROBERTO CERBINO, University of Milan, Milan, ETHAN TSAI, MARK MORAN, GREGORY SMITH, DAVID WALBA, NOEL CLARK, LCMRC, University of Colorado, Boulder, DIPARTIMENTO DI CHIMICA, BIOCHIMICA E BIOTECNOLOGIE, UNIVERSITY OF MILAN, MILAN COLLABORATION, LIQUID CRYSTAL MATERIALS RESEARCH CENTER, UNIVERSITY OF COLORADO, BOULDER COLLABORATION — Concentrated solutions of DNA oligomers (6 to 20 base pairs) organize into chiral nematic (NEM) and columnar (COL) liquid crystal (LC) phases. When the oligomer duplexes are mixed with single strands, LC phase formation proceeds through macroscopic phase separation, as a consequence of the combination of various self-assembly processes including strand pairing, reversible linear aggregation, demixing and LC ordering. We extended our investigation to the case of LC ordering in oligonucleotides whose sequences are partially or entirely randomly chosen, and we observed LC phases even in entirely random 20mers, corresponding to a family of $4^{20} \approx 10^{12}$ different sequences. We have tracked the origin of this behaviour: random sequences pair into generally defected duplexes, a large fraction of them terminating with stretches of unpaired bases (overhangs); overhangs promote linear aggregation of duplexes, with a mean strength depending on the overhang length; LC formation is accompanied by a phase separation where the duplexes with longer overhangs aggregate to form COL LC domains that coexist with an isotropic fluid rich in duplexes whose structure cannot aggregate.

Tuesday, February 28, 2012 11:15AM - 2:15PM —

Session J52 GSNP DFD: Focus Session: Extreme Mechanics - Plates 153C

11:15AM J52.00001 Radial stretching of thin sheets: A prototypical model for morphological complexity

, BENNY DAVIDOVITCH, UMass Amherst — The complex morphologies of thin sheets consist of wrinkles, crumples, folds, creases, and blisters. These descriptive words may sound lucid — but do they carry any quantitatively distinguishable content? Following the classical approach of pattern formation theory, we seek to impart a universal meaning to these modes of deformation as distinct types of symmetry-breaking instabilities of a flat, featureless sheet. This idea motivates us to consider the general problem of *axisymmetric stretching* of a sheet. A familiar realization of this problem is the “map maker’s conflict”: projecting a flat sheet onto a foundation of spherical shape. Another representative realization is the ‘Lame’ set-up: exerting a radial tension gradient on a sheet, which may be free-standing or resting on a solid or liquid foundation. I will introduce a set of *generic parameters: bendability, confinement, stiffness, adhesiveness*, that span a phase space for the morphology of radially stretched sheets. In this phase space, wrinkling, crumpling, folding, creasing and blistering could be identified as primary and secondary symmetry-breaking instabilities.

11:27AM J52.00002 Bending of a surface with spontaneous curvature

, CATHERINE QUILLIET, PHILIPPE MARMOTTANT, ALEXANDRE FARUTIN, CHAOUQI MISBAH, LIPhy, Univ. Grenoble, France — We interest to curvature deformations that can be described by Helfrich’s energy: a quadratic mean curvature term, and a gaussian curvature term. When the surface is not strictly incompressible and presents a nonzero spontaneous mean curvature, we focus on simple cases to show that a priori determination of key features (spontaneous curvature, equilibrium area) may be biased according the expression taken for the energy.

11:39AM J52.00003 Deformations of 2D Random Elastic Networks

, HENDRIK FLORIJN, M. VAN DEEN, HENK IMTHORN, MARTIN VAN HECKE, Leiden University, GRANULAR & DISORDERED MEDIA TEAM — We study the linear and nonlinear behavior of random 2D elastic networks at the desktop scale. We demonstrate how to fabricate random networks and characterize them with the lattice coordination number Z . We investigate experimentally if there is a relation between the mechanical response and the lattice coordination number Z of the network.

11:51AM J52.00004 Packing with a twist: from Wrinkles to Scrolls

, ARSHAD KUDROLLI, JULIEN CHOPIN, Department of Physics, Clark University — We discuss an experimental investigation of a thin elastic sheet in the form of a ribbon with clamped boundary conditions at both ends which is then subjected to a twist by rotating the ends through a prescribed angle. We find that a wrinkling instability appears even at a small twist angle which depends on the aspect ratio of the ribbon, its bending modulus and initial tension. Using x-ray tomography, we show that the pattern of this first instability has an impact on the folding at larger twist angles which can result in ordered configurations including Fermat scrolls. Still further twisting results in a highly compressive packing as in wringing a towel without application of direct radial compression. Implications for developing yarns with novel mechanical and transport properties [Lima, et al., Science 331, 51 (2011)] will be discussed.

12:03PM J52.00005 Geometry and Mechanics of Chiral Pod Opening¹, ERAN SHARON, SHAHAF ARMON, The Hebrew University of Jerusalem, EFI EFRATI, University of Chicago, RAZ KUPFERMAN, The Hebrew University of Jerusalem — We study the geometry and mechanics that drive the opening of Bauhinia seeds pods. The pod valve wall consists of two fibrous layers oriented at $\pm 45^\circ$ with respect to the pod axis. Upon drying, each of the layers shrinks uniaxially, perpendicularly to the fibers orientation. This active deformation turn the valve into an incompatible sheet with reference saddle-like curvature tensor and a flat (Euclidean) reference metric. These two intrinsic properties are incompatible. The shape is, therefore, selected by a stretching-bending competition. Strips cut from the valve tissue and from synthetic model material adopt various helical configurations. We provide analytical expressions for these configurations in the bending and stretching dominated regimes. Surface measurements show the transition from minimal surfaces (narrow limit) to cylindrical ones (wide limit). Finally, we show how plants use these mechanical principles using different tissue architectures.

¹Supported by ERC “soft Growth” project and by BSF grant #2008432

12:15PM J52.00006 Flat-twisted-helical transition in composed gel sheets and self assembled chiral molecules¹, SHAHAF ARMON, ERAN SHARON, Hebrew University, Jerusalem, EFI EFRATI, University of Chicago, RAZ KUPFERMAN, Hebrew University, Jerusalem — We recently presented a new chirality creating mechanism in elastic strips. In such frustrated bodies, the chiral configuration is determined in a competition between bending and stretching energies, controlled by a dimensionless parameter $\tilde{w} = w\sqrt{k}/t$, in which w is the strip's width, t – its thickness and k – the spontaneous curvature. I will show the geometrical and mechanical equivalence between such elastic strips and self assembled molecules made of twisted elements. I will also show experiments in responsive gels, showing how a continuous variation in $\tilde{w}$ yields an ordered shape transition from flat to twisted and helical shapes and to tubes. Similar transitions have been observed in self assembled macromolecules.

¹This work was supported by Eshkol scholarship of the Israeli ministry of Science and ERC “SoftGrowth” project.

12:27PM J52.00007 Curvature and defects in soft membranes with orientational order¹, THANH SON NGUYEN, JUN GENG, JONATHAN V. SELINGER, Liquid Crystal Institute, Kent State University — Previous research has demonstrated that soft membranes have a coupling between curvature and in-plane orientational order. Defects in the orientational order can induce curvature, and conversely, curvature leads to an effective geometrical potential acting on defects [1]. Recently, our group has done simulations which show that the interaction between curvature and defects depends on several important issues, including the baseline curvature of the membrane (flat, cylinder, sphere, torus), the phase of the defects (radial or tangential), and the relative contribution of in-plane (intrinsic) vs. out-of-plane (extrinsic) variations of the director [2]. To understand the simulations, we develop a theoretical approach that can address those issues. Using this approach, we calculate the energy of defect structures in curved geometries, and determine how the energy varies as a function of the defect position and separation and the membrane distortions. The interaction energy depends on the relative magnitude of intrinsic vs. extrinsic couplings, and on the mechanical properties of the membrane. This approach provides opportunities to design membranes that will relax into selected shapes. [1] AM Turner et al, Rev Mod Phys 82, 1301 (2010). [2] RLB Selinger et al, J Phys Chem B, in press.

¹This work was supported by NSF DMR-1106014.

12:39PM J52.00008 Capillary induced buckling of floating sheets, MIGUEL PINEIRUA, JOSE BICO, BENOIT ROMAN, PMMH-ESPCI, NARAYANAN MENON, UMass — When a water droplet is deposited over a thin floating sheet, radial wrinkles appear in the vicinity of the droplet as a result of capillary forces exerted at the contact line [1]. However, determining the stress state at the contact line is still challenging and limits the full description of the wrinkling pattern. In order to avoid this contact line ambiguities, we propose the experimental study of the buckling of a macroscopic annulus floating on the surface of water and submitted to a difference in surface tension between its inner and outer edges. This particular configuration allows to generate radial wrinkles on the membrane with well defined border conditions. The topography of the wrinkled patterns are precisely measured using a synthetic Schlieren technique. Based on the standard buckling theory, we develop scaling laws for the buckling threshold of the annulus as well as for the wave length and radial extension of the wrinkles, which are compared to our experimental results and numerical simulations.

[1] J. Huang, M. Juszkiwicz, W.H. de Jeu, E. Cerda, T. Emrick, N. Menon, and T.P. Russell. Capillary wrinkling of floating thin polymer films. Science, 317(5838):650-653, 2007.

12:51PM J52.00009 The wrinkle transition of a sheet on a drop, ROBERT SCHROLL, BENNY DAVIDOVITCH, HUNTER KING, NARAYANAN MENON, Physics Department, University of Massachusetts — A thin sheet subject to confinement will wrinkle in order to relieve compressive stress. We discuss the case of a circular sheet living on the surface of a liquid drop. The pressure of the drop forces the sheet to be non-planar, which may induce confinement along the outer edge of the sheet. We show that, in the limit of very thin, highly bendable sheets, the system is governed by a single confinement parameter. This parameter determines if and where wrinkles appear on the sheet. Comparison to experimental results provides the first detailed confirmation of a new far-from-threshold theory to describe such ultra-thin sheets. According to this model, the transition to the wrinkled state represents the loss of axisymmetry in the height field, while the stress field maintains its symmetry.

1:03PM J52.00010 Transition from Wrinkling to Crumpling in a Sheet Floating on a Drop¹, HUNTER KING, NARAYANAN MENON, ROBERT SCHROLL, BENNY DAVIDOVITCH, University of Massachusetts, Amherst — An ultrathin* circular polystyrene sheet floating on the surface of a water drop stretches radially and compresses along its circumference as the curvature of the drop increases. The compression is at first fully relaxed by a wrinkle pattern extending inward from the edge. When the wrinkles occupy too large a fraction of the area of the sheet, sharp, localized, crumpled features continuously emerge. We show that the onset of crumpling is a primary symmetry breaking transition of the stress field. We experimentally characterize this transition from wrinkling to crumpling by studying the distribution of gaussian curvature in the film, measured by optical profilometry. *Typical dimensions are tens of nanometers in thickness and millimeters in lateral size.

¹NSF DMR 0907245

1:15PM J52.00011 Supported conical defects, EFI EFRATI, University of Chicago — In this work we study the elastic equilibrium configurations of a hyperbolic conical defect (a flat disc with a single negative Gaussian curvature condensation), supported on a rigid plane. Originating from the study of strictureplasty, this problem which seems to be a natural extension to the D-cone problem displays a distinct behavior.

1:27PM J52.00012 Stamping and wrinkling of elastic plates, JEREMY HURE, JOSE BICO, BENOIT ROMAN, PMMH - ESPCI ParisTech — In classical Euler buckling a beam is found to buckle with the lowest mode as a compressive strain is applied. Higher modes are however observed if the amplitude of the out-of-plane displacement is bounded by geometrical constraints. What is the limit when the maximum amplitude prescribed is decreased to zero? We show that the wavelength tends towards a finite value dictated by the thickness of the beam. This one-dimensional model is used to describe the compression of a circular elastic plate into an hemispherical mold.

1:39PM J52.00013 Deterministic Wrinkling Patterns of Thin Polymeric Coatings on Soft Substrates, JIE YIN, Department of Mechanical Engineering, Massachusetts Institute of Technology, JOSE L. YAGUE, Department of Chemical Engineering, Massachusetts Institute of Technology, KAREN K. GLEASON, Department of Chemical Engineering, Massachusetts Institute of Technology, MARY C. BOYCE, Department of Mechanical Engineering, Massachusetts Institute of Technology — Wrinkling surface patterns in soft materials have become increasingly important for a broad range of applications including stretchable electronics, microfluidics, thin-film property measurement, wetting and adhesion, and other surface area and topology controlled phenomena. Thermal and swelling mismatch between the thin surface layer and the soft substrate lead to spontaneous formation of buckling-induced disordered labyrinth patterns, which exhibit a mechanistically-determined short wavelength, but an undetermined and highly varied long wavelength. In this paper, analytical and computational models are presented to create deterministic wrinkling patterns through directed buckling methods, which capture the physics of the instabilities governing the formation of multiple wavelength wrinkling patterns, providing a predictive tool for design of deterministic wrinkling patterns. The fabrication of the deterministic patterns is accomplished using novel chemical vapor deposition processes. The role of these patterns in providing multifunctional performance is illustrated and discussed.

1:51PM J52.00014 Wrinkles in reinforced membranes, ATSUSHI TAKEI, ESPCI, FABIAN BRAU, Université de Mons, BENOÎT ROMAN, JOSÉ BICO, ESPCI — We study, through model experiments, the buckling under tension of an elastic membrane reinforced with a more rigid strip or a fiber. In these systems, the compression of the rigid layer is induced through Poisson contraction as the membrane is stretched perpendicularly to the strip. Although strips always lead to out-of-plane wrinkles, we observe a transition from out-of-plane to in plane wrinkles beyond a critical strain in the case of fibers embedded into the elastic membranes. The same transition is also found when the membrane is reinforced with a wall of the same material depending on the aspect ratio of the wall. We describe through scaling laws the evolution of the morphology of the wrinkles and the different transitions as a function of material properties and stretching strain.

2:03PM J52.00015 Mechanics of Graphene Electronics¹, XUANHE ZHAO, Soft Active Materials Laboratory, Duke University — Graphene, a monolayer of tightly-packed carbon atoms, has demonstrated great academic and industrial promises for integrating superior properties of nanomaterials and nanostructures into novel macroscale devices. Here, we demonstrate a simple method to enable over 200% reversible deformation of continuous large-area graphene sheet (over 1cm × 1cm) on polymer substrates. By patterning large-area graphene on a pre-stretched polymer layer by 200%, the graphene film develops hierarchical patterns including wrinkles with wavelengths on the order 10~100 nm and delaminated buckles with wavelengths on the order of 1 μ m. If the polymer is stretched again (<100%), the wrinkled region relaxes and the graphene on this region becomes flat. As the stretch further increases (over 100%), the graphene on delaminated buckles slides toward the flat regions, decreasing the amplitude of the buckles. The relaxation of the wrinkles and buckles enables the large deformation of graphene electrode without fracture. We further demonstrate potential applications of the graphene electrodes capable of large deformation. For example, a polymer film can be sandwiched between two graphene electrodes. As a voltage is applied between the two graphene electrodes, the polymer can achieve an actuation strain over 200%.

¹Funding for this research was provided by the NSF's Research Triangle MRSEC (DMR-1121107) and Pratt School of Engineering at Duke University.

Tuesday, February 28, 2012 11:15AM - 2:15PM – Session J53 GSNP: Disordered Systems: Jamming 153B

11:15AM J53.00001 The contact percolation transition¹, TIANQI SHEN, Physics Department at Yale University, COREY O'HERN, Department of Mechanical Engineering & Materials Science, Yale University, MARK SHATTUCK, Benjamin Levich Institute and Department of Physics, City College of New York of the City University of New York — Typical quasistatic compression algorithms for generating jammed packings of athermal, purely repulsive particles begin with dilute configurations and then apply successive compressions with relaxation of the elastic energy allowed between each compression step. It is well-known that during isotropic compression athermal systems with purely repulsive interactions undergo a jamming transition at packing fraction ϕ_J from an unjammed state with zero pressure to a jammed, rigid state with nonzero pressure. Using extensive computer simulations, we show that a novel second-order-like, contact percolation, which signals the formation of a system-spanning cluster of mutually contacting particles, occurs at $\phi_P < \phi_J$, preceding the jamming transition. By measuring the number of non-floppy modes of the dynamical matrix, the displacement field between successive compression steps, and the overlap between the adjacency matrix, which represents the network of contacting grains, at ϕ and ϕ_J , we find that the contact percolation transition also heralds the onset of nontrivial response to applied stress. Highly heterogeneous, cooperative, and non-affine particle motion occurs in unjammed systems significantly below the jamming transition for $\phi_P < \phi < \phi_J$.

¹This research was supported by NSF Grant No. DMS-0835742.

11:27AM J53.00002 Constraint counting for frictional jamming, D.A. QUINT, University of California Merced, S. HENKES, J.M. SCHWARZ, Syracuse University — While the frictionless jamming transition has been intensely studied in recent years, more realistic frictional packings are less well understood. In frictionless sphere packings, the transition is predicted by a simple mean-field constraint counting argument, the isostaticity argument. For frictional packings, a modified constraint counting argument, which includes slipping contacts at the Coulomb threshold, has had limited success in accounting for the transition. We propose that the frictional jamming transition is not mean field and is triggered by the nucleation of unstable regions, which are themselves dynamical objects due to the Coulomb criterion. We create frictional packings using MD simulations and test for the presence and shape of rigid clusters with the pebble game to identify the partition of the packing into stable and unstable regions. To understand the dynamics of these unstable regions we follow perturbations at contacts crucial to the stability of the "frictional house of cards."

11:39AM J53.00003 Decoupling of Rotational and Translational Diffusion in a 2D Granular Experiment, NABIHA SAKLAYEN, GARY L. HUNTER, ERIC R. WEEKS, Emory University — We experimentally study the rotation and diffusion of granular clusters in a 2D binary granular system. Our apparatus vibrates a 2D system of densely packed granular bidisperse disks (to avoid crystallization) containing trackable 3-particle clusters. We use this system to mimic hard-sphere fluids and the clusters probe the system's local translational and rotational dynamics. As the area fraction of the bidisperse disks is increased, diffusion within the sample becomes slower, and above a critical area fraction, the sample behaves as a granular glass. We analyze the rotational and translational motions of the clusters to determine whether they decouple with changing area fraction of the system. As we approach the glass transition, we observe a decoupling between the two motions.

11:51AM J53.00004 Characterizing the clogging transition by individual grain behavior, CHARLES THOMAS, DOUGLAS DURIAN, University of Pennsylvania — Granular media clogs as it flows out of a hopper when the exit hole is appropriately small. However, when the hole is enlarged, the grains will never clog: there exists a well-defined transition between these two regimes at a particular critical hole size. To understand the origin of this clogging transition we follow the behavior of individual grains in the bulk. Using a quasi-2D hopper and a fast CCD, we can measure the positions of grains to sub-pixel accuracy. We then use this information to determine various local and global properties, including strain rate, velocity correlations, and dynamical heterogeneity time scales. We study how these quantities depend on the distance to the clogging transition, defined as the difference between the hole size and the critical hole size. This helps to explain the clogging transition and its relationship to the jamming transition.

12:03PM J53.00005 Jamming around fixed obstacles¹, AMY BUG, SAM BULLARD-SISKEN, Swarthmore College, CARL GOODRICH, University of Pennsylvania, LISA MANNING, Syracuse University, ANDREA LIU, University of Pennsylvania — Lattices of obstacles, such as microfluidic arrays, are capable of filtering or sorting particles like emulsion droplets, colloidal particles, and even cells. We study the jamming of soft, bidisperse discs placed within a lattice of fixed obstacles. Such obstacles provide a supporting structure for the jammed configuration, and their ability to alter a jamming threshold is of interest. Conjugate gradient methods are used to find minimum energy configurations, both with and without fixed obstacles. The likelihood of jamming as a function of disc volume fraction is calculated. If a configuration is jammed, the coordination number, energy, pressure, and other parameters of interest are calculated as a function of the obstacle size, number density, and configuration (hexagonal vs. square vs. random lattices).

¹Acknowledgement is made to the Donors of the Petroleum Research Fund administered by the American Chemical Society, a Eugene M. Lang Faculty Fellowship and the Division of Natural Sciences of Swarthmore College, and DOE grant DE-FG02-05ER46199.

12:15PM J53.00006 Frictional Jammed Packings: Classification, Protocol Dependence and the Phase Diagram, STEFANOS PAPANIKOLAOU, COREY O' HERN, Departments of Mechanical Engineering & Materials Science and Physics, Yale University, New Haven, Connecticut 06520, MARK D. SHATTUCK, Benjamin Levich Institute and Physics Department, The City College of the City University of New York, New York, New York 10031 — We probe the nature of the jamming transition in systems of frictional disks, where static friction is modeled geometrically using “bumpy-particles” with uniform circular asperities on the disks’ surface. First, we enumerate and classify the mechanically stable (MS) packings in small systems using exhaustive numerical simulations. We explicitly show that finite friction stabilizes packings that are unstable for frictionless particles, which causes the number of MS packings to increase strongly with the friction coefficient. MS packings for frictional particles are organized into low-dimensional geometric families in configuration space. We then calculate the critical behavior of the structural and mechanical properties near the jamming transition for frictional particles and as a function of protocol and show that friction drastically alters the nature of the transition.

12:27PM J53.00007 Jammed 2D circle packing reconsidered as a jigsaw puzzle, ERIC CORWIN, Department of Physics, University of Oregon, KENNETH DESMOND, ERIC WEEKS, Department of Physics, Emory University — Athermal random packings are inherently non-equilibrium structures. For a bidisperse jammed packing of N disks the global packing structure can be thought of as composed of N jigsaw pieces, each representing the local structure around a disk. We show that we can assign a unique identifier, termed a jigsaw number, to each local packing structure. We find that as the number of disks grows to infinity the number of different jigsaw numbers present in a packing remains finite. We report on the distribution of jigsaw numbers and find that certain local packing structures are more common than others, demonstrating that the non-equilibrium packing structure is incompatible with a flat measure over all configurations. We further report on the correlations present between jigsaw pieces.

12:39PM J53.00008 An experimental test of equilibration of temperature-like variables in jammed granular materials¹, JAMES PUCKETT, Dept. of Physics, North Carolina State University, BRIAN TIGHE, Process & Energy Laboratory, TU Delft, KAREN E. DANIELS, Dept. of Physics, North Carolina State University — Although jammed granular systems are athermal, a number of thermodynamic-like descriptions have been proposed which make predictions about the distributions of volume and stress fluctuations. We perform experiments with an apparatus designed to generate a large number of jammed two-dimensional configurations, which consists of a single layer of photoelastic disks supported by a layer of air driven through a microporous membrane. New configurations are automatically generated by alternately dilating the system (permitting large-scale rearrangements) and compressing it biaxially until a desired volume or pressure is reached. Within each configuration, a bath of $\gtrsim 10^3$ particles surrounds a smaller subsystem of particles with either the same or a different inter-particle friction coefficient than the bath. The use of photoelastic particles permits us to find all particle positions, and to numerically solve for the vector forces at each inter-particle contact. By comparing temperature-like quantities between subsystems, we test whether equilibration is observed under several proposed volume and stress ensembles.

¹We acknowledge support from NSF DMR-0644743.

12:51PM J53.00009 Energy decay of freely cooling granular gases in three dimensions, ZAHERA JABEEN, Department of Physics, University of Michigan, Ann Arbor, MI 48109-1040, SUDHIR N. PATHAK, RAJESH R., Institute of Mathematical Sciences, CIT Campus, Taramani Chennai-600 113, India — Freely cooling granular gases, wherein a dilute system of macroscopic particles with uncorrelated initial velocities lose energy through inelastic collisions, have been extensively studied both as a simple model for granular systems as well as a nonequilibrium system showing nontrivial coarsening at late times. As the system cools, inelasticity induces clustering, making the system inhomogeneous. While the form of energy decay ($E(t) \sim t^{-\theta}$) in the initial homogeneous regime is well established by Haff’s law ($\theta = 2$), the energy decay in the clustered regime is still unresolved in higher dimensions. Within mean field theory, $\theta = 2d/(d+2)$ (where d is the spatial dimension), while a correspondence to Burgers equation implies an exponent $\theta = 2/3$ ($d = 1$), $d/2$ ($d > 1$). In one and two dimensions, the two formulae predict the same exponents. By performing extensive event driven molecular dynamics simulations, we show that in three dimensions, the energy decays asymptotically with a power ≈ 1.2 , for all coefficients of restitution $r < 1$, consistent with the mean field exponent. However, we argue that the mean field arguments fail due to non local interactions between mass clusters.

1:03PM J53.00010 The Influence of Topology on Signal Propagation in Granular Force Networks¹, DANIELLE BASSETT, University of California Santa Barbara, ELI OWENS, KAREN DANIELS, North Carolina State University, MASON PORTER, Oxford University — Granular materials exhibit numerous rich and complex behaviours, which have been investigated from both continuum and particulate perspectives. In particular, sound propagation through granular materials is both heterogeneous and complicated, and understanding its features is important not only from the perspective of fundamental physics but also for practical applications such as the characterization and non-destructive testing of such materials. Unfortunately, continuum models of sound propagation have been unable to explain the full range of observed behaviours. Here we represent granular materials as spatially-embedded networks composed of nodes (particles) and weighted edges (contact forces between particles) located in Euclidean space, and we use network science to provide fundamental insights into how sound propagates. Using photoelastic particles, we quantitatively characterise the internal force structure and show that its meso-scale network structure plays a crucial role in sound propagation. These results might help to explain the failure of previous physical models, and illustrate that contact topology alone is insufficient to understand signal propagation in granular materials.

¹Supported in part by the David and Lucile Packard Foundation, Public Health Service Grant NS44393, the Institute for Collaborative Biotechnologies through Contract W911NF-09-D-0001 from the US Army Research Office.

1:15PM J53.00011 Jamming of Brownian disks in a channel with a constriction¹, ALEJANDRO BILBAO, JERZY BLAWDZIEWICZ, Texas Tech University — We investigate jamming dynamics of an externally driven system of Brownian particles in a two-dimensional channel with an abrupt constriction. Our numerical simulations reveal a rich dynamical behavior that results from an interplay between external driving forces, thermal excitations, and geometrical constraints due to confinement. In particular, we have observed that channel blockage arising from particle accumulation at the constriction entrance alternates with sudden unjamming events originating from thermal fluctuations. We have also found that the dependence of the average particle flux on the channel width is non-monotonic as a result of strong spatial particle-wall correlations. Under some conditions there exist spontaneous particle ordering and dynamic switching between phases with square and hexagonal symmetry. We expect that similar phenomena can be observed in confined granular flows and in suspension flows in microchannels.

¹We acknowledge financial support by NSF grant CBET 1059745.

1:27PM J53.00012 To be or not to be jammed, SIMON DAGOIS-BOHY, Kamerling Ohnes Laboratory - Leiden University, BRIAN TIGHE, TU Delft - 3mE, JOHANNES SIMON, Kamerling Ohnes Laboratory - Leiden University, SILKE HENKES, Syracuse University, MARTIN VAN HECKE, Kamerling Ohnes Laboratory - Leiden University — When are packings of soft athermal spheres jammed? Any experimentally relevant definition must at least require a jammed packing to resist compression and shear. Numerical algorithms usually rely on a global compression monitored by a parameter (like pressure) that signals whether the packing is jammed or not. Here we show that compression is not sufficient to ensure properly jammed packings: some of those packings have positive pressures and bulk moduli, but negative shear moduli, and even for large systems, the number of these “bad apples” diverges as the jamming point is approached. We will discuss how to understand this situation and propose as a remedy the boundary relaxation, that is including the boundary shape parameters as variables in the equilibration process; finally we will compare the distribution of shear moduli obtained for both methods.

1:39PM J53.00013 Jamming, Yielding and Rheology of Weakly Vibrated Granular Media, GEERT WORTEL, JOSHUA DIJKSMAN, University of Leiden, OLIVIER DAUCHOT, CEA-Saclay, MARTIN VAN HECKE, University of Leiden, GRANULAR AND DISORDERED MEDIA TEAM, GROUPE INSTABILITÉS ET TURBULENCE TEAM — We establish that the rheological curve of dry granular media is nonmonotonic, both in the presence and absence of external mechanical agitations. In the absence of vibrations, the nonmonotonic flow curve governs the yielding behavior of granular media. In the presence of weak vibrations, the nonmonotonic flow curves govern a hysteretic transition between slow but steady and fast, inertial flows. For large agitations, the transition becomes non-hysteretic. We probe the fluctuations near the point where the 1st order transition becomes of 2nd order.

1:51PM J53.00014 Dynamics near shear-jamming for a dense granular system¹, JIE REN, JOSHUA DIJKSMAN, ROBERT BEHRINGER, Duke University — This talk will present several systematic experimental studies of a two-dimensional, frictional dense granular system subjected to simple shear deformation. The first experiment consists of linear shear for densities smaller than the isotropic jamming point, and examines both the evolution of the average stress and the evolution of force network. These measures reveal three distinguishable regimes of the granular system with increasing shear strain: unjammed, fragile, and shear-jammed regimes. The second experiment uses small amplitude cyclic shear to probe the dynamical response of the states from the first experiment. For fragile or jammed regimes, cyclic shear drives the system through transient states that evolve towards relatively stable forces networks and system-averaged stress. The timescale of the transient increases rapidly as the system moves deeper into the fragile, or shear-jammed regimes. These experiments also involve particle tracking (displacements and rotations) to search for and characterize non-affine motion and spatial heterogeneity. There is a clear increase in particle diffusion with increasing density and shear strain amplitude, even when the system is still unjammed and experiences only minimal stress. When the system is fragile or jammed, the heterogeneity of particle displacements reveals subtle correlations with the force network.

¹This work is funded by NSF grants: DMR0906908, DMS0835571, NASA grant NNX10AU01G and ARO grant W911NF-11-1-0110.

2:03PM J53.00015 Tricriticality in constraint percolation, L. CAO, J. M. SCHWARZ, Physics Department, Syracuse University — Constraint percolation goes beyond ordinary percolation to include constraints on the occupation of sites/bonds. For instance, k -core site percolation implements a geometric constraint requiring each occupied vertex on a network have at least k occupied neighboring vertices. It turns out that the percolation transition in such a model is essentially equivalent to the study of a dynamical glass transition in the Fredrickson-Andersen model, one of the models underlying the kinetically-constrained approach to the glass transition. We study heterogeneous k -core bond percolation on a random network with f denoting the probability of a $k = 2$ -core vertex and $1 - f$ the probability of a $k = 3$ -core vertex. This model corresponds to a heterogeneous extension of the Fredrickson-Anderson model. For $f = 1$, the percolation transition is continuous, while for $f = 0$, it is discontinuous. Using a master equation approach, we show that there exists a tricritical point at $f = 1/2$ with a new order parameter exponent of unity. Our results are consistent with other mean field results obtained via a different method. We also look for tricriticality beyond mean field by investigating another constraint percolation model dubbed force-balance percolation.

Tuesday, February 28, 2012 11:15AM - 2:03PM –
Session J54 GSNP: Focus Session: Complex and Co-evolving Networks - Empirical Studies of Social Networks 152

11:15AM J54.00001 Modeling users' activity on Twitter networks: validation of Dunbar's number, BRUNO GONCALVES, NICOLA PERRA, ALESSANDRO VESPIGNANI, Northeastern University — Microblogging and mobile devices appear to augment human social capabilities, which raises the question whether they remove cognitive or biological constraints on human communication. In this paper we analyze a dataset of Twitter conversations collected across six months involving 1.7 million individuals and test the theoretical cognitive limit on the number of stable social relationships known as Dunbar's number. We find that the data are in agreement with Dunbar's result; users can entertain a maximum of 100-200 stable relationships. Thus, the “economy of attention” is limited in the online world by cognitive and biological constraints as predicted by Dunbar's theory. We propose a simple model for users' behavior that includes finite priority queuing and time resources that reproduces the observed social behavior.

11:27AM J54.00002 Entropy of dynamical social networks, KUN ZHAO, Northeastern University, MARTON KARSAI, Aalto University, Finland, GINESTRA BIANCONI, Northeastern University — Dynamical social networks are evolving rapidly and are highly adaptive. Characterizing the information encoded in social networks is essential to gain insight into the structure, evolution, adaptability and dynamics. Recently entropy measures have been used to quantify the information in email correspondence, static networks and mobility patterns. Nevertheless, we still lack methods to quantify the information encoded in time-varying dynamical social networks. In this talk we present a model to quantify the entropy of dynamical social networks and use this model to analyze the data of phone-call communication. We show evidence that the entropy of the phone-call interaction network changes according to circadian rhythms. Moreover we show that social networks are extremely adaptive and are modified by the use of technologies such as mobile phone communication. Indeed the statistics of duration of phone-call is described by a Weibull distribution and is significantly different from the distribution of duration of face-to-face interactions in a conference. Finally we investigate how much the entropy of dynamical social networks changes in realistic models of phone-call or face-to-face interactions characterizing in this way different type human social behavior.

11:39AM J54.00003 The nature and perception of fluctuations in human musical rhythms¹, HOLGER HENNIG, Harvard University, and Max Planck Institute for Dynamics and Self-Organization (MPIDS), Goettingen, Germany, RAGNAR FLEISCHMANN, MPIDS, ANNEKE FREDEBOHM, Institute of Psychology, University of Goettingen, YORK HAGMAYER, Kings College, London, UK, JAN NAGLER, ANNETTE WITT, MPIDS, FABIAN THEIS, Institute for Bioinformatics and Systems Biology, Helmholtz Zentrum Munich, Germany, THEO GEISEL, MPIDS — Although human musical performances represent one of the most valuable achievements of mankind, the best musicians perform imperfectly. Musical rhythms are not entirely accurate and thus inevitably deviate from the ideal beat pattern. Nevertheless, computer generated perfect beat patterns are frequently devalued by listeners due to a perceived lack of human touch. Professional audio editing software therefore offers a humanizing feature which artificially generates rhythmic fluctuations. However, the built-in humanizing units are essentially random number generators producing only simple uncorrelated fluctuations. Here, for the first time, we establish long-range fluctuations as an inevitable natural companion of both simple and complex human rhythmic performances [1]. Moreover, we demonstrate that listeners strongly prefer long-range correlated fluctuations in musical rhythms. Thus, the favorable fluctuation type for humanizing interbeat intervals coincides with the one generically inherent in human musical performances. [1] HH et al., PLoS ONE, 6, e26457 (2011)

¹We acknowledge financial support by the BCCN, grant no. 01GQ0430 (AW and TG).

11:51AM J54.00004 Structural and social aspects of human mobility, JAMES BAGROW, Northwestern University, YU-RU LIN, Northeastern University — Research on human mobility has been revolutionized by cellular phone data, capturing activity patterns across extensive populations. A number of interesting features have been discovered, including the ultra-slow growth of human mobility patterns, which cannot be reproduced by traditional random-walk models. However, the spatiotemporal flows and detailed microstructure of human mobility have not been well studied. Inferring complex mobility networks from country-wide data from mobile phone data, we find that human mobility is dominated by a small group of frequently visited and dynamically close locations, forming a primary “habitat” that captures typical behavior, along with subsidiary habitats representing additional travel. These habitats are both well separated and spatially compact. We find that motion within habitats exhibits distinct temporal scaling and that the time delay to enter subsidiary habitats is a primary factor in the spatiotemporal growth of human travel. Mobility is also coupled with social activity. Interestingly, many phone users possess habitats that occupy single temporal and social contexts and display high temporal and social predictability when occupying subsidiary habitats, revealing new connections between human activity and mobility dynamics.

12:03PM J54.00005 Temporal and spatial regularity of mobile-phone data¹, PHILIPP HOEVEL, TU Berlin, Germany, ALBERT-LASZLO BARABASI, CCNR, Northeastern University — Network science is a vibrant, interdisciplinary research area with strong connections to a plethora of different fields. As the amount of empirically obtained datasets increases more and more, approaches from network sciences continue to enhance our understanding, for instance, of human dynamics. The available data often consist of temporal as well as spatial information. In our case they originate from anonymized mobile-phone traces, which include information about the timing of the connections between two mobile phones and also their positions. Thus, the data contains an additional social component. In this study, we evaluate patterns of human behavior identifying both temporal and spatial regularity. This leads to a detailed mobility analysis on various timescales and contributes to a general theory of synchronization in complex, real-world networks.

¹This work is supported by a postdoctoral fellowship of the Deutsche Akademische Austauschdienst (DAAD).

12:15PM J54.00006 Scale-free correlations in the geographical spreading of obesity, LAZAROS GALLOS, City College of New York, PABLO BARTTFELD, Buenos Aires University, SHLOMO HAVLIN, Bar-Ilan University, MARIANO SIGMAN, Buenos Aires University, HERNAN MAKSE, City College of New York — Obesity levels have been universally increasing. A crucial problem is to determine the influence of global and local drivers behind the obesity epidemic, to properly guide effective policies. Despite the numerous factors that affect the obesity evolution, we show a remarkable regularity expressed in a predictable pattern of spatial long-range correlations in the geographical spreading of obesity. We study the spatial clustering of obesity and a number of related health and economic indicators, and we use statistical physics methods to characterize the growth of the resulting clusters. The resulting scaling exponents allow us to broadly classify these indicators into two separate universality classes, weakly or strongly correlated. Weak correlations are found in generic human activity such as population distribution and the growth of the whole economy. Strong correlations are recovered, among others, for obesity, diabetes, and the food industry sectors associated with food consumption. Obesity turns out to be a global problem where local details are of little importance. The long-range correlations suggest influence that extends to large scales, hinting that the physical model of obesity clustering can be mapped to a long-range correlated percolation process.

12:27PM J54.00007 Mining networks of human contact with wearable sensors, ALAIN BARRAT, CPT Marseille, CNRS, France & ISI Foundation, Torino, Italy — Due to the development of sensors of various types and the use of digital media and computational devices, we increasingly leave digital traces of our daily activities. The scale at which such data can be gathered and analyzed makes possible a novel, data-driven approach to the investigation of various aspects of human behavior. In this talk, I will focus on the research done within the SocioPatterns project (www.sociopatterns.org), in which we have developed the SocioPatterns sensing platform to obtain longitudinal datasets on face-to-face contact events between individuals in a variety of contexts ranging from scientific conferences to museum, schools or hospitals. The gathered data sets consists in dynamic networks of human contacts, and their analysis reveal interesting similarities and differences of human interaction patterns across contexts. I will also consider the impact of the temporal resolution, which allows to take into account causality constraints, on dynamical processes occurring on networks, such as spreading processes.

1:03PM J54.00008 Are we in our travel decisions self-determined?, CHRISTIAN SCHNEIDER, MIT, THOMAS COURONNE, ZBIGNIEW SMOREDA, Orange Labs, MARTA GONZALEZ, MIT — Mobile phone data, as saved by every phone provider worldwide, allows us to extract information about human mobility. It can be mainly used to study the locations and routes of each mobile phone user during entire months. In order to gain deeper understanding of the inherent travel decisions of the daily trips measured by phone data, we compare them statically with those extracted from 10,000 trajectories reported in a travel diary survey. We identify and compare from both data sets the underlying trip decisions networks or motifs. Interestingly, although millions of different motifs are possible, in both data sets we found similar motif distributions. Hence, we develop a simple model, which could reproduce not only the size distribution of the motifs, but the motifs themselves and answer the opening question.

1:15PM J54.00009 A cross-section test of Cobb-Douglass production function between market capitalization and GDP, ADAM AVAKIAN, Boston University, Boston, MA 02215, USA, BORIS PODOBNIK, Faculty of Civil Engineering, University of Rijeka, 51000 Rijeka, Croatia, H. EUGENE STANLEY, Boston University, Boston, MA 02215, USA — Most classical economic theories imply that both (a) economies with lower output (GDP) per person tend to grow faster in per capita terms and (b) economies with lower capital per person tend to grow faster in per capita terms. It is well-known that the former was found to be wrong. Taking market capitalization as a proxy for physical capital, we analyze a cohort of countries over a 17-year period (1994-2010) and we find the latter statement in agreement with empirical data implying a contradictory result that while capital data worldwide tend to converge, GDP data tend to diverge. However, for the countries analyzed, for which we have both market capitalization and GDP data, we find that even economies with lower output (GDP) per person tend to grow faster in per capita terms. The result that for all countries one obtains divergence while for a group of countries having both market capitalization and GDP data we have convergence is in contrast with the refutation of (a) but our results only apply to countries that have an exchange market, and are thus participating in globalization, indicating the convergent effect of globalization.

1:27PM J54.00010 Statistical Analysis on the Korean Transportation System, OKYU KWON, National Institute for Mathematical Sciences, GABJIN OH, Chosun University, WOO-SUNG JUNG, POSTECH — We investigate the Korean transportation system including subway, highway and express bus systems. The network topology and traffic pattern of the Korean transportation system is studied. We find the transportation have many complexity features such as scale-free property. We also find the relationship between the traffic flow, and the population and the distance.

1:39PM J54.00011 The Growth Dynamics of Words: How Historical Context Shapes the Competitive Linguistic Environment, JOEL TENENBAUM, Center for Polymer Studies, Department of Physics, Boston University, Boston, MA, ALEXANDER PETERSEN, IMT Lucca Institute for Advanced Studies, Lucca 55100, Italy, SHLOMO HAVLIN, Minerva Center and Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel, H. EUGENE STANLEY, Center for Polymer Studies, Department of Physics, Boston University, Boston, MA — Using the massive Google n-gram database of over 10^{11} word uses in English, Hebrew, and Spanish, we explore the connection between the growth rates of relative word use and the observed growth rates of disparate competing actors in a common environment such as businesses, scientific journals, and universities, supporting the concept that a language's lexicon is a generic arena for competition, evolving according to selection laws. We find aggregate-level anomalies in the collective statistics corresponding to the time of key historical events such as World War II and the Balfour Declaration.

1:51PM J54.00012 Voronoi Cell Patterns: Application of the size distribution to societal systems¹, RAJESH SATHIYANARAYANAN², DIEGO LUIS GONZÁLEZ³, ALBERTO PIMPINELLI⁴, T.L. EINSTEIN, U. of Maryland — In studying the growth of islands on a surface subjected to a particle flux, we found it useful to characterize the distribution of the areas of associated Voronoi (proximity or Wigner-Seitz) cells in terms of the generalized Wigner surmise⁵ and the gamma distributions. Here we show that the same concepts and distributions are useful in analyzing several problems arising in society.⁶ We analyze the 1D problem of the distribution of gaps between parked cars, assuming that successive cars park in the middle of vacant spaces, and compare with published data. We study the formation of second-level administrative divisions, e.g. French *arrondissements*. We study the actual distribution of *arrondissements* and the Voronoi tessellation associated with the chief town in each. While generally applicable, there are subtleties in some cases. Lastly, we consider the pattern formed by Paris Métro stations and show that near the central area, the associated Voronoi construction also has this sort of distribution.

¹Work at UMD supported primarily by NSF-MRSEC-DMR 05-20471, with partial support from DOE-BES-CMCSN and by CNAM at UMD.

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⁴Presently Science Attaché, French Consulate, Houston

⁵AP & TLE, PRL 99 (2007) 226102; PRL 104 (2010) 149602

⁶DLG et al., arXiv 1109.3994; RS, Ph.D. dissertation; RS et al., preprint

2:00PM - 2:00PM —
Session K1 Poster Session II (2:00-5:00PM) Exhibit Hall C

K1.00001 PHYSICS EDUCATION —

K1.00002 Integrated High Switch Test System to Determine Time-Dependent Dielectric Breakdown, HEATHER PETROCCIA¹, Villanova University — As a 2011 SPS summer intern, I worked for NIST in the Semiconductor Division learning about characterizing defects in MOSFETs. The lifetime and reliability of a MOSFET is directly related to the projected lifetime of an electronic device. By applying an increased stress voltage to the gate oxide, the lifetime of the MOSFET within an electronic device can be simulated. From this simulation, the reliability of the device can be determined from a mathematical extrapolation which is derived from breakdown data. Although time dependent breakdown has been thoroughly studied in the past in silicon dioxides, large statistical studies are still necessary to confirm the already accepted models for extrapolating mean lifetimes as well as increasing the accuracy of the projected lifetime. By creating an integrated high switch test system to determine time dependent dielectric breakdown, we hope to create a more affordable and efficient system to test copious numbers of oxides. This system is composed of set of highly parallel switches which apply a stress voltage to a total of 48 oxides. By implementing LabVIEW, the level of the stress voltage as well as the break down voltage and time can be determined. From this data further statistical analysis can be applied.

¹Society of Physics Students Intern

K1.00003 ABSTRACT WITHDRAWN —

K1.00004 Out of the Box Thinking: Kinematics from a 163 Million-Year-Old Dinosaur Trackway, SCOTT LEE, University of Toledo — Dinosaurs always grab the interest of students. Information about dinosaur locomotion is accessible from the trackways they left. In a unique connection to kinematics, evidence of the acceleration of a meat-eating dinosaur (theropod) is evident in Trackway 13 in Ardley Quarry in Oxfordshire, UK. This particular trackway is described by J.J. Day, D.B. Norman, P. Upchurch and H.P. Powell in Vol. 415 of Nature on pages 494 and 495, published in 2002. This particular theropod underwent an acceleration of about $g/3$. This example provides a fun and engaging exercise for students studying kinematics.

K1.00005 Polyaniline-Carbon Nanotubes Composite Actuators¹, SABRINA ROSA, University of Puerto Rico at Humacao, Humacao, Puerto Rico, CARLOS CAMARGO, Centre Nacional de Microelectronica, Barcelona, Spain, EVA CAMPO, University of Pennsylvania, PA, JAUME ESTEVE, Centre Nacional de Microelectronica, Barcelona, Spain, IDALIA RAMOS, University of Puerto Rico at Humacao, Humacao, Puerto Rico — The understanding of photoactuation in Carbon Nanotubes (CNT)-polymer composites can contribute to the development of micro- and nano-optical-mechanical systems for applications that include intracellular motors, artificial muscles, and tactile displays for blind people. The integration of CNTs into polymers combines the good processability of polymers with the functional properties of CNTs. CNTs-polymer composite fibers were fabricated using the electrospinning technique. electrospinning process orients the CNTs along the precursor stream and can contribute to enhance photo actuation properties. The addition of polyaniline, an electroactive conductive polymer is expected to enhance the actuation strain of the composite. aim of this research is to study photoactuation in MWCNT-Polyaniline electrospun fibers. fibers were characterized using Scanning Electron Microscopy, Atomic Force Microscopy, and X-Ray Diffraction. Results demonstrate evidence of photo-actuation after irradiating the fibers with visible light. tests are being conducted to understand the mechanisms of the composites response to light stimulation.

¹Research Sponsored by Partnership for Research and Education in Materials (NSF-DMR 0934195).

K1.00006 Using the IPAD as a Pedagogical Tool: Focus on Angular Motion Analysis with Real-World Applications¹, LEAH BUSH, ANGELA GARRIOTT, ROBERTO RAMOS, Indiana Wesleyan University — The IPAD is a portable, novel interface that has the potential to create a more interactive learning environment in undergraduate physics education, particularly in the introductory physics laboratory setting. We report our experience in using this pedagogical tool in an algebra-based physics laboratory course, focusing on its application in analysis of angular motion. Taking advantage of its portability, we use it to analyze motion not only using standard physics laboratory equipment but using it for analyzing motion in real-world applications such as with exercise equipment such as an exercise bicycle and an elliptical machine. We report on student response to this learning tool.

¹We acknowledge Indiana Wesleyan University for providing an IPAD minigrant to R. Ramos

K1.00007 Why Physics Programs are Slimming Down, SAMINA MASOOD, University of Houston Clear Lake — We study the Physics enrollment in the light of the current financial situation. Role of the Physics program in the growth of several programs in a university and the importance of a successful Physics program to prepare for the future needs of the time are analyzed in detail. The effect of shutting down of Physics programs will also be discussed.

K1.00008 Student Autonomy and its Effects on Student Enjoyment in a Traditional Mechanics Course for First-Year Engineering Students¹, JANAKI I. PERERA, BRENDAN T. QUINLIVAN, JENNIFER A. SIMONOVICH, EMILY TOWERS, OREN H. ZADIK, YEVGENIYA V. ZASTAVKER, F. W. Olin College of Engineering — In light of recent literature in educational psychology, this study investigates instructional support and students' autonomy at a small technical undergraduate school. Grounded theory is used to analyze twelve semi-structured open-ended interviews about engineering students' experiences in *Introductory Mechanics* that includes *Lecture*, *Recitation*, and *Laboratory* components. Using data triangulation with each course component as a unit of analysis, this study examines students' course enjoyment as a function of instructional support and autonomy. The *Lecture* utilizes traditional instructor-centered pedagogy with predominantly passive learning and no student autonomy. The *Recitation* creates an active learning environment through small group work with a moderate degree of autonomy. The *Laboratory* is designed around self-guided project-based activities with significant autonomy. Despite these differences, all three course components provide similar levels of instructional support. The data reveal that students enjoy the low autonomy provided by *Lecture and Recitations* while finding the *Laboratory* frustrating. Analyses indicate that the differences in autonomy contribute to students' misinterpretation of the three course components' value within the context of the entire course.

¹NSF HRD #0624738

K1.00009 Does requiring graded online homework improve physics exam performance?, NORMA CHASE, Massachusetts College of Pharmacy and Health Sciences — In a first experiment with using Mastering Physics in a first semester calculus-based course, homework and exam performance was tracked periodically during the semester. As expected, the use of novel technology (and its ability to track which students were persistently working at problem exercises) motivated many students to become more involved with work on assigned physics problems. Although there did appear to be a significant correlation between exam averages and homework scores in the upper half of the exam average distribution, individuals spanning the full range of exam averages (down to 45 percent) earned homework scores as high as those who had performed outstandingly well in exams. In this work, we present results and proposed plausible explanations for the apparent anomaly.

K1.00010 UNDERGRADUATE RESEARCH (SOCIETY OF PHYSICS STUDENTS ABSTRACTS) —

K1.00011 Preparation and characterization of optically-active metal probes for tip-enhanced Raman spectroscopy, JAE CHO, ISAAC RIISNESS, MICHAEL GORDON, University of California, Santa Barbara — Tip-enhanced Raman spectroscopy (TERS) has enabled spatially correlated topographic and chemical imaging of biomolecules, catalysts, photovoltaics, and materials on the nanoscale. Critical to the TERS experiment is the tip; tip size sets the spatial resolution, whereas tip material and shape determine how well far-field laser light couples to electron oscillations (plasmons) in the tip to create a tightly confined field that enhances Raman scattering of molecules in the tip-surface gap. Tips are typically prepared via electrochemical etching of metal wires in strong acid or base solutions. This etching process is not well understood, and the production of sharp, plasmonically active tips remains a key challenge in the TERS field. To address this issue, we developed an electrochemical etching cell with diagnostic system based on a tuning fork oscillator to evaluate the tip-etching process. We present initial study of oscillation dynamics during electrochemical tip etching under varying conditions.

K1.00012 Electrical and Magnetic Properties of Nanostructured Mo-Doped Yttrium Iron Garnet¹, S. KHANRA, A. LAUDARI, Department of Physics, Missouri State University, Springfield, MO 65897, Y. KOLEKAR, Department of Physics, Pune University, India, P. KAHOL, K. GHOSH, Department of Physics, Missouri State University, Springfield, MO 65897 — Yttrium Iron Garnet (YIG) is a synthetic garnet and ferromagnetic with the chemical formula $Y_3Fe_5O_{12}$. In YIG, five iron (III) ions occupy two octahedral and three tetrahedral sites, with yttrium (III) ions coordinated by eight oxygen ions in an irregular cube. The iron ions in the two coordination sites exhibit different spins, resulting in magnetic behavior. It is also transparent to infrared wavelengths over 600 nm. Nanostructured YIG has been synthesized systematically by solid state reaction method. The formation of pure YIG have been investigated through X-ray diffraction (XRD) beginning from weighing in molar proportions of Y_2O_3 and Fe_2O_3 , mixing and grinding, pre-sintering and final sintering at 1300 °C. XRD study shows that YIG exhibits cubic structure with lattice constant of about 12 Å. Magnetization with varying field and temperature has been measured using a SQUID magnetometer. Room temperature dielectric measurements indicate that the YIG shows the usual dielectric dispersion. Magnetic studies of Mo YIG has shown that it becomes diluted after doping and dielectric measurement have shown that dielectric constant of that sample has been reduced.

¹This work is supported by National Science Foundation (Award Number DMR-0907037).

K1.00013 Water on a Hydrophobic Surface: Contact Angle vs. Depletion Layer, CAITLYN NEIDIG, JACOB BREZINSKY, MENGJUE ZHOU, ADELE POYNOR, Allegheny College — Hydrophobic surfaces repel water. When this occurs, a depletion layer is formed between the water and the hydrophobic surface. We will be studying the effects from the contact angle, the angle at which the water droplet meets the surface, on the depletion layer. Larger contact angles create thicker depletion layers, which has lead us to determine if there is a direct relationship between the contact angle and depletion layer. In order to do this, we will be coating gold slides with a hydrophobic ODT solution, a hydrophilic Mercapto solution, and various mixtures of both of these solutions to create a large range of contact angles. We will be using Surface Plasmon Resonance to study to any depletion layer created by water on these surfaces.

K1.00014 SPS Fabric of the Cosmos Cafe¹, ANISH CHAKRABARTI, Drury University — Hosted by Brian Greene and based on his best-selling book of the same title, *The Fabric of the Cosmos* is a new four- part NOVA series that explores the deepest mysteries of space and time. The program was kicked-off by 30 “Cosmic Cafes” being held around the country funded by an NSF grant which allows SPS-NOVA to fund SPS chapters for these events. During the summer I assisted in planning this kick-off, reviewing and suggesting revisions of resources related to the NOVA series to make them relevant to an SPS audience. I also got to organize and moderate the first “Cosmic Cafe.” The Cosmic cafe that I organized was discussion based, with our speaker Dr. James Gates starting with a short talk and then opening the floor up for questions. By organizing a “Cosmic cafe,” I got real hand experience about the challenges an SPS chapter would face while organizing a cafe themselves. Based on my experience I shall also discuss the effectiveness of the first ever themed science cafe blitz. A science café is an informal discussion with an expert in a very casual location, usually a restaurant, coffee shop, or a bar. A science cafe is mostly discussion based, but has a lot of freedom for the format. A “Cosmic” cafe is a science cafe which is based around the topics discussed in the documentary “The Fabric of the Cosmos.”

¹Society of Physics Students

K1.00015 Water on a Hydrophobic surface, RYAN SCRUGGS, MENGJUE ZHU, ADELE POYNOR, Allegheny College — Hydrophobicity, meaning literally fear of water, is exhibited on the surfaces of non-stick cooking pans and water resistant clothing, on the leaves of the lotus plan, or even during the protein folding process in our bodies. Hydrophobicity is directly measured by determining a contact angle between water and an objects surface. Associated with a hydrophobic surface is the depletion layer, a low density region approximately 0.2 nm thick. We study this region by comparing data found in lab using surface plasmon resonance techniques to theoretical calculations. Experiments use gold slides coated in ODT and Mercapto solutions to model both hydrophobic and hydrophilic surfaces respectively.

K1.00016 Correlation between acoustic emission and mechanoluminescence of rock cores under quasistatic compression¹, RACHEL A. MILLER, TIMOTHY W. DARLING, Physics, University of Nevada, Reno — When a rigid solid undergoes mechanical deformation, locally accumulated strain energy can be released through multiple avenues including acoustic emission (AE) and light emission known as mechanoluminescence (ML). In AE, events within a stressed rock such as defect movement, grain boundary shifting, and crack propagation create pressure waves which can be detected at the rock surface. While AE is used extensively for rock evaluation in geophysics, civil engineering, and mining, ML by comparison has received little attention from the geoscience community. ML from stressed and fracturing rock has been observed in mines, earthquakes, and the laboratory, but the underlying mechanism behind ML is poorly understood. Possible candidates include defect movement, creation of charged surfaces during fracture, piezoelectrification, and triboluminescence. Observing whether a correlation exists between ML and AE will help determine the source of ML. We have designed an apparatus for AE and ML detection of rock cores under quasistatic compression. Using photomultiplier tubes and piezoelectric transducers, AE and ML events can be spatially and temporally observed and correlated. We present apparatus design and preliminary results.

¹Funding by University of Nevada, Reno College of Science Research/Instructional Enhancement Award

K1.00017 Harpoon-based sample Acquisition System, JAVIER BERNAL, Researcher, JOSEPH NUTH, DONALD WEGEL, Mentor — Acquiring information about the composition of comets, asteroids, and other near Earth objects is very important because they may contain the primordial ooze of the solar system and the origins of life on Earth. Sending a spacecraft is the obvious answer, but once it gets there it needs to collect and analyze samples. Conceptually, a drill or a shovel would work, but both require something extra to anchor it to the comet, adding to the cost and complexity of the spacecraft. Since comets and asteroids are very low gravity objects, drilling becomes a problem. If you do not provide a grappling mechanism, the drill would push the spacecraft off the surface. Harpoons have been proposed as grappling mechanisms in the past and are currently flying on missions such as ROSETTA. We propose to use a hollow, core sampling harpoon, to act as the anchoring mechanism as well as the sample collecting device. By combining these two functions, mass is reduced, more samples can be collected and the spacecraft can carry more propellant. Although challenging, returning the collected samples to Earth allows them to be analyzed in laboratories with much greater detail than possible on a spacecraft. Also, bringing the samples back to Earth allows future generations to study them.

K1.00018 AIP Career Pathways¹, AMANDA PALCHAK, University of Southern Mississippi — American Institute of Physics (AIP) Career Pathways is a new project funded by the National Science Foundation. One of the goals of AIP Career Pathways is to prepare students to compete for Science, Technology, Engineering, and Mathematics (STEM) careers with a bachelor's degree in physics. In order to do so, I reviewed and compiled useful resources on finding a STEM career with a bachelor's degree in physics. These resources not only supply the job seeker with job postings in STEM careers but also provide them with information on resumes, interviewing skills, and networking. Recently at the 2011 Industrial Physics Forum, I interviewed companies in the private sector to obtain a unique perspective on what types of skills potential employers expect an applicant to possess with a bachelor's degree in physics. Ultimately, these components will be used as supplements at student career workshops held at annual Society of Physics Students Zone Meetings.

¹National Science Foundation, American Institute of Physics

K1.00019 Simulation of a Tunable, Three-dimensional Resonant Cavity for Quantum Control and Measurement¹, RAVI NAIK, KATER MURCH, I. SIDDIQI, UC Berkeley, QNL — We present the design and simulation of a tunable, superconducting, three-dimensional resonant cavity for control and measurement of quantum systems. By adjusting the dimensions of the cavity appropriately, we create a photon resonant mode in the 4-8 GHz frequency band, typical of many current superconducting qubits. We simulate the resonance behavior of the cavity using a commercial three-dimensional finite-element solver to explore the effects of various modifications of the cavity boundaries and coaxial signal ports, as well as the insertion of dielectric materials and metallic control lines within the cavity. In particular, we find that the quality factor of the cavity resonance is exponentially dependent on the insertion depth of the port pins from the surface of the cavity. A weak dependence is observed for other modifications. By adjusting the pin depth, we can achieve a range of quality factors from a few hundred to a few million, as verified by experiment.

¹This research is supported by the IARPA CSQ program.

K1.00020 Suspended Particle Mass Determination from Transport Coefficients¹, DONOVAN MYERS, Louisiana State University Baton Rouge, PAUL RUSSO, Department of Chemistry, Louisiana State University — It has long been known that a suitable combination of transport coefficients can be used to determine particulate mass in suspensions. Advances in particle tracking make this straightforward and easier to apply to large numbers of particles. This poster will concern recent experiments along these lines, which are devoted to improved understanding of composite, hybrid, core-shell colloidal particles, without regard to shape.

¹Supported by NSF DMR 10055707

K1.00021 Electromagnetically Induced Transparency in a Four-Level W Scheme: Effect of Beam Intensity and Phase on Propagation, MATTHEW LEWIS, CHRISTOPHER NELSON, Department of Physics, Millersville University, Millersville, PA — Co-propagation of two circularly polarized lasers in an electromagnetically induced transparency four-level W scheme is investigated. Our four level system is produced using the ground state and three Zeeman levels of ultracold magnesium atoms. Parameters are determined such that co-propagation of the two incident optical fields will occur. Group velocities obtained by solving the density matrix master equation for the appropriate coherences are found to be periodic with respect to the phase angle of the Rabi frequency.

K1.00022 Fluorescent security markers on ZnO nanowires¹, KRISTY WARREN, MARIAN TZOLOV, None — Zinc oxide is an efficient emitter of light thanks to the large exciton binding energy of 60 meV. The narrow emission lines from ZnO nanowires can be used as an enhanced security feature in documents and can be easily recognized from the background originating from the paper itself. We have studied the emission properties of ZnO nanowires in the UV range and how they can be implemented into paper products for document security. The zinc oxide nanowires were synthesized by chemical vapor transport and postprocessed in solution. The nanowires were dispersed using a sonicator into nitric acid water solutions with a pH of 2 and 4, and ammonium hydroxide water solution with a pH of 5 and 7. The morphology of the dispersed ZnO nanowires was imaged under a scanning electron microscope. Fluorescence measurements have shown better light emission from the nanoparticles dispersed in the basic pH solution. This material was then implemented into crafted paper and viewed under UV lamps and with a spectrometer. We have studied the loading of the paper with ZnO nanoparticles. A comparison was done with equivalently processed material of ZnO in powder form. The implementation of zinc oxide nanowires into paper products can advance document security at a relatively low cost.

¹Lock Haven University of PA, Department of Physics

K1.00023 Noise correlations in quasi-1D conductors with different contact geometries¹, A. BELKADI, A.F. ISAKOVIC, Khalifa University - KUSTAR, Abu Dhabi, UAE — We nanofabricated end contacts to mesowires of NbSe₃ and tested for the presence of correlations in noise spectroscopy at various temperatures below Peierls transition temperature. We find that for $1/f$ -like, broadband noise (BBN), the degree of correlations in transport in two segments along a NbSe₃ mesowire can be tuned with electric field and temperature. For standard, bottom/top contacts geometries, we see a limited degree of correlations for narrow band noise (NBN) (typically 20-30%, except for a limited range of temperatures), but we also see that end contact geometry enhances the degree of correlations for NBN signal (closer to 50%). We believe this phenomenon is related to a better control of the CDW transport, such as weaker temperature dependence of condensate current. We also explore the issues of the overall energy transfer through such contacts.

¹The material growth and some of the measurements were done in Prof. R. E. Thorne lab at Cornell University. We acknowledge recent support from ATIC-SRC through contract 2011-KJ-2190 and KUSTAR.

K1.00024 Intensity dependent photoluminescence studies on zinc oxide nanowires, MARIAN TZOLOV, ANDREW EPPS, ERIC DRISCOLL, ZACHARY BARCIKOWSKI, Lock Haven University — The ZnO nanowires were grown by the chemical vapor transport method using a thin gold film as a catalyst. Their light emission in the visible and near UV spectral range was studied using excitation sources with large variation of the pump intensity, e.g. Xenon lamp, UV LEDs, nitrogen laser. The photoluminescence spectrum consists typically of the exciton emission band and a defect related band in the green spectral range. We have observed drastic change in the photoluminescence spectrum at high pump intensities with drastically decreased intensity of the defect related band. The results have been interpreted within a model accounting for the surface effects and associated band banding at the surface. Cathodoluminescence measurements of ZnO nanowires and bulk films were performed, which support the proposed model.

K1.00025 Specific Heat of Two-Gap Extreme Type-II Superconductors in High Magnetic Fields¹, TAMIRO VILLAZON, JULIAN IRWIN, SASHA DUKAN, Department of Physics and Astronomy, Goucher College, MD21204 — We present a numerical study of the quasiparticle contribution to the low-temperature specific heat of an extreme two-gap type-II superconductor at high magnetic fields. Within a T-matrix approximation for the self-energies in the mixed state of a homogeneous superconductor, the electronic specific heat is a linear function of temperature with a linear- T coefficient $\gamma(H)$ being a nonlinear function of magnetic field H . We compare our theoretical curve with available experimental data for the two-gap superconductors NbSe₂ and LuNi₂B₂C.

¹This work is supported by NSF grant no. DMR-0856415.

K1.00026 Changes in Ocean Color at Puerto Rico due to Tropical Storms¹, ANGELA FERRA, FERNADO GILBES, University of Puerto Rico at Mayaguez — In this research we analyze the impact of tropical storms in the ocean color of the Puerto Rico coast. The changes in ocean color are due to the absorption and scattering of light. It has been shown that remote sensing techniques are used as a fast and economical way to study the concentrations of phytoplankton and other water constituents at the ocean. Data from MODIS (Moderate Resolution Imaging Spectroradiometer) were used to generate images of ocean color. The images were downloaded from internet and processed using the program developed by NASA called SeaDAS. The processing involved the standard atmospheric correction and algorithm application. Dramatic changes in ocean color were detected due to tropical storms Earl and Jeanne. The results support the use of remote sensing in this type of assessments.

¹The research was done thanks for the support of the Physics Department at the University of Puerto Rico at Mayaguez.

K1.00027 High aspect ratio cell probes based on ZnO nanowires, MATTHEW KNARR, Lock Haven University, MARIAN TZOLOV, Lock Haven University, Department of Physics — ZnO is a useful and versatile material being used in nanotechnology and has many potential applications as a material in nanoscale biotechnological devices. The growth of ZnO nanowires using a gold catalyst has been extensively researched. In this project we propose an alternative growth method using electrophoretically deposited gold nanoparticles as a catalyst, rather than use of the more common gold thin film catalyst, in order to grow ZnO nanowires. Colloidal Au nanoparticles approximately 25 nm in diameter are used as the catalyst source and 0.003" diameter tungsten wire as the substrate. The gold nanoparticles were deposited on the tip of the tungsten wire by electrophoresis. The ZnO nanowires were deposited by chemical vapor transport process in a three zone tube furnace. Scanning electron microscopy was used to image the nanowires and energy dispersive X-ray spectroscopy to analyze the composition of the probes. We will illustrate our approach on electrically insulating the probe so that only the very tip can probe electrically the interior of biological cells.

**K1.00028 Laser Induced Fluorescence Studies of New Liquid Crystal C16-Fluorescent Dipyrri-
none** , SAMUEL BECK, DARREN NORTH, RICHARD RODE, CHRISTOPHER HEATH, AMY RENAUD, LOGAN TATE, Undergraduate, CHANDRA PRAYAGA, AARON WADE, MICHAEL HUGGINS, Faculty Advisor — A new liquid crystal, C-16 Fluorescent Dipyrri-
none, was synthesized and its absorption and fluorescence properties investigated near the phase transitions. A sample of the liquid crystal was dissolved in chloroform and deposited on a glass slide and housed in a temperature controlled environment. Fluorescence was induced by pumping the sample at 355nm from a frequency-tripled, pulsed ND:YAG laser and was analyzed using a monochromator and a 1GHz oscilloscope. The sample was held at each temperature, from 30 °C to 80 °C, with 1 mK precision before taking the spectra. The results show significant changes in the peak in the spectra near the phase transitions, allowing for precise measurement of the phase transitions. The samples were further characterized by measuring their absorption spectrum at different temperatures in the range of 30-60 °C was recorded over the spectral region 300-800 nm.

**K1.00029 Absorption and Fluorescence Study of New Liquid Crystal C14-Fluorescent Dipyrri-
none** , RICHARD RODE, SAMUEL BECK, DARREN NORTH, CHRISTOPHER HEATH, AMY RENAUD, LOGAN TATE, Undergraduate, CHANDRA PRAYAGA, AARON WADE, MICHAEL HUGGINS, Faculty Advisor — A new liquid crystal, C14-Fluorescent Dipyrri-
none, was synthesized and its fluorescence and absorption properties were studied near the phase transitions. A frequency-tripled, pulsed ND: YAG laser was used to induce fluorescence in the liquid crystal sample. The fluorescence spectra and decay times were studied as functions of temperature using a 1GHz oscilloscope, monochromator, and photomultiplier tube. This sample was tested over a temperature range of 30-60 °C with 1 mK resolution to allow precise determination of the phase transitions of the sample. The absorption spectra were recorded over the temperature range of 30 – 50°C using a HP 8453 UV-VIS spectrometer, on a sample of the liquid crystal dissolved in chloroform and dried on a quartz insert.

K1.00030 Resonance Circuit with a Nonlinear Liquid Crystal Capacitor , CHLOE RENFROE, SAMUEL BECK, Undergraduate, SAMI ALSHEIKH, Pensacola High School, CHANDRA PRAYAGA, TIM ROYAPPPA, Faculty Advisor — The liquid crystal 4'octyl-4-cyanobiphenyl (8CB) was injected into a commercially available liquid crystal capacitor cell (INSTEC, Inc). The cell was housed in a temperature-controlled environment constructed in the lab and a resonant circuit was assembled using the 8CB capacitor. The temperature of the capacitor was varied over the range 25 °C to 45 °C, covering the smectic, nematic, and isotropic phases. The sample was held at each temperature with a precision of 1mK before measuring the resonance curve with a network analyzer. The results showed a non-linearity in the resonance curve in the nematic phase, distorting the shape of the resonance curve. The corresponding curves for the smectic and isotropic phases were linear.

**K1.00031 Optical Absorption and Laser Induced Fluorescence Studies of Liquid Crystal C-
10 Fluorescent Dipyrri-
none** , DARREN NORTH, SAMUEL BECK, RICHARD RODE, CHRISTOPHER H, AMY RENAUD, LOGAN TATE, Undergraduate, CHANDRA PRAYAGA, AARON WADE, MICHAEL HUGGINS, Faculty Advisor — A newly synthesized liquid crystal C-10 Fluorescent Dipyrri-
none was dissolved in chloroform and allowed to dry on a glass slide. The slide was housed in a temperature controlled environment constructed in the lab. A frequency-tripled pulse ND: YAG laser (355 nm) was used to induce fluorescence in the liquid crystal sample, which was analyzed using a monochromator, photomultiplier tube, and a 1GHz oscilloscope. The sample was tested over a temperature range of 30-70°C. The temperature control was precise to within 1 mK, allowing precise determination of the phase transition temperatures. The area, fall time, and peak values of the fluorescence signal were studied as functions of wavelength and temperature. Absorption spectra in the spectral range 300 – 800 nm were also recorded using a commercial (HP8453) UV-VIS spectrometer.

**K1.00032 Analysis, Reconstruction, and Modeling of the Electrical Signal of the Weakly Elec-
tric Fish *Apteronotus Leptorhynchus*** , LORENZO SEWANAN, KENT DUNLAP, Trinity College — The weakly electric fish *Apteronotus leptorhynchus* uses approximately sinusoidal electrical signals to electrolocate and electrocommunicate. In particular, the complex electrical signals which are generated during dynamic interactions have been shown to impact the behavior and physiology of interacting fish. In order to study the specific features of these electrical signals that are biologically relevant, signals collected from fish under diverse conditions are analyzed using temporal and spectral techniques, specifically amplitude variation and frequency variation. Having characterized specific features of the signals, computational methods are then used to construct signals to mimic real electric fish signals. Constructed signals show close matching in relevant features when analyzed in the same manner as the original signals. From a different perspective, a two-dimensional dynamic model is formulated to simulate the generation of amplitude modulation in these signals based on the motion of a particle sampling a generalized field of time-varying points and found to generate some features of experimental electric fish signals. Work continues on both analysis, reconstruction, and modeling as well as actual playback experiments to determine the impact of these signals to influence fish neuroethology.

**K1.00033 The WASTED Resolutions: exploration of the spatial and energy limits of the
Webcam Alpha Spectrometer TEchnology Demonstrator** , JOSEPH FRYMAN, ARTHUR PALLONE, Northern Kentucky University — Scientists and engineers build simple, low-cost, webcam-based instruments for use in many disciplines. Analysis of the optical signal received through the three broadband color filters – red, green and blue – form the basis of many of those instruments. The CMOS sensors in webcam pixels also produce signals in response to ionizing radiations – such as alpha particles from a radioactive source. Simple alpha radiography has been demonstrated with an alpha source and a webcam modified to expose the sensors. The performance of the Webcam Alpha Spectrometer TEchnology Demonstrator (WASTED) built from such a modified webcam and a commercially available alpha source mounted to an optics rail is analyzed in terms of the energy upper-half-width-half-maximum and of the spatial modulation transfer function.

**K1.00034 Temperature and polarization dependent photoluminescence studies of WO₃ and
WO₃-x single crystals¹** , EMILY MAKOUTZ, Michigan Technological University, PRASENJIT DEY, DENIS KARAISKAJ, University of South Florida — WO₃ is an important material not only due to its interesting electronic properties but also due to applications in electrochromic devices and energy storage. The mechanism behind the electrochromic effect has been debated for several decades [1]. We have studied two WO₃ single crystals, a transparent and doped WO₃-x. A photoluminescence center around 865 nm is observed after sub-band gap excitation at 405 nm with relatively higher intensity in the crystal containing oxygen vacancies. The center appears as a broad transition of 35 nm FWHM and does not follow the band gap energy with temperature. However polarization dependent studies reveal at least two polarization dependent components of the center. To further investigate the polarization dependence for the two WO₃ crystals, we will use samples for which the orientation of the high axis of symmetry is known.

¹This work was supported by NSF REU program (award No DMR-1004873).

K1.00035 Raman spectroscopy investigation in the NWA 3118 meteorite: Implications for planet formation¹, BHUWAN GHIMIRE, The University of Utah and Westminster College MO, ANALÍA G. DALL'ASÉN, JORDAN M. GERTON, INESE I. IVANS, BENJAMIN C. BROMLEY, The University of Utah — Planet formation involves the coagulation of micron-scale dust into centimeter-meter scale objects. Explanation is sought of the adhesion property of the dust aggregates ultimately leading to the formation of structures like planetesimals. Confocal raman microscopy has been used to investigate carbon structures on the NWA 3118 meteorite. It is a carbonaceous type CV3 meteorite composed of micrometer scaled structures like chondrules and inclusions embedded in the matrix material. Raman mapping of meteorite samples with a laser of excitation wavelength 488nm was pursued, with a focus on the interfaces between chondrules and the matrix. Raman spectra of olivines and graphitic structures with corresponding optical and raman images of the spotted structures in the NWA 3118 are reviewed.

¹This work was supported by an internship grant from Nano-Optics lab at the Department of Physics and Astronomy, The University of Utah.

K1.00036 Formation of wave packets in electron diffraction on crystals, ROBERT LANNING, CRISTIAN BAHIRM, Department of Physics, Lamar University — Measurements of electron diffraction typically reveal the atomic structure of crystals and allow finding the length of chemical bonds. The effective electronic charge of each atom in the crystal acts upon the incident electron beam as a netting of narrow pinholes, and Fourier transforms the unique deBroglie wavelength of the projectile electron accelerated at fixed voltage into a wave packet. Using the uncertainty principle one can understand the mechanism that makes an incident electron to become a wave packet travelling inside the crystal at a group velocity identical with the initial speed of the projectile electron. Furthermore, the Pauli Exclusion Principle allows us to understand the fast passage of the projectile electron through the crystal and also, it allows the evaluation of the characteristic time for electron transmission. The project was sponsored by the STAIRSTEP program under the NSF-DUE grant# 0757057.

K1.00037 Exploring the limits of spin transport efficiency for spin ejection in spin photodiodes¹, K.P. SIMON, Olin College of Engineering, Needham, MA, USA, A. BELKADI, A.F. ISAKOVIC, Khalifa University - KUSTAR, Abu Dhabi, UAE — We examine several factors that affect the efficiency of the transport of optically excited, spin-polarized carriers in ferromagnet-semiconductor heterostructures. The process of optical excitation leads to the creation of the population of spin carriers in a III-V semiconductor [1], which faces a number of obstacles on its way out of the semiconductor. This poster addresses a hierarchy of problems that need to be addressed in order to improve the efficiency of spin ejection, with the goal of bringing it up to the efficiency level of the opposite process, the spin injection. Our approach is based on modeling the existing spin ejection data, in order to understand several spin relaxation processes and the transport across the interface between a semiconductor and a ferromagnet or other metal. Our results are based in part on Schokley-Queisser [2] approach for photodiodes efficiency. Our investigation shows that there is a considerable space for improvement of spin ejection transport efficiency, which opens up possibility of designing novel spintronics devices.

[1] A. F. Isakovic, D. M. Carr, J. Strand, *et al.*, Phys. Rev. B **64** 161304.

[2] W. Schokley, H. J. Queisser, J. Appl. Phys. **32** (3), 510.

¹K.P.S. acknowledges hospitality of KUSTAR in Spring 2011 and A. B. acknowledges support from Khalifa University.

K1.00038 Testing of Unfolding Algorithm Using Blind Data, EMY RIVERA, University of Puerto Rico Mayaguez, NATALIE MILKE, Technische Universität Dortmund — The RooUnfold package currently has available several different algorithms for the numerical solution of inverse problems or unfolding. Time-dependent Regularized Unfolding for Economics and Engineering, also known as TRUEE is an algorithm used to unfold and with time will be integrated to the RooUnfold package. Tests using simulated data in TRUEE were made with the goal to let future users know which parameters are ideal for their data. To test the TRUEE algorithm we used simulated data, with a known distribution and two different resolutions. The number of degrees of freedom and knots were found for different bin sizes. Chi square was then used to compare the unfolded and real distribution. The bin sizes with the smallest chi square were then used to unfold the blind data along with its parameters. Smaller bin sizes were used as well and then re-binned to see if the distributions matched. These re-binned distributions matched the unfolded distribution but did not match the known distribution.

K1.00039 Reconfiguration of the Receiver System for Sodium Doppler Wind/Temperature Lidar, VARDAN SEMERJYAN, Student, Utah State University, TAO YUAN, Research Assistant Professor, Utah State University — The newly established USU Na Lidar has the capability to measure neutral temperature and horizontal winds in the mesopause region (80-110 km in altitude) under clear sky condition in full diurnal cycle. Current system setup allows the observations of zonal (east-west) and meridional (north-south) winds, but lacks the coverage of the wind speed in zenith direction, which is essential to estimate the vertical wind perturbations. Since such perturbations are most likely associated with the atmospheric gravity waves (bouncy waves) breaking events and the related energy, momentum transfer, this upgrade of the Na Lidar system will provide further detailed information to the ongoing studies of such gravity wave dynamics and the induced atmospheric instabilities in the MLT (mesosphere and lower thermosphere) region. The proposed addition of the fourth channel and the associated new design of the Lidar receiving system will not only enable the data acquisition of the zenith channel but, the same time, will produce a more compact and robust structure than the current design. The new design will accommodate four high quantum efficiency(40%) Hamamatsu PMTs in the Lidar receiver, therefore, increase the system signal/noise(S/N) ratio by a factor of two.

K1.00040 Surface adhesion and confinement variation of Escherichia coli on SAM surfaces¹, KARISA BOWERSOX, KRISTA SITLER, JOSEPH CALABRESE, Lock Haven University of Pennsylvania, RESHANI SENEVIRATHNE, Don's Food Products, INDRAJITH SENEVIRATHNE, Lock Haven University of Pennsylvania — Controlled surface adhesion of non - pathogenic gram negative bacterial strain, Escherichia coli, DH5 alpha is interesting as a model system due to possible development of respective biosensors for prevention and detection of the pathogenic strain Escherichia coli and further as a study in biological and monolayer interactions. Self Assembled Monolayers (SAM) with engineered surfaces of linear thiols on Au(111) were used as the substrate. Sub cultured E. coli were used for the analysis. The SAM layered surfaces were dipped in varying concentrations of 2 – 4 Log/ml E. coli solutions. Subsequent surface adhesion at different bacterial dilutions on surfaces will be discussed, and correlated with quantitative and qualitative adhesion properties of bacteria on the engineered SAM surfaces. The bacteria adhered SAM surfaces were investigated using intermittent contact, noncontact, lateral force and contact modes of Atomic Force Microscopy (AFM).

¹Lock Haven University Nanotechnology Program

K1.00041 Aligned Single-Walled Carbon Nanotube Cantilevers, ALEXANDER RUYACK, Materials Science and Engineering, Cornell University, Ithaca NY, SAMANTHA ROBERTS, Department of Physics, Cornell University, Ithaca NY, IVE SILVESTRE, Department of Physics, Universidade Federal de Minas Gerais, Brazil, ARTHUR BARNARD, School of Applied and Engineering Physics, Cornell University, Ithaca NY, RODRIGO LACERDA, Department of Physics, Universidade Federal de Minas Gerais, Brazil, PAUL MCEUEN, Department of Physics, Kavli Institute at Cornell for Nanoscale Science, Cornell University, Ithaca NY — Researchers are striving to make smaller cantilever sensors with higher resonant frequencies in an effort to enhance force, position and mass detection sensitivity. With its minimal mass and high Young's modulus, a single wall carbon nanotube (SWNT) cantilever is suggested to represent the ultimate limit of this trend. We will present a novel nanolithography method that has been developed utilizing highly aligned SWNT's grown via chemical vapor deposition which are then transferred to a silicon/silicon dioxide substrate planarized with chemical mechanical polishing. This method allows us to create arrays of ~ 1 nanometer diameter aligned SWNT cantilevers of tunable length (typically 75 to 700 nanometers) with densities on the order of one cantilever per micrometer. Details about the nanofabrication process analyzed via imaging techniques such as scanning electron microscopy and atomic force microscopy will be discussed. Our future work will include characterization of the mechanical properties of these cantilevers and possible applications in biological sensing.

K1.00042 Parallel Performance Analysis between Free Response Environments and the Force Concept Inventory in Introductory Mechanics Courses, NICOLE BOBBITT, AARON WADE, CHANDRA PRAYAGA, University of West Florida — This paper reports our attempts to: 1) find a way to model and predict common thought processes that cause typical misconceptions identified by the Force Concept Inventory (FCI), 2) create a problem solving situation that folds in both kinematics and force discussions, and 3) accurately assess the students' ability to interpret a kinematic graph. Two pen and paper test questions were designed with these goals in mind, both broken into specific elements, not only to allow for partial credit, but also to arrive at a quantifiable fragmentation of the necessary thought processes required to solve the problem. These results were compared to pre- and post-FCI data to analyze the common misconceptions as defined by FCI and their correlation to mistakes in the thought processes in answering the designed questions. Ultimately this, and any future questions, would become a tool in the classroom to pinpoint the critical ideas with which a typical student struggles during a mechanics course.

K1.00043 Surface engineering and adhesion modification of SAM surfaces of 1-mercaptopundecanoic acid 1-undecanethiol: confining *Bacillus subtilis*¹, ROSE PASQUALE, LAUREN SWIGER, JOSEPH CALABRESE, RESHANI SENEVIRATHNE, INDRAJITH SENEVIRATHNE, Lock Haven University of Pennsylvania — Engineering surfaces for adhesion and confinement of bacteria is interesting towards development of respective biosensors, and to understand the interactions between biological systems and molecular layers. Investigation was focused on modification of surfaces towards confinement and entrapment of the nonpathogenic strain *Bacillus subtilis* or *Bacillus pathogenic/non pathogenic* variants and to study surface engineering. Clean, flat Au(111) on mica surfaces were used for self assembly for Self Assembled Monolayers (SAM). 1-mercaptopundecanoic acid and 1-undecanethiol were used at total 5 mM solutions in varying ratios, in 200 proof Ethanol solution. Resulting SAM layers were investigated for surface corrugation, morphology and structure variation at different thiol ratios. Observations will be discussed, quantitatively and qualitatively. Eventual mixture ratios were so selected towards optimum conditions for confining *Bacillus subtilis* as a model system. SAM surfaces were investigated using intermittent contact, noncontact, lateral force and contact modes of Atomic Force Microscopy (AFM).

¹Lock Haven University Nanotechnology Program

K1.00044 Light Scattering Characterization of Salt Dependent Thermoreversible Micelles Synthesized from Elastin-Like Polypeptides¹, KAITLIN VANDEMARK, ALI GHOORCHIAN, KIRIL STRELETZKY, NOLAN HOLLAND, Cleveland State University — Environmentally responsive nanoparticles synthesized from Elastin-Like Polypeptides (ELP) present a promising system for applications such as biosensors, drug delivery vehicles, and viscosity modifiers. These nanoparticles undergo a transition from a soluble state at T_{room} to micellar aggregates above the transition. The ELP micelles have been found to be sensitive to various outside stimuli including pH, salt concentration, and solvent. Dynamic and Static Light Scattering were used to study structure and dynamics of ELP nanoparticles below the transition and of formed ELP micelles above the transition. Micelles were found to generally depend strongly on solution pH, however, in the pH window of 10.1-10.4 their size stayed constant. The apparent radius and molecular weight of micelles in this pH range strongly depend on salt concentration with three apparent regimes. At low salt (0-15mM), largely spherical micelles were found with $R_h=15nm$, which corresponds to the size of folded ELP hydrophilic tail; and molecular weight of 5000-6000kg/mol. At the intermediate salt (15-30mM) the observed particles are spherical micelles that increase in size (by about 3 fold) and molecular weight (by about 50 fold) as salt concentration increases. At high salt concentrations (30-60mM), $R_g/R_h \sim 1.3$, indicating the micelles behave as elongated particles with $R_h \sim 75nm$ that corresponds to the size of a stretched ELP chain with an apparent molecular weight of 300000-600000kg/mol.

¹Supported by NSF (DMR-0908795) & CSU Summer Undergrad Research.

K1.00045 Fluorescence studies of gram-positive and gram-negative bacteria, BRITNI BLUST, None, TRACY SWINGER COLLABORATION¹, DR. MARIAN TZOLOV COLLABORATION², DR. JOSEPH CALABRESE COLLABORATION³ — Autofluorescence is a relatively unexplored technique for identification. It is nondestructive, noncontact, fast, and has the potential to be integrated in small handheld devices. On the other hand, the autofluorescent signal is sometimes very weak, or it can be overwhelmed by the emission of a surrounding medium. We are exploring the possibility to develop an optical method for identification of the Gram-type of bacterial cultures based on the autofluorescence. We have enhanced the detectivity of a standard fluorimeter using combination of bandpass and long pass filters. In this particular study, we are investigating if the previously observed difference in the autofluorescent spectra of Gram-positive and Gram-negative bacteria is dependent on the age of the culture. We have selected two types of bacteria, *Kocuria rhizophila* and *Alcaligenes faecalis*, and we have monitored in equal time intervals of their development the autofluorescence spectra. The stages of development were monitored separately by measuring the turbidity and creating a growth curve. The goal of this study is to find out if the previously observed difference in the autofluorescence spectra of Gram-positive and Gram-negative bacteria is dependent on the stage of the development of the bacterial culture.

¹Student whom participated in research along with me

²Research Advisor

³Research Super Advisor

K1.00046 Surface engineering and adhesion modification of SAM surfaces of 1-dodecanethiol, and 3-mercapto-1-propanol: confining Escherichia coli¹, KRISTA SITLER, KARISA BOWERSOX, JOSEPH CALABRESE, Biology, Lock Haven University, Lock Haven PA 17745, United States, RESHANI SENEVIRATHNE, Don's Food Products, Schwenksville, PA 19473, United States, INDRAJITH SENEVIRATHNE, Geology and Physics, Lock Haven University, Lock Haven PA 17745, United States — Engineering surfaces for adhesion and confinement of bacteria is interesting towards development of respective biosensors, and correlation of biological systems and molecular layers. Investigation was focused towards modification of surfaces towards confinement and entrapment of the nonpathogenic strain Escherichia coli or similar pathogenic strains and to study surface engineering. Clean, flat Au(111) on mica surfaces were used for self assembly for Self Assembled Monolayers (SAM). 1-dodecanethiol, and 3-mercapto-1-propanol were used at total 5 mM solutions in varying ratios, in 200 proof Ethanol solution. Resulting SAM layers were investigated for surface corrugation, morphology and structure variation at different thiol ratios. Observations will be discussed, quantitatively and qualitatively. Eventual mixture ratios were so selected towards optimum conditions for confining Escherichia coli as a model system. SAM surfaces were investigated using intermittent contact, noncontact, lateral force and contact modes of Atomic Force Microscopy (AFM).

¹Lock Haven University Nanotechnology Program

K1.00047 Surface adhesion and confinement variation of Staphylococcus aureus on SAM surfaces, ALICIA AMROSKI, MORGAN OLSEN, JOSEPH CALABRESE, Lock Haven University of Pennsylvania, Lock Haven PA 17745, United States, RESHANI SENEVIRATHNE, Don's Food Products, Schwenksville, PA 19473, United States, INDRAJITH SENEVIRATHNE, Lock Haven University of Pennsylvania, Lock Haven PA 17745, United States — Controlled surface adhesion of non - pathogenic gram positive strain, Staphylococcus aureus is interesting as a model system due to possible development of respective biosensors for prevention and detection of the pathogenic strain methicillin resistant Staphylococcus aureus (MRSA) and further as a study for bio-machine interfacing. Self Assembled Monolayers (SAM) with engineered surfaces of linear thiols on Au(111) were used as the substrate. Sub cultured S. aureus were used for the analysis. The SAM layered surfaces were dipped in 2 – 4 Log/ml S. aureus solution. Subsequent surface adhesion at different bacterial dilutions on surfaces will be discussed, and correlated with quantitative and qualitative adhesion properties of bacteria on the engineered SAM surfaces. The bacteria adhered SAM surfaces were investigated using intermittent contact, noncontact, lateral force and contact modes of Atomic Force Microscopy (AFM).

K1.00048 Precipitant diffusion and surface segregation in Al Alloys near melting point: Al 2024¹, AUSTIN MOHNEY, INDRAJITH SENEVIRATHNE, Lock Haven University of Pennsylvania — Industrial Al alloys are precipitant hardened with an impurity phase. Micro precipitants introduce various novel physical properties to the systems system. The diffusion of these constituents under thermal gradient was studied by sequentially increasing temperatures near melting point as it was observed to better facilitate the migration of precipitants. Study is based on Al 2024, age hardened, high strength AL alloy, annealed at incremental temperatures near melting point of 500 C and was observed in Scanning Electron Microscopy (SEM) and Energy Dispersive X ray Spectroscopy (EDX). Solvent cleaned near surface region of the alloy was investigated with observation of differential migration of constituent Cu, Fe Mg and Zn precipitants. The migrations were modeled in terms of diffusion coefficients and established literature of the participating species. Study will attempt to correlate the elemental concentration variation with applied elevated heat stress in industrial settings.

¹Lock Haven University Nanotechnology Program

K1.00049 Entanglement in Quantum Harmonic Chains¹, NOEL KLINGLER, NATHAN HARSHMAN, American University — We study interparticle entanglement in finite chains of coupled harmonic oscillators as a function of the vibrational mode, excitation number, and bipartition of oscillators. Harmonic chains are used as a model in quantum information theory for ion traps and simple solid state systems, and our results extend previous work for the Gaussian ground state to excited states. Entanglement is analyzed by calculating the purity of the reduced density matrix of the combined wavefunctions of the oscillators in the chain tracing, over subensembles. We present analytic and numerical results for a varying effective spring constants between the particles and number of particles in the chain. Our entanglement results show interesting correlations between the symmetries of the modes and the symmetries of the partitions.

¹The District of Columbia NASA Space Grant Consortium

K1.00050 Computational Design of Druglike Small Molecule Plk1 PBD Inhibitors, SEAN VANADIA, The College of New Jersey (TCNJ) Undergraduate — Polo-like Kinase 1 (Plk1) participates in regulation of the cell cycle and is often overexpressed in cancers. Inhibition of Plk1 was found to suppress cancer development. Most known kinase inhibitors interact with highly conserved ATP binding sites of the kinases. This makes the design of Plk1-specific inhibitors difficult. However, Plk1 has another active site, the Polo-Box Domain (PBD). PBD is not present in other kinases that were studied here. In this research, the PBD site of Plk1 was used as a target for designing small molecules that could potentially bind Plk1. A previously designed small molecule, Purpurogallin (PPG), was found to bind only the PBD of Plk1 and a highly similar site of LYN kinase, but no other kinases. The PPG structure was used as a template to design new putative Plk1-specific inhibitors. Druglike properties of the new molecules were evaluated with the Osiris Property Explorer program. Interactions of the molecules with Plk1, LYN, and eight other kinases were studied using the Argus Lab docking program. Further search for Plk1-specific inhibitors that could potentially target cancers with overexpressed Plk1 is discussed.

K1.00051 Experimental and Numerical Study of the Role of Disorder on Contact Angle Hysteresis¹, ANGELINA N. SAMS, VICTORIA E. MERTEN, MICHAEL S. PETTERSEN, Washington and Jefferson College — Hysteretic behavior of the contact angle of a liquid on a solid is often ascribed to topographic or chemical heterogeneity of the surface. Recent experiments by Rolley and Guthmann² on liquid hydrogen on cesium suggest that both the hysteresis and the contact line dynamics might be explained in terms of the mesoscale structure of the cesium surface. We have investigated a room temperature system with similar wetting and structural properties, tetradecane on dodecanethiol-treated evaporated gold films, and compare the results with a model of the expected hysteresis due to the topographical heterogeneity as measured by AFM, and reported disorder in the thiol film.³

¹Supported by NSF grant 0959373 and the Washington and Jefferson DDF fund

²E. Rolley and C. Guthmann, *Phys. Rev. Lett.* **98**, 166105 (2007).

³E. Delamarche, B. Michel, H. Kang and C. Gerber, *Langmuir* **10**, 4103 (1994).

K1.00052 Surface adhesion and confinement variation of *Bacillus subtilis* on SAM surfaces, LAUREN SWIGER, ROSE PASQUALE, JOSEPH CALABRESE, INDRAJITH SENEVIRATHNE, Lock Haven University — Controlled surface adhesion of non-pathogenic gram positive strain, *Bacillus subtilis* is interesting as a model system due to possible development of respective biosensors for prevention and detection of the pathogenic variants *B. anthracis* and *B. cereus*. Further as a study for bio-machine interfacing systems. Self Assembled Monolayers (SAM) with engineered surfaces of linear thiols on Au(111) were used as the substrate. Sub cultured *B. subtilis* were used for the analysis. The SAM layered surfaces were dipped in 2 – 5 Log/ml *B. subtilis* solution. Subsequent surface adhesion at different bacterial dilutions on surfaces will be discussed, and correlated with quantitative and qualitative adhesion properties of bacteria on the engineered SAM surfaces. The bacteria adhered SAM surfaces were investigated using intermittent contact, noncontact, lateral force and contact modes of Atomic Force Microscopy (AFM).

K1.00053 Micromechanical and structural study of ambient grown Au nanostructures on P doped Si(100)¹, INDRAJITH SENEVIRATHNE, JOSHUA TATHAM, Department of Geology and Physics, Lock Haven University, Lock Haven, PA — Au nanostructure have wide application potential due to their noble nature, plasmonic, catalytic and specific conductive properties. Such nanostructures grown on substrate support under ambient conditions are complex but provides unique opportunities in dirty systems. In this model system Au was self assembled on solvent cleaned P doped Si(100) surface giving rise to near spherical geometry. Self assembly was initiated by magnetron sputter deposited Au at RT (300K) under high vacuum, on Si(100) which subsequently exposed to atmosphere. The micromechanical properties of the structures were measured by contact mode force curves in Atomic Force Microscopy (AFM). Both the stiffness and young modulus was measured for the nanostructures assembled and annealed at different temperatures. Initial plasticity of the nano structures was observed to reduce at annealing. Au nano structures were likely Stranski - Krastanov growth mode. Observed structure and their variations when annealed at successively higher temperatures will also be discussed. All measurements were taken by the AFM in contact intermittent contact and non-contact modes.

¹Lock Haven University Nanotechnology Program

K1.00054 Open-frame external cavity diode laser for teaching and research¹, JASEN SCARAMAZZA, TYLER DONATO, ZACHARY BUCK, BRITTANY CURRAN, MICHAEL LIM, Dept. of Physics and Astronomy, Rowan University — We have constructed an open-frame, low-power, tunable external cavity diode laser suitable for both teaching and research purposes. We adapt the design of [1, 2] to an open, 4-rod frame composed entirely of commercially available parts. The laser can be quickly disassembled and reassembled by undergraduate students, while its open architecture provides an intuitive demonstration for students learning about laser physics. The laser will be used for atomic absorption spectroscopy.

[1] X. Baillard, et al., *Opt. Comm.* **266**, 609 (2006)

[2] M. Gilowski, et al., *Opt. Comm.* **280**, 443 (2007)

¹Supported in part by NSF PHY0613659.

K1.00055 Surface engineering and adhesion modification of SAM surfaces of 1-hexanethiol and 1-decanethiol: confining *Staphylococcus aureus*¹, MORGAN OLSEN, ALICIA AMROSKI, Department of Chemistry, Lock Haven University, PA 17745, JOSEPH CALABRESE, Department of Biology, Lock Haven University, PA 17745, RESHANI SENEVIRATHNE, Don's Food Products, Schwenksville, PA 19473, INDRAJITH SENEVIRATHNE, Department of Geology and Physics, Lock Haven University, PA 17745 — Engineering surfaces for adhesion and confinement of bacteria is interesting towards development of respective biosensors, and bio machine interfacing. Investigation was focused towards modification of surfaces towards confinement and entrapment of the nonpathogenic strain *Staphylococcus aureus* or similar pathogenic strains and to study surface engineering. Clean, flat Au(111) on mica surfaces were used for self assembly for Self Assembled Monolayers (SAM). 1-hexanethiol, and 1-decanethiol were used at total 5 mM solutions in varying ratios, in 200 proof Ethanol solution. Resulting SAM layers were investigated for surface corrugation, morphology and structure variation at different thiol ratios. Observations will be discussed, quantitatively and qualitatively. Eventual mixture ratios were so selected towards optimum conditions for confining *Staphylococcus aureus* as a model system. SAM surfaces were investigated using intermittent contact, noncontact, lateral force and contact modes of Atomic Force Microscopy (AFM).

¹Lock Haven University Nanotechnology Program

K1.00056 Scanning electron microscopy studies of bacterial cultures¹, TRACY SWINGER, BRITTNI BLUST, JOSEPH CALABRESE, MARIAN TZOLOV, Lock Haven University — Scanning electron microscopy is a powerful tool to study the morphology of bacteria. We have used conventional scanning electron microscope to follow the modification of the bacterial morphology over the course of the bacterial growth cycle. The bacteria were fixed in vapors of Glutaraldehyde and ruthenium oxide applied in sequence. A gold film of about 5 nm was deposited on top of the samples to avoid charging and to enhance the contrast. We have selected two types of bacteria *Alcaligenes faecalis* and *Kocuria rhizophila*. Their development was carefully monitored and samples were taken for imaging in equal time intervals during their cultivation. These studies are supporting our efforts to develop an optical method for identification of the Gram-type of bacterial cultures.

¹Lock Haven University Nanotechnology Program

K1.00057 Electrical Characterization of Temperature Dependent Resistive Switching in $\text{Pr}_{0.7}\text{C}_{0.3}\text{MnO}_3$, MELINDA LOPEZ, CHRISTOPHER SALVO, STEPHEN TSUI, California State University San Marcos — Resistive switching offers a non-volatile and reversible means to possibly create a more physically compact yet larger access capacity in memory technology. While there has been a great deal of research conducted on this electrical property in oxide materials, there is still more to be learned about this at both high voltage pulsing and cryogenic temperatures. In this work, the electrical properties of a PCMO-metal interface switch were examined after application of voltage pulsing varying from 100 V to 1000 V and at temperatures starting at 293 K and lowered to 80 K. What was discovered was that below temperatures of 150 K, the resistive switching began to decrease across all voltage pulsing and that at all temperatures before this cessation, the change in resistive switching increased with higher voltage pulsing. We suggest that a variable density of charge traps at the interface is a likely mechanism, and work continues to extract more details.

K1.00058 Preparation and Characterization of C-16 and C-10 Fluorescent Dipyrinone Liquid Crystal Langmuir-Blodgett Films , GIOVANNI DELUCA¹, ALEXANDER CARROLL², CHANDRA PRAYAGA³, AARON WADE⁴, Physics Department, University of West Florida, CHRISTOPHER HEATH⁵, AMY RENAUD⁶, MICHAEL HUGGINS⁷, Chemistry Department, University of West Florida — A new C-16 and C-10 Fluorescent Dipyrinone Liquid Crystal has been synthesized by the University of West Florida's Chemistry department. The liquid crystals have amphiphilic properties with their dipyrinone polar heads and long hydrocarbon nonpolar tails. This led to the preparation and characterization of their Langmuir and Langmuir-Blodgett Film, using a Nima Langmuir-Blodgett Trough. The influence of the length of the hydrocarbon tail on the behavior of the pressure-area isotherm of the Langmuir film is studied. There is considerable difference in the behavior of the C-16 and C-10 Fluorescent Dipyrinone Liquid Crystal Films prepared. Ellipsometric characterization of the films, using an ellipsometer built by the Physics department, is used to further study the Liquid Crystal films.

¹ Undergraduate student

² Undergraduate student

³ Faculty mentor

⁴ Faculty mentor

⁵ Undergraduate student

⁶ Undergraduate student

⁷ Faculty mentor

K1.00059 Characterization of Acryl amide Resins Using Static Light Scattering , SUMIT LIBI, DAVID NORWOOD, Southeastern Louisiana University — Our research is based on the use of light scattering technique for the characterization of known and unknown particles within a liquid. The research focused specifically on the detection of resin polymer that may be present in the given samples using static light scattering. The sample was delivered into a high performance liquid chromatography system with static light scattering, refractive index and viscosity detectors. Static Light scattering measures the intensity of the light scattered as the function of scattering angle and polymer sample concentration. Based on these results the molecular weight and radius of gyration of the given sample can be calculated.

K1.00060 SUPERCONDUCTIVITY —

K1.00061 Synthesis and properties of a new superconducting compound (ZrNi_xS₂) , ARTHUR SCARAMUSSA, Escola de Engenharia de Lorena - Universidade de Sao Paulo, ZACHARY FISK, Departments of Physics and Astronomy, University of California at Irvine, ANTONIO JEFFERSON MACHADO, Escola de Engenharia de Lorena - Universidade de Sao Paulo, DEPARTMENTS OF PHYSICS AND ASTRONOMY, UNIVERSITY OF CALIFORNIA AT IRVINE - IRVINE, CA 92697, USA COLLABORATION — Since the discovery of superconductivity in chalcogenides in Fe-Se system and in iron pnictides much attention have been give for synthesis of new materials which can exhibit superconductivity. Within this context in this work we show results which suggest that ZrNi_xS₂, where x can assume 0.3, 0.5 and 0.8 values, is a new superconductor material. This compound crystallizes in a new crystallographic structure with hexagonal symmetry belongs to the space group R – 32/m. Indeed this compound is a variation of the Zr₃S₄ which can be considered as the prototype structure of this new compound (ZrNi_xS₂). In this prototype structure zirconium atoms may occupy two different sites in the structure. Thus, nickel atoms substitute zirconium in a specific site of the structure. These results suggest that superconducting critical temperature is dependent of the nickel content in this new compound. The optimum Ni content yield to T_c ~ 9.8 K.

K1.00062 Superconductivity in the T₂ phase of the Ta-Ge-B system , LUCAS EDUARDO CORRÊA, CARLOS NUNES, GILBERTO COELHO, ANTONIO AUGUSTO SILVA, ZACK FISK, ANTONIO JEFFERSON MACHADO, None, UNIVERSITY OF CALIFORNIA AT IRVINE COLLABORATION — In the Ta-Ge system the α-Ta₅Ge₃ phase is not superconductor. Considering the high solubility of this phase for boron, in this work it has been evaluated the effect of boron doping in α-Ta₅Ge₃ on the electrical, heat capacity and magnetic properties of the produced materials. It has been shown that boron doping promoted superconductivity for some specific composition. The Ta₅GeB₂, also named T₂ phase, crystallizes in the tetragonal symmetry with Cr₅B₃ prototype structure. In this composition the sample presented the maximum superconducting critical temperature (3.4 K). Others systems that exhibit the existence of the T₂ phase present superconductivity such as Mo₅SiB₂ (T_c ~5.5 K), Nb₅Si_{3-x}B_x (T_{cmax} ~7.8 K) and W₅SiB₂ (T_c ~5.5 K). Thus, Ta₅GeB₂ is more one example.

K1.00063 Evidence of the superconductivity in the Zr-Pt-Te system , SERGIO RENOSTO, Escola de Engenharia de Lorena, Universidade de São Paulo, P.O. Box 116, Lorena, SP, Brasil, TED GRANT, ZACHARY FISK, Departments of Physics and Astronomy, University of California at Irvine, Irvine, CA 92697, USA, ANTONIO MACHADO, Escola de Engenharia de Lorena, Universidade de São Paulo, P.O. Box 116, Lorena, SP, Brasil — Layered transition metal dichalcogenides MetalX₂ are well-known CDW conductors, with low dimensionality properties. The structure of layered TMDC can be regarded as a stacking of covalent coupled M-X-X sandwiches, and the coupling between layers X-X is of weak van der Waals type. The intercalation of metallic atoms into the weak coupled region between the X-X layers leads to significant modification of electronic properties. In this work results suggest that the Pt intercalation is able to induce superconductivity in the matrix compound (ZrTe₂). The critical temperature at 6.5 K is revealed through of magnetization, resistivity and specific heat measurements. Heat-capacity measurements show unambiguously a bulk superconductivity behavior. However, the x-ray diffraction results reveal that ZrPt_xTe₂ can crystallize in the LiCrS₂ prototype structure. Thus, we had shown that the superconductivity is induced by intercalation of Pt atoms.

K1.00064 Superconductivity in Zr_{1-x}V_xB₂ , LUIS HENRIQUE CONSOLINE, SERGIO RENOSTO, Escola de Engenharia de Lorena, Universidade de São Paulo, ZACHARY FISK, Departments of Physics and Astronomy, University of California at Irvine, ALEX COSTA, ANTONIO JEFFERSON MACHADO, Escola de Engenharia de Lorena, Universidade de São Paulo, UNIVERSITY OF CALIFORNIA AT IRVINE COLLABORATION — Since the discovery of superconductivity in MgB₂, much attention has been give for research in new diboride with potential for exhibit superconductivity. There are many diboride of refractory metals which crystallize in the same prototype structure than MgB₂ (AlB₂ prototype structure). However, only NbB₂ can exhibit superconductivity with superconductor critical temperature close to 3.5 K on the optimum composition. Some authors have been reported superconductivity in ZrB₂ with critical temperature close to 5.5 K, but this result was not reproduced for other research groups. In this work we present results which show that small substitution of Zr by V in the Zr_{1-x}V_xB₂ is able to induce superconductivity in the matrix phase (ZrB₂). The best composition gives a superconducting critical temperature close to 8.5 K.

K1.00065 Superconductivity in ZrVGe and HfVGe compounds , ANTONIO JEFFERSON MACHADO, Escola de Engenharia de Lorena, Universidade de São Paulo, P.O. Box 116, Lorena, SP, Brazil, ZACHARY FISK, Departments of Physics and Astronomy, University of California at Irvine, Irvine, CA 92697, USA — In the Zr-V-Ge and Hf-V-Ge there are two ternary phases of ZrVGe and HfVGe compositions which crystallize in a tetragonal symmetry. Both structures crystallize in the UGeTe prototype with space group I4/mmm. The lattice parameters of the two compounds are a = 3.72 Å and c = 14.34 Å for HfVGe and a = 3.75 Å and c = 14.48 Å for ZrVGe. In this structure the elements are arranged in layers in which obey V-RM-Ge sequence, where RM represents the refractory metal like Zr or Hf. In this work we show that both compounds are bulk superconductor with superconducting critical temperature at 4.8 K for HfVGe and 6.0 for ZrVGe.

K1.00066 Superconductivity in ZrAg_xTe_2 , HELTON SANTANA, SERGIO RENOSTO, ANTONIO JEFFERSON MACHADO, Escola de Engenharia de Lorena, Universidade de Sao Paulo — Layered transition metal dichalcogenides of the type MX_2 (M is transition metal, X = S, Se, Te) have been studied for their electronic properties due to low dimensionality. In these materials each layer correspond to the hexagonal transition metal intercalated by two similar chalcogen sheets. In ZrTe_2 the prototype structure is CdI_2 . The interaction of layers is weak as van der Waals bonding between chalcogen element (X). In general charge density wave and superconductivity coexist in these of materials. Indeed, various compounds of this material class exhibits this coexistence such as 2H-TaS_2 , 2H-NbS_2 etc. Some results reported in literature about the electrical properties of ZrTe_2 show that this material presents metallic behavior at a temperature interval from 4.0 K to 300 K. In this work we present results about intercalation of silver in the ZrTe_2 compound. The results suggest that the intercalation of Ag also is able to induce superconductivity in this compound. The superconducting critical temperature close to 9.0 K is revealed through of magnetization and resistivity measurements. The x-ray result reveals a new compound, originating from Ag intercalation and crystallizes in the LiCrS_2 prototype structure.

K1.00067 Superconductivity in ZrCu_xTe_2 , NAIARA BAPTISTA, Escola de Engenharia de Lorena, Universidade de Sao Paulo, TED GRANT, University of California at Irvine, SERGIO RENOSTO, Escola de Engenharia de Lorena, Universidade de Sao Paulo, ZACK FISCH, University of California at Irvine, ANTONIO JEFFERSON MACHADO, Escola de Engenharia de Lorena, Universidade de Sao Paulo, UNIVERSITY OF CALIFORNIA AT IRVINE COLLABORATION — Layered transition metal dichalcogenides of the type MX_2 (M is transition metal, X = S, Se, Te) have been studied for their electronic properties due to low dimensionality. In these materials each layer correspond to the hexagonal transition metal intercalated by two similar chalcogen sheets. In ZrTe_2 the prototype structure is CdI_2 . The interaction of layers is weak as van der Waals bonding between chalcogen element (X). In general charge density wave and superconductivity coexist in these of materials. Indeed, various compounds of this material class exhibits this coexistence such as 2H-TaS_2 , 2H-NbS_2 etc. Some results reported in literature about the electrical properties of ZrTe_2 show that this material presents metallic behavior at a temperature interval from 4.0 K to 300 K. Thus, in this work we present results about intercalation of Cu in the ZrTe_2 compound. The results suggest that the intercalation of Cu is able to induce superconductivity in this compound. The superconducting critical temperature close to 10.2 K is revealed through of magnetization and resistivity measurements. The x-ray result reveals a new compound, originating from Cu intercalation and crystallizes in the LiCrS_2 prototype structure.

K1.00068 Synthesis and properties of a new superconducting compound (ZrCu_xSe_2) , ANA CAROLINA GENEROSO, NAIARA BAPTISTA, SERGIO RENOSTO, ANTONIO JEFFERSON MACHADO, Escola de Engenharia de Lorena, Universidade de Sao Paulo — Since the discovery of superconductivity in chalcogenides in Fe-Se system and in iron pnictides much attention have been give for synthesis of new materials which can exhibit superconductivity. Within this context in this work we show results which suggest the existence of a new selenite intercalate with copper atoms in the ZrCu_xSe_2 nominal composition, where x is $0.1 \leq x \leq 0.4$ interval. A superconductor behavior begins in the $\text{ZrCu}_{0.3}\text{Se}_2$ with superconducting critical temperature close to 9.0 K. ZrSe_2 is a compound which crystallize in the hexagonal symmetry with CdI_2 prototype structure belongs to the space group $P-32/m1$. Indeed, copper is intercalating between Se-Se which have van der Waals interaction in the ZrSe_2 compound. This intercalation with copper atoms, produce superconductivity in the matrix compound (ZrSe_2) which is not superconductor. The copper intercalation in the matrix compound crystallizes in a LiCrS_2 prototype structure.

K1.00069 Superconductivity in a new compound of Zr_2CuSb_3 composition , RAFAEL TEBECHERANI, SERGIO RENOSTO, LUCAS CORREA, Escola de Engenharia de Lorena, Universidade de Sao Paulo, ZACHARY FISK, Departments of Physics and Astronomy, University of California at Irvine, ANTONIO JEFFERSON MACHADO, Escola de Engenharia de Lorena, Universidade de Sao Paulo, UNIVERSITY OF CALIFORNIA AT IRVINE COLLABORATION — In the Zr-Cu-Sb system there is a phase of Zr_2CuSb_3 composition which represents a ternary compound. This phase crystallize in a new prototype structure Zr_2CuSb_3 which have a tetragonal symmetry with space group $P-4m2$. The lattice parameters are $a=3.9404 \text{ \AA}$ and $c=8.6971 \text{ \AA}$. This structure can be represented as sequence of $1\text{Zr}_4\text{Sb}_2\text{Cu}_2\text{Sb}$ and (4Sb) which form like layer compound. However, the literature is very poor in results about the properties of this compound. Thus, in this work we show results which suggest the existence of superconductivity with superconducting critical temperature close to 8.0 K. These conclusions were obtained through X-ray diffraction, magnetization, and resistivity measurements.

K1.00070 Microscopic description of vortices in nanoscale superconductors , LIVIU CHIBOTARU, BART DELOOF, VICTOR MOSHCHALKOV, University of Leuven — The results of Bogolyubov-de Gennes calculations for thin superconducting discs and squares in applied magnetic field will be presented. The paramagnetic effect is taken fully into account. The vortex phase diagrams for the samples of nanoscopic size will be constructed and compared with the predictions of the Ginzburg-Landau theory. The size limitations for the entering of one and several vortices as function of material parameters will be established. Several unusual vortex transformations during the vortex pattern evolutions as function of temperature and field will be discussed.

K1.00071 Hexagonal pnictide SrPtAs ; the role of spin-orbit interaction and locally broken inversion symmetry¹ , S.H. RHIM, Northwestern U., S.J. YOUN, Gyeong Sang Natl. U., M.H. FISCHER, LASSP and Cornell U., D.F. AGTERBERG, U. Wisconsin-Milwaukee, M. SGRIST, ETH-Zuerich, M. WEINERT, U. Wisconsin-Milwaukee, A.J. FREEMAN, Northwestern U. — The first hexagonal pnictide superconductor SrPtAs which consists of stacked PtAs layers has been studied using the FLAPW method² and tight-binding methods. The single PtAs layer forms a honeycomb structure that exhibits: (1) locally broken inversion symmetry despite the presence of the global inversion center, and (2) strong spin-orbit interaction, for which physical consequences are nontrivial. Based on these findings, we predict significant enhancement of both the spin susceptibility and the paramagnetic limiting field with respect to the usual s wave superconductors. Further, we suggest an increase of T_C by electron doping of a van Hove singularity.

¹DOE (DE-FG02-88ER45382)

²Wimmer, Krakauer, Weinert, and Freeman, Phys.Rev.B. **24**, 864 (1981)

K1.00072 Superconductivity and structural variation of the electron-correlated layer systems $\text{Sr}(\text{Pd}_{1-x}\text{Te}_x)_2\text{Ge}_2$ ($T = \text{Co, Ni, or Rh}$; $0 \leq x \leq 1$)¹ , H.C. KU, J.W. WANG, I.A. CHEN, Y.B. YOU, C.Y. LIN, C.H. HUANG, S.J. WANG, Department of Physics, National Tsing Hua University, Y.Y. HSU, Department of Physics, National Taiwan Normal University — Superconductivity variations in the pseudoternary $\text{Sr}(\text{Pd}_{1-x}\text{Te}_x)_2\text{Ge}_2$ layer system ($\text{Pd}(4d^8)$, $T = \text{Co}(3d^7)$, $\text{Ni}(3d^8)$, or $\text{Rh}(4d^7)$; $0 \leq x \leq 1$) are reported. For the BaFe_2As_2 -type tetragonal structure, the degenerate nd^7 or nd^8 orbital of transition metal T is splitted by c -axis squeezed $T\text{Ge}_4$ tetrahedral crystal field in the T -Ge layer. For the isoelectronic $\text{Sr}(\text{Pd}_{1-x}\text{Ni}_x)_2\text{Ge}_2$ system, superconducting transition temperature T_c decreases monotonically from 3.12 K for $4d$ -band SrPd_2Ge_2 to 0.92 K for $3d$ -band SrNi_2Ge_2 , where major contribution of conduction electrons was from the half-filled dispersive 3D-like upper-lying $nd_{xz,yz}$ bands. For the $\text{Sr}(\text{Pd}_{1-x}\text{Rh}_x)_2\text{Ge}_2$ system, T_c decreases to 2.40 K with 25% of $4d^7$ Rh substitution. For the $\text{Sr}(\text{Pd}_{1-x}\text{Co}_x)_2\text{Ge}_2$ system, T_c decreases sharply to 2.58 K with only 3% of $3d^7$ Co substitution. The lower T_c of the present electron-overdoped (nd^7 or nd^8) compound is due to dispersive 3D-like $nd_{xz,yz}$ conduction bands with weak electron correlation.

¹This work was supported by NSC98-2112-M-007-013-MY3 and NSC99-2112-M-003-007.

K1.00073 Local antiferromagnetic exchange and collaborative Fermi surface as key ingredients of high temperature superconductors, JIANGPING HU, Purdue University, HONG DING, Institute of Physics, Chinese Academy of Sciences — Cuprates, ferropnictides and ferrochalcogenides are three classes of unconventional high-temperature superconductors, who share similar phase diagrams in which superconductivity develops after a magnetic order is suppressed, suggesting a strong interplay between superconductivity and magnetism, although the exact picture of this interplay remains elusive. Here we show that there is a direct bridge connecting antiferromagnetic exchange interactions determined in the parent compounds of these materials to the superconducting gap functions observed in the corresponding superconducting materials. High superconducting transition temperature is achieved when the Fermi surface topology matches the form factor of the pairing symmetry favored by local magnetic exchange interactions. Our result offers a principle guide to search for new high temperature superconductors. References: Jiangping Hu and Hong Ding, Arxiv:1107.1334 (2011)

K1.00074 Electronic structure of iron-based superconductors from DFT+DMFT: the important role of Hund's coupling and correlations, ZHIPING YIN, KRISTJAN HAULE, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University — The iron pnictide and chalcogenide compounds are a subject of intensive investigations due to their surprisingly high temperature superconductivity. Density functional theory (DFT) has been widely used in the theoretical study but often suffers from significant discrepancy with experimental observations. The fundamental reason is that the low energy electrons in many iron-based superconductors, while displaying nice Fermi-liquid behavior, form quasiparticles and acquire sizable masses. Thus the actual low energy electronic states are strongly renormalized compared to DFT bands. We show that the combination of DFT and dynamic mean field theory (DFT+DMFT), which incorporates the detail electronic structure and local electronic correlations, overcomes most of DFT limitations and describe well the trends in all the physical properties such as the ordered moments, effective masses, Fermi surfaces, x-ray spectroscopy, optical conductivity, magnetic excitations and so on across all families of iron-based compounds, and find them in good agreement with various different experiments. We stress that Hund's blocking mechanism and electronic correlations are crucial in determining the electronic structures of iron-based superconductors.

K1.00075 Chlorine-doping effects on crystal structure and superconductivity in $\text{FeSe}_{1-x}\text{Cl}_x$ ¹, H.H. SUNG, R.R. HU, S.C. CHEN, W.H. LEE, National Chung Cheng University, W.H. LEE TEAM — According to the assessed Fe-Se phase diagram,² the FeSe compound could crystallize either in tetragonal Pb-O type structure with space group P4/nmm (called β FeSe) or hexagonal Ni-As type structure with space group P6₃/mmc (called δ FeSe) depending on the materials preparation process. In general, different starting composition of FeSe_x results in a mixture of superconducting phase with almost identical T_c and different amounts of magnetic impurity, therefore, it was proposed that the tetragonal β -FeSe superconducting phase ($T_c \sim 8$ K) only exists in a very narrow Se-deficiency range.³ Our experimental data indicated that the single hexagonal δ phase sample could be obtained by carrying out the low-temperature (400 °C) annealing for FeSe_xCl_y after reaction at 680 °C. This result is contrary to what is observed in the FeSe system in which the tetragonal β phase is the predominant stable one at the low annealing temperature 400 °C. As compared with the β -FeSe superconductor reported in the literature, higher T_c values (> 8 K) and larger superconducting volume fraction could be achieved by suitable tuning and heat treatments in the FeSe_xCl_y system.

¹Supported by the National Science Council of Republic of China under Contract Numbers NSC 99-2112-M-194-006-MY3 and NSC 100-2811-M-194-015.

²"Binary Alloy Phase Diagrams" 2nd edition, ASM International, Editor-in-Chief: Thaddeus B. Massalski, pp 1769-1770 (1992).

³Zhaofei Li, et. al., J. Phys. & Chem. Solids, **71**, 495-498 (2010).

K1.00076 Effective five band analysis on the lattice structure effect in iron pnictides, HIDETOMO USUI, KAZUHIKO KUROKI, The University of Electro-Communications — The discovery of superconductivity in the iron pnictides[1] and its T_c up to 55K[2] has given great impact to the field of condensed matter physics. From the early stage, much attention has been paid to the correlation between T_c and the lattice structure[3]. In the present study, we focus on the condition for optimizing superconductivity in the iron pnictides, varying hypothetically the lattice structure of LaFeAsO . Studying the band structure of the hypothetical lattice structure of LaFeAsO , the hole Fermi surface multiplicity is found to be maximized around the Fe-As-Fe bond angle regime where the arsenic atoms form a regular tetrahedron. Superconductivity is optimized within this three hole Fermi surface regime, thereby providing a natural explanation as to why T_c is optimized around the regular tetrahedron angle. Combining also the effect of the varying the Fe-As bond length, we provide a guiding principle for obtaining high T_c . [1]Y.Kamihara *et al.*, J. Am. Chem. Soc. **130**, 3296 (2008). [2]Z-A Ren *et al.*, Chinese Phys. Lett. **25**, 2215 (2008). [3]C.H. Lee *et al.*, J. Phys. Soc. Jpn. **77**, 083704 (2008).

K1.00077 The origin of the electron-hole asymmetry of the spin fluctuations and the effect on superconductivity in iron-based superconductors, KATSUHIRO SUZUKI, HIDETOMO USUI, KAZUHIKO KUROKI, University of Electro-Communications — Development of the spin fluctuation has been considered as one of the important features in the iron-based superconductors. One of interesting observation is the electron-hole asymmetry in its incommensurability, which appears in the neutron scattering experiments. In the present study, we study the origin of this electron-hole asymmetry, and its effect on the superconducting gap form. We first obtain a 10 orbital model for 122 iron-based superconductors from first principle calculation and obtain 5 orbital model in the unfolded Brillouin zone, which can only be done approximately in 122 systems. We apply the random phase approximation to these models to obtain the spin susceptibility, and solve the Eliashberg equation for the spin-fluctuation-mediated superconductivity. We find that the origin of the electron-hole asymmetry of the spin fluctuations is the multi-orbital nature of the Fermi surfaces. The multi-orbital nature of the Fermi surface is also found to be important in the appearance of horizontal nodes in the superconducting gap found in the calculation for 122 systems.

K1.00078 Re-entrant Resistance and Transport Anomalies in P-doped Eu Pnictide: $\text{EuFe}_2(\text{As}_{0.7}\text{P}_{0.3})_2$, with coexisting superconducting and ferromagnetic phases¹, NICHOLAS CORNELL, Nanotech Institute, University of Texas at Dallas, TIAN SHENG, HUIQIU YUAN, GUANGHAN CAO, SHENGGAO XU, ZHU'AN XU, Department of Physics, Zhejiang University, AUSTIN HOWARD, NATHANIEL MAYO, MYRON SALAMON, ANVAR ZAKHIDOV, Nanotech Institute, University of Texas at Dallas — The doping of Eu 122 pnictides by Phosphorus has been shown to result in superconductivity which coexists with ferromagnetism of spins ordered in Eu sites. Recently, in the course of exploring Fe-based superconductors, we observed both SC associated with Fe-3d electrons and ferromagnetism due to the long-range ordering of Eu-4f moments in $\text{EuFe}_2(\text{As}_{0.7}\text{P}_{0.3})_2$ and in similar compound with lower P-doping, at 0.27 the $R(T)$ peak appears at $T \sim 19$ K [1]. This $R(T)$ peak is associated with suppression of superconductivity by ferromagnetism and a re-entrance of resistance at low temperature. This presentation further investigates the pnictides at different P doping levels with transport measurements, correlated with magnetic and ESR data. Pnictides were made with a Solid state reaction method including the flux method to grow the single crystals. The dependence of the transition temperature and the behavior of the re-entrant $R(T)$ peak at 18-19 K on magnetic field and amount of dopant are addressed. [1]Amir Ahmed, M. Itou, Shenggao Xu, Zhu'an Xu, Guanghan Cao, Y. Sakurai, James Penner-Hahn, Aniruddha Deb, Phys. Rev. Letters **105**, 207003 (2010)

¹AFOSR grant FA 9550-09-10384

K1.00079 First principles Study on Transparent High-Tc Superconductivity in hole-doped Delafossite CuAlO₂, AKITAKA NAKANISHI, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University — The CuAlO₂ is the transparent *p*-type conductor without any intentional doping. Transparent superconductivity and high thermoelectric power are suggested in *p*-type CuAlO₂ [1]. Katayama-Yoshida *et al.* proposed that it may cause a strong electron-phonon interaction and a superconductivity. But, the calculation of superconducting critical temperature T_c is not performed. We performed the first principles calculation about the T_c of hole-doped CuAlO₂ by shifting the Fermi level rigidly. In lightly hole-doped CuAlO₂, the Fermi level is located at Cu and O anti-bonding band. The electrons of this band strongly interact with the A₁L₁ phonon mode because the direction of O-Cu-O dumbbell is parallel to the oscillation direction of the A₁L₁ phonon mode. As a result, T_c of lightly hole-doped CuAlO₂ is about 50 K. We also discuss the materials design to enhance the T_c based on the charge-excitation-induced negative effective U system.

[1] H. Katayama-Yoshida, T. Koyanagi, H. Funashima, H. Harima, A. Yanase: Solid State Communication **126** (2003) 135.

[2] A. Nakanishi and H. Katayama-Yoshida: Solid State Communication, in printing. (arXiv:1107.2477v3)

K1.00080 Synthesis of the electron-doped copper superconductors Eu_{2-*x*}Ce_{*x*}CuO_{4-*y*} and their physical property characterization using the X-ray powder diffraction and high pressure¹, GUOQING WU, WILLIAM NELSON, LUIS FLORES, SEAN HEFFERNAN, CHRISTOPHER WECKERLY, Dept. of Physics, University of West Florida, 32514, USA — The electron-doped copper superconductors Eu_{2-*x*}Ce_{*x*}CuO_{4-*y*} ($0 \leq x \leq 0.25$) were synthesized successfully using a solid state reaction method under a series of annealing and reduction procedures. X-ray diffraction and high hydrostatic pressure were used for their structure and electrical property characterization. Preliminary results show that the samples are in a single phase and the T_c drops as the pressure increases with a rate in sign opposite to the hole-doped counterparts and in magnitude apparently smaller than other cuprate superconductors.

¹UWF Scholarly Creative Activity Award and UWF Research Academy Award 2011

K1.00081 Investigation of Un-reacted, Multi-phase, Solution-Derived Targets for Pulse Laser Deposition (PLD) of High T_c Superconducting Y₂Ba₄Cu₈O₁₆ (Y248) In-Situ, Epitaxial Thin Films, GRACE YONG, RODNEY DIXON, STEPHEN MONK, VERA SMOLYANINOVA, RAJESWARI KOLAGANI, Towson University — Y₂Ba₄Cu₈O₁₆ (Y248) is known to be robust in terms of O stability and is characterized by the absence of twin formation, and no structural phase transitions. It is stable in ambient atmosphere, resisting H₂O (and possibly even CO₂ exposure). These characteristics make Y248 more attractive for several applications of thin film superconductors as compared to Y₁Ba₂Cu₃O_{7- δ} (Y123). In addition, Y248 is very likely to have a much lower 1/f electrical noise level than Y123. (Electrical noise in Y123 has been shown to arise from mobile O defects). This would be an important advantage, since it has been established that electrical noise is a performance limiting parameter for Y123 devices. Limited past work on Y248 films has shown that a traditional approach to the growth of thin films by PLD that use stoichiometric, fully reacted, single phase targets has not been successful in achieving in-situ, epitaxial Y248 films. Such studies have also indicated the potential for achieving in-situ, epitaxial, PLD Y248 films using an un-reacted, multi-phase, solution-derived target. We will present results of our work towards obtaining high quality, in-situ, epitaxial thin films of Y248 via PLD employing non-traditional targets.

K1.00082 Superconductivity via Two-Phase Condensation of Localized Electrons, STEVEN KAPLAN, Yorktown Heights, NY, ALAN KADIN, Princeton Junction, NJ — Superconductivity is believed to occur via the formation of bound Cooper pairs of charge $2e$, and Bose condensation of the pairs. Recently, a fundamentally different approach [1] was developed that combines two novel aspects. First, a “distortion lattice” akin to an incommensurate dynamic charge-density wave is induced by the electron-phonon interaction. This localizes individual electrons on the scale of the coherence length by diffraction at the Brillouin zone of this distortion lattice, thus forming an energy gap. Second, these localized electrons are packed together with others of the same energy in two interlocked close-packed sublattices, analogous to ions in an ionic crystal. The electron wavefunctions in each sublattice are coherently in phase with each other, but out of phase with those in the other sublattice. The two sublattices together constitute a stable condensed structure compatible with the Pauli principle, which maintains long-range order of the quantum phase of the localized electrons. This structure can move coherently without pinning or resistance, manifesting itself as a supercurrent. Remarkably, the electron localization gap maps onto the BCS gap equation, and the flux quantum $h/2e$ is reproduced, without the presence of bound electron pairs. Moreover, this picture is easily extended to electron localization mediated by spin waves or other excitations. Experimental approaches to distinguish this new picture from conventional theories will be discussed.

[1] A.M. Kadin, <http://arxiv.org/abs/0909.2901>; <http://arxiv.org/abs/1007.5340>.

K1.00083 Theory of High- T_c Superconductivity: Accurate Predictions of T_c , DALE HARSHMAN, Physikon Research Corporation, Lynden, WA 98264 USA; U. Notre Dame, Notre Dame, IN 46556 USA, ANTHONY FIORY, New Jersey Institute of Technology, Newark, NJ 07102 USA — The superconducting transition temperatures of high- T_c compounds based on copper, iron, ruthenium and certain organic molecules is discovered to be dependent on bond lengths, ionic valences, and Coulomb coupling between electronic bands in adjacent, spatially separated layers [1]. Optimal transition temperature, denoted as T_{C0} , is given by the universal expression $k_B T_{C0} = e^2 \Lambda / \ell \zeta$; ℓ is the spacing between interacting charges within the layers, ζ is the distance between interacting layers and Λ is a universal constant, equal to about twice the reduced electron Compton wavelength (suggesting that Compton scattering plays a role in pairing). Non-optimum compounds in which sample degradation is evident typically exhibit $T_c < T_{C0}$. For the 31+ optimum compounds tested, the theoretical and experimental T_{C0} agree statistically to within ± 1.4 K. The elemental high- T_c building block comprises two adjacent and spatially separated charge layers; the factor e^2/ζ arises from Coulomb forces between them. The theoretical charge structure representing a room-temperature superconductor is also presented.

1. doi:10.1088/0953-8984/23/29/295701

K1.00084 Two-orbital analysis on the material dependence of T_c in the single-layered cuprates, HIROFUMI SAKAKIBARA, HIDETOMO USUI, KAZUHIKO KUROKI, The University of Electro-Communication, RYOTARO ARITA, HIDEO AOKI, The University of Tokyo — The significant material dependence of T_c in the cuprates remains an important puzzle, even within the single-layer family. A recent paper[1] has demonstrated, with a two-orbital model, that, while the usual wisdom is to consider the cuprate as a one-band ($d_{x^2-y^2}$) system, a hybridization with the second (d_{z^2}) one around the Fermi energy significantly affects T_c in the spin-fluctuation mediated pairing. There, the energy offset (ΔE) between the two orbitals has been shown to govern the extent of the d_{z^2} mixture, hence T_c . Here we further extend this line of approach to identify the key factors that determine ΔE in the cuprates, focusing on the structural difference among broader (La, Hg, Bi, and Tl) single-layer cuprates. We have revealed that the apical oxygen height (h_O) above the CuO₂ plane and the separation (d) between the CuO₂ planes are the important parameters that determine ΔE , thereby causing the material dependence of T_c . This picture enables us to capture the T_c variation among the single-layered cuprates in a simple lattice-parameter space. [1]H. Sakakibara *et al.* Phys. Rev. Lett. **105**, 057003 (2010)

K1.00085 Specific heat of cuprate superconductors¹, P. SALAS, Posgrado en Ciencia e Ingeniería de Materiales, UNAM, M. FORTES, F.J. SEVILLA, M.A. SOLIS, Instituto de Física, UNAM — We model cuprate superconductors as a fluid of electrons able to create pairs within an infinite layered structure. The paired electrons (Cooper pairs) coexist with the unpaired electrons in almost two dimensional slabs stacked in their perpendicular direction. Electron pairs are considered as noninteracting zero spin bosons with a linear dispersion relation, and inter-slab penetrable planes are simulated by Kronig-Penney delta potential taken in one dimension, while paired and unpaired electrons are free to move in the other two dimensions. We introduce the slab thickness and the plane “impenetrability”, using real parameters of YBaCuO_{7-x} cuprates. Paired electrons develop a boson condensate with a jump in the specific heat at the superconductor critical temperature. After summing the electronic contributions, paired plus unpaired, we obtain a linear behavior of the electronic specific heat over temperature, C_e/T . By adding the lattice specific heat (phonons) C_l , we are able to qualitatively reproduce the total specific heat. We also obtain a theoretical value for the electronic specific heat constant γ_e , which is in agreement with the experimental values reported.

¹We thank support from grant PAPIIT IN105011, IN117010 and CONACYT 104917

K1.00086 How to measure the spatial characteristics of the Kosterlitz- Thouless transition in disordered systems?, AMIR EREZ, YIGAL MEIR, Ben Gurion University of the Negev — The effect of disorder on the Kosterlitz-Thouless (KT) transition in two dimensions is unresolved. Here we propose and simulate an experiment to probe the spatial nature of the KT transition in such disordered systems, by studying the effects of cutting individual bonds in the disordered classical two-dimensional XY model. This will allow, similar to experiments carried out on quasi one-dimensional and on quantum Hall systems, to probe the channels through which global phase coherence propagates. We analyze the spatial distribution of these bonds and discuss implications towards a percolation description of the KT transition in superconducting thin films.

K1.00087 ABSTRACT WITHDRAWN —

K1.00088 Determination of superconducting parameters of Gd-123 phase added with Co₂FeO₄ nano ferrite from Excess conductivity and magneto conductivity analysis, ALY ABOU-ALY, NAYERA MOHAMMED, RAMADAN AWAD, Alexandria University, HUSSEIN MOTAWEH, DOAA BAKEER, Damanhur University — Excess conductivity and magneto conductivity data of the Gd-123 added with Co₂FeO₄ nano ferrite were analyzed in terms of Aslamazov-Larkin and Maki-Thompson models for layered superconductors. Co₂FeO₄ nano ferrite was prepared by Co-perceptions method with grain size of about 20 nm. The concentrations of Co₂FeO₄ nano ferrite were varied from 0.0 to 0.1 % wt. of the total sample's weight. The superconducting parameters such as superconducting transition temperature, coherence lengths along *ab*-plane and along *c*-direction at 0K and phase breaking time at 100 K were determined as a function of Co₂FeO₄ nano ferrite concentrations. The superconducting transition temperature decreased from 91.7 K to 79.3 K as Co₂FeO₄ nano ferrite concentrations increased from 0.0 to 0.1 % wt. of the total sample's weight, confirming with the decrease of phase breaking time at 100 K from 2.7×10^{-14} sec to 1.93×10^{-14} sec. The superconducting anisotropy parameter was calculated as a function of Co₂FeO₄ nano ferrite concentrations and its value varied from 6.7 to 8.3.

K1.00089 Magnetothermoelectric effects in Fe_{1+d}Te_{1-x}Se_x¹, MARCIN MATUSIAK, Institute of Low Temperature and Structural Research, PAS, KAZIMIERZ CONDER, Laboratory for Developments and Methods, Paul Scherrer Institute — We report data on resistivity as well as Hall, Seebeck and Nernst coefficients for the Fe_{1+d}Te_{1-x}Se_x single crystals with $x = 0, 0.39$, and 0.40 . The parent compound Fe_{1.04}Te exhibits a Fermi surface reconstruction at $T = 61$ K, which is ascribed to the onset of the antiferromagnetic order. Two very closely doped samples: Fe_{1.01}Se_{0.39}Te_{0.61} (Se39) and Fe_{1.01}Se_{0.4}Te_{0.6} (Se40) are superconductors with $T_c = 13.4$ K and 13.9 K, respectively. Properties of these two single crystals are almost identical at high temperatures, but start to diverge below $T \approx 80$ K. Despite there is no magnetic transition in neither Se39 nor Se40, the observed differences seem to be a consequence of varying with selenium content spin correlations.

¹This work was supported by a grant No. N N202 130739 of the Polish Ministry of Science and Higher Education.

K1.00090 Magnetism in EuBCO and YBCO vortex states near and below T_c , R. SCHWARTZ, San Jose State University, M.C. BROWNE, SLAC National Accelerator Laboratory, C. BOEKEMA, San Jose State University — By means of MaxEnt- μ SR [1] analysis, we investigate transverse field μ SR data [2] of EuBa₂Cu₃O_{7- δ} EuBCO; $T_c = 93$ K). Our focus is on a temperature interval near T_c to search for precursor effects, [3] and for predicted [4a] pseudogap loop currents above and below T_c , already observed [4b] above T_c for GdBCO. Further, we continue to study the field-direction dependence of the predicted [5a] and observed [5b] antiferromagnetism (AF) below $0.5T_c$ for the vortex states in *c*-axis-oriented YBCO. This AF in and near the vortex cores is likely three-dimensional. In sum, magnetic roots of cuprate superconductivity are well plausible. Research is supported by LANL-DOE, REU-NSF and AFC.

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K1.00091 Confinement induced anisotropy of superconducting films onto porous anodized aluminum oxide, QIONG LUO, ZHILI XIAO, Northern Illinois University, Argonne National Lab, WAI-KWONG KWOK, Argonne National Lab — We investigate the matching effect observed in superconducting Nb films sputtered on anodized aluminum oxide substrates containing regular arrays at various external magnetic field orientations. We find that both the magnetoresistance and the transition temperature exhibits two strong anisotropic effects: Little-Parks oscillations whose period varies with field direction superimposed on a smooth background arising from one dimensional confinement by the finite lateral space between neighboring holes, revealing the anisotropy change due to the confinement effect of artificial holes.

K1.00092 Theoretical Study of Tunneling Conductance in Normal-Metal/Insulator/PrOs₄Sb₁₂ and Ferromagnet/Insulator/PrOs₄Sb₁₂ Junctions¹, SEYYED SAEED BOHLOUL, STEPHANIE CURNÖE, Memorial University of Newfoundland — We theoretically investigate the tunnel conductance in normal-metal/insulator/superconductor and ferromagnet/insulator/superconductor junctions for the unconventional superconductor PrOs₄Sb₁₂. Using several pair potentials provided by group theoretical considerations, the conductance is calculated for singlet as well as triplet pairing. The result shows that the direction of the electric tunneling current and the relative orientation of the superconductor (i.e. position of point nodes) are two main factors that determine the shape of conductance spectrum for a junction. In addition, comparison with experimental results provide useful information regarding the actual symmetry of the pair potential in the superconducting phase of PrOs₄Sb₁₂.

¹This work is supported by NSERC of Canada.

K1.00093 Scattering from incipient stripe order in the high-temperature superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ ¹, EDUARDO H. DA SILVA NETO, COLIN PARKER², PEGOR AYNAJIAN, AAKASH PUSHUP³, Princeton University, JIN-SHENG WEN, ZHIJUN XU, GENDA GU, Brookhaven National Laboratory (BNL), ALI YAZDANI, Princeton University — We use spectroscopic mapping with the scanning tunneling microscope to probe modulations of the electronic density of states in single crystals of the high temperature superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ as a function of temperature. We show that the Cu-O bond-oriented modulations, with periodicity near four lattice constants ($4a$), that form below the pseudogap temperature have a temperature-dependent energy dispersion displaying different behaviors in the superconducting and pseudogap states. We demonstrate that quasiparticle scattering off impurities does not capture the experimentally observed energy- and temperature-dependence of these modulations. Instead, a model of scattering of quasiparticles from short-range stripe order is necessary to reproduce the experimentally observed energy dispersion of the bond-oriented modulations and its temperature dependence across the superconducting critical temperature, T_c .

¹This work is funded by a DOE-BES grant. Infrastructure at the Princeton Nanoscale Microscopy Laboratory are also supported by grants from NSF-DMR, Keck Foundation, and NSF-MRSEC.

²Currently at The University of Chicago

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K1.00094 STM/STS Study of Li_xCoO_2 Single Crystals, KATSUYA IWAYA, TAKETOSHI MINATO, Tohoku University, KIYOTAKA MIYOSHI, JUN TAKEUCHI, Shimane University, YOUSOO KIM, RIKEN, TARO HITOSUGI, Tohoku University, TOHOKU UNIVERSITY COLLABORATION, RIKEN COLLABORATION, SHIMANE UNIVERSITY COLLABORATION — We have performed low temperature scanning tunneling microscopy/spectroscopy (STM/STS) measurements on Li_xCoO_2 ($x=0.66$) single crystal surfaces. A (1×1) hexagonal lattice was clearly observed and found to be moved by changing bias-voltage polarity, indicating that this could be associated with Li ions on the surface. Under the (1×1) hexagonal lattice, we imaged almost randomly distributed bright dots that were strongly dependent on bias-voltage, with insulating spectroscopic features. Different area on the surface showed a (2×2) hexagonal lattice that could be related to an ordering of Co^{3+} and Co^{4+} ions. These results suggest the electronic structure of Li_xCoO_2 surface is inhomogeneous possibly due to segregation of Li ions.

K1.00095 Scanning tunneling microscopy at 70 mK in the dichalcogenide superconductor TaSe_2 , JOSE GALVIS, HERMANN SUDEROW, SEBASTIAN VIEIRA, Laboratorio de Bajas Temperaturas, Departamento de Física de la Materia Condensada, Facultad de Ciencias, Universidad Autónoma de Madrid, Spain — We present scanning tunneling microscopy and spectroscopy measurements of the layered dichalcogenide 2H-TaSe_2 , performed in a dilution refrigerator cryostat equipped with a three axis superconducting magnet. In this compound superconductivity and charge density wave (CDW) ordering coexist below 200mK . We find CDW order corresponding to hexagonal ($2H$) symmetry, but we also find areas where CDW order corresponding to trigonal ($1T$) symmetry appears. We study the superconducting density of states as a function of position and magnetic field at 70mK and relate the results to the CDW patterns.

K1.00096 Long-Range Superharmonic Josephson Current, LUKA TRIFUNOVIC, University of Basel — We consider a long superconductor-ferromagnet-superconductor junction with one spin-active region. It is shown that an *odd* number of Cooper pairs cannot have a long-range propagation when there is *only one* spin-active region. When temperature is much lower than the Thouless energy, the coherent transport of two Cooper pairs becomes dominant process and the *superharmonic* current-phase relation is obtained ($I \propto \sin 2\phi$).

K1.00097 Ground Capacitance in Josephson Junction Arrays¹, ZLATKO MINEV, IOAN POP, NICHOLAS MASLUK, ARCHANA KAMAL, MICHEL DEVORET, Yale University, QLAB — Josephson junction arrays (JJAs) have gained popularity in modern experiments. They find employment as high impedance “superinductance” elements in fluxonium type qubits [Manucharyan et al. Science 326, 113 (2009)] or in the study of Bloch oscillation. However this high impedance behavior is limited at high frequencies by the junction array capacitance to ground. We investigate the dependence of JJAs impedance on frequency. The JJA behaves as a linear inductance for frequencies sufficiently below the array self resonance. The maximum number of junctions in the array is thus limited by the ground capacitance. We study the dependence of the ground capacitance of JJAs on their geometry, and extract general design principles which will reduce this parasitic coupling and maximize the number of junctions in the superinductance.

¹Work supported by IARPA, ARO, NSF

K1.00098 Bias current effect on inverse spin-switch behavior in Permalloy/Nb/Permalloy trilayers, DONG HO KIM, TAE-JONG HWANG, Yeungnam University — We investigated the effect of bias current on the inverse spin-switch (ISS) effect in Permalloy(Py)/Nb/Permalloy trilayers. Samples grown by using dc magnetron sputtering methods were patterned in the bar shape of $5\text{ }\mu\text{m}$ wide and $120\text{ }\mu\text{m}$ long, and their magnetoresistance (MR) in the superconducting transition region were measured in sweeping magnetic fields. The MR measured in the transition region of Nb at the antiparallel domain (AD) states of two outer Py layers showed a rapid increase compared to the MR at the parallel (P) states with increasing current density. At high enough bias current densities exceeding 10^5 A/cm^2 , we found a temperature window where the MR at the AD states returned to the normal state resistance whereas the MR at the P state remained superconducting. This ideal ISS effect is assumed to be originated in massive flux flow triggered by the onset of flux motion inside Nb layer due to the large Lorentz force exerting on flux lines where the magnetic flux were induced by the normal component of the stray field from the domain walls in the AD state of Py layers.

K1.00099 Thermal fluctuations and flux-tunable barrier in proximity Josephson junctions, JIAN WEI, Peking University, P.R. China, PAUL CADDEN-ZIMANSKY, Columbia University, VENKAT CHANDRASEKHAR, Northwestern University, PAULI VIRTANEN, University of Wurzburg — The effect of thermal fluctuations in Josephson junctions is usually analysed using the Ambegaokar-Halperin (AH) theory in the context of thermal activation. We report measurements of micron-scale normal metal loops contacted with thin superconducting electrodes, where the unconventional loop geometry enables tuning of the junction barrier with applied flux. We observe stronger “enhanced” fluctuations when the flux threading the normal metal loop is near an odd half-integer flux quantum, and for devices with thinner superconducting electrodes. These findings suggest that the activation barrier, which is the Josephson coupling energy of the proximity junction, is different from that for conventional macroscopic Josephson junctions. Simple one dimensional quasiclassical theory is used to predict the interference effect due to the loop structure, but the exact magnitude of the coupling energy cannot be computed without taking into account the details of the sample dimensions. In this sense, the physics of nanoscale proximity junctions can be related to the thermally activated phase slips (TAPS) model for thin superconducting wires, and indeed our data can be better fitted with TAPS model than AH theory.

K1.00100 Enhancement of shot noise due to the fluctuation of Coulomb interaction, DUO LI, LEI ZHANG, FUMING XU, JIAN WANG, Department of Physics, The University of Hong Kong, DEPARTMENT OF PHYSICS AND THE CENTER OF THEORETICAL AND COMPUTATIONAL PHYSICS TEAM — We have developed a theoretical formalism to investigate the contribution of fluctuation of Coulomb interaction to the shot noise based on Keldysh non-equilibrium Green's function method. We have applied our theory to study the behavior of dc shot noise of atomic junctions using the method of nonequilibrium Green's function combined with the density functional theory (NEGF-DFT). In particular, for atomic carbon wire consisting 4 carbon atoms in contact with two Al(100) electrodes, first principles calculation within NEGF-DFT formalism shows a negative differential resistance (NDR) region in I-V curve at finite bias due to the effective band bottom of the Al lead. We have calculated the shot noise spectrum using the conventional gauge invariant transport theory with Coulomb interaction considered explicitly on the Hartree level along with exchange and correlation effect. Although the Fano factor is enhanced from 0.6 to 0.8 in the NDR region, the expected super-Poissonian behavior in the NDR region is not observed. When the fluctuation of Coulomb interaction is included in the shot noise, our numerical results show that the Fano factor is greater than one in the NDR region indicating a super-Poissonian behavior.

K1.00101 Flux-charge duality and quantum phase fluctuations in one-dimensional superconductors¹, ANDREW KERMAN, MIT Lincoln Laboratory — It has long been thought that superconductivity breaks down in one dimension due to enhanced quantum phase fluctuations. However, the exact mechanism for this is still an active research area. One common feature of existing theories is the idea of “quantum phase-slip” (QPS): quantum tunneling of the superconducting order parameter between states where the relative phase between the wire ends differs by $\pm 2\pi$. Many experiments have been carried out to investigate QPS, and a wide range of phenomena have been observed, including resistive fluctuations well below T_C and an apparent quantum phase transition to an insulating state in the narrowest wires. Although these are all likely connected to QPS, a unified understanding has not yet been possible. I will describe a theory for QPS which is based on the idea that flux-charge duality, a classical symmetry of Maxwell's equations, relates the phase fluctuations associated with QPS to the well-known charge fluctuations associated with Josephson tunneling, at a microscopic level. The predictions of this theory compare favorably with a wide range of experimental observations, and may also provide a conceptual link to 2D phase fluctuation phenomena and insulating transitions in thin films.

¹This work is sponsored under Air Force Contract Number FA8721-05-C-0002. Opinions, interpretations, conclusions, and recommendations are those of the author and are not necessarily endorsed by the United States Government.

K1.00102 Intermediate state of strongly disordered superconductors, IVAN SADOVSKYY, LEV IOFFE, Rutgers University — We study theoretically the superconductor-insulator transition in disordered Josephson junction arrays. Our numerical simulations suggest the existence of the intermediate state between superconducting and insulating states across the SIT that appears in a relatively narrow range of Josephson couplings. In this state the long range order parameter is absent but the excitations have a significant decay rate. We discuss the relation this finding to the experimental data that show the existence of the “bad metal” state characterized by a large temperature-independent resistance (J. Paramanandam, M.T. Bell, L.B. Ioffe, and M.E. Gershenson).

K1.00103 Cooper pair islanding model of insulating nanohoneycomb films, S.M. HOLLEN, E. RUDISAILLE, J. SHAINLINE, Brown University, Department of Physics, J.M. XU, Brown University, Division of Engineering, J.M. VALLES, JR., Brown University, Department of Physics — Nanohoneycomb (NHC) amorphous Bi thin films, made by thermal evaporation onto substrates that contain a nanometer-scale array of holes and regular surface height variations, exhibit an insulating phase of localized Cooper pairs. Recently, we described how thickness variations induced by the substrate height variations can give rise to superconducting island formation.¹ Here, we will present an extension of this analysis to suggest how the island sizes evolve through the magnetic field-driven superconductor-insulator transition. Using this islanding picture, we will discuss the applicability of a granular array model to explain the appearance and behavior of the CPI phase in these films. Finally, we will discuss recent experimental tests of this proposal for thickness-undulation-driven Cooper pair localization.

¹Hollen et. al., Phys. Rev. B, 84(6), August 2011. This work is supported by the AAUW, the NSF through Grant No. DMR-0605797 and No. DMR-0907357, by the AFRL, and by the ONR.

K1.00104 INSULATORS AND DIELECTRICS —

K1.00105 Large ferroelectric polarization in the new double perovskite NaLaMnWO₆ induced by non-polar instabilities, TETSUYA FUKUSHIMA, Graduate School of Engineering Science, Osaka University, 1-3 Machikaneyama, Toyonaka, Osaka 560-8531, Japan, ALESSANDRO STROPPA, SILVIA PICOZZI, Consiglio Nazionale delle Ricerche-Institute for Superconducting and Innovative Materials and Devices (CNR-SPIN), 67100 L'Aquila, Italy, J. MANUEL PEREZ-MATO, Dept de Física de la Materia Condensada, Facultad de Ciencia y Tecnología, Universidad del País Vasco, Apartado 644, E-48080 Bilbao, Spain — Based on density functional theory and group theoretical analysis, we have studied NaLaMnWO₆ compound. At low temperature, the structure has monoclinic $P2_1$ symmetry, with layered ordering of the Na and La ions and rocksalt ordering of Mn and W ions. By comparing the low symmetry structure with a parent phase of $P4/nmm$ symmetry, two distortion modes are found dominant. They correspond to MnO₆ and WO₆ octahedron tilt modes, often found in many simple perovskites. While in the latter these common tilting instabilities yield non-polar phases, in NaLaMnWO₆ the additional presence of the Na-La cation ordering is sufficient to make these rigid unit modes a source of the ferroelectricity. Through a trilinear coupling with the two unstable tilting modes, a polar distortion is induced, although the system has no intrinsic polar instability. The calculated electric polarization is as large as $16 \mu\text{C}/\text{cm}^2$. Despite its secondary character, this polarization is coupled with the dominant tilting modes and its switching is bound to produce the switching of one of two tilts, enhancing in this way a possible interaction with the magnetic ordering.

K1.00106 InGaZnO₄ based thin film transistors with sputter-deposited PMMA/ BaSrTiO₃ stacked gate dielectrics on flexible substrate, DONG HUN KIM, Massachusetts Institute of Technology, IL-DOO KIM, Korea Advanced Institute of Science and Technology — This study reports the enhanced electrical properties of InGaZnO₄ TFTs with sputter-deposited PMMA/BST stacked gate dielectrics. A noticeable reduction in the leakage current density was achieved by coating a PMMA over-layer. With the introduction of sputter-deposited PMMA film with a high electrical breakdown strength and a smooth surface morphology, the leakage current characteristics were greatly enhanced. The calculated field effect mobility of the InGaZnO₄ TFTs with the PMMA (30 nm)/BST (270 nm) and PMMA (50 nm)/BST (250 nm) gate dielectrics were 10.2 cm²/V-s and 7.4 cm²/V-s, respectively. The noticeable increase of the field effect mobility is thought to have stemmed from an interface improvement that was caused by the addition of the smooth sputter-deposited PMMA layer. The threshold voltages of the InGaZnO₄ TFTs with the PMMA (30 nm)/BST (270 nm) and PMMA (50 nm)/BST (250 nm) gate dielectrics were reduced to 1.1 V and 1.6 V compared to that (1.8 V) of the TFTs with the pure BST gate dielectric. The InGaZnO₄ TFTs using only sputter-deposited PMMA (300 nm) gate insulators exhibited an on/off current ratio of 4.1×10^6 , field effect mobility of 36.1 cm²/V-s at 10 V of VDS, and a relative large threshold voltage of 3.1 V.

K1.00107 Transient absorption and nonlinear refractive index changes in thermally reduced nominally pure LiNbO₃ by sub-100-fs light pulses¹, HOLGER BADORRECK, VOLKER DIECKMANN, MIRCO IMLAU, Department of Physics, University of Osnabrueck, Osnabrueck, Germany — Due to its polaronic features nominally undoped lithium niobate—as grown and thermally reduced—is of great interest for ultrafast optical devices. With formation times in the sub-ps-range short-lived small polarons can be generated in thermally reduced lithium niobate by optical gating of bipolarons due to single photon absorption. Simultaneously, formation of small hole polarons by two-photon-absorption is observed. In this work nonlinear absorption and refractive index changes due to exposure to sub-100-fs light pulses of 488 nm are presented with thermally reduced crystals as an example. It is found that the two-photon absorption coefficient is not affected by the thermal reduction procedure, whereas the nonlinear refractive index change is considerably smaller in the reduced sample. We further present our results on the study of the transient absorption in the blue and NIR spectral range by means of fs-pump-probe technique. The influence of the thermal reduction procedure on lifetime and densities of electron and hole polarons is discussed.

¹Financial support by the DFG (IM 37/5, INST 190/137-1) is gratefully acknowledged.

K1.00108 In-situ Characterization of Laser-Induced Crystallization in Glass Using Raman Spectroscopy¹, BRIAN KNORR, PRADYUMNA GUPTA, ADAM STONE, HIMANSHU JAIN, VOLKMAR DIEROLF, Lehigh University — We report crystallization and other structural changes in glasses (such as LaBGeO₅) due to laser-induced localized heating. This heating process is a result of non-radiative decay after a photon absorption process. We explore linear absorption due to both band-to-band excitation or intentionally doped transition metal or rare earth ions using CW lasers as well as nonlinear absorption induced by high-intensity pulsed lasers. The ability to precisely position the laser on the μm length scale makes the crystallization interesting for photonic and optical applications such as waveguides and 3-D active functional devices. To better understand and control the crystallization process we are developing a combined CW laser-writing setup/confocal Raman microscope. This system will allow in-situ monitoring of the Raman emission during the crystallization. The data yielded will help elucidate the relationship between the phase, composition, and structure of the modified glass regions as a function of experimental variables, which include, but are not limited to, writing speed, irradiation time, heating rates, and defect concentration.

¹Supported by NSF-DMR 0906763

K1.00109 Magnetoelastic coupling in doped multiferroic YCrO₃, YOGESH SHARMA, Materials Science Programme, Indian Institute of Technology Kanpur, SOMDUTTA MUKHERJEE, RAJEEV GUPTA, Department of Physics, Indian Institute of Technology Kanpur, ASHISH GARG, Materials Science and Engineering, Indian Institute of Technology Kanpur — Recent years have witnessed a renewed interest in ABO₃ structured perovskites due to possibility of combining ferroelectric and ferromagnetic order parameters in a single phase. Here we show an experimental study on one such material namely YCrO₃ which shows a phase transition from paramagnetic to a canted antiferromagnetic state at $T_N \sim 142\text{K}$ and a ferroelectric transition at $T_C \sim 473\text{K}$. The material has an orthorhombic crystal structure (S.G.Pbnm). In the present work, we prepared polycrystalline samples of $\text{YCr}_{1-x}\text{X}_x\text{O}_3$ (X = V or Ni) by conventional solid-state-reaction method. X-ray diffraction shows the formation of single phase material. DC magnetic measurements exhibit a magnetic transition at $T_N \sim 140\text{K}$ and the presence of magnetic hysteresis below this temperature. Above T_N , the susceptibility follows the Curie-Weiss law with the corresponding effective magnetic moment μ_{eff} of $3.75\mu_B$ close to the theoretically expected value of $3.87\mu_B$. Further, we investigated the magneto-elastic coupling in the material using temperature dependent Raman scattering. We observe 16 phonon modes below T_C . Phonon modes at 145, 403 and 422cm^{-1} showed pronounced deviation from the expected anharmonic behavior below T_N , suggesting a spin-phonon coupling below T_N . Further, we also look at the effect of doping at the Cr site on the magnetoelastic coupling strength in this material.

K1.00110 Magnetodielectric consequences in double perovskite Pr₂CoMnO₆, J.H. ZHANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, S. MUKHERJEE, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan., H.C. WU, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, J.Y. LIN, Institutes of Physics, National Chiao Tung University, Hsinchu 30010, Taiwan, A.N. VASILIEV, Department of Low temperature Physics, Moscow State University, Moscow 119991, Russia, H.D. YANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan — We report an intriguing colossal dielectric and magnetodielectric (MD) response on double perovskite Pr₂CoMnO₆(PCMO) system. At the highest applied magnetic field 9T, the giant dielectric constant around $T_m \sim 175\text{K}$ is enhanced almost $\sim 22\%$ (at 10 kHz frequency) compare with that at zero field. The observed positive MD effect is considered to be associated with the direct consequence of negative magnetoresistance changes ($\sim -15\%$ at 175 K). Concomitantly, a pronounced ferromagnetic ordering is observed near $T_C \sim 175\text{K}$ coinciding with T_m of $\epsilon'(T)$. These experimental results suggest that the magnetoresistive MD response is very much conditioned by magnetic property of PCMO.

K1.00111 Enhanced ferromagnetism in co-doped BiFeO₃ ceramics, HARSH TRIVEDI, DEEPA SINGH, Materials Science Programme, Indian Institute of Technology Kanpur, RAJEEV GUPTA, Department of Physics, Indian Institute of Technology Kanpur, ASHISH GARG, Materials Science Engineering, Indian Institute of Technology Kanpur — BiFeO₃ (BFO) is the most studied multiferroic material with high ferroelectric polarization as well as above room temperature transition temperatures. Studies have shown significant improvements in the electrical and magnetic properties of BFO upon atomic substitutions at Bi (A) and Fe (B) sites. While enhanced ferromagnetism upon A-site doping is attributed to the suppression of cycloidal spin ordering of Fe moments, B site substitution reduces leakage current by eliminating oxygen vacancies. This study aims to combine these two aspects by co-doping the material at A- and B- sites using La³⁺ and V³⁺/V⁵⁺ respectively and to investigate the electrical and magnetic characteristics of co-doped BFO. La-doped La_xBi_{1-x}FeO₃ and co-doped La_xBi_{1-x}V_yFe_{1-y}O₃ (x = .05, 0.1, 0.15, 0.2; y = 0.03) samples were prepared solid-state reaction method. While La-doped samples show only reduced leakage without any discernible change in the magnetic characteristics, co-doped samples (La³⁺ & V⁵⁺) show significant enhancements in magnetic properties in addition to reduced leakage attributed to the elimination of oxygen vacancies. Improvement in the magnetic characteristics can be understood as a consequence of enhanced double exchange interaction between adjacent Fe ions. This argument is further strengthened by our observation that co-doped samples made by substitution of Fe with V³⁺ show a magnetic response equivalent to that of only La-doped BFO samples.

K1.00112 Dielectric properties and electrical conduction of high-k LaGdO₃ ceramics¹, SHOJAN PAVUNNY, REJI THOMAS, ASHOK KUMAR, RAM KATYAR, Department of Physics and Institute for Functional Nanomaterials, University of Puerto Rico, San Juan, PR, USA — The temperature and frequency dependent dielectric properties and leakage conduction mechanism in LaGdO₃ (LGO) ceramics have been studied and this material has been identified as a potential high-k candidate for the future complementary metal-oxide-semiconductor (CMOS) and dynamic random access memory (DRAM) technology nodes. The dielectric constant and the loss tangent at 100 kHz were ~ 21.5 and ~ 0.003 respectively at ambient conditions without any significant temperature and voltage dependence. The ac conductivity showed the typical features of universal dynamic response (UDR) and obey the double power law $\sigma_{ac} = \sigma_{dc} + A\omega^{n_1} + B\omega^{n_2}$ with three types of temperature dependent conduction processes involved; i) a dc plateau ($< 3\text{kHz}$) due to long range translational hopping, ii) a mid frequency region due to the short range hopping (3 – 100 kHz), and iii) a high frequency region due to localized or reorientational hopping (100 – 1000kHz). The temperature dependent dc conductivity followed the Arrhenius relation with activation energies of 0.05eV in the 200 – 400 K range and 0.92 eV in the 400 – 600 K range. The leakage current behavior revealed bulk limited Poole-Frenkel (PF) conduction mechanism with very low leakage current density (2 nA / cm² at 5.7 kV/cm).

¹Acknowledgement: NSF Grant NSF-RII-0701525 and NSF-IFN doctoral fellowship

K1.00113 Electronic, Magnetic and Thermal Properties of Electron Doped YMnO_3 ¹, TIAN YU, PENG GAO, TREVOR A. TYSON, New Jersey Institute of Technology — The thermal, magnetic and electronic properties of the electron doped $\text{Y}_{1-x}\text{Zr}_x\text{MnO}_3$ system were measured at both low and high temperatures. Correlations are made with structural studies on multiple length scales. Raman and IR measurements were performed at room temperature to track the changes in the phonons with doping. The effect of doping on the ferroelectric transition is examined. This work is supported by DOE Grant DE-FG02-07ER46402.

¹DOE Grant DE-FG02-07ER46402

K1.00114 Electrical properties of $\text{NaSr}_2\text{Nb}_5\text{O}_{15}$ ferroelectric ceramic, BANARJI BEHERA, School of Physics, Materials Research Laboratory, Sambalpur University, Jyoti Vihar, Burla - 768 019, Odisha, India, NIHAR PRADHAN, University of Massachusetts, Amherst and Mount Holyoke College, Massachusetts, USA, P. NAYAK, School of Physics, Materials Research Laboratory, Sambalpur University, Jyoti Vihar, Burla - 768 019, Odisha, India — Since the discovery of ferroelectricity, tungsten bronze (TB) ferroelectrics has been a rapid progress in search of new TB-type materials for applications such as capacitors, actuators, transducers, ferroelectric random access memory and display technologies. The materials with TB structure have potential advantages for devices because of their high dielectric constant and low tangent loss. In view of the above importance we have studied the electrical properties of $\text{NaSr}_2\text{Nb}_5\text{O}_{15}$ (NSN) ferroelectric ceramic. The polycrystalline $\text{NaSr}_2\text{Nb}_5\text{O}_{15}$ (NSN) was prepared by mixed oxide method at high temperature. Electrical properties of NSN have been studied using complex impedance spectroscopy (CIS) with wide range of frequency (10^2 - 10^6 Hz) and temperature. The complex impedance plot reveals the main contribution of bulk effect. The bulk resistance has been decreased with rise in temperature. The negative temperature coefficient of resistance (NTCR) manifests a semiconductor like behavior. The ac conductivity spectrum was found to obey Jonscher's universal power law.

K1.00115 Domain walls of ferroelectric BaTiO_3 within the Ginzburg-Landau-Devonshire model¹, P. MARTON, I. RYCHETSKY, J. HLINKA, Institute of Physics, Academy of Sciences of the Czech Republic — Mechanically compatible and electrically neutral domain walls in tetragonal, orthorhombic, and rhombohedral ferroelectric phases of BaTiO_3 are systematically investigated in the framework of the phenomenological Ginzburg-Landau-Devonshire (GLD) model. Domain wall thicknesses, energy densities are derived analytically and evaluated numerically for several temperatures. Apart from simple Ising-type solutions of the model we also discuss more complicated solutions (two-dimensional approximation in polarization - curved polarization path). The calculations indicate that the lowest energy structure of the 109-degree domain wall and few other domain walls in the orthorhombic and rhombohedral phases resemble Bloch-like walls known from magnetism.

¹The authors are grateful to prof. V. Janovec for helpful discussions. The work has been supported by the Czech Science Foundation (Projects Nos. P204/10/0616 and 202/09/0430)

K1.00116 Growth of CaIrO_3 and $\text{Gd}_2\text{Ir}_2\text{O}_7$ by MBE¹, YUEFENG NIE, RAINER HELD, SHOUVIK CHATTERJEE, ERIC MONKMAN, DANIEL SHAI, JOHN HARTEY, BULAT BURGANOVA, CAROLINA ADAMO, Laboratory of Atomic and Solid State Physics, Department of Physics, Cornell University, Ithaca, NY 14853, USA, DARRELL SCHLOM, Department of Materials Science and Engineering, Cornell University, Ithaca, New York 14853, USA, KYLE SHEN, Laboratory of Atomic and Solid State Physics, Department of Physics, Cornell University, Ithaca, NY 14853, USA — Recently, it was pointed out that the 5d transition metal iridium oxides (iridates) are promising candidates to realize topological insulators, which provide a unique platform in studying the interplay of Coulomb interactions, spin-orbit coupling, and the band topology of solids. We successfully grew epitaxial perovskite CaIrO_3 and pyrochlore $\text{Gd}_2\text{Ir}_2\text{O}_7$ films by reactive molecular-beam epitaxy (MBE). A range of biaxial strains for epitaxial CaIrO_3 films was achieved by growing on different substrates. Angle-resolved photoemission spectroscopy (ARPES) will be used to investigate the electronic structure of the epitaxial CaIrO_3 and $\text{Gd}_2\text{Ir}_2\text{O}_7$ films.

¹The work is supported by the Cornell Center for Materials Research through the National Science Foundation.

K1.00117 Epitaxial growth of polar magnetic PbVO_3 thin films on LaAlO_3 substrates, R.H. SHIN, S.H. OH, W. JO¹, Department of Physics, Ewha Womans University, Seoul, 120-750, Korea, Y.-S. SEO, J.S. AHN, Department of Physics, Pusan National University, Pusan 609-735, Korea — Layered perovskite PbVO_3 (PVO) is a curious polar magnetic material, which has a potential of room temperature multiferroics. A sintered PbVO_x ceramic target was prepared for pulsed-laser deposition. To obtain a stoichiometric single-phase PbVO_3 thin-film, it is known that control of oxygen partial pressure during the deposition is critical. With a base pressure of 10^{-6} Torr, the deposition pressure was maintained as low as 10^{-5} Torr, which is a severe reducing condition for most of oxide thin-films. We used $\text{LaAlO}_3(001)$ substrates, of which lattice constant is 0.379 nm. Substrate temperature was changed from 450 to 650°C. X-ray diffraction studies show that all the films show (001) oriented PbVO_3 growth but parasitic peaks are found near 39 and 42°, which are presumably linked with the chervetite $\text{Pb}_2\text{V}_2\text{O}_7$ phase. In addition, the c-axis lattice constant of the PbVO_3 cell is decreasing and the grain size becomes bigger as the growth temperature increases. Microscopic analysis and optical measurements have been performed to investigate their local structures. However, the plume in the low pressure would generate a disperse shape of ablated ions and molecules. We will discuss how to improve the structure of the films via a new set of process parameters and their electrical properties including polarization switching and charge conduction.

¹a corresponding author

K1.00118 Nanoscale Periodic Modulations on Sodium Chloride Induced by Surface Charges¹, KENDAL CLARK, SHENGYONG QIN, XIAO GUANG ZHANG, JOHN WENDELKEN, AN-PING LI, Oak Ridge National Laboratory — The sodium chloride surface is one of the most common platforms for the study of catalysts, thin film growth, and atmospheric aerosols. Here we report a nanoscale periodic modulation pattern on the surface of a cleaved NaCl single crystal, revealed by non-contact atomic force microscopy with a tuning fork sensor. The surface pattern shows two orthogonal domains, extending over the entire cleavage surface. The spatial modulations exhibit a characteristic period of 5.4 nm, commensurate with the atomic rows of the NaCl surface. The modulations are robust in vacuum, not affected by the tip-induced electric field or gentle annealing (<300 °C); however, they are eliminated after exposure to water and an atomically flat surface can be recovered by subsequent thermal annealing after water exposure. A strong electrostatic charging is revealed on the cleavage surface and the modulations appear to reflect a surface structural reconstruction facilitated by surface charges.

¹This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Office of Basic Energy Sciences, U.S. Department of Energy.

K1.00119 Theoretical study of defects in $c\text{-BC}_2\text{N}$, ONYEKWE LU OKEKE, Harvard University — Periodic supercells with 64 atoms using a zincblende stoichiometry for $c\text{-BC}_2\text{N}$ are generated for various native point defects and random distribution of boron and carbon atoms in B-C-N compound. The atomic structures of these systems were relaxed by first-principles density functional theory. The elastic properties including the bulk modulus, shear modulus, and Young's modulus of the bulk $c\text{-BC}_2\text{N}$ crystals and the defective systems were examined and compared

K1.00120 Charge trapping/de-trapping in nitrided SiO₂ dielectrics and its influence on device reliability, KENNETH KAMBOUR, SAIC, HAROLD HJALMARSON, Sandia National Laboratories, DUC NGUYEN, CAMRON KOUHESTANI, RODERICK DEVINE, AFRL/RVSE — Field effect devices with insulator gate dielectrics are excellent test vehicles to probe the physics of defects and charge trapping in the insulator/ semiconductor structure. p-channel field effect device reliability under negative bias stressing has been identified to originate from at least two terms: a) charged defect generation at the Si substrate/SiO_xNy interface and b) charge trapping at neutral defect pre-cursors in the “bulk” of the SiO_xNy beyond the interface. Measurements of transistor characteristics enable extraction of the two terms. We report the results of such measurements and demonstrate that short time effects are associated primarily with electric field assisted tunneling of holes from the inversion layer to neutral traps. This is confirmed by bias stressing measurements at different frequencies in the range 1 Hz to 2 MHz. First principles modeling of the tunneling/trapping phenomena is presented. K.Kambour worked under contract FA9453-08-C-0245 with the Air Force Research Laboratory/RVSE. Sandia National Labs is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

K1.00121 Structural, electronic, and magnetic properties of cation mixed (Ga,Mn)(As,N) and (In,Mn)(As,N) quaternaries and (Ga,Mn)N, and (In,Mn)N ternaries, AHMAD ALSAAD, ABDULLAH SHUKRI, Jordan University of Science and Technology, DR. I.A.QATTAN, KHALIFA UNIVERSITY OF SCIENCE, TECHNOLOGY AND RESEARCH TEAM — ABINIT simulation package with local density approximation, generalized gradient approximation, and spin local density approximation have been used to investigate the structural, electronic, and magnetic properties of cation mixed (Ga,Mn)(As,N) and (In,Mn)(As,N) quaternaries contain equal and fixed compositions of Ga,In, and Mn atoms. In particular, total energy minimization approach have been used to compute the equilibrium structural parameters of zinc-blende (GaAs, InAs, and MnAs), wurtzite (GaN, InN, and MnN) binary parent compounds, as well as, the corresponding equilibrium parameters of the two (Ga,Mn)(As,N) and (In,Mn)(As,N) quaternary systems. The band structures of zinc-blende GaAs, InAs and MnAs binary parent compounds have been computed and analyzed. Spin polarized band structures of the cation mixed (Ga,Mn)(As,N) and (In,Mn)(As,N) quaternaries contain equal compositions of Ga, In, and Mn cations have been computed and analyzed using spin local density approximation based calculations. Moreover, the magnetic properties of (Ga,Mn)(As,N) and (In,Mn)(As,N) quaternaries for equal concentration of Ga, In, and Mn cations have been investigated. Our simulations indicate that the two quaternary systems are nonmagnetic. This unusual result has been interpreted and explained. In addition, the magnetic properties of (Ga,Mn)N and (In,Mn)N diluted magnetic semiconductors will be presented.

K1.00122 First Principle Ab-initio Study of TiO₂¹, CHINEDU EKUMA, MARK JARRELL, JUANA MORENO, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA, DIOLA BAGAYOKO, Southern University and A&M College, Baton Rouge, LA 70803, USA — We report results from first principle computations of electronic properties of rutile TiO₂ within the local density functional approximation (LDA). Our first principle, non-relativistic and ground state calculations employed a local density functional approximation (LDA) potential and the linear combination of atomic orbitals (LCAO) – utilizing a self-consistently obtained, optimized basis set. We solved self-consistently both the Kohn-Sham equation and the equation giving the ground state charge density in terms of the wave functions of the occupied states. Our calculated band structure shows that there is significant O_{2p}-Ti_{3d} hybridization in the valence bands. These bands are well separated from the conduction bands by an indirect band gap of 2.95 eV, from Γ to R. Consequently, this work predicts that rutile TiO₂ is an indirect band gap material, as all other gaps from our calculations are larger than 2.95 eV. A slightly larger, direct band gap of 3.05 eV is found at the Γ point, in excellent agreement with experiment. Our structural optimization led to lattice parameters of 4.65 Å and 2.97 Å for a_o and c_o , respectively, with a u parameter of 0.3051, and a bulk modulus of 215 GPa.

¹This work was funded in part by the the National Science Foundation (Award Nos. 0754821, EPS-1003897, and NSF (2010-15)-RII-SUBR), the Department of the Navy, Office of Naval Research (ONR, Award No. N00014-04-1-0587), and Ebonyi State, Nigeria

K1.00123 Optically induced transient absorption related to formation of small polarons in Sn₂P₂S₆ in the sub-100-fs time domain¹, VOLKER DIECKMANN, HOLGER BADORRECK, MIRCO IMLAU, Department of Physics, University of Osnabrueck, Osnabrueck, Germany, ALEXANDR SHUMELYUK, Institute of Physics, National Academy of Science, Kyiv, Ukraine — The interaction of sub-100-fs light pulses with single crystals of nominally undoped Sn₂P₂S₆ is studied in the NIR spectral range (590 – 1630 nm). A predominant contribution of two-photon absorption (TPA) is verified. Scans over the photon energy show that the TPA coefficient increases in a superlinear way for photon energies exceeding $E_g/2$; for any photon energy it is nearly independent of propagation direction and polarization of the incident beam. The coefficient saturates at a maximum value of $\beta \approx 8 \text{ cm GW}^{-1}$ at $E_p \approx 1.8 \text{ eV}$. It drops when reaching the bandgap E_g . The TPA coefficients are higher by a factor of two than the values reported for other wide bandgap ferroelectrics, such as LiNbO₃, while being lower in comparison to semiconductor crystals. Using fs-pump-probe measurements at 626 nm, a transient absorption is observed that persists for probe pulse delays much longer than the pump pulse duration, up to 2.5 ns. Such transients are typical for a variety of wide bandgap ferroelectrics, where they are described by optically generated polaronic states. We discuss our results in the frame of the microscopic structure of Sn₂P₂S₆ with emphasis on the optical generation of S⁻ small hole polarons.

¹Financial support by the DFG (IM 37/9-1, INST 190/137-1) is gratefully acknowledged.

K1.00124 Mapping topological order in coordinate space, RAFFAELE RESTA, RAFFAELLO BIANCO, Phys. Dept., Univ. of Trieste — Topological insulators are distinguished from normal ones by the manner in which the electronic ground state is knotted in k-space. But topological order also reflects a peculiar organization of the electrons even when the concept of k-space does not make any sense, for e.g. inhomogeneous systems and finite systems within open boundary conditions. Here we only address Chern vs. normal insulators, within an independent-electron scheme in 2d. We introduce a “topological marker” in the form of a local Chern number, which may vary in different regions of the same sample. Since our marker samples the electron distribution locally, the boundary conditions (either periodic or open) are irrelevant. Actual simulations based on the model Haldane Hamiltonian, all of them adopting open boundary conditions, demonstrate the power of our approach. We provide perspicuous plots of our topological marker for crystalline and disordered samples, either normal or Chern insulators. We also monitor the Chern number switching in two cases: varying the Hamiltonian parameters in homogeneous samples, and addressing heterojunctions where two homogeneous regions (having different order) are joined. In all test cases our marker provides an unmistakable signature of the actual topological order.

K1.00125 ABSTRACT HAS BEEN MOVED TO T24.00016 —

K1.00126 Vacancy-induced bound states in topological insulators, WENYU SHAN, JIE LU, HAIZHOU LU, SHUNQING SHEN, Department of Physics, The University of Hong Kong, Pokfulam Road, Hong Kong — We present an exact solution of a modified Dirac equation for topological insulator in the presence of a hole or vacancy to demonstrate that vacancies may induce bound states in the band gap of topological insulators. They arise due to the Z_2 classification of time-reversal invariant insulators, thus are also topologically-protected like the edge states in the quantum spin Hall effect and the surface states in three-dimensional topological insulators. Coexistence of the in-gap bound states and the edge or surface states in topological insulators suggests that imperfections may affect transport properties of topological insulators via additional bound states near the system boundary.

K1.00127 Electron transmittivity and reflectivity through a barrier in 2D and 3D topological insulators¹, ANDRII IUROV, Hunter College and Graduate Center, City University of New York, GODFREY GUMBS, OLEKSIY ROSLYAK, Hunter College, City University of New York, DANHONG HUANG, USAF Research Lab (AFRL/RVSS) — We investigated theoretically the tunneling through a square potential barrier for both 2D and 3D topological insulators and their relationship to the well-known anomalous tunneling effect in graphene. Additionally, we analyzed the way in which both surface and bulk states are affected by the application of circularly-polarized light in comparison with electron dressed states in graphene where the electron-photon interaction led to the formation of an energy gap and chiral symmetry breaking of the electron eigenstates. We compare our results for topological insulators with recently obtained data for graphene. The difference arising from the presence of the bulk state energy spectrum will be analyzed and discussed in detail.

¹This research was supported by contract # FA 9453-11-01-0263 of AFRL. DH would like to thank the Air Force Office of Scientific Research (AFOSR) for its support.

K1.00128 Electronic structure of $\text{Ti}_2\text{Hg}_3\text{Te}_4$ and related systems - possible topological insulators, ANDREW BACZEWSKI, S.D. MAHANTI, Michigan State University, MERCOURI KANATZIDIS, Northwestern University — Topological insulators (TI) have attracted considerable interest in condensed matter physics in recent years. The origin of TI behavior in 3D systems is band inversion at time reversal invariant points throughout the Brillouin zone, induced by a strong spin-orbit interaction (SOI). Motivated by this physics, we have looked at the electronic structure of $\text{Ti}_2\text{Hg}_3\text{Te}_4$ and related systems focusing on the physics of band gap formation, parentage of near-gap states, and the influence of SOI. Calculations within the GGA give a band gap of 0.48 (0.33) eV in the absence (presence) of SOI, in reasonable agreement with a recent band structure calculation¹. However, there is no SOI-induced band inversion at the Γ point because the lowest conduction band (LCB), which is mainly Hg s, lies below a TI p band, suggesting that $\text{Ti}_2\text{Hg}_3\text{Te}_4$ is probably not a TI. Replacing Hg by other divalent atoms may make the TI p band the LCB, resulting in a system that may be a TI. To this end, we will discuss the electronic structures of several possible candidates. [1] S. Johnsen, et. al., Chem. Mater., 2011, 23 (19), pp 4375 to 4383

K1.00129 ABSTRACT WITHDRAWN —

K1.00130 ENERGY RESEARCH AND APPLICATIONS —

K1.00131 The Effect of Secondary Phase on Thermoelectric Properties of Zn_4Sb_3 Compound, GAOHUA ZHU, WEISHU LIU, Boston College, GANG CHEN, MIT, ZHIFENG REN, Boston College, BOSTON COLLEGE TEAM, MIT TEAM — Zn_4Sb_3 is a promising thermoelectric material because of its high thermoelectric performance and the abundance of Zn and Sb in nature. Samples of Zn_4Sb_3 with ZnSb or Zn as the minor phase were prepared to optimize the figure-of-merit (ZT). The effects of ZnSb or Zn secondary phase on the thermoelectric properties of Zn_4Sb_3 were investigated. The highest peak ZT of about 1.3 was achieved at 400 °C in the sample with single Zn_4Sb_3 phase, which has the lowest thermal conductivity. Transmission electron microscopy observations of the nanostructures suggest that the precipitated ZnSb, Zn-rich nanoparticles, and nano voids, caused by volatile Zn diffusion, all contribute to the extraordinarily low thermal conductivity.

K1.00132 Figure of Merit ZT achieved in Nanostructured Half Heusler alloys, DI WU, Department of Physics, University of Virginia, SONG ZHU, WENJIE XIE, Department of Physics and Astronomy, Clemson University, JOSEPH POON, Department of Physics, University of Virginia, TERRY TRITT, Department of Physics and Astronomy, Clemson University, PETER THOMAS, RAMA VENKATASUBRAMANIAN, Center for Solid State Energetics, RTI International, Research Triangle Park, NC — Half-Heusler (HH) phases have recently gained attention due to their high temperature thermoelectric performance, especially in the environment of growing concern over the dependence on the limited fossil fuels for energy production. These materials are investigated from the perspective of thermal and electronic transport properties for enhancing the dimensionless figure of merit (ZT) at 800-1000 K. Refinement on grain sizes and embedment of nanoparticles in HH alloy hosts were employed to produce fine-grained as well as nanocomposites and monolithic nanostructured materials. Present experiments indicated that HH alloys and their nanoparticles-embedded phases can attain $\text{ZT} \sim 1$, or slightly higher near 900-1000K. The observed ZT enhancements could be attributed to multiple origins. HH alloy hosts of nano-sized grains with/without embedment of different nanoparticles are also being investigated to further improve their thermoelectric performance.

K1.00133 Simulation of Photon, Exciton and Charge Transports in Organic Photovoltaics based on the Dynamic Monte Carlo Method coupled with the Maxwell Equation¹, BUYOUNG JUNG, School of Mechanical Engineering, Yonsei University, Korea, JUNGWON KIM COLLABORATION, KANGMIN KIM COLLABORATION, WOCHUL KIM COLLABORATION — Organic photovoltaics (OPVs) have received increasing attention as alternatives to inorganic solar cells. To understand the physics of OPVs, the dynamic Monte Carlo (DMC) method for simulating exciton and charge carrier movements has been regarded as a suitable method. However, simulation of light absorption has been ignored. We presented a simulation of the performance of OPVs by DMC method with solving the Maxwell equation for light absorption. We especially focused on the ordered bulk heterojunction (OBHJ) OPV which is composed of P3HT and PCBM. Our analysis indicated that locations of light absorption are different at different wavelength, which suggests that the simulation of light absorption is essential. In the wavelength of 300 to 400 nm, light absorption occurred dominantly nearby the interface between the P3HT and PCBM. This implies that the generated exciton can be more efficiently dissociated into the free charges. For wavelength longer than 400 nm, most of light are absorbed away from the interface between the P3HT and PCBM. As a result of this, the internal quantum efficiencies gradually decrease from 44.6% to 30.2% as the wavelength increases from 300 to 700 nm.

¹This work was supported by the Priority Research Centers Program through the Korea (NRF)(2010-0093823), by the Human Resources Development(20104010100500)

K1.00134 Fabrication of nanostructured CIGS solar cells¹, HONGWANG ZHANG, Department of Physics, University at Buffalo-SUNY, FANG WANG, Shanxi Normal University & University at Buffalo-SUNY, JAMES PARRY, SAMANTHE PERERA, HAO ZENG, Department of Physics, University at Buffalo-SUNY — We present the work on $\text{Cu}(\text{In,Ga})(\text{Se,S})_2$ based nanostructured solar cells based on nanowire arrays. CIGS as the light absorber for thin-film solar cells has been widely studied recently, due to its high absorption coefficient, long-term stability, and low-cost of fabrication. Recently, solution phase processed CIGS thin film solar cells attracted great attention due to their extremely low fabrication cost. However, the performance is lower than vacuum based thin films possibly due to higher density of defects and lower carrier mobility. On the other hand, one dimensional ordered nanostructures such as nanowires and nanorods can be used to make radial junction solar cells, where the orthogonality between light absorption and charge carrier separation can lead to enhanced PV performance. Since the charge carriers only need to traverse a short distance in the radial direction before they are separated at the heterojunction interface, the radial junction scheme can be more defect tolerant than their planar junction scheme. In this work, a wide band gap nanowire or nanotube array such as TiO_2 is used as a scaffold where CIGS is conformally coated using solution phase to obtain a radial heterojunction solar cell. Their performance is compared that of the planar thin film solar cells fabricated with the same materials.

¹Research supported by NSF DMR1104994 and NYSTAR.

K1.00135 Electronic properties and mechanism of superionic conductivity in Li_3N , MASARU AOKI, Shizuoka Sangyo University, KAZUO TSUMURAYA, Meiji University — Lithium nitride is a superionic conductor with high Li conductivity. The compound has been studied intensively because of its potential utility as electrolyte in solid-state batteries. Though it is known that the charge carriers responsible for conduction are Li vacancies in the Li_2N plane, the mechanism of the high mobility remains unsolved. To clarify the origin of the mobility we simulate the dynamics in the Li_3N crystal with the first principles molecular dynamics method. We have found the existence of the cooperative dynamics of Li ions in the Li_2N plane.

K1.00136 Light-induced degradation in gallium-doped silicon, JEANETTE LINDROOS¹, MARKO YLI-KOSKI, ANTTI HAARAHILTUNEN, Aalto University, Department of Micro and Nanosciences, MARTIN C. SCHUBERT², Fraunhofer Institute for Solar Energy Systems (ISE), HELE SAVIN, Aalto University, Department of Micro and Nanosciences — Light-induced degradation (LID) is a lifetime-decreasing effect in silicon solar cells attributed to the formation of B-O defect complexes during illumination [1-2]. However, Savin et al. [3] have recently observed degradation similar to LID in B- and P-doped Si contaminated with Cu, suggesting that Cu might be the cause of LID. Since Ga-doped Si is considered a degradation-free option to conventional B-doped Si [2], lifetime stability should also be studied in Cu-contaminated Ga-Si. Hence, in this paper, we intentionally contaminated high-oxygen 0.41 and 10.1 Ωcm Ga-doped Cz-Si with Cu and subjected the material to illumination. No lifetime degradation was measured with μ -PCD in clean Ga-Si or at low Cu levels, which is in agreement with the previously reported LID-free behavior of Ga-Si [2]. However, at higher Cu levels (20 ppb), a clear lifetime degradation was observed in Ga-Si. This lifetime degradation increased with increasing Cu concentration or with increasing wafer resistivity. [1] J. Schmidt, A.G. Aberle and R. Hezel, 26th IEEE PVSC, Anaheim, CA, USA, p.13-18 (1997). [2] S.W. Glunz, S. Rein, W. Warta, J. Knobloch and W. Wettling. Sol. Energ. Mat. Sol. C. 65, 219-229 (2001). [3] H. Savin, M. Yli-Koski and A. Haarahiltunen. Appl. Phys. Lett. 95, 152111 (2009).

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K1.00137 Simulation of thin nanowires for solar energy conversion: Operation as photoelectrodes and with discrete ohmic-selective contacts, MICHELLE PRICE, JUSTIN FOLEY, STEPHEN MALDONADO, University of Michigan — Nanostructured, high aspect ratio form factors can dramatically improve the performance of solar energy conversion devices made from low cost, earth-abundant materials that are otherwise limited by poor carrier transport properties. This poster presentation identifies and more precisely defines the limiting factors in the operation of thin nanowire photoelectrodes to facilitate their design and synthesis. Results from finite-element simulations used to model the key features of thin nanowire photoelectrodes under low-level injection conditions are shown that illustrate the respective effects of nonuniform doping, tapering along the length, variation in charge carrier mobilities and lifetimes, changes in nanowire radius, and changes in the density of surface defects on the photocurrent-potential responses. Also reported are results from simulations of nanostructures featuring near-intrinsic doping densities and discrete, ohmic-selective contacts operating under high-level injection conditions. The sensitivity of device operation to contact size, carrier mobility, surface recombination velocity, doping density and illumination intensity are reported. The presented work will address the hypothesis that the discrete, ohmic-selective contact photoelectrode design affords large solar energy conversion efficiencies with thin, lightly doped semiconductor nanowires.

K1.00138 Multiple Exciton Generation in Si Nanoparticles under pressure¹, STEFAN WIPPERMANN, Dep. of Chemistry, University of California (UC), Davis, MARTON VOROS, Dep. of Atomic Physics, Budapest University of Technology and Economics (T&E), DARIO ROCCA, Dep. of Chemistry, UC Davis, ADAM GALI, Dep. of Atomic Physics, Budapest University of T&E, GERGELY ZIMANYI, Dep. of Physics, UC Davis, GIULIA GALLI, Dep. of Chemistry, UC Davis — Multiple exciton generation (MEG) in semiconductor nanoparticles (NPs) is a promising path towards surpassing the Shockley-Queisser limit in solar energy conversion efficiency. Recent theoretical and experimental studies demonstrate MEG to be more efficient in semiconductor NPs than in the bulk material [1]. However, the increased efficiency is observed only on a relative energy scale in units of the gap, as the quantum confinement effects believed to be responsible for efficient MEG in NPs also lead to a significant increase of their gap with respect to the bulk. For successful device applications, it is necessary to identify NPs with enhanced MEG rates on an absolute energy scale. We propose that Si nanoparticles with a core structure resembling that of high pressure Si phases may be promising candidates to exhibit enhanced MEG rates on an absolute scale. In the bulk, upon compression the Si gap is reduced and a recent experimental study demonstrated successful fabrication of Si NPs in the BC8 phase. In the present study we investigate the electronic structure and MEG rates of Si NPs made from the beta-tin, R8, BC8 and hexagonal diamond Si phases from first principles.

[1] M. Beard, J. Phys. Chem. Lett. 2, 1282 (2011)

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K1.00139 Crosslinkable P3HT as Hole Transport Layer of Polymer Based Solar Cells, JUNG-KEUN KIM, Department of Polymer Science and Engineering, University of Massachusetts Amherst, MA 01002, JAE WOONG JUNG, Department of Materials Science and Engineering, Seoul National University, Seoul 151-742, Korea, WON HO JO, 2Department of Materials Science and Engineering, Seoul National University, Seoul 151-742, Korea, THOMAS P. RUSSELL, None — A photocrosslinkable bromine-functionalized poly(3-hexylthiophene) (P3HT-Br) copolymer was synthesized and used as the hole transport layer in polymer solar cells based on poly(3-hexylthiophene), and low band gap polymer, poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']dithiophene)-alt-4,7-(2,1,3-benzothiadiazole)] (PCPDTBT) with [6,6]-phenyl-C61-butyric acid methyl ester. Electrochemical stability of crosslinked P3HT-Br is superior to poly(3,4-ethylenedioxythiophene): poly(styrenesulfonate) (PEDOT:PSS), which has widely been used as the hole transport material in polymer solar cells.

K1.00140 First-principles calculations of covalently-bonded 3D networks of graphitic boron-nitride for hydrogen storage, SANGHOON LEE, Department of Physics, POSTECH, SEUNG-HOON JHI, Department of Physics and Division of Advanced Materials Science, POSTECH — Graphitic nanomaterials such as carbon nanotube (CNT) and covalently-bonded graphene (CBG) have attracted great attention due to their large surface area for high-capacity hydrogen storage. We carried out first-principles calculations based on density functional theory of covalently-bonded 3D networks of hexagonal boron nitride (hBN) layers and investigated the metal dispersion and subsequent hydrogen adsorption inside the networks. We performed a comparative analysis of stability, metal dispersion, and hydrogen sorption between graphene, CNT, hBN single layer, and 3D hBN networks.

K1.00141 Simultaneous description of strong and weak H_2 adsorption sites coexisting in MOFs, MOON-HYUN CHA, KYUNG-SUK KIM, School of Engineering, Brown University, JISOON IHM, Department of Physics and Astronomy, Seoul National University — In designing hydrogen-storage materials, it is a wide-spread practice to introduce transition-metal atoms into the MOF structures in order to increase the binding energy of H_2 . In such systems, it is necessary to understand and describe the H_2 binding behaviors at both strong and weak binding sites. Here, we propose a model that quantitatively characterizes the hydrogen gas adsorption in the presence of different kinds of adsorption sites. Based on equilibrium thermodynamics, this model enables us to figure out the number of H_2 molecules adsorbed to each adsorbing site and the corresponding heat of adsorption. When the present model is applied to real experimental data, different binding sites are identified and the contribution of each term to the storage capacity is obtained. While the virial equation gives the isosteric heat of adsorption averaged over the system, our model gives the heat of adsorption at each adsorbed site. Furthermore, by analyzing the results of fitting, we can estimate the volume occupied by adsorbed H_2 molecules.

K1.00142 Interaction of Cellulose Chains with Ionic Liquids and Water via MD simulations¹, AHMED ISMAIL, BROOKS RABIDEAU, RWTH Aachen University — One promising route for combustible fuel sources which are both renewable and have a low environmental impact is the conversion of waste biomass into tailor-made fuels. An important aspect of this process is the low-energy separation of cellulose from the biomass. Ionic liquids (ILs) have proven to be very good in dissolving cellulose with the added benefit of being essentially non-volatile making them ideal for “green” processing. IL research, however, remains relatively new, with many parts of this dissolution process remaining uncertain. We examine the behavior of cellulose with the ionic liquids [BMIM]Cl, [EMIM]Ac and [DMIM]DMP as well as water via MD simulation. All three ionic liquids have been observed to dissolve cellulose quite well yet have differently sized anions. We explore these differences and the impacts they have on their interactions with cellulose. First we examine the dynamics of a single cellulose strand in these ionic liquids. We determine the radius of gyration and the hydrogen bonds that are formed between the anions and cellulose. Next, we probe the dissolution mechanism of multiple, bound cellulose strands examining of multiple, bound cellulose strands examining interactions at the IL/cellulose interface and the breakup of inter-cellulose hydrogen bonds.

¹This work was performed as part of the Cluster of Excellence “Tailor-Made Fuels from Biomass,” which is funded by the Excellence Initiative by the German federal and state governments to promote science and research at German universities.

K1.00143 Synthesis and Electrochemical Performance of SiOC-Carbon Nanotube Composite Coatings, ROMIL BHANDAVAT, Kansas State University, MARCO COLOGNA, RISHI RAJ, GURPREET SINGH, University of Colorado at Boulder — Rechargeable battery anodes made from crystalline Si-based nanostructures have been shown to possess high experimental first cycle capacities (3000 mAh/g), but face challenges in sustaining these capacities beyond initial cycles mainly due to large volume expansion (400 percent) and chemical degradation (pulverization). Polymer-derived ceramic SiOC due to its high thermodynamic stability and nano domain structure could present a viable alternative. Additionally, functionalization of SiOC with carbon nanotubes could result in increased electronic and ionic conductivities in the ceramic. Here, we demonstrate synthesis and electrochemical characterization of SiOC-CNT composite coatings for use in Li-ion battery anode. Materials characterization performed using electron microscopy, Infrared (FT-IR), and X-ray photoelectron spectroscopy suggests non-covalent functionalization of CNT with oxygen moieties in SiOC. Sustained battery capacities of over 700 mAh/g and first cycle coulombic efficiencies of about 75 percent were achieved. Future work will involve determination of lithium ion intercalation sites characterized by electron microscopy whereas cyclic voltammetry analysis will access the sequential change in anode chemistry.

K1.00144 Polymer-derived Ceramic SiCN-MoS₂ Nanosheet Composite for Lithium Ion Battery Anodes¹, ROMIL BHANDAVAT, GURPREET SINGH, Kansas State University — We demonstrate synthesis of a novel SiCN-MoS₂ nanosheet composite for use as Li-ion battery anode for high power applications. The nanosheet composite was prepared by thermal decomposition of polysilazane (SiCN precursor) on exfoliated MoS₂ surfaces. The morphology and chemical structure was studied using a range of spectroscopy techniques that revealed a sidewall functionalization of exfoliated MoS₂ by the polymeric precursor. The thermodynamic stability of SiCN-MoS₂ nanosheets was also confirmed by thermo-gravimetric analysis (1000 degree C). Batteries assembled using MoS₂-SiCN nanosheets as active anode material showed that lithium can be reversibly intercalated in the voltage range of 0-2.5 V with first cycle discharge capacity of 620 mAh/g at a current density of 100 mA/g.

¹State of Kansas, National Science Foundation

K1.00145 First principles MD simulations of proton diffusion in cubic perovskite BaZrO₃, MARCO FRONZI, YOSHITAKA TATEYAMA, National Institute for Material Science, NICOLA MARZARI, École Polytechnique Fédérale de Lausanne, ENRICO TRAVERSA, National Institute for Material Science — The development of highly proton conductive and chemically stable ceramic materials, including doped barium zirconate, is particularly important for the fabrication of high performance solid oxide fuel cell (SOFCs) operating at intermediate-low temperature (550-900K). In this work, extensive first-principles molecular dynamics simulations have been employed to analyze proton self-diffusion in cubic perovskites BaZrO₃. Simulations have been performed at 1300K, that are typical fuel-cells' working conditions. The runs were carried out for the stoichiometric system in unit cells of 40 atoms, and in the canonical ensemble. We also studied the effect of applied compressive and tensile stresses on the proton motion finding a non linear effect on the proton mobility as a function of the strain. Enhanced diffusion has been found for an isotropic compression of 2% in the lattice parameter. On the other hand, the presence of a tensile strain does not seem to affect the proton diffusion, compared to the equilibrium case. The power spectrum obtained by the velocity-velocity correlation function for the proton shows no significant change in the vibrational frequencies for the strains studied.

K1.00146 Effect of Surfactants on the Physical Properties and Electrochemical Performance of LiFePO₄ Cathode Material for Lithium Ion Batteries, K. BAZZI, Wayne State University, M. NAZRI, Applied Sciences Inc., P. VAISHNAVA, Kettering University, V.M. NAIK, University of Michigan-Dearborn, G.A. NAZRI, R. NAIK, Wayne State University — The lithium iron phosphate chemistry is plagued by the poor electronic conductivity and slow lithium ion diffusion in the solid phase. In order to solve these problems, various research groups have adopted different strategies including decreasing the particle size, covering the particles with carbon, and adding dopants to the cathode material. Here, we report synthesis of C-LiFePO₄ cathode materials using 0.25M lauric, myristic, and oleic acid as surfactants. The phase purity of all three C-LiFePO₄ was confirmed by x-ray diffraction. SEM and TEM investigations reveal that the surfactants coat the LiFePO₄ particles uniformly with carbon and the coating reduces the particle size to 20-30 nm. Due to high electrical conductivity, controlled particle size and suitable microstructure, among the three LiFePO₄ coated samples, the sample with 0.25M lauric acid exhibited superior electrochemical performance in terms of specific capacity, the cycling stability and delivered high discharge capacity of 155, 150 and 123 mAhg⁻¹ at 0.5 C, 1C and 5C, respectively. The correlation between the ratio of the intensities of the D and G bands observed by micro-Raman spectroscopy, conductivity and electrochemical characteristics will be presented.

K1.00147 Block Copolymer Membranes for Biofuel Purification, ALI EVREN OZCAM, NITASH BALSARA, UC Berkeley, EBI TEAM — Purification of biofuels such as ethanol is a matter of considerable concern as they are produced in complex multicomponent fermentation broths. Our objective is to design pervaporation membranes for concentrating ethanol from dilute aqueous mixtures. Polystyrene-*b*-polydimethylsiloxane-*b*-polystyrene block copolymers were synthesized by anionic polymerization. The polydimethylsiloxane domains provide ethanol-transporting pathways, while the polystyrene domains provide structural integrity for the membrane. The morphology of the membranes is governed by the composition of the block copolymer while the size of the domains is governed by the molecular weight of the block copolymer. Pervaporation data as a function of these two parameters will be presented.

K1.00148 Toyota Prius Hybrid Plug-in Conversation and Battery Monitoring system, MICHAEL MCINTYRE, ROBERT KESSINGER, MAEGAN YOUNG, JOSEPH LATHAM, KRISHNANUNNI UNNIKANNAN, Department of Engineering, Western Kentucky University, Bowling Green, KY 42101 — The objective of the project was to analyze the performance of a Toyota Hybrid. We started off with a stock Toyota Prius and taking data by driving it in city and on the highway in a mixed pre-determined route. The batteries can be charged using standard 120V AC outlets. First phase of the project was to increase the performance of the car by installing 20 Lead (Pb) batteries in a plug-in kit. To improve the performance of the kit, a centralized battery monitoring system was installed. The battery monitoring system has two components, a custom data modules and a National Instruments CompactRIO. Each Pb battery has its own data module and all the data module are connected to the CompactRIO. The CompactRIO records differential voltage, current and temperature from all the 20 batteries. The LabVIEW software is dynamic and can be reconfigured to any number of batteries and real time data from the batteries can be monitored on a LabVIEW enabled machine.

K1.00149 Response of High Optical Heterogeneity in Three Dimensional Solar Cells , YUAN LI, Wake Forest University, XIANG WAN, University of Virginia, WENXIAO HUANG, WANYI NIE, Wake Forest University, HUIHUI HUANG, Wuhan University, DAVID CARROLL, Wake Forest University — The incident light throughout the cavity of three dimensional photovoltaic architecture is heterogeneous, and it may influence the cell's outputs, including the open circuit voltage, short current density, and fill factor and corresponding efficiency. In this work, an equivalent circuit for three dimensional solar cells was derived by an infinitesimal method, to model the response at different light distribution. Using this model, an upper bound was given to estimate the difference between two distributions, and this can show heterogeneous light has a similar effect on open circuit voltage (Voc) as well as that from homogeneous light while low heterogeneity. We further provided a method to predict the accurate Voc on very high optical heterogeneity, such that the optimum architecture can be found to design the three dimensional solar cells.

K1.00150 FLUIDS —

K1.00151 Soft, Hydrodynamically Coupled Particles in a Hele-Shaw Channel¹ , WILLIAM USPAL, Physics, Massachusetts Institute of Technology, PATRICK DOYLE, Chemical Engineering, Massachusetts Institute of Technology — Control of flowing suspensions is central to many emerging microfluidic applications. For instance, manipulation of small clusters is important in the synthesis of functional particles. Via theory and simulations, we study small clusters confined in a microchannel with thin cross section and subject to an external flow. We show that many-body hydrodynamic interactions sustain long-lived bound states with complex dynamics. As these interactions are sensitive to confinement, we investigate modulation of channel geometry as a means to perform sequential operations in a continuous process. We also probe the effects of shape and elasticity via a Lattice Boltzmann/Lattice Spring code, finding spontaneous excitation of elastic waves ("flapping"), and enriched behavior through the orientational effects of shape. Our results demonstrate phenomena that could be exploited for assembly of soft colloids in microchannels.

¹Supported by the Institute for Collaborative Biotechnologies through grant W911NF-09-0001 from the U.S. Army Research Office.

K1.00152 Nanoparticle transport and binding dynamics in blood flow , YALING LIU, JIFU TAN, ANTONY THOMAS, Lehigh University — Nanoparticle systems have been widely used in diagnostic imaging and targeted therapeutic applications in recent years. Most current studies on nanoparticle drug delivery considered a Newtonian fluid with suspending spherical nanoparticles. However, blood is a complex biological fluid composed of deformable cells, proteins, platelets, and plasma. For blood flow in capillary, arterioles and venules, the particulate nature of the blood need to be considered in the delivery process. Non-Newtonian effects such as the cell-free-layer and nanoparticle-cell interaction will largely influence both the dispersion and binding rates, thus impact targeted delivery efficacy. A 3D multiscale particle-cell hybrid model is developed to model nanoparticle transport, dispersion, and adhesion dynamics in blood suspension. The motion and deformation of red blood cell is captured through Immersed Finite Element method. The motions and bindings of individual nanoparticles of various shapes are tracked through Brownian adhesion dynamics and molecular ligand-receptor binding kinetics. Nanoparticle dispersion and binding coefficients are derived from the developed model under various rheology conditions. The influences of vascular flow rate, geometry, nanoparticle size on nanoparticle distribution and delivery efficacy are characterized. A non-uniform nanoparticle distribution profile with higher particle concentration near the vessel wall is observed. Such distribution leads to 50% higher particle binding rate compared to the case without RBC considered. The tumbling motion of RBCs in the core region of the capillary is found to enhance nanoparticle dispersion. The modeled binding results are validated through designed experiments in microfluidic devices.

K1.00153 Fabrication of Out-of-Plane Electrodes for ACEO Pumps¹ , YEHYA SENOUSY, CINDY HARNETT, University of Louisville — This abstract reports the fabrication process of a novel AC Electroosmosis (ACEO) pump with out of plane asymmetric interdigitated electrodes. A self-folding technique is used to fabricate the electrodes, that depends on the strain mismatch between the tensile stressed film (metal layer) and the compressive stress film (oxidized silicon layer). The electrodes roll up with a well-defined radius of curvature in the range of 100-200 microns. Two different electrical signals are connected to alternating electrodes using an insulating silicon nitride barrier that allows circuits to cross over each other without shorting. Electroosmotic micropumps are essential for low-cost, power-efficient microfluidic lab-on-chip devices used in diverse application such as analytical probes, drug delivery systems and surgical tools. ACEO pumps have been developed to address the drawbacks of the DCEO pumps such as the faradic reaction and gas bubbles. The original ACEO microfluidic pump was created with planar arrays of asymmetric interdigitated electrodes at the bottom of the channel. This rolled-up tube design improves on the planar design by including the channel walls and ceiling in the active pumping surface area of the device.

¹This project is supported from KY EPSCOR grant: "Engineering Platforms for Exploring Cellular and Molecular Processes."

K1.00154 Design and Simulation of Optically Actuated Bistable MEMS , THOMAS LUCAS, EVGENIYA MOISEEVA, CINDY HARNETT, University of Louisville — In this project, bistable three-dimensional MEMS actuators are designed to be optically switched between stable states for biological research applications. The structure is a strained rectangular frame created with stress-mismatched metal-oxide bilayers. The devices curl into an arc in one of two directions tangent to the substrate, and can switch orientation when regions are selectively heated. The heating is powered by infrared laser, and localized with patterned infrared-resonant gold nanoparticles on critical regions. The enhanced energy absorption on selected areas provides switching control and heightened response to narrow-band infrared light. Coventorware has been used for finite element analysis of the system. The numerical simulations indicate that it has two local minimum states with extremely rapid transition time ($\ll 0.1$ s) when the structure is thermally deformed. Actuation at laser power and thermal limits compatible with physiological applications will enable microfluidic pumping elements and fundamental studies of tissue response to three-dimensional mechanical stimuli, artificial-muscle based pumps and other biomedical devices triggered by tissue-permeant infrared light.

K1.00155 Reactant consumption analysis in microchannel based fuel cells , JOSEPH D'ALESSANDRO, PETRU FODOR, Cleveland State University, Department of Physics — In this work a miniaturized fuel cell design based on microchannels using liquid fuel and oxidizer streams is optimized for improved fuel usage. This particular design exploits the laminar nature of the fluid flow at small Reynolds numbers to keep the fuel and oxidizer confined in the vicinity of the corresponding electrodes without the need of a proton exchange membrane. Thus typical issues associated with the proton exchange membrane, such as reactant crossover, membrane dry-out and fouling are avoided. While the long term functional degradation effects associated with a physical membrane are eliminated, for an arbitrarily chosen geometry the slow thermal diffusion limits the efficiency of the cell due to the formation of depletion layers close to the electrodes. The performance of the cell is sensitive to geometry and rate of fluid flow with high aspect ratio cells operated at high Peclet number regimes being the most efficient.

K1.00156 High-throughput single-cell PCR using microfluidic emulsions¹ , MIRA GUO, LINAS MAZUTIS, JEREMY AGRESTI, MORTEN SOMMER, GAUTAM DANTAS, GEORGE CHURCH, PETER TURNBAUGH, DAVID WEITZ, Harvard University — The human gut and other environmental samples contain large populations of diverse bacteria that are poorly characterized and unculturable, yet have many functions relevant to human health. Our goal is to identify exactly which species carry some gene of interest, such as a carbohydrate metabolism gene. Conventional metagenomic assays sequence DNA extracted in bulk from populations of mixed cell types, and are therefore unable to associate a gene of interest with a species-identifying 16S gene, to determine that the two genes originated from the same cell. We solve this problem by microfluidically encapsulating single bacteria cells in drops, using PCR to amplify the two genes inside any drop whose encapsulated cell contains both genes, and sequencing the DNA from those drops that contain both amplification products.

¹Supported by NSF and Harvard MRSEC.

K1.00157 Competition in the condensation of immiscible vapors on a cold substrate¹, JOSÉ GUADARRAMA-CETINA, WENCESLAO GONZÁLEZ-VIÑAS, University of Navarra — We report experimental results on the breath figures which appear upon condensation of a mixture of vapors on a cold substrate (5° C). Both fluids have similar contact angles on the chosen substrate (72° vs 90°) and are immiscible. After getting the occupation diagram, we focus on the range of experimental conditions where we can see a relevant competition between the two species during the condensation. In the set of experiments, we measure the growth laws and compare them to the case of pure fluids. Also, we study the morphology of the patterns, by paying attention to the relative occupation factors and other related statistical quantities [1].

[1] J. Guadarrama-Cetina & W. González-Viñas, in preparation.

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K1.00158 Adsorption kinetics of surfactants at liquid-solid and liquid-vapor interfaces from atomic-scale simulations¹, EUGENIYA K. ISKRENOVA, Propulsion Directorate, Air Force Research Laboratory, Wright Patterson Air Force Base, OH 45433, USA and UES, Inc., Dayton, OH 45432, USA, SOUMYA S. PATNAIK, Propulsion Directorate, Air Force Research Laboratory, Wright Patterson Air Force Base, OH 45433, USA — Nucleate pool boiling of pure liquid is a complex process involving different size- and time-scale phenomena. The appearance of the first nanobubble in the liquid at the bottom of a hot pan, the detachment of the bubble from the solid surface, its subsequent coalescence with other bubbles, all represent complex multiscale phenomena. Surfactants added to water increase the complexity of the process by contributing to the dynamic surface tension at the liquid-vapor and liquid-solid interfaces and thus affecting the heat and mass transfer at those interfaces. We apply molecular dynamics simulations to study the adsorption kinetics of anionic, cationic, and non-ionic surfactants at liquid/solid and liquid/vapor interfaces. The all-atom vs. united-atom approaches for the solid and surfactants are surveyed in view of their applicability at near boiling temperatures and a range of model water potentials is assessed for reproducing the thermal properties of water at boiling conditions.

¹The authors gratefully acknowledge the Air Force Research Laboratory DoD Supercomputing Resource Center for computing time.

K1.00159 Experiment links the afterbounce instability and period doubled emission in single-bubble sonoluminescence, MOGENS LEVINSSEN, Niels Bohr Institute, University of Copenhagen — We report the first direct and long time stable observation for a single sonoluminescing bubble of the afterbounce instability that is believed to be one of the ways for a sonoluminescing bubble to lose stability and eventually break up. Furthermore we show that the instability is directly linked to the curious phenomenon of flash by flash period doubling of the sonoluminescent emission as the afterbounce instability is always period doubled whenever the emission is. This lends credit to a hot core picture coupled with refraction in the surface of the bubble. A theoretical understanding of this peculiar coupling is still missing.

K1.00160 Electrohydrodynamic simulation of an electrospray in a colloid thruster, MANISH JUGROOT, MARTIN FORGET, CECILE MALARDIER-JUGROOT, Royal Military College of Canada — A precise understanding of electrosprays is highly interesting as the complexity of micro-technology (such as nano-material processing, spacecraft propulsion and mass-spectrometers) systems increases. A multi-component CFD-based model coupling fluid dynamics, charged species dynamics and electric field is developed. The simulations describe the charged fluid interface with emphasis on the Taylor cone formation and cone-jet transition under the effect of a electric field. The goal is to recapture this transition from a rounded liquid interface into a Taylor cone from an initial uniform distribution, without making assumptions on the behaviour, geometry or charge distribution of the system. The time evolution of the interface highlights the close interaction among space charge, coulombic forces and the surface tension, which appear as governing and competing processes in the transition. The results from the coupled formalism provide valuable insights on the physical phenomena and will be applied to a colloid thruster for small spacecrafts.

K1.00161 Reaction Force of Micro-scale Liquid Droplets Constrained Between Parallel Plates through CFD, ROBERT FREE, HAIDER HEKIRI, TAKUMI HAWA, School of Aerospace and Mechanical Engineering, The University of Oklahoma — Micro-scale liquid droplets responding to depression between parallel plates are investigated analytically and numerically. The functional dependence of the reaction force accrued in such droplets on droplet size, surface tension, depression amount, and contact angle is explored. For both the 2D and 3D case, an analytical model is developed based on first principles. Computational fluid dynamics is then utilized to evaluate the validity of these models. The reaction force is highly nonlinear, initially increasing very slowly with increasing depression of the droplet, but eventually moving asymptotically to infinity. The force scales linearly with both the droplet free radius and surface tension of the liquid, but has a much more complicated dependence on the contact angle and depression. Explicit expressions for the reaction force have been determined, showing these dependencies. The 3D model has been largely supported by the CFD results. It very accurately predicts the reaction force on the upper plate as the droplet is crushed, accounting for the effect of contact angle, surface tension, and droplet size.

K1.00162 Dynamics control of micro-sized droplets for fluid-based electrothermal management¹, DUSTIN BAKER, TAKUMI HAWA, HAIDER HEKIRI, School of Aerospace and Mechanical Engineering, The University of Oklahoma — Heat transfer rate across a micro-scale liquid droplet constrained in two parallel plates at various contact angles are investigated numerically. Electrowetting is used to change how fluids wet solid surfaces, and two plates are at different temperatures. Computational fluid dynamics (FLUENT) is utilized to understand the heat transfer mechanism between two plates and to evaluate the combinations of design parameters needed to produce effective electrowetting thermal management systems. When the high-thermal conductivity fluid does not wet the plates, it functions as a high thermal resistance layer, allowing limited contact surface area for heat transfer through the high-thermal conductivity fluid between the plates. However, when wettability is altered so the high-thermal conductivity fluid wets the plates, the contact area is increased substantially, leading to heat transfer action between the plates. Understanding the dynamics of fluid rearrangement as long as the heat transfer phenomena associated with the fluid rearrangement is particularly important for this system.

¹BP

K1.00163 A comparative study of phase separation dynamics of sulfur hexafluoride under fine and coarse temperature quenching in microgravity¹, CATHLEEN WISE, ANA OPRISAN, SORINEL A. OPRISAN, College of Charleston, JOHN J. HEGSETH, University of New Orleans, CAROLE LECOUTRE, YVES GARRABOS, University of Bordeaux, DANIEL BEYSENS, University of Grenoble — Phase separation is determined by thermal quenches that break the symmetry of the homogeneous supercritical phase and leads to the formation of inhomogeneous structures with important implications for the mechanical, thermal, and electrical properties of materials. Sulfur hexafluoride (SF₆) heated about 1 K above its critical temperature then quenched below the critical temperature formed gas and liquid domains in microgravity conditions. Full view and microscopic view images were analyzed to determine the changes in the size distribution of droplets. For the first time, we provided experimental evidences regarding the existence of dimple and nose coalescence mechanisms in pure supercritical fluids under microgravity conditions. We recorded data for two different thermal quenches of 3.6 mK and 0.3mK, respectively. Our results indicate that, during the late stage of phase separation, the number of the liquid clusters decreases due to the coalescence events. We estimated the power law growth of the droplets/clusters and fitted it to a universal curve.

¹Acknowledged support from NASA-SCSGC and Research and Development grant from the College of Charleston to AO, NSF-CAREER award IOS 1054914 to SAO, and NASA grants NAG3-1906 and NAG3-2447 to JJH.

K1.00164 Microfluidic migration of soft particles in shear and Poiseuille flow, YENG-LONG CHEN, Institute of Physics, Academia Sinica, YA-YU HEW, University of Texas-Arlington — We investigate the migration of deformable particles in shear flow and Poiseuille flow due to the competition between shear forces, particle elasticity, particle diffusion, and particle inertia. At low particle Reynolds number ($Re < 1.0$), the soft particles migrate towards the channel center due to the coupling of particle elasticity and wall-induced hydrodynamic interactions. The competition between the shear forces and particle diffusivity, characterized by the Peclet number Pe , is found to affect whether the particles concentrate in the channel center of in an off-center position. As particle Reynolds number increases to moderate values ($Re \geq 1.0$), the particle concentration profile has two maxima at off-center positions. The migration effect is also found to be enhanced for softer particles with longer elastic relaxation time. The variation of particle concentration profiles leads to non-linear variations of the mixture viscosity and the average flow rate.

K1.00165 Surface Design for Efficient Capturing of Rare Cells in Microfluidic Device, YALING LIU, ANTONY THOMAS, Lehigh University, CHI-MON CHEN, SHU YANG, University of Pennsylvania — This work aims to design, fabricate, and characterize a micro-patterned surface that will be integrated into microfluidic devices to enhance particle and rare cell capture efficiency. Capture of ultralow concentration of circulating tumor cells in a blood sample is of vital importance for early diagnostics of cancer diseases. Despite the significant progress achieved in development of cell capture techniques, the enhancement in capture efficiency is still limited and often accompanied with drawbacks such as low throughput, low selectivity, pre-diluting requirement, and cell viability issues. The goal of this work is to design a biomimetic surface that could significantly enhance particle/cell capture efficacy through computational modeling, surface patterning, and microfluidic integration and testing. A PDMS surface with microscale ripples is functionalized with epithelial cell adhesion molecule (EPCAM) to capture prostate cancer PC3 cells. Our microfluid chip with micropatterns has shown significantly higher cell capture efficiency and selectivity compared to the chips with plane surface or classical herringbone-grooves.

K1.00166 A Look at Long Term Trends and Short Term Transition Zones (Fronts) in the Atmosphere using Fourier and Wavelet Analysis, JOSEPH TROUT, Richard Stockton College of New Jersey — An atmospheric front can be defined as sloping zones of pronounce transition of thermal and or wind fields in the atmosphere. This study uses Fourier analysis to look at the long term trends in atmospheric data and uses Wavelet Analysis to analyze the short term transition zones. These transition zones are characterized by a strong horizontal temperature gradient and/or large horizontal wind shear. They also may have large static stability and vertical wind shear. The signature of the front is evident as a large horizontal temperature gradient and moisture gradient. The compact nature of the wavelets make them perfect candidates for analyzing the short term transition zones in the thermal and wind fields that comprise the fronts. The frequency, intensity and shape of these transition zones are analyzed.

K1.00167 Sediment ripple profiles, ABIGAIL KOSS, JUSTIN KAO, TAYLOR PERRON, Massachusetts Institute of Technology — Sand ripples are a commonly observed phenomenon in shallow-water environments with oscillatory flow. Ripple morphology reflects patterns of sediment transport and turbulence across the bottom of the bed, providing easily measurable information about the mathematical form of sediment transport laws. A set of flume experiments has been conducted to record equilibrium ripple profiles produced by a wide range of wave orbital diameters and bed shear stresses. Results indicate that normalized ripple profiles are similar across the experimental range of wave conditions: i.e., that any ripple profile can be predicted from a standard ripple shape scaled by wave orbital diameter and bed shear stress. These experiments have also quantified ripple profile asymmetry and the nonlinear relationship between ripple wavelength and amplitude.

K1.00168 BIOLOGICAL PHYSICS —

K1.00169 Optical properties of large amyloid spherulites, MICHAEL SMITH, JAMES SHARP, University of Nottingham — Amyloid Spherulites, consisting of a central core surrounded by radially oriented birefringent fibres (known as amyloid fibrils), have been found to occur in certain pathologies, such as Alzheimer's disease. Typically ~5 30 m in diameter they can be observed by optical microscopy and easily distinguished by their characteristic maltese cross pattern, seen when viewed under crossed polarisers. Here we report the existence of much larger amyloid spherulites formed from bovine insulin, which grow under a particular set of conditions (10 mg/ml-1 BPI, pH ~2.8, T ~67°C, 25mM NaCl) to diameters of up to ~500 m. These huge spherulites when viewed under crossed polarisers in addition to the maltese cross feature beautiful coloured rings which change with the size and density of the spherulite. Such rings have been observed in other systems such as fish eye lenses and nematic liquid crystal drops and appear to be related to the rather unusual radially oriented birefringence of their internal structure. Using a ray tracing technique we model the optical path of rays through these spherulites. Taking into account refraction and the radially oriented birefringence of the amyloid fibrils, we elucidate the origin of these beautiful patterns.

K1.00170 FTIR and RRS Study of the Archaeorhodopsin-3 Optogenetic Neural Silencer and Transmembrane Voltage Sensor, ERICA SAINT CLAIR, JOHN OGREN, SERGEY MAMAEV, Boston University, Department of Physics, JOEL KRALL, Harvard University, Chemistry and Chemical Biology, KENNETH ROTHSCCHILD, Boston University, Department of Physics — Archaeorhodopsin-3 (AR3) is a light driven proton pump from *H. Sodomense* with a 74% sequence homology to the more extensively studied bacteriorhodopsin (BR) from *H. Salinarum*. Recent studies show that the wild type (WT) AR3 functions as a high-performance, genetically targetable optical silencer of neuronal activity and the mutant D95N functions as a transmembrane fluorescence voltage sensor. In order to understand the molecular similarities and differences between AR3 and BR, we compared light-activated structural changes using resonance Raman spectroscopy (RRS) and Fourier transform infrared (FTIR) difference spectroscopy. RRS pH titration and H/D exchange of WT AR3 showed that the retinylidene chromophore structure and Schiff base hydrogen bond strengths are almost identical to BR. RRS of the mutant D95N revealed a mixture of an N-like and O-like species at a pH greater than 7, unlike WT AR3. Low-temperature and rapid-scan time-resolved FTIR difference spectroscopy of WT AR3 revealed conformational changes during formation of the K, M and N intermediates similar but not identical to BR. Positive/negative bands in the region above 3600 cm⁻¹, which have been assigned to changes in weakly hydrogen bonded internal water molecules, differed substantially between AR3 and BR. These results indicate molecular differences between the AR3 and BR proton pumps which may underlie the ability of AR3 to function as a neurophotonic switch and sensor.

K1.00171 Polymorphic Ab protofilaments exhibit distinct conformational dynamics as calculated by normal mode analysis, MATTHEW ARMBRUSTER, PATRICIA SOTO, Creighton University — This project proposes to test the hypothesis that the physicochemical milieu modulates the conformational dynamics of synthetic Alzheimer's Ab protofilament structures, the main component of Alzheimer's senile plaques. To this end, 3D solid-state NMR structures of Ab protofilaments were used as initial structures for molecular dynamics simulations in explicit water and a water/hexane environment. The initial structures of the simulations and representative structures from the simulation-generated trajectories were taken to perform computational normal mode analysis. We developed a code in python with a graphical user-friendly interface. The program incorporated the ProDy (0.7.1) package. With the application, we examined cross-correlation plots of Ca positions of the 2-fold Ab protofilaments along the most collective mode and the slowest mode. The protofilament structures were highly correlated in the water environment. We hypothesized the protofilament would move as one in water because of the viscosity. The square fluctuation of Ca positions was calculated for the slowest mode for the hexane model and the MD generated ensemble. The two plots match up until midway through the structure. At the midway point a phase shift emerged between the two structures most likely where the surrounding changes. The in-house developed code made it easy to perform analysis and will be used by other students in the research group.

K1.00172 A simple system for the identification of fluorescent dyes capable of reporting differences in secondary structure and hydrophobicity among amyloidogenic protein oligomers, EMMA YATES, University of Cambridge — Thioflavin T and Congo Red are fluorescent dyes that are commonly used to identify the presence of amyloid structures, ordered protein aggregates. Despite the ubiquity of their use, little is known about their mechanism of interaction with amyloid fibrils, or whether other dyes, whose photophysics indicate that they may be more responsive to differences in macromolecular secondary structure and hydrophobicity, would be better suited to the identification of pathologically relevant oligomeric species in amyloid diseases. In order to systematically address this question, we have designed a strategy that discretely introduces differences in secondary structure and hydrophobicity amidst otherwise identical polyamino acids. This strategy will enable us to quantify and compare the affinities of Thioflavin T, Congo Red, and other, incompletely explored, fluorescent dyes for different secondary structural elements and hydrophobic motifs. With this information, we will identify dyes that give the most robust and quantitative information about structural differences among the complex population of oligomeric species present along an aggregation pathway between soluble monomers and amyloid fibrils, and correlate the resulting structural information with differential oligomeric toxicity.

K1.00173 A new multiplexing single molecule technique for measuring restriction enzyme activity, ALLISON HARBOTTLE, JILLIAN CAVANAUGH, Emmanuel College, Boston, MA, WENDY GORDON, JOSEPH LOPARO, Harvard Medical School, Boston, MA, ALLEN PRICE, Emmanuel College, Boston, MA — We present a new multiplexing single molecule method for observing the cleavage of DNAs by restriction enzymes. DNAs are attached to a surface at one end using a biotin-streptavidin link and to a micro bead at the other end via a digoxigenin-antidigoxigenin link. The DNAs are stretched by applying a flow. After introduction of the restriction enzyme, the exact time of cleavage of individual DNAs is recorded with video microscopy. We can image hundreds to thousands of DNAs in a single experiment. We are using our technique to search for the signature of facilitated diffusion in the measured rate dependence on ionic strength.

K1.00174 ABSTRACT WITHDRAWN —

K1.00175 Plasmon-Enhanced Single-Molecule Fluorescence for Sub-Diffraction-Limited Imaging, ESTHER WERTZ, JESSICA DONEHUE, JULIE BITEEN, University of Michigan — Super-resolution microscopy is a powerful tool for noninvasively imaging biological structures below the standard diffraction limit of light. One such technique, single-molecule fluorescence (SMF) imaging, achieves this resolution gain based on localizing isolated fluorophores. The accuracy of such localizations increases as the number of photons collected from each fluorophore increases. The ability to engineer the fluorescence quantum yield, radiative decay rate, and photostability of emitters will therefore greatly enhance the image resolution. In this work, we control SMF by coupling emission to plasmon resonances in metallic nanoparticles. These localized surface plasmons are confined charge density oscillations, and the local enhanced electromagnetic field they generate can be used to reduce the radiative lifetime and improve fluorophore brightness and photostability. We explore the effects of particle plasmons on the fluorescence properties of single dye molecules through wide-field single-molecule microscopy and fluorescence lifetime imaging microscopy experiments. All measurements are made both in the presence and absence of gold plasmonic structures. We observe up to ten-fold enhancements in photostability upon coupling to nanostructured gold, indicating that plasmon-enhanced imaging is a promising means to increase the resolution of single-molecule microscopy. We will extend our current experiments on dyes and quantum dots to fluorescent proteins.

K1.00176 Fluorescence Correlation Spectroscopy of Tryptophan-containing Proteins in Sugar Solutions using Two Photon Excitation¹, YULI WANG, NATHAN HOLMAN, DAVID SIDEBOTTOM, MICHAEL NICHOLS, ERIC HAAS, Creighton University — Sugars are common ingredients for many commercial cryopreserving agents yet their function in this role is poorly understood. Some believe that sugars preferentially bind with a protein surface thereby replacing hazardous, ice-forming water. In an attempt to test idea, we have undertaken studies of the diffusion of proteins and protein-coated nanospheres using fluorescence correlation spectroscopy in an effort to determine if the hydrodynamic size is influenced by the addition of sugars. Some novelty of our approach lies in exploiting the native fluorescence of tryptophan (a common fluorophore found in many proteins) by use of two-photon excitation.

¹This research supported by funding from NIH grant number 1R01EB009644-01

K1.00177 Laser Stimulated Genomic Exchange in Stem Cells. Laser Non-cloning Techniques¹, V.ALEXANDER STEFAN, Institute for Advanced Physics Studies, Stefan University — I propose a novel technique for a pluripotent stem cell generation. Genomic exchange is stimulated by the beat-wave free electron laser, (B-W FEL), frequency matching with the frequencies of the DNA² eigen-oscillations. B-W FEL-1³ scans entire stem cell; B-W FEL-2 probes the chromosomes. The scanning and probing lasers: 300-500nm and 100-300nm, respectively; irradiances: the order-of-10s mW/cm² (above the threshold value for a particular gene structure); repetition rate of few-100s Hz. A variety of genetic-matching conditions can be arranged. Genomic glitches, (the cell nucleus transfer⁴), can be hedged by the use of lasers.

¹Supported by the Tesla Labs, Stefan University

²J.D. Watson and F. H. C. Crick, *Nature*, 171, 737-738 (1953).

³V. Stefan, B.I.Cohen, C. Joshi *Science*, **243**,4890, (Jan 27,1989); Stefan, et al., Bull. APS. 32, No. 9, 1713 (1987); Stefan, APS March-2011, #S1.143; APS- March-2009, #K1.276.

⁴Scott Noggle et al. *Nature*, 478, 70-75 (06 October 2011).

K1.00178 A one-dimensional model of Nucleosome distribution in DNA, BRENDAN OSBERG, University of Munich, WOLFRAM MOEBIUS, University of Munich, Harvard University, KIEN NGUYEN, ULRICH GERLAND, University of Munich, UNIVERSITY OF MUNICH STATISTICAL PHYSICS GROUP TEAM — Nucleosome positioning along DNA is neither random nor precisely regular. Genome-wide maps of nucleosome positions in various eukaryotes have revealed a common pattern around transcription start sites, involving a nucleosome-free region flanked by a periodic pattern in the average nucleosome density. We take a quantitative mathematical description of the nucleosome pattern, and incorporate specifically bound transcription factors. Our model assumes a dense, one-dimensional gas of particles, however, instead of previous work which assumes fixed-size particles interacting only by exclusion, our model explicitly accounts for transient unwrapping of short segments of nucleosomal DNA. Hence, such particles no longer have a fixed size, but interact by an effective repulsive potential. This model has been successfully used, by us, to provide a unified description of 12 *Hemiascomycota* yeast species with a single unified set of model parameters. We incorporate into this model, specifically bound particles, or transcription factors (TF), which serve an important role in gene regulation. Nucleosome distribution patterns have an important influence on TF binding, and can even mediate interactions between transcription factors at a distance. This interaction can account for cooperative or competitive binding between these proteins, and we will discuss the implications this can have on gene regulation.

K1.00179 Unified physical model for statistical nucleosome positioning in different yeast species, WOLFRAM MÖBIUS, Department of Physics, Harvard University, Cambridge, MA, BRENDAN OSBERG, Arnold Sommerfeld Center for Theoretical Physics, LMU Munich, Munich, Germany, ALEXANDER M. TSANKOV, Broad Institute of MIT and Harvard and Department of Electrical Engineering and Computer Science, MIT, Cambridge, MA, OLIVER J. RANDO, Department of Biochemistry and Molecular Pharmacology, University of Massachusetts Medical School, Worcester, MA, ULRICH GERLAND, Arnold Sommerfeld Center for Theoretical Physics, LMU Munich, Munich, Germany — Recent genome-wide maps of nucleosome positions in different eukaryotes have revealed a common pattern around transcription start sites, involving a nucleosome-free region flanked by a pronounced periodic pattern in the average nucleosome density. For the yeast *S. cerevisiae*, a gas of hard rods, known as Tonks gas and equivalent to the statistical positioning mechanism of Kornberg and Stryer, can be used to describe the experimentally observed pattern. Here, we consider 12 *Hemiascomycota* yeast species, each of which displays a distinct nucleosome pattern. Since the mechanisms underlying the formation of the patterns are expected to be related, we undertake a data-driven search for a unified quantitative description. We find that the simple one-dimensional gas model needs to be extended to take into account transient unwrapping of short segments of nucleosomal DNA, such that the particles no longer have a fixed size. Chromatin behavior in all but one species is well described by this generalized gas model, with a single unified set of model parameters where only the average nucleosome density is a species-dependent variable.

K1.00180 Dynamics of Chromatin Silencing at Telomeres: Deterministic and Stochastic Aspects, MANJUL APRATIM, Dept. of Physics and Astronomy, Rutgers University, ADEL DAYARIAN, KITP, University of California, Santa Barbara, EDUARDO SONTAG, Dept. of Mathematics, Rutgers University, ANIRVAN SENGUPTA, BioMaPS Institute and Dept. of Physics and Astronomy, Rutgers University — Epigenetic silencing modifications are often associated with well-defined domains. We study potential mechanisms of formation of boundary of silenced regions. We specially focus on the possibility that some telomeric silencing boundaries are formed in a self-organized manner, as opposed to being defined by specific boundary elements. In particular, we examine systems where a titration-induced feedback can stabilize the boundary of the silenced region. A consequence of having multiple such boundaries is large stochastic cell-to-cell variation of boundary locations. We proceed to make an argument about the nature of the fall-off of the average silencing protein occupancy, coming from such variability, and test the predictions against HA-Sir3 ChIP-seq data from experiments performed on yeast.

K1.00181 Static Magnetic Field Induced Stochastic Resonance in Gene Expression, MEGAN BRADY, Binghamton University, PAUL FRISCH, Memorial Sloan-Kettering, KENNETH MCLEOD, CRAIG LARAMEE, Binghamton University — Biological systems are naturally complex, making singular responses difficult to detect. However, when the emergent behavior is investigated, the collective properties may be observed and characterized. These responses to external stimuli are often evident at the genomic level. When an optimal dose of external noise is used to perturb the system, it may work in synergy with the system's intrinsic noise to produce a change in stable state. This phenomenon, known as stochastic resonance (SR), is responsible for shifts in gene expression. This paper proposes that static magnetic fields (SMFs) elicit a SR genomic response in biological systems under environmentally relevant exposures. Using single reporter biomarkers as well as gene expression microarrays, the responses of three cell model systems (MCF-10A; Rat-1; Caco-2) to SMF exposure were examined. Results show that while responses for a single gene do occur, they are difficult to replicate and are near the detection cutoff limits. However, the system as a whole displays a shift in the pattern of gene expression. The replication of this pattern across different experimental platforms provides evidence that the cells are responding to the noise presented by the SMFs.

K1.00182 Membrane Fusion Mediated by pH-Low-Insertion-Peptide (pHLIP)¹, JENNIFER DANIELS, University of Rhode Island, LAN YAO, Binghamton University, DONALD ENGELMAN, Yale University, OLEG ANDREEV, YANA RESHETNYAK, University of Rhode Island — Liposomes are traditionally used as drug delivery carriers. The major mechanism of liposome entry into cell is endocytotic. First, the endocytotic pathway of cellular entry is non-specific: the delivery of therapeutics occurs to cells in both diseased and healthy tissues. Second, liposomes are usually trapped in endosome/lysosome, which prevents delivery of therapeutics to cytoplasm. We proposed to use pHLIP (pH-Low-Insertion-Peptide) to promote selective delivery of the liposome content to cytoplasm of cancer cells. We showed that liposomes coated with PEG polymer and pHLIP peptide enhance membrane fusion in acidic environments. pHLIP promotes fusion between lipid bilayer of liposome and plasma membrane or membrane of endosome/lysosome, which results in intracellular delivery of payload. Liposomes composed of 5 % pHLIP and 5 % PEG were ideal for the delivery. Since cancer and other pathological states produce an acid extracellular environment, this allows the liposome to target diseased tissue while avoiding healthy tissue (with neutral pH in extracellular space). The work is supported by NIH grants CA133890 to OAA, DME, YRK.

¹Supported by NIH grants CA133890 to OAA, DME, YRK.

K1.00183 Wide-field Time Resolved Microscopy for in-situ Lipid Phase Dynamics¹, NEDA DADASH-VAND, FELIX SCHUPP, CHRISTINA OTHON, Wesleyan University — We have developed a new time-resolved fluorescence platform which enables us to follow the molecular orientation and dynamics of a lipid monolayer at the air – water interface. Confocal microscopy is limited in its ability to characterize dynamic orientation changes within cellular membranes. By implementing an all reflective Cassegrain objective we minimize dispersion while eliminating the restriction of collinear excitation. We investigate the miscibility transition of a ternary lipid mixture, DPPC / DOPC / Cholesterol, using a combination of fluorescence imaging and spectroscopy. The technique affords unprecedented dynamic characterization for lipid orientation as the monolayer is forced from the liquid to the gel phase. We demonstrate the applicability of this device by contrasting the time-resolved fluorescence signal of three different lipid probes (NBD-PC), (BIODIPY), (DiI) which show different orientation and dynamic freedom when bound to the lipid layer for a range of lipid phases. Using this technique we can resolve highly dynamic processes such as the insertion of peptide and proteins into the lipid membrane.

¹Wesleyan grants in support of scholarship

K1.00184 Aggregation of Phosphoinositides at Physiological Calcium Concentrations¹, ADOLPHE KAZADI BADIAMBILE, Physic Department, Syracuse University,, MARTIN B. FORSTNER, Syracuse Biomaterials Institute, Syracuse University — Phosphoinositides play a crucial role in many cellular functions such as calcium signaling, endocytosis, exocytosis and the targeting of proteins to specific membrane sites. To maintain functional specificity, it has been suggested that phosphoinositides are spatially organized in “pools” in the cellular plasma membrane. A possible mechanism that could induce and regulate such organization of phosphoinositides is their interaction with Ca²⁺ ions. Understanding the physicochemical mechanism that can regulate membrane structure is a crucial step in the development of adaptive biomimetic membrane systems. Using Langmuir monolayers, we investigated the effect of bivalent calcium and magnesium cations on the surface pressure-area/lipid isotherm of monolayers of phosphatidylinositol (PI), phosphatidylinositol bisphosphate (PIP2) and dioleoylphosphatidylglycerol (DOPG) and dipalmitoylphosphatidylcholine (DPPC). It is found that the decrease of area per lipid, i.e. the increase in aggregation, is dependent on both the lipid's head group charge, the bivalent cation and temperature. However, electrostatics are not sufficient to account for all experimental observations. Thus additional interactions between ions and phosphoinositides need to be considered.

¹The National Science Foundation (NSF)

K1.00185 ABSTRACT WITHDRAWN —

K1.00186 How evolvable are polarization machines?, LIEDEWIJ LAAN, ANDREW MURRAY, FAS Center for Systems Biology, Harvard University — In many different cell types proper polarization is essential for cell function. Polarization mechanisms however, differ between cell types and even closely related species use a variety of polarization machines. Budding yeast, for example, depends on several parallel mechanisms to establish polarity. One mechanism (i) depends on reaction and diffusion of proteins in the membrane. Another one (ii) depends on reorganization of the actin cytoskeleton. So why does yeast use several mechanisms simultaneously? Can yeast also polarize robustly in the absence of one of them? We addressed these questions by evolving budding yeast in the absence of mechanism (i) or (ii). We deleted a mechanism by deleting one or two genes that are essential for its function. After the deletion of either mechanism the growth rate of cells was highly decreased (2-5 fold) and their cell shape was highly perturbed. Subsequently, we evolved these cells for 10 days. Surprisingly, the evolved cells rapidly overcame most of their polarity defects. They grow at 0.9x wildtype growth rate and their cell shape is significantly less perturbed. Now we will study how these cells rescued polarization. Did they fix the deleted mechanism, strengthen other mechanisms or evolve a completely new one?

K1.00187 Myosins V and VI increase actin filament flexural rigidity through a weak to strong binding transition, BRANNON MCCULLOUGH, WENXIANG CAO, ENRIQUE DE LA CRUZ, Yale University — Myosins are ATPase molecular motors that couple ATP hydrolysis with force generation along actin filaments. Myosin alters the torsional dynamics of actin filaments, which may contribute to aspects of force generation and nucleotide-dependent stability of the actin-myosin complex. We measured how biochemical ATPase-cycle intermediate states of high-duty myosins V and VI affect the flexural rigidity of actin filaments by analyzing the angular correlation of thermally driven shape fluctuations. Both myosins increase the flexural rigidity of actin filaments in a manner that depends on the chemical state of bound adenine nucleotide. High binding affinity states increase the flexural rigidity of actin filaments more than weak binding states. These results indicate that actin filaments may flex during myosin cycling to allow bound motors to coordinate stepping.

K1.00188 Time-temperature-transformation curves in chemical reactions regulated by cytoskeletal activity, BHASWATI BHATTACHARYA, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India, ABHISHEK CHAUDHURI, University of Oxford, UK, KRIPA GOWRISHANKAR, University of California, Davies, SATYAJIT MAYOR, National Centre for Biological Sciences-TIFR, Bangalore, India, MADAN RAO, Raman Research Institute/National Centre for Biological Sciences-TIFR, Bangalore, India — Efficient and reproducible construction of signaling and sorting complexes, both on the surface and within the living cell, is contingent on local regulation of biochemical reactions by the cellular milieu with active components. We have recently proposed that in many cases this spatiotemporal regulation can be mediated by interaction with components of the dynamic cytoskeleton, where the interplay between active contractility and remodeling of the cytoskeleton results in transient focusing of passive molecules to form clusters, leading to a dramatic increase in the reaction efficiency and output levels. In this presentation, we discuss the implications of actin dynamics by introducing an “effective temperature,” which can work as a regulatory parameter for signaling replacing the details of actin dynamics. We show this in time-temperature-transformation plots, with the proposed “effective temperature” as a parameter, which paves way for discussion of active chemical thermodynamics.

K1.00189 Elastic Coupling in Bipedally Crawling Cells¹, ALEX LOOSLEY, JAY TANG, Brown University — Periodic shape changes during cell migration are recorded in fast moving fish epithelial keratocytes where sticking and slipping at opposite sides of the cell's broad trailing edge generate bipedal locomotion and oscillatory lateral displacement of the nucleus. We use a two-dimensional finite element model to study the mechanical coupling, adhesion forces, and cell shapes that recapitulate the dynamics of these crawling cells. The model consists of elastically coupled point-like elements representing regions of the cell: leading edge, opposite sides of the trailing edge, and the nucleus. Based on simple assumptions, such as cell symmetry and localization of each element to a specific cellular region, we determine that there are only four viable permutations of elastic couplings between these four elements. We compare the four configurations and find that centralized elastic coupling to the cell nucleus and wide aspect ratio of the shape is necessary to mechanically generate realistic bipedal shape dynamics and lateral displacement of the nucleus. We suggest one configuration that is most realistic. The dynamics of this configuration are strongly dependent on the elasticity between peripheral elements, but not on the elasticity between these elements and the nucleus.

¹National Science Foundation CMMI 0825873, Natural Sciences and Engineering Research Council of Canada Post Graduate Scholarship D (AJL).

K1.00190 Delivery of imaging and therapeutic agents to tumor using pHILIP, DAYANJALI WIJESINGHE, ANNA MOSHNIKOVA, BETHANY ROSSI, Department of Physics, University of Rhode Island, DONALD ENGELMAN, Department of Molecular Biophysics and Biochemistry, Yale University, OLEG ANDREEV, YANA RESHETNYAK, Department of Physics, University of Rhode Island — We are developing a novel technology for selective delivery of imaging probes and membrane-impermeable molecules to cancer cells. It is based on action of water-soluble membrane peptide, pHILIP® (pH [Low] Insertion Peptide), which has ability to insert and fold in cellular membrane at slightly acidic environment, which is a characteristic for various pathological states including cancer. The insertion of the peptide is unidirectional: C-terminus moves inside the cell across membrane, while N-terminus flags outside. Thus pHILIP possess dual delivery capability. Imaging agents (fluorescent, PET, SPECT or MRI) could be attached to the N-terminus of the peptide to mark tumor mass and tumor margins with high precision. At the same time, therapeutic molecules attached to the C-inserting end, could be moved across membrane to reach cytoplasmic target. Among translocated molecules are synthetic cyclic peptides, gene regulation agent (peptide nucleic acid) and phallo- and amanita toxins with hydrophobicity tuned by attachment of fatty acids for optimum delivery. Currently we have family of pHILIP peptides for various applications. The work is supported by NIH grants CA133890 to OAA, DME, YRK.

K1.00191 The mechanics of cellular compartmentalization as a model for tumor spreading¹, ANATOL FRITSCH, STEVE PAWLIZAK, MAREIKE ZINK, JOSEF A. KAES, University of Leipzig, Division of Soft Matter Physics — Based on a recently developed surgical method of Michael Höckel, which makes use of cellular confinement to compartments in the human body, we study the mechanics of the process of cell segregation. Compartmentalization is a fundamental process of cellular organization and occurs during embryonic development. A simple model system can demonstrate the process of compartmentalization: When two populations of suspended cells are mixed, this mixture will eventually segregate into two phases, whereas mixtures of the same cell type will not. In the 1960s, Malcolm S. Steinberg formulated the so-called differential adhesion hypothesis which explains the segregation in the model system and the process of compartmentalization by differences in surface tension and adhesiveness of the interacting cells. We are interested in to which extent the same physical principles affect tumor growth and spreading between compartments. For our studies, we use healthy and cancerous breast cell lines of different malignancy as well as primary cells from human cervix carcinoma. We apply a set of techniques to study their mechanical properties and interactions. The Optical Stretcher is used for whole cell rheology, while Cell-cell-adhesion forces are directly measured with a modified AFM. In combination with 3D segregation experiments in droplet cultures we try to clarify the role of surface tension in tumor spreading.

¹Funding from ESF and Graduate School BuildMoNa

K1.00192 Contour instabilities and micro-structures in early tumor growth models, MARTINE BEN AMAR, Ecole Normale Supérieure, PASQUALE CIARLETTA, Université Pierre et Marie Curie, CLÉMENT CHATELAIN, THIBAUT BALOIS, Ecole Normale Supérieure — Clinical diagnosis of skin cancers is based on several morphological criteria, among which growth, color, border instabilities and microstructures (e.g. dots, nests) sparsely distributed within the tumor lesion. We use the multiphase mixture models adapted to the skin to explain various patterning occurring in the avascular phase. Restricting to a simple but realistic version of these models with an elastic cell-to-cell interaction and a growth rate dependent on diffusing nutrients, we prove analytically that the tumor cell concentration at the border acts as a control parameter inducing a bifurcation with loss of circular symmetry which explains the instabilities of the tumor border. The finite wavelength at threshold has the size of the proliferating peritumoral zone. We apply our predictions to melanoma growth since these instabilities are crucial for the early diagnosis. The same model is used to show the existence of micro-structures. Taking into account a reaction-diffusion coupling between nutrient consumption and cellular proliferation, we show that two-phase models may undergo a spinodal decomposition even when considering mass exchanges between the phases. The cell-nutrient interaction defines a typical diffusive length in the problem, which is found to control the saturation of a growing separated domain, thus stabilizing the microstructural pattern. The distribution and the evolution of such emerging cluster morphologies are successfully compared to the clinical observation of microstructural patterns in tumor lesions.

K1.00193 Smart-design of Tunable Nanomaterials for Enhancing Cancer Diagnosis and Radiation Therapy, TABBETHA DOBBINS, CRISTINA IFTODE, Rowan University — Gold nanoparticles (AuNPs) will be studied for both cancer diagnosis and treatment. At present, protocols are being established using benign fibroblast cell phenotype. The diagnosis hypothesis is that approaches may be developed to examine differences in intracellular matrices of healthy and tumor cells (or to examine cell metabolic activity) via understanding the absorption and agglomeration state of intracellular AuNPs. The treatment hypothesis is that the efficacy of irradiation with laser light (and monochromatic x-rays) at killing cells after attachment of AuNPs to the external cell wall has a fundamental mechanism which may not be accounted for solely by particle heating under irradiation. It remains unclear whether quantum effects also play a role. This work will ultimately explore phonon-phonon coupling or electron-phonon coupling at the surface of the AuNP and its contribution to the observed enhanced cell death upon irradiation. Early results will be presented.

K1.00194 Magnetic Hyperthermia in ferrofluid-gel composites¹, HUMESHKAR NEMALA, ANSHU WADEHRA, Wayne State University, MI, AMBESH DIXIT, IIT Rajasthan, India, RAJESH REGMI, Sloan-Kettering Cancer Center, NY, PREM VAISHNAVA, Kettering University, MI, GAVIN LAWES, RATNA NAIK, Wayne State University, MI — Magnetic hyperthermia is the generation of heat by an external magnetic field using superparamagnetic nanoparticles. However, there are still questions concerning magnetic hyperthermia in tissue; in particular the confinement of the nanoparticles at mesoscopic scales. We used Agarose and Alginate gels as models for human tissue and embedded magnetic nanoparticles in them. We report the synthesis and characterization of dextran coated iron oxide (Fe₃O₄) nanoparticles. Characterization of these nanoparticles was done using X-ray diffraction, transmission electron microscopy, magnetometry, and hyperthermia measurements. Temperature dependent susceptibility measurements reveal a sharp anomaly in the ferrofluid sample at the freezing temperature. This is conspicuously absent in the ferrofluid-gel composites. Heat generation studies on these superparamagnetic gel-composites revealed a larger heat production in the ferrofluids (~4W/g) as compared to the gels (~1W/g), which we attribute to a reduction in Brownian relaxation for the nanoparticles embedded in Agarose and Alginate.

¹Research was supported by the Richard J. Barber Fund for Interdisciplinary research.

K1.00195 Predicting tumor sizes of ductal carcinoma in situ from immunohistochemical images using a novel approach of mathematical pathology: preliminary results, potentials and challenges ahead¹, YAO-LI CHUANG, University of New Mexico, Dept. Pathology, MARY EDGERTON, University of Texas, MDACC, Dept. Pathology, PAUL MACKLIN, University of Southern California, Center for Applied Molecular Medicine, WEI YANG, University of Texas, MDACC, Dept. Radiology, ELAINE BEARER, University of New Mexico, Dept. Pathology, VITTORIO CRISTINI, University of New Mexico, Dept. Pathology and Dept. Chemical Engineering — Differential equation models have recently drawn increasing attentions as a useful tool to help advance the knowledge in cancer research. However, challenges remain for applying such models to clinical practices on a patient-specific basis to assist surgical decisions. Clinical diagnoses essentially at a single time point are often insufficient to fully constrain the time-dependent differential equations. Here we present a novel mathematical pathology approach, identifying robust indicators for time-invariant predictions of the model that can be used for surgical planning. We demonstrate this approach by predicting the sizes of ductal carcinoma in situ by calibrating model parameters from immunohistochemical images. Our preliminary studies of 17 excised tumor cases resulted in a better agreement with the actual measured sizes than the other estimates available to us, showing the potential of our approach for patient-specific cancer diagnosis. Conversely, our studies also revealed challenges to overcome before we can take this approach to the next level.

¹Supported by Cullen Trust for Health Care, NIH 2P30CA016672, NINDS NS046810

K1.00196 Preventing biosensor non-specific adsorption: Static to dynamic interfaces, LUCY HARWOOD, NEAL HOPKINS, Dstl — Biosensors are currently being developed for the detection of a wide range of analytes in a variety of scenarios. One such area is that of environmental monitoring for the presence of biological threats, from toxins through to viruses and bacteria. Environmental samples will contain a wide variety of contaminants, dependent on the location and prevalent environmental conditions. The sensing surfaces employed by biosensor instruments must be capable of resisting non-specific adsorption (NSA) of the contaminants whilst specifically capturing targets of interest. The ability to do so reduces the incidence of false positives and negatives increasing confidence in the system. We have assessed a range of biosensor surface chemistries of both two and three dimensional topography using a commercial BIAcore™ platform, for ability to prevent NSA of soluble materials of medical and military significance. This has highlighted that future solutions may benefit from dynamic interfaces as opposed to the conventional static interface often employed.

K1.00197 Vertical nanowire electrode array: a highly scalable platform for intracellular interfacing to neuronal circuits, MARSELA JORGOLLI, Department of Physics, Harvard University, JACOB ROBINSON¹, ALEX SHALEK, Department of Chemistry and Chemical Biology, Harvard University, MYUNG-HAN YOON, Gwangju Institute of Science and Technology, RONA GERTNER, Department of Chemistry and Chemical Biology, Harvard University, HONGKUN PARK, Department of Chemistry and Chemical Biology and Department of Physics, Harvard University — Interrogation of complex neuronal network requires new experimental tools that are sensitive enough to quantify the strengths of synaptic connections, yet scalable enough to couple to a large number of neurons simultaneously. Here, we will present a new, highly scalable intracellular electrode platform based on vertical nanowires that affords parallel interfacing to multiple mammalian neurons. Specifically, we show that our vertical nanowire electrode arrays can intracellularly record and stimulate neuronal activity in dissociated cultures of rat cortical neurons and be used to map multiple individual synaptic connections. This platform's scalability and full compatibility with silicon nanofabrication techniques provide a clear path toward simultaneous high-fidelity interfacing with hundreds of individual neurons, opening up exciting new avenues for neuronal circuit studies and prosthetics.

¹Equal Contributor

K1.00198 1/f Noises as a Superposition of First Order Autoregressive Model, TAKAYUKI FUJITA, AKIRA TSUKAMOTO, SHIGERU TADA, National Defense Academy — In various physical and physiological systems, power spectrum densities (PSD) of temporal sequences appear to be inversely proportion to the frequency. Those systems include the fluctuations of resistances in semiconductors, heart beats and membrane currents. Those inverse proportions of PSD to frequency are so called 1/f noises. One of the mechanisms with which 1/f noises are generated is superimposition of Ornstein-Uhlenbeck processes. Although this superimposition of Ornstein-Uhlenbeck processes, sequential temporal sequences, successfully generate 1/f noises, temporal sequences in physical and physiological systems are rarely measured sequentially. Instead, those temporal sequences are usually measured discretely. In this study, 1/f noises were attempted to generate with AR(1) processes, one example of discrete temporal sequences. As a result, PSD of superimposed AR(1) processes was inversely proportion to the frequency under some limitations. Those limitations include uniformly distribution of model parameter for AR(1) processes and white noise of driving noise. Thus, it was suggested that 1/f noises could be generated by superimposing discrete temporal sequences.

K1.00199 Population dynamics on heterogeneous bacterial substrates, WOLFRAM MOBIUS, Department of Physics and FAS Center for Systems Biology, Harvard University, Cambridge, MA, ANDREW W. MURRAY, FAS Center for Systems Biology and Department of Molecular and Cellular Biology, Harvard University, Cambridge, MA, DAVID R. NELSON, Department of Physics and FAS Center for Systems Biology, Harvard University, Cambridge, MA — How species invade new territories and how these range expansions influence the population's genotypes are important questions in the field of population genetics. The majority of work addressing these questions focuses on homogeneous environments. Much less is known about the population dynamics and population genetics when the environmental conditions are heterogeneous in space. To better understand range expansions in two-dimensional heterogeneous environments, we employ a system of bacteria and bacteriophage, the viruses of bacteria. Thereby, the bacteria constitute the environment in which a population of bacteriophages expands. The spread of phage constitutes itself in lysis of bacteria and thus formation of clear regions on bacterial lawns, called plaques. We study the population dynamics and genetics of the expanding phage for various patterns of environments.

K1.00200 Inter- and intracellular signaling induced by magnetomechanical actuation of plasma membrane channels, ELINA A. VITOL, Argonne National Laboratory, Materials Science Division and Center for Nanoscale Materials, ELENA A. ROZHKOVA, Argonne National Laboratory, Center for Nanoscale Materials, VALENTYN NOVOSAD, Argonne National Laboratory, Materials Science Division, SAMUEL D. BADER, Argonne National Laboratory, Materials Science Division and Center for Nanoscale Materials — Magnetic particles allow for non-invasive control over their spatial orientation and motion which makes them ideally suitable for studying real-time processes in living cells. Lithographically defined ferromagnetic disks with spin-vortex ground state have the advantage of zero net magnetization in remanence. This eliminates long-range magnetic forces which otherwise lead to the interaction between particles and their agglomeration. Moreover, magnetically soft permalloy particles have high magnetization of saturation thus requiring very low external field for inducing high magnetomotive force, compared to superparamagnetic particles. Our group has previously demonstrated that micron-sized permalloy disks can be used for destruction of cancer cells (D.-H. Kim, E. A. Rozhkova, I. V. Ulasov, S. D. Bader, T. Rajh, M. S. Lesniak, V. Novosad, Nat. Mater. 9, 165-171 (2010)). In this work, we investigate the effects of magnetomechanical stimulation of human brain cancer cells with these particles. It will be shown that the actuation of ion channels in cell plasma membrane induces, on the one hand side, intracellular signaling triggering cell apoptosis and, on the other hand, it stimulates the energy transfer between the cells which carries the information about apoptotic signal.

K1.00201 Bacterial sensing using phage-functionalized whispering gallery microcavities, HALA GHALI, Department of Engineering Physics, École Polytechnique de Montréal, HICHAM HIBLI, Biomedical Engineering Department, McGill University, PABLO BIANUCCI, Department of Engineering Physics, École Polytechnique de Montréal, JAY NADEAU, Biomedical Engineering Department, McGill University, YVES-ALAIN PETER, Department of Engineering Physics, École Polytechnique de Montréal — Whispering gallery optical microcavities are structures which can efficiently confine light at the micro scale. This confinement is based on total internal reflection of light at the interface between the cavity and the surrounding medium. Devices based on optical microcavities have a wide range of applications, such as microlasers, quantum optical devices and much more. In this work, we describe a biosensing application of these optical microcavities for the label-free detection of bacteria. In order for the sensor to be specific to a particular species of bacteria, we need to properly functionalize its surface so that only that kind of bacteria will produce a signal. The microcavity surface is first functionalized using PEGylated aminosilane. We then introduce phage-derived proteins that are specific to the bacteria we want to detect. The binding between the bacteria and the phage proteins creates a perturbation to the cavity field that leads to a thermo-optic effect. This effect is then observed as a shift in the resonance features of the transmission spectrum. We performed experimental measurements using a tapered fiber to couple the light from red laser (635 nm) into the resonator.

K1.00202 ABSTRACT WITHDRAWN —

K1.00203 Flow-controlled densification in E. Coli suspension¹, GASTÓN MIÑO, PMMH-ESPCI - University Pierre et Marie Curie, France, ERNESTO ALTSHULER, LENIN DEL RIO, CARLOS PEREZ-PENICHET, Dept of Physics, University de la Havana, Cuba, ANKE LINDNER, ANNIE ROUSSELET, ERIC CLEMENT, PMMH-ESPCI - University Pierre et Marie Curie, France — Bacterial suspensions are paradigmatic examples of “active matter.” Each bacterium can be regarded as a self-propelled particle that interact hydrodynamic ally with other bacteria or the suspension boundaries. As we know, in confined environments such as micron size channels or porous systems, solid boundaries act as traps for the bacterial motion and modify drastically the macroscopic transport properties of the suspension [1]. In this presentation, we show a new phenomenon concerning E. Coli suspensions flowing through a funnel-like constrictions between two micro-fluidic channels. The applied flow induces a counter-intuitive symmetry breaking in the bacteria concentration which increases strongly past the funnel. The enhancement persists over large distances. The density dissymmetry increases linearly with the flow rate and disappears at larger flow values. The effect is reversible with the flow. We explain these observations by emerging anomalous dispersion properties due to bacterial swimming trajectories and interactions between the bacteria and the channel boundaries. This experiment opens the possibility to control the bacterial concentration in microfluidic channels by simply tuning the flow of the suspending fluid. [1] Mino et al. Phys.Rev.Lett. 106, 048102(2011).

¹Supported by CNRS-UMR7636, PGDG foundation and SESAME-IdF

K1.00204 Small angle scattering study of the structure and organization of RNA and protein in Brome Mosaic Virus (BMV)¹, NARAYAN C. DAS, Center for the Exploration of Energy and Matter, GARFIELD T. WARREN, SI CHENG, Department of Physics, C. CHENG KAO, PENG NI, Department of Molecular and Cellular Biochemistry, BOGDAN DRAGNEA, Department of Chemistry, PAUL E. SOKOL, Center for the Exploration of Energy and Matter & Department of Physics, Indiana University — Brome mosaic virus (BMV) is a small icosahedral of the alpha virus-like superfamily of RNA with a segmented positive-strand RNA genome and a mean diameter $\sim 268\text{\AA}$ that offers high levels of RNA synthesis and virus production in plants. BMV also tightly regulates the packaging of its four RNAs (RNA1 through RNA4) into three separate particles; RNA1 and RNA2 are encapsidated separately while one copy each of RNA3 and RNA4 are normally packaged together. Small angle neutron scattering (SANS) and small angle X-ray scattering (SAXS) were applied to study the size, shape and protein-RNA organization of BMV. D₂O/H₂O mixture was used to enhance contrast in SANS measurement. The radial distribution of BMV from the Fourier transform of scattering spectrum gives a clear indication of RNA packing, and distribution and their structure in the BMV. The result reveals that the virus is about 266 Å in diameter and is composed of RNA inside the virion coated with a protein shell.

¹Construction of LENS was supported by the NSF grants DMR-0220560 and DMR-0320627, the 21st Century Science and Technology fund of Indiana, Indiana University, and the Department of Defense. Operation of LENS is supported by Indiana University.

K1.00205 Measuring the Rate of Conjugal Plasmid Transfer and Phage Infection in a Bacterial Population Using Quantitative PCR, ZHENMAO WAN, The Graduate Center, CUNY, NOEL GODDARD, Hunter College, CUNY — Horizontal gene transfer between species is an important mechanism for bacterial genome evolution. In *Escherichia coli*, conjugation is the transfer from a donor(F⁺) to a recipient(F⁻) cell through cell-to-cell contact. We demonstrate a novel qPCR method for quantifying the transfer kinetics of the F plasmid in a population by enumerating the relative abundance of genetic loci unique to the plasmid and the chromosome. This approach allows us to query the plasmid transfer rate without the need for selective culturing with unprecedented single locus resolution. It also allows us to investigate the inhibition of conjugation in the presence of filamentous bacteriophages M13. Experimental data is then compared with numerical simulation using a mass action, resource limited model.

K1.00206 Pressure-temperature dependence of growth bottlenecks and phenotypic transitions of *Escherichia coli*, PRADEEP KUMAR, ALBERT J. LIBCHABER, Center for studies in Physics and Biology, Rockefeller University, New York, NY — A vast majority of bacteria and archaea can grow in diverse environmental conditions. The range of those conditions include high pressures, high temperature, low temperature, high salinity, low and high pH etc. We investigate the growth bottlenecks and phenotypic transitions of *Escherichia coli* (*E. coli*), a mesophilic bacterium, as a function of pressure and temperature. We find that *E. coli* can grow and proliferate in a wide range of pressures (1-400 atm) and temperatures (23-40 deg C). Moreover, we find that the division time of *E. coli* increases monotonically upon increasing pressure and exhibits a sharp increase in division time at pressures between 250-400 atm for all the temperatures investigated in our experiments. The sharp change in division time is followed by a sharp change in phenotypic transition of *E. coli* at high pressures where bacterial cells switch to an elongating cell type. We propose that this phenotypic changes in bacteria at high pressures is an irreversible stochastic process whereas the switching probability to elongating cell type increases with increasing pressure. Furthermore, we propose an irreversible stochastic model of cell phenotype switching. We find that model fits well the experimental data. We discuss our experimental results in the light of structural and so the functional changes in proteins and structural changes in membranes at different pressure and temperature.

K1.00207 Quantifying *E. coli* chemotaxis at the population level, with high spatial and temporal resolution, LAURENCE WILSON, RONGJING ZHANG, The Rowland Institute at Harvard — The response of microorganisms to an external chemical stimulus is key to their survival in the wild, and so has obvious connotations for natural selection. Although much is now known about the biochemical signaling pathways that allow bacteria to respond to fluctuating levels of chemoattractant in their environment, the implications for the group behavior of cells are unknown. Previous microscopic studies have focused on single-cell behavior to build up a picture of how cells adapt to changing environmental conditions. Instead of taking this approach, we borrow ideas from light scattering, and apply them to video microscopy data in a manner similar to differential dynamic microscopy (DDM). This approach places emphasis on the local density of bacteria, allowing us to study the collective behavior of around 5000 cells simultaneously with excellent spatial and temporal resolution. We use this new method in conjunction with other techniques developed in the lab to provide a comprehensive and highly automated characterization of bacterial behavior in the presence of a chemical stimulus.

K1.00208 ABSTRACT WITHDRAWN —

K1.00209 Novel Dynamics Observed in a Spiking Neural Network Model of the NTS in the Rat Hind-brain, JINGYI ZHOU¹, J. DAVID SCHAFER², PATRICIA DILORENZO³, CRAIG LARAMEE⁴, Binghamton University — The Nucleus of the Solitary Tract (NTS) is a hind-brain structure in the rat that is the first way-station in taste processing. Its structure and function are poorly understood. Recently our group produced a model, implemented as a spiking neural network (SNN), that successfully replicated experimental data. The model's topology was manually devised and the parameters were set by a genetic algorithm. In order to better understand its information processing capabilities, we probed the model with a variety of input spike patterns and observed a striking winner-take-all decision-making dynamic. We show how the topology and tuned parameters enable this decision to depend on precise spike timing events. It is curious that the experimental data upon which the model was originally evolved did not include winner-take-all examples; this was an emergent capability. It remains for additional experiments on rats to confirm or reject this model prediction.

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K1.00210 Criticality in Neuronal Networks, NIR FRIEDMAN, Department of Physics, University of Illinois at Urbana-Champaign, SHINYA ITO, Department of Physics, Indiana University, BRADEN A. W. BRINKMAN, Department of Physics, University of Illinois at Urbana-Champaign, MASANORI SHIMONO, Department of Physics, Indiana University, R.E. LEE DEVILLE, Department of Physics, University of Illinois at Urbana-Champaign, JOHN M. BEGGS, Department of Physics, Indiana University, KARIN A. DAHMEN, Department of Physics, University of Illinois at Urbana-Champaign, TOM C. BUTLER, Department of Physics, Massachusetts Institute of Technology — In recent years, experiments detecting the electrical firing patterns in slices of in vitro brain tissue have been analyzed to suggest the presence of scale invariance and possibly criticality in the brain. Much of the work done however has been limited in two ways: 1) the data collected is from local field potentials that do not represent the firing of individual neurons; 2) the analysis has been primarily limited to histograms. In our work we examine data based on the firing of individual neurons (spike data), and greatly extend the analysis by considering shape collapse and exponents. Our results strongly suggest that the brain operates near a tuned critical point of a highly distinctive universality class.

K1.00211 Multidimensional representations of the phase response curve for both type 1 and type 2 membrane excitability¹ , ROBERT RAIDT, ANDREW J. SMITH, SORINEL A. OPRISAN, Department of Physics and Astronomy, College of Charleston — Neurons are complex excitable cells with a highly nonlinear response to external perturbations, such as presynaptic inputs and biological noise. Single-cell activity is determined by the properties of ionic channels and the ionic makeup of cell's environment and is mathematically described by coupled and nonlinear evolution equations. The phase resetting curve (PRC) reduces the complexity of the biophysical mechanisms involved in generating action potentials to tabulating advances or delays of subsequent spikes of a neuron due to an external perturbation. The PRC is widely used to predict the activity of large neural networks that by replacing the computationally intensive integration of evolution equations with lookup tables. The fundamental assumption of the PRC approach in predicting phase-locked modes in coupled neural networks is that the transient PRC measured for isolated and bursting neurons (open-loop) remains the same under the recurrent inputs of a phase-locked mode (close-loop). The novelties of our approach are: 1) the use of discrete sine transforms (DST's) to store the PRC's as a series of coefficients, and 2) the use of multidimensional stacks to represent multidimensional objects.

¹RR and AJS acknowledge HHMI summer fellowships through a College of Charleston grant. SAO acknowledges the NSF-CAREER award IOS 1054914 support.

K1.00212 Hamiltonian Dynamics of a Forced Two-Degree-of-Freedom Arm with Viscoelastic Muscles Executing Planned Motions¹ , SAYAN PATRA, GREG OJAKANGAS, ANDREW CHASE, ANISH CHAKRABARTI, DALTON SIVILS, EVAN JOHNSON, KIEFER BARRETT, MASON NORTH, PRESTON JULIAN, None — In order to improve our understanding of how the brain controls the human arm both in the presence and absence of gravity, we have developed a two-degree-of-freedom robotic arm which is driven by six servo-actuated viscoelastic muscles. The computer-controlled servos mimic the contractive action of the sarcomeres in actual muscles, sections of elastic tubing represent the elastic behavior of actual muscles, while the behavior of tendons is represented by inelastic strings. The servos receive instructions to move from the visual C++ platform in the computer and the actual motion of the arm is recorded with optical encoders built into each joint axis. This experiment is a purely feed-forward system, and our goal is to determine whether our equations of motion, formulated using Hamiltonian dynamics, when numerically integrated, will predict the observed motion of the arm within experimental uncertainties. Our research was selected as one of 12 teams chosen nationwide as part of NASA Grant Us Space Reduced Gravity Program, to fly and perform experiments aboard NASA's Weightless Wonder aircraft in Summer 2011.

¹This research wouldn't have been possible without funding and support from Drury University Physics Department and Dr. Greg Ojakangas

K1.00213 Modeling the Force Frequency Relation of a Cardiac Cell , DUYN MANH LE, Department of Physics and Graduate Institute of Biophysics, National Central University, Jhongli City 320, Taiwan, ALEXEY V. DVORNIKOV, Nizhny Novgorod State University, Russia, PIK-YIN LAI, Department of Physics and Graduate Institute of Biophysics, National Central University, Jhongli City 320, Taiwan, CHI-KEUNG CHAN, Institute of Physics, Academia Sinica, Nankang, Taipei 115, Taiwan — Recent pacing experiments with hearts of rat have discovered that the contractile response of the hearts can have an unexpected slow non-monotonic response. This later observation cannot be explained by the existing excitation-contraction coupling model. A new discrete map model of the EC coupling is developed to understand these experimental findings. It is found that the biphasic response and the slow time scale can be reproduced when a calcium feedback based on calcium regulation mechanism of the cell is introduced. Furthermore, this model can also reproduce the nonlinear dynamical properties of the system; such as the period doubling in the response of the contractile forces during a step change in the pacing period. The force frequency relation curve generated by the model also compare well with previous published data. Our findings suggest that the feedback is really needed to understand the calcium transient when pacing frequency is changed and the calcium regulation is very important for the calcium handling of cardiac myocytes.

K1.00214 Simulating Growth Dynamics of Neurons on Substrates , SAWYER BERNATH, CRISTIAN STAIL, TIMOTHY ATHERTON, Tufts University — We present computer simulations of neuron growth in which growth cones both create and are guided by growth promoter molecules which move diffusively. Our model predicts several features of the trajectories that are experimentally measurable, including arclength and curvature as functions of time. By comparing these predictions to time-lapse microscopy experiments of axon growth in a controlled environment, we gain new insights into neuronal growth and connectivity.

K1.00215 Controlling growth and electrical connectivity of neuronal cells patterned on surfaces , ROSS BEIGHLEY, ELISE SPEDDEN, Physics and Astronomy, Tufts University, JAMES WHITE, Physics and Astronomy and Biomedical Engineering, Tufts University, CRISTIAN STAIL, Physics and Astronomy, Tufts University — In the developing brain biochemical and geometrical cues are an essential source of information used by neurons when wiring up the nervous system. However, our current understanding of the mechanisms by which various guidance factors control the path that growing axons/dendrites follow to reach their targets and form functional electrical connections remains qualitative. A current limitation for the study of neural network formation is the ability to precisely control the growth and interconnectivity of small numbers of neurons. Here we present a combined Atomic Force Microscopy - Fluorescence Spectroscopy approach for patterning neurons on 2-dimensional substrates and precisely controlling their location, growth and interconnectivity. We demonstrate that this approach allows one to: a) form simple neuronal circuits in well-controlled geometries; b) guide the formation of functional synapses between neurons, and c) measure the electrical activity of small groups of neurons. We also discuss the implications of these results for our current understanding of the fundamental mechanisms that govern the development of electrical connections between neurons.

K1.00216 Are the laws of nature Markovian? , ROBERT JONES, Emporia State University — The present laws of physics are Markovian. The state of the world at the current time step, t , depends only on the state of the world at the previous time step, $t-1$. (If there happen to exist closed timelike curves in our world then general relativity suggests that this may not be true even in physics.) But other sciences may propose laws which are nonMarkovian. Biology (evolution) has the memories stored in DNA, cognitive science has long term and short term memories, economics may exhibit behavior (cooperation) that depends on a memory of past events, etc.

K1.00217 Optical properties of thylakoid stacks , PAVEL SHIBAYEV, Princeton University, PETR SHIBAEV, Fordham University — Optical properties of grana are simulated by means of 4x4 matrix approach (Berreman method). The results of calculations lead to a conclusion that even small degree of chirality, that may be present in a granum structure, results in the dramatic changes of its optical properties. Depending on the birefringence and degree of chirality in granum organization the reflection of left or right handed circularly polarized light can be greatly suppressed. This can explain the light induced difference in the growth of pea and lentil shoots irradiated by left and right handed circularly polarized light [1].

[1] Pavel P. Shibayev, R.G. Pergolizzi, The effect of circularly polarized light on the growth of plants, International journal of botany, 7, 113 (2011)

K1.00218 CHEMICAL PHYSICS —

K1.00219 ABSTRACT WITHDRAWN —

K1.00220 The Use of Magnetite as a Polarisable Anode in the Electrolysis of Water¹, BJORN BERTSON, Imperial College London, J. WOODS HALLEY, ANDY SCHOFIELD, University of Minnesota — We have studied the oxidation of magnetite to Fe_2O_3 in an electrolytic cell in which the cathode is magnetite and the anode is platinum. We report cyclic voltammogram data consistent with the hypothesis that magnetite, without oxygen gas production but with hydrogen gas production at the anode, is occurring. The reaction occurs at a potential at the cathode of about 0.3V vs SCE in 1M NaOH electrolyte, consistent with colloid experiments which also estimated the equilibrium potential of the hypothesized reaction. We find currents on the order of a milliamp per gram of magnetite electrode with the pelletized magnetite powder electrodes which we are using. Electrode characterization results using BET, XDS and macroscopic volume and mass measurements are reported, as well measurements of the amount of hydrogen gas generated per unit current. The quantity of gas generated is also consistent with our hypothesis concerning the electrode chemistry. Some samples exhibit evidence of two oxidation reactions occurring at the cathode and a possible interpretation of these is also discussed.

¹This work was supported by a grant from the Center for Urban and Regional Affairs at the University of Minnesota and by the University of Minnesota Supercomputing Institute.

K1.00221 Interfacial Electron Transfer from a PbSe Ququantum Dot into the TiO_2 Surface¹, RUN LONG, Department of Chemistry, University of Rochester, NY 14627 USA; School of Chemical & Bioprocess Engineering, University College Dublin, Ireland, OLEG PREZHDO, Department of Chemistry, University of Rochester, NY 14627 — We report an *ab initio* nonadiabatic molecular dynamics (NAMD) simulation of ultrafast photoinduced electron transfer (ET) from a PbSe quantum dot (QD) into the rutile TiO_2 (110) surface. The simulation supports the observation that the ET successfully competes with energy losses due to electron-phonon relaxation. The ET proceeds by the adiabatic mechanism due to strong donor-acceptor coupling. High frequency polar vibrations of both QD and TiO_2 promotes the ET, since these modes can rapidly influence the donor-acceptor state energies and coupling. Low frequency vibrations generate a distribution of initial conditions for ET, which shows a broad variety of scenarios at the single-molecule level. The system exhibits diverse scenarios for individual electron injection events, involving a complex interplay of ET mechanisms, time scales, and phonon dynamics.

¹R.L. thanks the IRCSET-Marie Curie International Mobility Fellowship in Science, Engineering and Technology (reference no. PD/2010/INSP/1485). O.P. acknowledges the NSF Grant CHE-1050405 dedicated to the method development and the DOE Grant DE-FG02-05ER15

K1.00222 Semiconducting (Half-Metallic) Ferromagnetism in Mn(Fe) Substituted Pt and Pd Nitrides, SAMIR MATAR, ICMCB-CNRS, Université de Bordeaux, France, VOLKER EYERT, www.materialsdesign.com — Using first principles calculations as based on density functional theory, we propose a class of so far unexplored diluted ferromagnetic semiconductors and half-metals. Here, we study the electronic properties of recently synthesized *4d* and *5d* transition metal dinitrides. In particular, we address Mn- and Fe-substitution in PtN_2 and PdN_2 . Structural relaxation shows that the resulting ordered compounds, $\text{Pt}_{0.75}(\text{Mn,Fe})_{0.25}\text{N}_2$ and $\text{Pd}_{0.75}(\text{Mn,Fe})_{0.25}\text{N}_2$, maintain the cubic crystal symmetry of the parent compounds. On substitution, all compounds exhibit long-range ferromagnetic order. While both $\text{Pt}_{0.75}\text{Mn}_{0.25}\text{N}_2$ and $\text{Pd}_{0.75}\text{Mn}_{0.25}\text{N}_2$ are semiconducting, Fe-substitution causes half-metallic behavior for both parent materials.

K1.00223 Time-dependent Partition Density-functional Theory, MARTIN MOSQUERA, ADAM WASSERMAN, Purdue University — We present an extension of time-dependent density functional theory that allows to partition the time-dependent external potential in terms of localized molecular fragment potentials. As a consequence, localized time-dependent densities arise for each molecular fragment. To enforce the condition that the sum of fragments must add up to the exact total density, a new quantity termed “time-dependent partition potential” is introduced. The Runge-Gross theorem is employed to show that there is a quasi one-to-one correspondence between the partition potential and the electronic density. The corresponding quantum-mechanical actions are derived by using the van Leeuwen’s action and are used to derive a decomposition of the partition potential which allows for practical approximations. Linear response formulas are deduced to obtain the transition energies, and an approximation is suggested to obtain localized excitations in large molecular systems. Finally, numerical illustration of our theory is shown for one-dimensional fermions under the influence of a laser field.

K1.00224 A Density Functional Approach to High Harmonic Generation¹, MICHAEL MACK, DANIEL WHITENACK, Purdue University, ADAM WASSERMAN, Purdue University, THE SUSPENDERS TEAM — The role of the asymptotic behavior of the ground state exchange-correlation (xc) potential is examined for the case of high harmonic generation (HHG) in N_2 via Time-dependent Density Functional Theory (TDDFT) within the adiabatic approximation. High harmonic generation (HHG) is a high-energy phenomenon that has been theoretically investigated using the strong-field approximation (SFA) within the single active electron approximation (SAEA) for small molecules. In the case of N_2 , experimental results for characteristic features of the harmonic emission suggest a breakdown of those approximations. TDDFT bypasses the need for such approximations as it accounts for all the electrons in the system; however, it requires approximations to the xc-potential. We investigate how asymptotic corrections to the Local Density Approximation (LDA) xc-potential influence the HHG spectrum.

¹Purdue Research Foundation

K1.00225 Measuring the Performance of Generalized Gradient Approximations in Solids, ZACHARY NAULT, A.C. CANCIO, Ball State University — There recently have been a number of generalized gradient approximations (GGA’s) developed to address a major limitation of the approach—the inability to model both energies and structural constants at the same time. We examine the performance for bulk systems of four different GGA exchange-correlation (XC) functionals: the PBE functional, best for energy calculations in molecules, the PBEsol functional developed to improve calculations of solid structures, the SOGGA functional developed to improve lattice constant calculations, and the VMT1 functional developed to improve atomization energy calculations without a loss in lattice constant accuracy. These XC functionals are tested on a set of 12 solids composed of metals, semiconductors, ionic metals, and transition metals. The plane-wave DFT code ABINIT was used to calculate the cohesive energy for each solid using each XC approximation. The bulk moduli and lattice constants were determined by fitting to the Murnaghan equation of state. We look particularly into how the use of a pseudopotential will effect the predictions of each model in comparison to experiment.

K1.00226 Investigating optical properties of Atmospheric gases using multi-color collocated Laser system: an application of elastic and inelastic backscattering, WATHEQ AL-BASHEER, KEVIN STRAWBRIDGE, Science and Technology Branch, Environment Canada, Center for Atmospheric Research Experiments, 6248 eight line, Egbert, ON, Canada L0L 1N0, SCIENCE AND TECHNOLOGY BRANCH, ENVIRONMENT CANADA, CENTER FOR ATMOSPHERIC RESEARCH EXPERIMENTS TEAM — The application of nanosecond pulsed lasers to probe optical properties of atmospheric gases by the application of elastic and inelastic backscattering mechanisms, is one of the most effective tools to investigate atmospheric gases effect on short and long term climate changes. Capabilities, properties, and limitations of newly built multi-color lidar (light detection and ranging) system at the CARE facility, Ontario, Canada, will be presented and thoroughly discussed. CARE’s setup utilizes elastic and inelastic backscattered signals of the second (532 nm), third (355 nm), and forth (266 nm) harmonic outputs of simultaneously employed YAG lasers, which are manipulated to investigate optical properties of ozone, water vapor, and nitrogen molecules up to 25 km geometrical altitude. In particular, by employing inelastic backscattering lidar signals of Raman nitrogen channel (386.7 nm) and Raman water vapor channel (407.5 nm), vertical profiles of water vapor mixing ratio (WVMR) from the near ground up to 12 km geometrical altitude are deduced, calibrated, and compared against WVMR profiles obtained from collocated radiosonde launches. Furthermore, a detailed theoretical treatment to the lidar technique will be presented and related to recent experimental findings.

K1.00227 Nonspherical structure of aqueous organic nanodroplets¹, BARBARA E. WYSLOUZIL, HARSHAD PATHAK, Ohio State University, FAWAZ HRAHSEH, GERALD WILEMSKI, Missouri University of Science and Technology — The structure of nanodroplets plays a critical role in many natural phenomena involving atmospheric nucleation and aerosol formation. Here, we review our experimental and theoretical work on the structure of nonane/water nanodroplets. The experiments involve small angle x-ray scattering (SAXS) of nanodroplets formed in supersonic nozzles. Classical density functional theory (DFT) calculations of species density profiles are made in cylindrical coordinates, which allows for the possibility of non-spherical droplets under appropriate conditions. One key theoretical result is the occurrence of a nonspherical Russian-Doll (RD) structure at low temperatures that is confirmed by molecular dynamics (MD) simulations. Some, but not all, of the measured SAXS spectra can be well-fit by a simple RD model, but the poor x-ray contrast between nonane and deuterated water generally makes it difficult to distinguish among well-mixed, core-shell, and RD structural models.

¹Supported by National Science Foundation Grant Nos. CBET-1033439 and CBET-1033387.

K1.00228 Investigation of Forces Exerted During the Expansion of Nanomechanically Tensioned Organosilica Materials, THERESA ALBON, PAUL EDMISTON, SUSAN LEHMAN, The College of Wooster, Wooster, OH — Osorb® is a sol-gel derived organosilica that instantaneously swells up to four times in volume with organic liquids. The nanoporous glass-like material is hydrophobic and does not swell in water but absorbs non-polar organic solutes from aqueous solution. Swelling due to absorption of organic solutes, liquids, or gases leads to the generation of substantial mechanical force, presumably derived from the relaxation of the interconnected network of organosilica nanoparticles that comprise the material. We have investigated the force exerted by placing a powdered sample in a cylinder with a freely movable piston. As solvent percolates into the cylinder from below, the exerted force is measured by a load cell. The piston is then gradually moved upward to allow the material to expand. As the sample just begins to swell, we have routinely observed forces in excess of 500 N per gram; the exerted force then decreases as the volume is allowed to increase. The relationship between the exerted force and sample volume is shown to be exponential, and we define the exponential decay constant as the characteristic volume V_C . We also determine the absorption capacity and fractional change in volume of the organosilica samples, and correlate these with changes in V_C .

K1.00229 2D IR Spectroscopy of Nucleic Acid Bases and the Folding of DNA Aptamers, CHUNTE SAM PENG, KEVIN C. JONES, CARLOS BAIZ, MICHAEL E. REPPERT, HELENA DE PUIG GUIXE, KIMBERLY HAMAD-SCHIFFERLI, ANDREI TOKMAKOFF, MIT, TOKMAKOFF COLLABORATION, HAMAD-SCHIFFERLI COLLABORATION — DNA can adopt a wide variety of conformations that have important roles in their biological functions, such as DNA packaging, replication, and protein recognition. Vibrational spectroscopy is known to reflect DNA conformation, and basic assignments of resonances in the IR and Raman spectra of nucleic acids have existed for decades. However, traditional spectral assignments are based on simple local vibrational mode basis such as C=O and C=N double bond stretches, although computational studies describe highly delocalized vibrations. We acquired polarization dependent 2D IR spectra of the base vibrations of five nucleotide monophosphates (NMPs) as the building blocks for developing a model of DNA and RNA vibrational spectroscopy. The distinctive cross-peaks between the vibrational modes of NMPs, such as ring vibrations and C=O stretches, indicate that these vibrational modes are strongly coupled anharmonic oscillators. We have characterized the eigenstate energies, vibrational anharmonicities, transition dipole strengths, and their relative orientations through the analysis and modeling of the experimental 2D IR spectra. We are currently applying this knowledge to study the folding of some G-rich DNA aptamers.

K1.00230 Intense-field ionization of heterocyclic organic molecules: fragmentation and metastable states¹, DAVID FOOTE, TIM SCARBOROUGH, CORNELIS UITERWAAL, University of Nebraska, Lincoln — Pyridine and the diazine molecules (pyridazine, pyrimidine, and pyrazine) are ionized by intense-field, ultrafast (50 fs), 800 nm laser pulses, and the resulting ion mass spectra are recorded as a function of laser intensity (ranging from $\sim 10^{13}$ W/cm² to $\sim 10^{15}$ W/cm²). Log-log plots of ion yield vs. intensity suggest resonance-enhanced multiphoton ionization (REMPI) mechanisms. These measurements are made possible by a unique tuning of the time of flight mass spectrometer that eliminates the focal volume effect in the ion yields. We also report on the fragmentation of the molecular ions under these same conditions. Fragment ion yields vary greatly when measured from different molecular parents, even those coming from the same mass. Furthermore, we observe evidence of metastable decays in the ion mass spectrometer, and measure the decay product mass by deliberately detuning the potentials on the time of flight mass spectrometer. This result is presented as a method of determining the nature of the metastable fragments—their masses and kinetic energy distributions.

¹This material is based upon work supported by the National Science Foundation under Grant Nos. PHY-0855675 and PHY-1005071.

K1.00231 Photoionization cross sections of atomic impurities in spherical quantum dots¹, CHIH-YUAN LIN, Y.K. HO, Institute of Atomic and Molecular Sciences — Quantum dots with atomic impurities have attracted considerable attention due to not only its theoretical but also practical significance. The confinement potentials associated with the structure of quantum dots are often described by the rectangular potential well or harmonic oscillator potential. However, the non-parabolic shape at the center for the rectangular well and the infinite depth for the harmonic oscillator potential make the models unrealistic in practical applications. Recently, the finite oscillator and Gaussian potentials are proposed to mimic the spherical quantum dots, which are defined respectively as $V_{FO}(r) = -A(1 + Br/\sqrt{A}) \exp(-Br/\sqrt{A})$ and $V_G(r) = -C \exp(-r^2/D^2)$ with the confining strengths A and C, and the radii of quantum dots 1/B and D. In this work, the method of complex-coordinate rotation in the finite-element discrete variable representation is implemented to study the photoionization of atomic impurities in spherical quantum dots. We explore the energy spectra and photoionization of atomic impurities influenced by the quantum confinement. The shifting of Cooper minima caused by the quantum confinement is observed.

¹Supported by NSC of Taiwan

K1.00232 A DFT Study of Palladium Clusters and their Reactions with H₂ and O₂: Application to catalyzed H₂O₂ synthesis¹, ADAM PELZER, Central Michigan University/Argonne National Lab, KOBLAR JACKSON, Central Michigan University, JULIUS JELLINEK, Argonne National Lab — Adsorption of oxygen and hydrogen in both atomic and molecular forms on small Pd_n clusters (n=2-13 and 19) is investigated using density functional theory. An extensive search for the energetically preferred structural forms and spin states of the clusters is performed. The geometries and energetics of the cluster-adsorbate systems and their transition states are mapped out as well. Cases of both single and multiple adsorptions are considered, and trends in the saturation coverage of the clusters versus cluster size are examined. Edge sites are found to be energetically preferred for O₂ adsorption, whereas the atop sites favor binding of H₂. Atomic adsorption of hydrogen is examined as well and limits to the number of H atoms that can be dissociated on each size cluster are found. In order to understand how trends in the results extend to larger cluster sizes, limited calculations have also been performed for Pd₅₅. The role of Pd_n clusters as catalysts for production of H₂O₂ from H₂ and O₂ is discussed as well.

¹AWP and KAJ were supported by the Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences, U.S. Department of Energy under Award Number: DE-SC0001330. JJ was supported by the Office of Basic Energy Sciences, Division

K1.00233 Morphologies of an anisotropic diffusion limited growth model to study electroless deposition¹, STEPHEN M. KUEBLER, Department of Chemistry and The College of Optics and Photonics, University of Central Florida, CHRISTOPHER J. CLUKAY, Department of Chemistry, University of Central Florida, ANIRUDDHA DUTTA, Department of Physics, University of Central Florida, CHRISTOPHER N. GRABILL, Department of Chemistry, University of Central Florida, HELGE HEINRICH, Department of Physics and The Advanced Materials Processing and Analysis Center, University of Central Florida, ANIKET BHATTACHARYA, Department of Physics, University of Central Florida — We report results of Monte Carlo simulation of a model which mimics certain aspects of electroless deposition of metals on polymeric surfaces. In the proposed model growth germinates from certain “active” particles residing on a flat surface. Further growth occurs via sticking of a diffusing particle while it is within the range of one of these active particles. Once within the attractive range of an “active” particle, the motion of the approaching particle is considered ballistic. This newly adsorbed particle then acts as an “active” site for further growth and the process continues. We monitor the layer by layer density variation, the pair correlation function and the structure factor as a function of the initial density of the particles and the range of the reaction, and comment on the fractal aspect of the morphology.

¹Supported by a grant from NSF-Chemistry.

K1.00234 ABSTRACT WITHDRAWN —

K1.00235 ABSTRACT WITHDRAWN —

K1.00236 Magneto-optical contrast in liquid-state optically-detected NMR spectroscopy, DANIELA PAGLIERO, CARLOS MERILES, Physics Department. City College of New York. CUNY — We use optical Faraday rotation (OFR) to probe nuclear spins in real time at high-magnetic field in a range of diamagnetic sample fluids [1]. This technique is shown to spectiate functional groups with the same chemical shifts as is seen in conventional NMR, however, the intensities of the OFR-NMR peaks are influenced by optical detuning and hyperfine couplings. We investigate protons at chemically-distinct sites and other lower-gyromagnetic-ratio nuclei including carbon, fluorine and phosphorous [2]. Binary mixtures for protonated systems were also tested and the results suggest that the present approach is sensitive to the solvent-solute dynamics in ways complementary to those known in inductive NMR.

[1] D. Pagliero, W. Dong, D. Sakellariou and C. A. Meriles. *J. Chem. Phys.* 133, 154505 (2010).

[2] D. Pagliero and C. A. Meriles. *Proc. Natl. Aca. Sci. USA* (2011) in press.

K1.00237 Hypo/hyperchromy in orthorhombic molecular crystals: Fluorene, and Dibenzofuran¹, ZAHRA NASROLLAHI, Department of Physics, University of Florida, Gainesville, Florida 32611, USA, LENINA NAKHIMOVSKY, Chemistry Department, Stony Brook University, Stony Brook, NY 11794, USA, JOHN TRUNK, Biology Department, Brookhaven National Laboratory, Upton, NY 11973, USA, D.B. TANNER, Department of Physics, University of Florida, Gainesville, Florida 32611, USA — The transmission of Fluorene and Dibenzofuran molecular crystals was measured over the near ultraviolet to vacuum ultraviolet (4-10 eV) range at the National Synchrotron Light Source. Polarized spectra were measured for both *a* and *b* crystallographic axes, and the spectrum in the *c* direction was found using the spectrum of a 40° rotated sample. Oscillator strengths were calculated by fitting the data to the Drude-Lorentz model. Comparison of the oscillator strength in the gas phase and in crystal show significant differences. These differences are attributed to the effect of intermolecular interaction in these molecular crystals.

¹Supported by the US DOE through contract DE-FG02-02ER45984

K1.00238 Superradiant light source for atmospheric remote sensing, DMITRI VORONINE, ANDREW TRAVERSO, RODRIGO SANCHEZ-GONZALEZ, LUQI YUAN, MICHAEL GRUBB, KAI WANG, ALEXEI ZHELTIKOV, Texas A&M University, College Station, TX 77843, ARTHUR DOGARIU, JAMES MICHAEL, RICHARD MILES, Princeton University, Princeton, NJ 08544, YURI ROSTOVTSSEV, University of North Texas, Denton, TX 76203, VLADIMIR SAUTENKOV, ALEXEI SOKOLOV, SIMON NORTH, MARLAN SCULLY, Texas A&M University, College Station, TX 77843 — We have studied coherent emission from ambient air and demonstrated efficient generation of laser-like beams directed both forward and backward with respect to a nanosecond ultraviolet pumping laser beam. The generated optical gain is a result of two-photon photolysis of atmospheric O₂, followed by two-photon excitation of atomic oxygen. We have analyzed the temporal shapes of the emitted pulses and have thereby shown that a large atomic coherence may well be responsible for the observed temporal structures. Our results suggest that the emission process is coherence brightened in its nature, and is to be compared with ordinary lasing where atomic coherence remains small on the one hand and cooperative Dicke superradiance where atomic coherence is maximized on the other. The collective coherence in this process adds insight as to the optical emission physics. The present superradiant source holds promise for remote sensing techniques employing nonlinear spectroscopy.

K1.00239 Estimating the contributions to the Low Energy Tail in Cu and Ag (100) using Positron Annihilation Auger Electron Spectroscopy¹, K. SHASTRY, P.V. JOGLEKAR, S. SATYAL, A.H. WEISS, Univ of Texas at Arlington — Low energy Auger lineshapes are difficult to measure because they sit on a large background due to secondary electrons arising from loss processes unrelated to the Auger mechanism. In this poster we discuss the implications of our Positron Annihilation Auger electron Spectroscopy (PAES) measurements of the ratio of the integrated Auger Peak and integrated low energy tail (LET) intensities for comparisons between theoretical and measured values of the Auger intensities. The experiments were carried out at university of Texas at Arlington on Ag (100) crystal. The various contributions to the low energy tail are highlighted in terms of processes intrinsic and extrinsic to the Auger mechanism. Our conclusions regarding the importance of the LET in determining the ratio of electrons in the Auger peak to the number of initial core holes are discussed in light of the electron stimulated Auger results obtained by Seah et al. using monte carlo simulations on various elements.

¹NSF DMR 0907679

K1.00240 Peroxynitrous Acid Dimer: Ab Initio Density Functional Study, RAJEEV PATHAK, Department of Physics, University of Pune, Pune 411007, MH, India — Peroxynitrous acid (PNA) HOONO, isomeric to nitric acid, is a very strong oxidant. A novel *dimeric* hydrogen-bonded cluster of peroxynitrous acid (PNA-D) is proposed herein; *ab initio* quantum chemical investigations performed whereupon lead to several stable structures that have a direct bearing on the reactivity of the participating monomers, quantified in terms of the molecular electrostatic potential. The electron-correlation lending stability to PNA and its dimers is gauged through several density functionals namely B3LYP, B3PW91, M06-2X, M06-L, and ω -B97X, etc.; as well as from popular wave-function based second order Møller-Plesset (MP2) perturbation theory, using the basis sets 6-311++G(d,p) and 6-311++G(2d,2p). The infra-red vibrational spectra reveal spectral shifts and intensity redistribution after dimerization. While the lowest energy PNA-D has a perfect inversion symmetry; the other stable dimers emerge as combinations of monomers in different orientation.

K1.00241 High resolution infrared spectra of protonated benzene isolated in solid parahydrogen, YU-JONG WU, National Synchrotron Radiation Research Center, MOMO BAHOU, YUAN-PERN LEE, Department of Applied Chemistry, National Chiao Tung University, NSRRC COLLABORATION, NCTU COLLABORATION — Identification of infrared (IR) spectra of protonated polyaromatic hydrocarbons (PAH) is important in understanding the unidentified IR bands of interstellar media. We demonstrate a new method that is superior to the Ar-tagging IR photodissociation or the IR-multiphoton-dissociation (IRMPD) methods currently used. The protonated benzene ($C_6H_7^+$) was produced on electron bombardment of a mixture of benzene (C_6H_6) and *para*-hydrogen ($p\text{-}H_2$) during deposition. IR features of $C_6H_7^+$ and C_6H_7 were identified by observing the change in intensity upon photolysis and comparison with theoretical calculations. Lines of $C_6H_7^+$ decreased in intensity when the matrix was irradiated with light at 365 nm, those of C_6H_7 increased in intensity. Similar experiments were performed for a sample of $C_6D_6/p\text{-}H_2$ and the production of $C_6D_6H^+$ was confirmed. Observed wavenumbers, relative IR intensities and deuterium isotopic shifts agree with those predicted for $C_6H_7^+$ and C_6H_7 . Compared with previous methods, this method provides a wider spectral coverage with much narrower lines and more accurate relative IR intensities, and may be readily applied to larger protonated and neutral PAH.

K1.00242 Pressure-temperature surface phase diagrams of $LaMnO_3$ surfaces in oxidative environments from first principles based kinetic Monte Carlo simulations¹, GHANSHYAM PILANIA, R. RAMPRASAD, University of Connecticut — Perovskite oxide surfaces catalyze many important oxidation reactions. They are also promising for oxygen ion conducting cathode materials in solid oxide fuel cells and efficient catalytic components for removal of NO_x gases in auto exhausts. Oxygen interaction with perovskite surfaces is of central importance in all such above mentioned technologically relevant examples. Here, we have employed first-principles based kinetic Monte Carlo (kMC) simulations to investigate the relative stability of the clean as well as molecular and atomic oxygen covered $LaMnO_3$ surfaces over a vast range of temperatures and oxygen partial pressures. The energetics as well as the activation energies of various surface reactions (adsorption, desorption, surface dissociation, and the surface diffusion of molecular and atomic oxygen) were computed and used in large-scale kMC simulations to predict the surface oxygen content and configuration at various combinations of temperature and pressure, thereby yielding a surface phase diagram. Owing to the state-of-the-art theory, algorithms and computations employed, these results are believed to represent the real situation with high fidelity. The phase boundaries as predicted by our kMC simulations are identified to be the catalytically active regions.

¹This research is based upon work supported by the Office of Naval Research. Computational support was provided through a National Science Foundation Teragrid Resource Allocation.

K1.00243 A New Technique for the Direct Determination of the Quasi-free Electron Energy in Dense Fluids, YEVGENIY LUSHTAK, CHERICE EVANS, Queens College – CUNY and the Graduate Center – CUNY, New York, NY, GARY FINDLEY, University of Louisiana at Monroe, Monroe, LA — Previous experimental studies of the quasi-free electron energy $V_0(\rho)$ in fluids of density ρ either directly measured $V_0(\rho)$, using photoemission from an electrode immersed in the fluid, or extracted $V_0(\rho)$ from field ionization of a dopant dissolved in the fluid. We present a new method to determine $V_0(\rho)$ directly, namely field enhanced photoemission. We show that this new method yields data of comparable quality to those obtained from dopant field ionization, thereby greatly improving on prior direct photoemission studies. Moreover, unlike dopant field ionization, field enhanced photoemission is not limited by the solubility of a dopant in the fluid of interest.

The experimental measurements reported here were performed at the University of Wisconsin Synchrotron Radiation Center (NSF DMR-0537588). This work was supported by grants from the Petroleum Research Fund (45728-B6) and from the National Science Foundation (NSF CHE-0956719).

K1.00244 Nonequilibrium Phase Transitions in Supercooled Water, DAVID LIMMER, DAVID CHANDLER, University of California, Berkeley — We present results of a simulation study of water driven out of equilibrium. Using transition path sampling, we can probe stationary path distributions parameterize by order parameters that are extensive in space and time. We find that by coupling external fields to these parameters, we can drive water through a first order dynamical phase transition into amorphous ice. By varying the initial equilibrium distributions we can probe pathways for the creation of amorphous ices of low and high densities.

K1.00245 Investigating the Glass Transition Temperature of Water using a Variety of Models and Methods via Molecular Dynamics Simulation, JOHN MURYN, Baldwin-Wallace College, GARY LEUTY, MESFIN TSIGE, Department of Polymer Science, The University of Akron — In everyday life, we think of solid water existing as crystalline ice. The majority of water in the universe, however, exists as an amorphous solid or “glassy” form. This glassy form has garnered significant interest and sparked sizable debate in recent years over the nature and conditions surrounding the transition from liquid to amorphous solid, not the least of which centers on the determination of the glass transition temperature. Previous experimental studies have suggested a glass transition temperature below the temperature at which water undergoes homogeneous nucleation, thus making experimental determination of the glass transition temperature difficult because of the need to avoid ice formation. In this study, we have used molecular dynamics simulation to study the structure, order and dynamics of water molecules at small timescales and under rapid cooling conditions to elucidate the formation of the amorphous solid and better understand the glass transition. Constant-pressure and constant-volume simulations have been performed in order to examine convergence or divergence of water dynamics under differing conditions. In addition, the van der Waals energy of simulation systems has been examined in an attempt to identify the glass transition temperature in a way that, to our knowledge, has not previously been used. Results suggest a glass transition temperature higher than previous widely accepted values but comparable to more recent results.

K1.00246 Ion size effects on the electrokinetics of spherical particles in salt-free concentrated suspensions¹, RAFAEL ROA, FELIX CARRIQUE, Fisica Aplicada I, Universidad de Malaga, EMILIO RUIZ-REINA, Fisica Aplicada II, Universidad de Malaga — In this work we study the influence of the counterion size on the electrophoretic mobility and on the dynamic mobility of a suspended spherical particle in a salt-free concentrated colloidal suspension. Salt-free suspensions contain charged particles and the added counterions that counterbalance their surface charge. A spherical cell model approach is used to take into account particle-particle electro-hydrodynamic interactions in concentrated suspensions. The finite size of the counterions is considered including an entropic contribution, related with the excluded volume of the ions, in the free energy of the suspension, giving rise to a modified counterion concentration profile. We are interested in studying the linear response of the system to an electric field, thus we solve the different electrokinetic equations by using a linear perturbation scheme. We find that the ionic size effect is quite important for moderate to high particles charges at a given particle volume fraction. In addition for such particle surface charges, both the electrophoretic mobility and the dynamic mobility suffer more important changes the larger the particle volume fraction for each ion size. The latter effects are more relevant the larger the ionic size.

¹Work supported by Junta de Andalucia, Spain (Project P08-FQM-3779) and MICINN, Spain (Project FIS2010-18972), co-financed with FEDER funds by the EU.

K1.00247 Modeling the transport of binary fluid/nanoparticle mixtures through microchannels with ciliated walls, YONGTING MA, AMITABH BHATTACHARYA, OLGA KUKSENOK, University of Pittsburgh, Pittsburgh, PA 15261, DENNIS PERCHAK, Kodak Research Laboratories, Rochester, NY 14650, ANNA C. BALAZS, University of Pittsburgh, Pittsburgh, PA 15261 — We study the dynamic behavior of nanoparticle-filled binary fluids that are driven through a microchannel with ciliated walls. To carry out these studies, we use a hybrid computational approach that combines the lattice Boltzmann model for binary fluids and a Brownian dynamics model for the nanoparticles. The ciliated walls of the microchannels are composed of flexible filaments that are modeled as beads connected by elastic springs. This hybrid model allows us to capture the interactions between the binary fluids, nanoparticles, and the hairy walls. We show that the process of capillary filling of such microchannels strongly depends on the rigidity of the hairs, their grafting density, and their affinity to the fluid components and nanoparticles. We demonstrate that by tailoring the properties of the nanoparticles, one can effectively control not only the velocities of the capillary filling, but also the deposition of nanoparticles on the hairy walls, and hence dynamically alter the properties of these ciliated surfaces. Our findings provide fundamental insights into the dynamics of this complex system, as well as potential guidelines for technological processes involving capillary filling with nanoparticles in a structured flexible porous medium.

K1.00248 Roles of Low Molecular Weight Amide on Crystallization Behavior of Poly (L-lactic acid)¹, XIA DONG, QIAN XING, XIUQIN ZHANG, DUJIN WANG, Institute of Chemistry Chinese Academy of Sciences — Organic nucleating agents play an important role in enhancing the crystallization rate of polymers. The aim of this study is to investigate the effect of low molecular weight aliphatic amides on the crystallization behavior and mechanism of poly (L-lactic acid) (PLLA). The crystallization rate of PLLA during non-isothermal crystallization and isothermal crystallization has been significantly improved with the addition of N, N'-ethylenebis (12-hydroxystearamide) (EBH) and/or N, N'-ethylenebisstearamide (EBSA), and EBH exhibits stronger nucleating ability. Time-resolved FTIR spectra illustrate the chain conformational changes and the crystallization kinetics during isothermal crystallization of PLLA mixtures and pure PLLA, especially in the early stages. The formation of interchain conformational-ordered structure and intrachain 103 helix structure for amide-doped PLLA precedes that of pure PLLA, suggesting a stimulatory nucleating effect of EBH and EBSA. In the case of PLLA/EBH, the interchain interactions of -(COC+CH3) and -CH3 groups are faster than the -(CH3+CC) intrachain interactions, while the interchain interactions and the intrachain 103 helix formation are nearly synchronous for PLLA/EBSA, indicating that EBH has an improved effect on the nucleating ability and crystallization kinetics of PLLA, compared to EBSA. The possible mechanism has been discussed, which may be attributed to the hydrogen bond interaction between hydroxyl groups in EBH and the carbonyl groups in PLLA.

¹The funding support from NSFC No.50925313.

K1.00249 Ion Energy Distribution Studies of Ions and Radicals in an Ar/H₂ Radio Frequency Magnetron Discharge During a-Si:H Deposition Using Energy-Resolved Mass Spectrometry, SAMUEL MENSAH, University of Arkansas, HUSAM ABU-SAFE, Labanese American University, Byblos, HAMEED NASEEM, University of Arkansas, MATT GORDON, Denver University — Ion energy distributions of sputtered Si particles have been measured by an energy-resolved mass spectrometer, and we correlate the results with measured thin film properties. The plasmas have been generated in a conventional magnetron chamber powered at 150W, 13.56MHz at hydrogen flow rates ranging from 0-25sccm. Various H_n⁺, SiH_n⁺, SiH_n fragments (with n = 1, 2, 3) together with Ar⁺ and ArH⁺ species were detected in the discharge. The most important species for the film deposition is SiH_n with n = 0,1,2, and H fragments affect the hydrogen content in the material. The flux of Ar⁺ decreases and that of ArH⁺ increases when the hydrogen flow rate was increased. However both fluxes saturate at hydrogen flow rates above 15sccm. Plasma parameters, such as plasma potential V_p, electron density n_e and electron energy T_e, are measured with the Langmuir probe. The ion energy distribution (IED) of all prominent species in the plasma is measured with an energy resolved mass analyzer. The plasma parameters decreased with increasing hydrogen flow rate; V_p, n_e and T_e decreased from 36.5V, 7.2x10¹⁵ m⁻³, 5.6eV to 32.8, 2.2x10¹⁵ m⁻³ and 3.8eV respectively. The ion energy of the heavy species, Ar, Ar⁺, ArH, ArH⁺, SiH and SiH_n⁺ radicals have ion energies comparable to the plasma potential. Analysis of the IEDs shows an inter-dependence of the species and their contribution to the thin film growth and properties.

K1.00250 Calculation of exciton binding energy and electron-hole recombination probability in quantum dots using explicitly correlated electron-hole wavefunction based method, ARINDAM CHAKRABORTY, Syracuse University — Accurate description of electron-hole correlation plays a central role in describing optical properties of quantum dots. This talk will focus on development of explicitly correlated wavefunction based methods for accurate treatment of electron-hole correlation. In this method, the wavefunction depends explicitly on the electron-hole inter-particle distance (R12) term and electron-hole wavefunction is obtained using variational procedure by minimizing the total energy. In inclusion of R12 term allows for a better description of wavefunction at small electron-hole distances and is found to be crucial for calculation of accurate electron-hole recombination probability and binding energy. The 2-particle electron-hole reduced density matrix (2-RDM) is obtained from the optimized wavefunction and the electron-hole recombination probability is computed from the diagonal elements of the 2-RDM. The developed method is applied to InGaAs/GaAs, CdSe/ZnS, and InP/InGaP quantum dots and exciton binding energy and electron-hole recombination probability are computed for a range of dot sizes. The computed results are compared with experimental results and path-integral Monte Carlo and configuration interaction calculations.

K1.00251 The Use of Confocal Raman Spectroscopy to Quantitatively Study the Interactions Between Immersive Water and Graphene/Graphene Oxide Surfaces, HANNAH NARCROSS, BYUNG HO JEON, JONG-WON LEE, CHANG YEOL RYU, Rensselaer Polytechnic Institute — The unique mechanical, chemical, optical, and electrical properties of graphene allow for many potential applications in biomaterials. Understanding and quantifying the surface interactions between graphene/graphene oxide and aqueous liquid is essential for the design of such graphene-based nanocomposites. Graphene sheets were produced by the mechanical exfoliation of graphite. We have used depth Confocal Raman Spectroscopy (CRM) profiles to measure graphene wettability using a water immersive objective lens, and demonstrated how surface energy between graphene/graphene oxide and immersive aqueous liquid can be affected to simultaneously measure the depth image profiles. Contact angles were also measured to further investigate the compatibility between graphene/graphene oxide and its environment.

K1.00252 Preparation and anisotropy of large-scale lyotropically aligned functionalized multilayer graphene, QIZHEN LIANG, XUXIA YAO, WEI WANG, C.P. WONG, Georgia Institute of Technology — Comparing with ballistic electron and phonon transport along graphene sheets, phonon and electron transferring traversing stacked graphene layers are conducted by weak Van der Waals forces and hopping conduction so that inevitably debate mechanical, electrical and thermal properties in "out-of-plane" direction. Alignment of graphene sheets can orient covalent chemical bonds in these parallel planes, resulting in a strong anisotropy of the large-scale materials from various graphitic forms with optimized mechanical, electrical and thermal properties. Moreover, systematic characterizations of the anisotropy of the ordered structures are rarely available due to their low profile in thickness directions. Here, conductors with highly ordered lamellar structure in large scale are prepared at room temperature from functionalized multilayer graphene (fMGs) by a lyotropical alignment methodology. Distinct difference in mechanical, electronic and thermal properties between lateral (in-plane) and thickness (out-of-plane) directions of the aligned fMGs indicates a strong anisotropy. Benefiting from the anisotropy, ultrahigh electrical and thermal conductivities in lateral direction are obtained, without aid of any chemical or thermal reduction. The finding facilitates the potential large-scale preparation and application of multilayer graphenes in photonic and electronic components, electrodes for energy collectors, conductive polymeric adhesives and composites.

K1.00253 Using computational chemistry to understand proton transfer in Green Fluorescent Protein¹, CHRISTA HOSKIN, PAUL CHAMPION, TIMOTHY SAGE, ABDELKRIM BENABBAS, ALEXANDER DEMIDOV, BRIDGET SALNA, Northeastern University, JASPER VAN THOR COLLABORATION², LEE THOMPSON COLLABORATION³ — Green Fluorescent Protein has been studied experimentally by the scientific community for years yet frustratingly little is known about the underlying proton transfer process that produces the green fluorescence. We are trying to elucidate more about this process using Density Functional Theory to prepare and run various calculations on GFP that we compare with kinetics data, Raman and vibrational coherence spectra. I am building a model of wild type GFP that is realistically sized for our computational power, yet still contains key residues that might affect the proton transport process. I will compare my results to those of the E222D GFP mutant. This comparison will allow us to see any differences in energy and normal modes that give insights regarding the proton transfer process. For example, how does it depend on a variety of factors such as temperature, buffer, pH, mutations, etc.? We also plan to examine if the proton transfer propagates through the three donor-acceptor pairs of the “proton wire” consecutively versus the three protons on the wire transferring simultaneously. Finally, we will consider how quantum tunneling may be involved in the proton transfer.

¹Special thanks to NSF grant CHE-1026369

²Imperial College London

³Imperial College London

K1.00254 ABSTRACT WITHDRAWN —

K1.00255 ATOMIC, MOLECULAR AND OPTICAL PHYSICS —

K1.00256 MEST-The quantum space-time explain some questions of quantum mechanics, DAYONG CAO, Beijing Natural Providence Science & Technology Development Co., Ltd — The probability of displacement and period of wave are the quantum space-time. The paper explain of the two-slit interference and the uncertainty relation. (1) $S = P(r) = P(\lambda) = f^2$. According to the Benford's law, (2) $T = P(t) = \ln(1 + \frac{1}{t}) = \nu$. Among it, S: the quantum space, f: the amplitude, r: the displacement, T: the quantum time, t: the period, ν : the frequency, λ : the wavelength, P(x): the probability function. (3) $E'\psi = i\hbar \frac{\partial \psi}{\partial t}$. (4) $m'\psi = i\hbar \frac{\partial \psi \partial t}{(\partial x)^2}$, equation (3) over equation (4), substituting equation (1) and (2) into it, (5) $E'\psi = m'\psi c'^2 = m'\psi \frac{(\partial f^2)^2}{(\partial \nu)^2}$, getting the energy-wave and mass-wave equation, (6) $E' = i\hbar \frac{\partial f^2}{\partial \nu}$. (7) $m' = i\hbar \frac{\partial \nu}{\partial f^2}$. (8) $\Delta E' \Delta \nu = \Delta E' \Delta t = i\hbar \Delta f^2$, ($\Delta f^2 \geq \frac{1}{2}$). (9) $\Delta p' \Delta f^2 = \Delta p' \Delta \lambda = i\hbar \Delta f^2$, ($\Delta f^2 \geq \frac{1}{2}$). Among it, E' : the energy of wave, m' : the mass of wave, c' : the velocity of light, ψ : the Wave Functions, f^2 : the probability. Here, the equation (8) and (9) are new uncertainty relation. In the two-slit interference, because (10) $c' = \frac{\lambda}{t} = \frac{f^2}{t}$, so (11) $f^2 = \lambda(\text{the wavelength})$, so (12) $\lambda \geq d$ (the width of the slits). Measuring the time of light at one slit(1) and its energy at other slit(2) together. And the measuring probability, if (13) $f_1^2 \geq \frac{1}{2}, f_2^2 \geq \frac{1}{2}, f_1^2 = f_2^2, (f_1^2 + f_2^2) \leq 1$, then (14) $f_1^2 = f_2^2 = \frac{1}{2}$.

K1.00257 Initial-state dependence of the quench dynamics in integrable quantum systems¹, MATTIAS FITZPATRICK, Middlebury College, MARCOS RIGOL, Georgetown University — We identify and study classes of initial states in integrable quantum systems that, after the relaxation dynamics following a sudden quench, lead to near-thermal expectation values of few-body observables. In the systems considered here, those states are found to be insulating ground states of lattice hard-core boson Hamiltonians. We show that, as a suitable parameter in the initial Hamiltonian is changed, those states become closer to Fock states (products of single site states) as the outcome of the relaxation dynamics becomes closer to the thermal prediction. At the same time, the energy density approaches a Gaussian. Furthermore, the entropy associated with the generalized canonical and generalized grand-canonical ensembles, introduced to describe observables in integrable systems after relaxation, approaches that of the conventional canonical and grand-canonical ensembles. We argue that those classes of initial states are special because a control parameter allows one to tune the distribution of conserved quantities to approach the one in thermal equilibrium. This helps in understanding the approach of all the quantities studied to their thermal expectation values.

¹This work was supported by the Office of Naval Research and the National Science Foundation under Grant No. DMR-1004268.

K1.00258 Many-body physics of optically excited, frozen Rydberg gases¹, DOMINIK MUTH, ACHIM LAUER, Fachbereich Physik und Forschungszentrum OPTIMAS, TU Kaiserslautern, Germany, JOHANNES OTTERBACH, Department of Physics, Harvard University, Cambridge, MA, USA, MICHAEL FLEISCHHAUER, Fachbereich Physik und Forschungszentrum OPTIMAS, TU Kaiserslautern, Germany — We discuss the many-body physics of an ensemble of optically excited Rydberg atoms with van der Waals dipole-dipole interactions [1]. Starting from a fully quantized model of the optical excitation we show that Rydberg excitations always possess a finite kinetic energy mediated by photon exchange even if the motion of the atoms can be disregarded. The kinetic energy competes with the repulsive vdW interactions. Using discretization and DMRG, we calculate the many-body ground state in the one-dimensional case. It is correlated much more strongly than possible for any local interaction, i.e., with a Luttinger parameter $K \ll 1$. In the presence of an additional lattice, a fractal phase diagram [2] emerges with Mott-insulating phases at any rational filling fraction. [1] see e.g. H. Weimer, R. Löw, T. Pfau, and H. P. Büchler; Phys. Rev. Lett. 101, 250601 (2008) [2] F. J. Burnell, M. M. Parish, N. R. Cooper, and S. L. Sondhi; Phys. Rev. B 80, 174519 (2009)

¹We gratefully acknowledge financial support by the DFG through the SFB TR 49 project.

K1.00259 Topological insulators in cold-atom gases with non- Abelian gauge fields: the role of interactions, PETER P. ORTH, Karlsruhe Institute of Technology (KIT), DANIEL COCKS, MICHAEL BUCHHOLD, Institut fuer Theoretische Physik, Goethe Universitaet, 60438 Frankfurt/Main, Germany, STEPHAN RACHEL, Yale University, KARYN LE HUR, 1 Center for Theoretical Physics, Ecole Polytechnique, 91128 Palaiseau Cedex, France, 2 Yale University, WALTER HOFSTETTER, Institut fuer Theoretische Physik, Goethe Universitaet, 60438 Frankfurt/Main, Germany — With the recent technological advance of creating (non)- Abelian gauge fields for ultracold atoms in optical lattices, it becomes possible to study the interplay of topological phases and interactions in these systems. Specifically, we consider a spinful and time-reversal invariant version of the Hofstadter problem. In addition, we allow for a hopping term which does not preserve S_z spin symmetry and a staggered sublattice potential. Without interactions, the parameters can be tuned such that the system is a topological insulator. Using a combination of analytical techniques and the powerful real-space dynamical mean-field (R-DMFT) method, we discuss the effect of interactions and determine the interacting phase diagram.

K1.00260 Composite-pulse magnetometry in the solid-state , CLARICE AIELLO, MASASHI HIROSE, PAOLA CAPPELLARO, Department of Nuclear Science and Engineering, Massachusetts Institute of Technology — The sensitivity yielded by magnetometry schemes at the quantum level is limited by experimental imperfections in the interrogation pulses and, especially in the solid-state, by relatively short dephasing times. We investigate the use of composite-pulse magnetometry sequences as a means of addressing both limitations. We perform proof-of-principle experiments on magnetometry and noise characterization through a continuous sequence of rotary echoes applied to a single qubit in the nitrogen-vacancy center in diamond. The rotary echo is the simplest unit of a composite pulse sequence, consisting of two consecutive pulses of identical nominal rotation angle applied with opposite excitation phases. Unlike other composite sequences, the rotary echo corrects for excitation field, but not for static field, inhomogeneities. The presented scheme is flexible in that a suitable choice of rotation angle compensates for different scenarios of noise strength and origin (dephasing or fluctuations in excitation intensity). Obtained sensitivities are in the range between those obtained with the widely used Ramsey spectroscopy sequence and the recently implemented method relying on frequency beats in Rabi oscillations.

K1.00261 Atoms talking to SQUIDS¹ , J.E. HOFFMAN, J.A. GROVER, S. RAVETS, K.D. VOIGT, J. LEE, Z. KIM, A.K. WOOD, I. SCHOCH, J.R. ANDERSON, A.J. DRAGT, M. HAFEZI, C.J. LOBB, L.A. OROZCO, S.L. ROLSTON, J.M. TAYLOR, F.C. WELLSTOOD, Joint Quantum Institute, Department of Physics and National Institute of Standards and Technology, University of Maryland, College Park, MD 20742 — We present our advances towards a hybrid quantum system of ⁸⁷Rb atoms coupled to a superconducting flux qubit through the magnetic dipole transition. We plan to trap atoms in the evanescent field outside a 500 nm nanofiber. This will allow us to bring the atoms less than 5 μ m above the surface of the superconductor without producing excessive heating or changing magnetic fields. As an intermediate step, we plan on coupling the atoms to a superconducting LC resonator. Current progress includes production of nanofibers with >98% transmission, and a tunable high-Q superconducting resonator. Additionally, we show how to use our system as a unified interface for microwave and optical photons, in which the atoms act both as a quantum memory and transduce excitations between the two frequency domains. Using coherent control techniques, we examine conversion and storage of quantum information between microwave photons in superconducting resonators, ensembles of ultracold atoms, and optical photons as well as a method for transferring information between two resonators.

¹Work supported by the NSF through the PFC at JQI , and the ARO Atomtronics MURI.

K1.00262 Nonequilibrium steady state for strongly-correlated many-body systems: a variational cluster approach¹ , MICHAEL KNAP, WOLFGANG VON DER LINDEN, ENRICO ARRIGONI, Graz University of Technology — The understanding of the nonequilibrium behavior of strongly correlated quantum many-body systems is a long standing challenge, both in theory as well as in experiments. Here, we present a new numerical approach that allows to calculate nonequilibrium steady state properties of strongly correlated quantum many-body systems. The approach is formulated in the framework of Keldysh Green's functions and is based on the ideas of the variational cluster approach (VCA), which has been successfully applied to a variety of strongly correlated many-body systems in equilibrium. As in equilibrium VCA, one crucial aspect appears to be the variational procedure, consisting in a self-consistent adjustment of the equilibrium reference system to the nonequilibrium target state. We apply the presented approach to non-linear transport across a strongly correlated quantum wire described by the fermionic Hubbard model.

¹Financial support from the Austrian Science Fund (FWF) under Project No. P18551-N16, and the Austrian Marshall Plan Foundation are gratefully acknowledged.

K1.00263 Two dimensional analysis of a free oscillation atom interferometer , RUDRA KAFLE, ALEX ZOZULYA, Worcester Polytechnic Institute, Worcester, MA 01609 — In a free oscillation atom Michelson interferometer, a Bose Einstein condensate in the ground state of a harmonic oscillator potential is split by a sequence of laser pulses and then the split wave packets are allowed to undergo a free oscillation. The wave packets are recombined at the splitting location after they make one or more full cycle oscillations. The motion of the wave packets becomes two dimensional if they are misaligned from the axis of the wave guide at the time of splitting. The dynamics of the split condensates becomes more complicated in this situation than a purely one dimensional oscillation. We develop a simple two dimensional model to analyze the effects of a slightly misaligned atomic wave packets on interferometry.

K1.00264 Exciton-polariton Vortex-Antivortex lattices in two-dimensional hexagonal potential geometries , NA YOUNG KIM, Stanford University, KENICHIRO KUSUDO, National Institute of Informatics, SVEN HOEFLING, ALFRED FORCHEL, University of Wuerzburg, YOSHIHISA YAMAMOTO, Stanford University — Microcavity exciton-polaritons possess the duality nature of wave and particle associated with the constituent particles, cavity photons and quantum well excitons. They are quantum bosons in the dilute density limit at low temperatures, exhibiting Bose-Einstein condensation (BEC) as a testbed to explore fundamental nature of physics. In particular, they are confined in two-dimensional plane, where exotic physical phenomena appear. Here, we discuss how to form vortex-antivortex lattices formed by exciton-polariton condensates trapped in two-dimensional hexagonal potential landscapes: triangular-, honeycomb- and Kagome- geometries. This will provide insights to investigate the BEC to Berenskii-Kosterlitz-Thouless transition.

K1.00265 Tunable Spin-orbit Coupling and Quantum Phase Transition in a Trapped Bose-Einstein Condensate , YONGPING ZHANG, GANG CHEN, CHUANWEI ZHANG, Department of Physics and Astronomy, Washington State University, Pullman, WA, 99164 USA — Spin-orbit coupling (SOC), the intrinsic interaction between a particle spin and its motion, is responsible for various important phenomena, ranging from atomic fine structure to topological condensed matter phenomena. While the SOC strength in typical solid state materials is much smaller than the Fermi velocity of electrons, it can reach the same order or even beyond the Fermi velocity of atoms in a recent breakthrough experiment that realizes SOC for ultra-cold atoms. However, the SOC strength in the experiment, determined by the applied laser wavelengths, is not tunable. Here we propose a scheme for tuning the SOC strength through a fast modulation of the laser intensities. We find that tuning SOC strength can drive a quantum phase transition (QPT) from a spin-balanced to a spin-polarized state in a harmonic trapped Bose-Einstein condensate (BEC). The QPT is similar as that in the long-sought Dicke model in quantum optics, which has important applications in quantum information. We characterize the QPT using the periods of collective oscillations (center of mass motion and scissors mode) of the BEC, which show pronounced peaks and damping around the quantum critical point.

K1.00266 Non-equilibrium spin dynamics in an ultra-cold gas , JEFFREY MCGUIRK, DORNA NIROOMAND, LYDIA ZAJICZEK, Simon Fraser University — We study spin dynamics in an out-of-equilibrium quantum gas. Using an optical technique, we imprint arbitrary one-dimensional spin structures in a trapped gas of Rb-87 atoms near quantum degeneracy. These spin structures can exhibit instabilities or lead to spin wave oscillations. The spin system has a highly nonlinear nature, and these spin waves can lead to collapse and revival of coherence. In particular, we measure spin currents in the ultra-cold gas, observe spatially localized collapse and revival of Ramsey fringe contrast, and show how the pattern of coherence depends on the strength of the spin-wave excitation. Lastly, we explore instabilities in the non-equilibrium spin system that can lead to spontaneous amplification of coherence.

K1.00267 Calculation of BEC transition using the Mathieu equation¹, QINQIN LU, Louisiana State University, KELLY PATTON, Seoul National University, DANIEL SHEEHY, Louisiana State University — While most calculations of the properties of bosons in optical lattices focus on the tight-binding Hubbard model regime, generally the single-particle states of bosons in an optical lattice satisfy the Mathieu equation. We have developed a formalism for studying bosons in an optical lattice using the Mathieu equation. The Mathieu equation formalism provides a natural way to explore physics in regimes where the Hubbard model description breaks down. We use this formalism to compute the momentum distribution of bosons in an optical lattice as probed in time-of-flight expansion, as well as finite size effects and signatures of the phase transition.

¹This work has been supported by the Louisiana Board of Regents, under grant LEQSF (2008-11)-RD-A-10.

K1.00268 A Theory of BCS-BEC Crossover, YASEMIN GURCAN, CUNY Graduate Center, J.L. BIRMAN, Distinguished Prof., CCNY, CUNY Graduate Center — In ultracold atomic fermions, the sign and the magnitude of pairing interactions can be controlled by using the magnetically-tuned Feshbach resonances to achieve a continuous transition between Cooper pairs of dilute fermi gas to BEC of diatomic molecules, which is known as the “BCS-BEC crossover.” At present, although several models have been proposed, there is still no exact analytical solution of the many-body problem of BCS-BEC crossover region. The standard BCS mean-field theory of superconductivity was used to describe the whole crossover resulting a useful approximation. In our studies, we introduced solvable models for an exact analytical solutions of BCS-BEC crossover region at $T = 0$ using the generalized $SU(2) \times SU(1,1)$ coherent states.

K1.00269 Boson gas in a periodic array of tubes¹, P. SALAS, Posgrado en Ciencia e Ingenieria de Materiales, UNAM, F.J. SEVILLA, M.A. SOLIS, Instituto de Fisica, UNAM — We report the thermodynamic properties of an ideal boson gas confined in an infinite periodic array of channels modeled by two, mutually perpendicular, Kronig-Penney delta-potentials. The particle's motion is hindered in the x - y directions, allowing tunneling of particles through the walls, while no confinement along the z direction is considered. It is shown that there exists a finite Bose-Einstein condensation (BEC) critical temperature T_c that decreases monotonically from the 3D ideal boson gas (IBG) value T_0 as the strength of confinement P_0 is increased while keeping the channel's cross section, $a_x a_y$ constant. In contrast, T_c is a non-monotonic function of the cross-section area for fixed P_0 . In addition to the BEC cusp, the specific heat exhibits a set of maxima and minima. The minimum located at the highest temperature is a clear signal of the confinement effect which occurs when the boson wavelength is twice the cross-section side size. This confinement is amplified when the wall strength is increased until a dimensional crossover from 3D to 1D is produced.

¹We thank support from grant PAPIIT IN105011, IN117010, IN106908, CONACyT 104917

K1.00270 Dynamics and evaporation of defects in Mott-insulating clusters of boson pairs¹, DOMINIK MUTH, FB Physik und Forschungszentrum OPTIMAS, TU Kaiserslautern, Germany, DAVID PETROSYAN, Institute of Electronic Structure and Laser, FORTH, Heraklion, Crete, Greece, MICHAEL FLEISCHHAUER, FB Physik und Forschungszentrum OPTIMAS, TU Kaiserslautern, Germany — Repulsively bound pairs of particles in a lattice governed by the Bose-Hubbard model can form stable clusters corresponding to finite-size Mott insulators. Here we study the dynamics of hole defects in such clusters corresponding to unpaired particles which can resonantly tunnel out of the cluster into the lattice vacuum. Because of bosonic statistics, the unpaired particles have different effective mass inside and outside the cluster, and “evaporation” from the cluster boundaries is allowed only when their quasi-momenta are within a certain range of transparency. We show that quasi-thermalization of hole defects occurs in the presence of catalyzing defects of triple occupied sites which thereby purify the Mott insulating clusters. We study the dynamics of 1D systems, verifying the analytical reasoning by numerically exact t-DMRG simulations. We derive an effective strong-interaction model that enables simulations of the system dynamics for longer times and allows checking with a higher number of defects. We also discuss a more general case of two bosonic species which for equal tunneling rates reduces to the special case of the fermionic Hubbard model in the strong interaction limit, where dynamical purification has been discussed before [2].

¹We gratefully acknowledge financial support by the DFG through the SFB TR 49 project and by the Humboldt Foundation.

K1.00271 Experimental witnessing of the initial correlation between an open quantum system and its environment¹, CHUAN-FENG LI, JIAN-SHUN TANG, YU-LONG LI, GUANG-CAN GUO, Key Laboratory of Quantum Information, University of Science and Technology of China, Chinese Academy of Sciences, Hefei 230026, P. R. C. — System-environment correlations, which determine the (non-)Markovian character of a dynamical process, is an area of intense interest in the study of open quantum systems. We send photons emitted from a quantum dot sample into a 15-m polarization-maintaining optical fiber to generate different system-environment correlated states and then witness the correlations by observing the growth of trace distances. This experimental scheme of correlation witnessing based on system-environment information flow can also be used for other similar systems.

¹We thank J. Piilo, H. P. Breuer, and E. M. Laine for their helpful discussions. This work is supported by the National Fundamental Research Program, National Natural Science Foundation of China (Grants No. 60921091, No. 10874162, and No. 10734060).

K1.00272 Time-dependent Hamiltonian identification, ALEXEI GOUN, Postdoctoral researcher — It is demonstrated that the time dependence of the Hamiltonian operator can be extracted by measurement of the evolution operator of the quantum system for a set of control parameters. For the case where the time dependence is weak and can be treated as a perturbation it is possible to express the inversion procedure in an analytic form. In the case of general time dependence, the iterative procedure is developed and its stability is analyzed.

K1.00273 Open Optomechanical Whispering Gallery Mode Resonators, DAVID AVELINE, LUKAS BAUM-GARTEL, NAN YU, Jet Propulsion Laboratory, California Institute of Technology — We have investigated open cavity Whispering Gallery Mode Resonators (WGMR) suitable for optomechanical coupling, and we present our initial demonstrations of structurally modified WGMR using microfabrication techniques. There has been strong interest in WGMR technology due to its extremely high optical quality and its compact robust nature. These monolithic optical resonators offer many advantages over mirror-based Fabry-Perot cavities that typically require special optical coatings. Standard WGMR, however, are constrained because only a tiny portion of the mode volume is externally accessible, limited to the perimeter of the disk where the evanescent field exists slightly outside the resonator. We have applied focused ion beam milling to augment WGMR discs with open structure, which allows direct access to the internal optical fields. By incorporating a mechanical cantilever inside the cavity, the coupled optomechanical system can yield extremely high sensitivity to displacement and acceleration, which would be well suited for miniature accelerometers and gyroscopes. This novel open cavity WGMR scheme could lead to many innovative applications that are unviable within the closed structure of conventional WGMR, including inertial sensors, trace gas detection, and laser sources.

K1.00274 Local Structural Study of Prussian Blue Analog $Fe_3(Co(CN)_6)_2 \cdot nD_2O$, JOE PETERSON, SOURAV ADAK, HEINZ NAKOTTE, New Mexico State University, LUKE DAEMEN COLLABORATION, KATHERINE PAGE COLLABORATION — The family of Prussian Blue analogs (PBA) is of interest, in part, because a number of them have been shown to exhibit negative thermal expansion. $Fe_3(Co(CN)_6)_2 \cdot nH_2O$ is particularly interesting because, when fully hydrated, it has been shown to have both positive and negative thermal expansion in the region from 80-298K while its partially dehydrated form demonstrates a linear-like negative thermal expansion over the same temperature region. To investigate the role local structural properties play in these systems we conducted temperature varying neutron pair distribution function (PDF) analysis on both the fully hydrated and partially dehydrated $Fe_3(Co(CN)_6)_2 \cdot nD_2O$.

K1.00275 Reduced-Density-Matrix Description for Multi-Photon Processes in Quantized Electronic Systems¹ , VERNE JACOBS, ALEX KUTANA, Naval Research Laboratory — A reduced-density-matrix description is developed for multi-photon processes in quantized many-electron systems, taking into account environmental electron-photon and electron-phonon interactions. Using a perturbation expansion of the frequency-domain Liouville-space self-energy operator, the spectral-line widths and shifts are evaluated in the isolated-line and short-memory-time (Markov) approximations. Applications of interest include spectral simulations for single-photon and two-photon absorption processes in atomic, molecular, and solid-state systems.

¹Work supported by the Office of Naval Research.

K1.00276 Ab Initio Calculations for Electronic Relaxations in Molecules and Solids Due to Scattering by Phonons¹ , ALEX KUTANA, VERNE JACOBS, Naval Research Laboratory, CENTER FOR COMPUTATIONAL MATERIALS SCIENCE TEAM — We carry out first-principles calculations for relaxations of excited electrons in molecules and solids due to scattering by phonons. Density matrix theory (DMT) is employed, which allows for a rigorous evaluation of electronic lifetimes, line widths and shifts, entirely from first principles. The three main ingredients in these calculations – electronic energy levels, dipole-transition matrix elements, and electron-phonon coupling matrix elements – are obtained from configuration interaction (CI) and density functional theory (DFT). Combining DMT, CI, and DFT allows one to avoid the use of the empirical line widths, as commonly employed in most previous investigations, and instead calculate their values from first principles. The calculated line widths and shifts are used to construct theoretical linear absorption spectra, which are then compared with experimental results.

¹Work supported by the Office of Naval Research. Part of this work was performed under the ASEE program at NRL.

K1.00277 Creation of superposition states in many-body systems by scattering , JAMES DOUGLAS, KEITH BURNETT, University of Sheffield — When quantum systems interact with the environment the interaction typically leads to decoherence of the system's quantum state. Here we show that one mechanism of interacting with the environment—uncontrolled scattering of probe particles by a many-body system—can instead lead to coherent superpositions of the system particles. For a system of two particles scattering leads to relative localization of the particle positions, while for more than two particles the system particles localize relative to one another in a pairwise fashion allowing superpositions in position space. We simulate scattering and the creation of these superposition states for many-body systems in free space and trapped in optical lattices. The different superpositions created are signaled in the scattering distributions and could be detected by allowing the particle wavefunctions to expand and interfere.

K1.00278 Analysis of Low-Z EUV Spectra from “Sparky” Laboratory Plasma Experiments , PENKA WILCOX, ALLA SAFRONOVA, VICTOR KANTSIREV, University of Nevada Reno — This study provides an analysis of recent experimental EUV and soft X-ray laser plasma spectra from the compact laser facility “Sparky”, generated under various plasma conditions. The developed non-LTE kinetic models of low-atomic number elements, such as C, O, F, etc., based on the Flexible Atomic Code data, are utilized. By matching the features of experimental spectra to the predictions of our atomic and plasma models, whose parameters are studied and precisely specified, the conditions of source plasmas can be inferred. The emitted EUV radiation we examine generally falls in the 90 Å to 260 Å wavelength range. In addition, the most intense lines from He-like ions of C and O in the soft X-ray region (20 Å - 40 Å) are observed. The most diagnostically significant temperature and density sensitive spectral lines are identified and proposed to use in plasma diagnostics for various applications including fusion research. This work is supported by DOE under grant DE-FG02-08ER54951.

K1.00279 Smart Combinatorial Research Equipment (SmartCoRE) for Sample Environmental Control and Automated Analysis with Optical Methods¹ , MATTHEW CHURCH, XIAODONG DING, NORMAN NANTEL, Jema Science Inc., SMARTCORE TEAM — Combinatorial research (CR) has revolutionized the way research is done in every major chemistry, physics and material science laboratory. We propose to bring the same success of automation and capabilities of CR to a widely used technique, small- and wide- angle x-ray scattering (SAXS/WAXS) through our development of a small, modular sample environmental chamber with embedded control electronics that can easily be used in large arrays. The device however is not restricted to a SAXS/WAXS techniques as it can easily be adapted to almost any kind of small volume sample prep or optical analysis technique requiring control of basic sample environmental parameters such as temperature, atmosphere, light and electromagnetic fields. The prototype has the following capabilities: 1. Automated switching of external electronic instrumentation between modules. 2. Thermoelectric temperature control from -50 to 200 C. 3. Ports for gas flow through or evacuation of sample environment. 4. Sealed sample environment using minimally scattering window material. 5. 90 degree field of view of both sides of sample. 6. Optional fiber-optic connections for UV-Vis spectroscopy. 7. Optional GISAXS mounting geometry. 8. Optional liquid sample flow cell.

¹SmartCoRE is supported by a DOE SBIR grant.

K1.00280 QUANTUM INFORMATION, CONCEPTS AND COMPUTATION —

K1.00281 Non-Perturbative and Moments Methods Applied to the Morse Potential , NATHAN WALSH, Fordham University, ERIC ASHENDORF, Kingsborough College of CUNY, JOHN TOLAND, Stevens Institute of Technology, VASSILIOS FESSATIDIS, Fordham University, JAY D. MANCINI, Kingsborough College of CUNY, SAMUEL P. BOWEN, Chicago State University — The well-known Morse potential has been well known to both physicists and quantum chemists for a number of years and has been used to model the behavior of diatomic molecules. Explicitly it may be written as

$$V(r) = D_e \left(e^{-2a(r-r_e)} - 2e^{-a(r-r_e)} \right) + D_e$$

where r is the inter-atomic separation, r_e is the (equilibrium) bond length and D_e is the depth of the potential well. The width of the well is given by $a^2 = k_e/2D_e$ with k_e the effective spring constant. Here we wish to study both the ground state energy (using both the Connected Moments Expansion and the Generalized Moments expansion) as well as the entire spectrum using a Lanczos scheme. Our results will be compared with other well-established results.

K1.00282 Low Frequency Perturbations, Adiabatic Ground States and Wave Function Collapse, SAMUEL P. BOWEN, Chicago State University, JAY D. MANCINI, Kingsborough College of CUNY, VASSILIOS FESSATIDIS, Fordham University — It is a well known and established fact that Time Dependent Perturbation Theory (TDPT) predicts that non- resonant time dependent perturbations will provoke no change in the excited state probability amplitudes of quantum systems. In this work we study a number of quantum systems wherein, at low frequencies, a response is indeed generated (by non-resonant perturbations) causing the system to respond adiabatically and hence resulting in the creation of instantaneous (time-dependent) ground states. These instantaneous time-dependent ground states are a linear combination of both the ground state and the excited states. The wave-function collapse of these adiabatic ground states calls into question the common wisdom that off-resonant perturbations can have no effect on quantum systems.

K1.00283 Topologically Protected Quantum State Transfer in a Chiral Spin Liquid, NORMAN YAO, CHRIS LAUMANN, Harvard University, ALEXEY GORSHKOV, California Institute of Technology, HENDRIK WEIMER, Harvard University, LIANG JIANG, California Institute of Technology, J. IGNACIO CIRAC, Max Planck Institute for Quantum Optics, PETER ZOLLER, University of Innsbruck, MIKHAIL LUKIN, Harvard University — Topology plays a central role in ensuring the robustness of a variety of physical phenomena. Notable examples range from the robust current carrying edge states associated with the quantum Hall and the quantum spin Hall effects to proposals involving topologically protected quantum memory and quantum logic operations. In this talk, I will describe a topologically protected channel for the transfer of quantum states between remote spin-based quantum registers. In our approach, state transfer is mediated by the edge-mode of a chiral spin liquid. I will demonstrate that the proposed method is intrinsically robust to realistic imperfections associated with disorder and decoherence. Possible experimental implementations and applications to the detection and characterization of spin liquid phases will be discussed.

K1.00284 Landau-Zener-Stückelberg Interference of Microwave Dressed States in a Superconducting Phase Qubit, GUOZHU SUN, RISE, Nanjing University, China, XUEDA WEN, School of Physics, Nanjing University, China, BO MAO, University of Kansas, YANG YU, School of Physics, Nanjing University, China, JIAN CHEN, WEIWEI XU, LIN KANG, PEIHENG WU, RISE, Nanjing University, China, SIYUAN HAN, University of Kansas — Landau-Zener-Stückelberg (LZS) interference is a well-known quantum phenomenon in a variety of physical systems, including atoms and solid-state systems. However, all the previous works were performed in simple systems having avoided level crossings in their energy diagrams. From both theoretical curiosity and practical significance it is important to know whether LZS interference can be observed in the dressed states, usually generated from the interaction between photons and atoms. We present the observation of LZS interference of the dressed states arising from a macroscopic quantum object, a superconducting phase qubit, interacting with a microwave field. The dependence of LZS interference fringes on the microwave power, microwave frequency, and the initial state of the qubit agrees quantitatively very well with the theoretical prediction. Such LZS interferometry involving the dressed states enables us to control the quantum states of multipartite systems with ease. In fact, this method is applicable to ANY quantum systems, which have avoided level crossings resulting from interaction between the individual constituents and photons.

K1.00285 Switching Phenomena in Bifurcation Amplifiers, WILLIAM SOO, ANDREW DOHERTY, School of Physics, University of Sydney, NSW 2006 — Recent experiments have seen high fidelity single shot measurement of superconducting qubits using the latching readout of a bifurcation amplifier. In these measurements, the coupling of the qubit to a nonlinear resonator correlates the qubit state with bistable states of the resonator. So qubit state discrimination, and hence readout quality, is ultimately governed by the dynamics of switching between the resonator states. In order to investigate how the quality of the measurement depends on system parameters, we study the physical mechanism of this probabilistic switching between the bistable resonator states. Recent simulations have shown that the switching rate can be very accurately obtained from a quantum trajectory model of the dynamics. We study Arrhenius formulae to model the switching rate and look to a Gaussian variational solution to the trajectory equations in order to gain an improved qualitative picture of the dynamics of these switching events.

K1.00286 Towards Realization of a Tunable Josephson Superinductor, MATTHEW BELL, IVAN SADOVSKYY, LEV IOFFE, MICHAEL GERSHENSON, Department of Physics and Astronomy, Rutgers, the State University of New Jersey, ALEXEI KITAEV, Institute for Quantum Information, Caltech — Many Josephson circuits intended for quantum computing would benefit from the realization of the Josephson “superinductor”: a phase-slip-free element whose inductive impedance at the plasma frequency exceeds the quantum of resistance, $h/(2e)^2$. With this aim, we have fabricated a chain of cells whose Josephson coupling can be frustrated by the magnetic field. These asymmetric dc-SQUID-like cells have several large Josephson junctions (JJs) in one arm shunted by a single small JJ in the other arm. The phase slips in this chain are suppressed by the phase rigidity across larger JJs, which remains strong even when the cell is frustrated by the magnetic field (while its Josephson inductance increases). Numerical simulations which explicitly take into account quantum fluctuations were used to optimize the JJ parameters. The inductance and phase rigidity of the device was probed by measuring the microwave response of the array coupled to a lumped-element microwave resonator. The resonance frequency of this circuit, f_r , and its quality factor Q were measured as functions of the magnetic field B. The observed dependences $f_r(B)$ and $Q(B)$ which reflects the variations of the Josephson inductance and phase rigidity of the array, will be compared with numerical simulations.

K1.00287 Collective Phenomena in a Capacitively-Coupled Transmon Array, ARTHUR SAFIRA, DEVIN UNDERWOOD, WILLIAM SHANKS, JAMES RAFTERY, ANDREW HOUCK, Princeton University — The manifestation of condensed matter physics phenomena in interacting photon systems has been of recent theoretical interest. Under the circuit quantum electrodynamics (cQED) architecture, light-matter interactions can be engineered into a strong coupling regime and many-body interacting photon systems can be fabricated. In this experiment, we create a triangular array of 100 niobium transmon qubits on a sapphire substrate. Photon-mediated interactions are facilitated through capacitive coupling among the transmons, each with a charging energy of approximately 200MHz. Collective quantum behavior of the Josephson-junction array is explored by measuring transmission across the array through input-output ports on the device itself as well as through a 3D cavity. This experiment is an important step towards realizing many-body, interacting quantum phenomena with photons.

K1.00288 Compact superconducting coplanar microwave beam splitters¹, A. BAUST, N. KALB, M. HAE-BERLEIN, J. GOETZ, E. HOFFMANN, E.P. MENZEL, M. SCHWARZ, F. WULSCHNER, L. ZHONG, F. DEPPE, A. MARX, R. GROSS, Walther-Meißner-Institute and TU Muenchen, Garching, Germany, SUPERCONDUCTING QUANTUM CIRCUITS AND NANOMECHANICS TEAM — The recent evolution of circuit quantum electrodynamics with standing-wave microwave modes towards setups for propagating quantum microwaves has triggered the need for low-loss superconducting microwave beam splitters. Such a device should have ports obeying the coplanar geometry relevant for circuit QED and, at the same time, be compact for the sake of scalability. This combination presents a serious challenge. In this work, we present an experimental characterization of various compact superconducting coplanar microwave beam splitters. In addition, we briefly discuss efforts towards a tunable beam splitter.

¹This work is supported by the DFG via SFB 631 and by the German Excellence Initiative via NIM.

K1.00289 Design and measurement of a silicon double quantum dot qubit with dispersive microwave readout¹, EDWARD HENRY, ANDREW SCHMIDT, UC Berkeley, QNL, MATHEW HOUSE, UCLA, YAO-TSENG WANG, CHEUK LO, UC Berkeley, HONG PAN, XIN XIAO, UCLA, HANHAN LI, LOREN GREENMAN, BIRGITTA WHALEY, UC Berkeley, HONGWEN JIANG, UCLA, ELI YABLONOVITCH, JEFFREY BOKOR, UC Berkeley, I. SIDDIQI, UC Berkeley, QNL — The electronic states of a semiconductor quantum dot are a promising candidate for quantum information processing. We describe a circuit QED qubit architecture in which a semiconductor qubit in silicon is capacitively coupled to a 6 GHz superconducting resonator. Silicon is an attractive material on account of the long electron spin lifetime. We discuss the design and operation of both the laterally defined double quantum dot qubit as well as the balanced coplanar stripline resonator. We focus in particular on the chip design and the specifics of the measurement setup, including both low and high frequency filtering. We also discuss the possibility of operating this device as a spin qubit by way of applying an inhomogeneous magnetic field.

¹This work is supported by the DARPA-QuEST program.

K1.00290 Improved rf-SSET Performance using On-Chip Superconducting LC Matching Networks on Si/Ge¹, ZHEN YANG, MINGYUN YUAN, CHUNYANG TANG, A.J. RIMBERG, Dartmouth College, M.A. ERIKSSON, D.E. SAVAGE, University of Wisconsin-Madison, RIMBERG TEAM, ERIKSSON COLLABORATION — The radio-frequency superconducting single electron transistor (rf-SSET) has been demonstrated to be a nearly quantum-limited charge sensor [1]. Building upon previous successful coupling of an aluminum SSET in the vicinity of quantum dots (QDs) on Si/SiGe using an off-chip inductor [2], we now developed on-chip matching networks to improve the charge sensing of Si/SiGe double quantum dots. Here, we report measurements in superconducting rf-SSETs, where the SET is directly fabricated with an on-chip inductor, giving enhanced sensitivity at our operating temperature of 0.3K. Recent experimental results including the investigation of the range of in-plane magnetic field compatible with RF-SET operation will also be discussed.

[1] W.W.Xue et al, Nature Phys. 5, 660 (2009);

[2] M.Y.Yuan et al, Appl. Phys. Lett. 98, 142104 (2011)

¹This work was supported by NSA, LPS and ARO.

K1.00291 Observable measure of quantum correlations, GERARDO ADESSO, DAVIDE GIROLAMI, University of Nottingham, School of Mathematical Sciences — The correlations of multipartite quantum states have nonclassical features that go beyond entanglement. A full theoretical and experimental characterization of these features is necessary to understand their foundational role in quantum theory, and to explore the usefulness of such nonclassical resources for quantum computation and communication. We introduce a measure of general bipartite quantum correlations for arbitrary two-qubit states, expressed as a state-independent polynomial function of the density matrix elements. The amount of quantum correlations can be quantified experimentally by measuring the expectation value of a small set of observables on up to four copies of the state, without the need for a full tomography. We extend the measure to $2 \times d$ systems, providing its explicit form in terms of observables for the relevant class of multiqubit states employed in the DQC1 model for quantum computation. Finally, we study the evolution of quantum correlations between two qubits embedded in a bosonic bath, showing that our measure can reliably identify the transition between weak and strong system-environment coupling regimes. This leads us to propose an experimentally friendly signature of non-Markovianity based on quantum correlations dynamics.

K1.00292 New Families of Coherent States for the Supersymmetric Oscillator¹, MORDECHAI KORNBLUTH, FREDY ZYPMAN, Yeshiva University, New York; Department of Physics — Supersymmetry is a viable theoretical framework to provide a unified picture of fermionic and bosonic fields. The subjacent supersymmetric algebra intrinsically transforms bosonic degrees of freedom into fermionic ones and vice-versa. Aside from physical realizations, the mathematical objects of supersymmetry (e.g. superspace, supertransformations) have proved fruitful for solving quantum problems based on the concept of partner Hamiltonians. The harmonic oscillator has been extensively studied in this context; a result of particular interest is the vanishing zero-point energy. The supercoherent states were first introduced 25 years ago [1], defined as eigenstates of a generalized annihilation operator that mixes fermionic and bosonic degrees of freedom. Here we extend that original annihilation operator to a family of complex 3-parameter annihilation operators. Our presentation shows the properties of those new operators as well as the properties of the corresponding eigenstates. In particular, after explicitly calculating the eigenstates in parameter space, we present a subspace with bounded uncertainty, for both the Heisenberg and entropic formulations of uncertainty. [1] Supercoherent States, C. Aragone and F. Zypman, Published in J. Phys. A 2267 (1986)

¹Funded by Kressel Research Scholarship and Gamson Fund of Yeshiva University

K1.00293 Room-temperature solid-state quantum memory using pairs of nuclear spins in diamond, NIR BAR-GILL, STEPHEN DEVIENCE, DAVID LE SAGE, CHINMAY BELTHANGADY, LINH PHAM, RONALD WALSWORTH, Harvard University — We propose a robust, room-temperature solid-state quantum memory scheme using a pair of nuclear spin impurities in diamond. The memory qubit is encoded in a decoherence-free subspace of this nuclear spin pair, which protects it from noise originating from the surrounding environment. In addition, nuclear spins close to a Nitrogen-Vacancy (NV) color center experience a significant electron-mediated coupling, which further suppresses decoherence of the qubit. We obtain coherence times on the order of a second, along with fast manipulation and readout through the coupling of the nuclear spins to the NV electronic spin. We show that through engineering of the diamond sample this scheme could offer scalability to a many-qubit memory, and could be used as a basic building block for hybrid quantum networks and quantum computing architectures.

K1.00294 Novel quantum behavior generated by traveling across a quantum phase transition¹, O.L. ACEVEDO, F.J. RODRIGUEZ, L. QUIROGA, Universidad de los Andes, N.F. JOHNSON, University of Miami — We report novel dynamical behavior in a multi-qubit-light system described by the Dicke model, which is being driven across its thermodynamic quantum-phase boundary. Analyzing the system's quantum fidelity, we find that the near-adiabatic regime exhibits the richest phenomena, with a strong asymmetry in the internal collective dynamics depending on which phase is the starting point. Depending on the quenching regime a highly non-trivial behavior emerges in both the qubit and radiation subsystems. For the former, we find that for some paths in parameter space the final fidelity of the near-adiabatic process does not depend on the direction of the trajectory, but depends only on the *speed* at which the path is traveled. This behavior is contrasted with Landau-Zener tunneling and the Kibble-Zurek mechanism. Furthermore, for some qubit subsystems, we identify purification and screening effects which could be used for quantum control. By contrast, the evolution of the Wigner function shows the radiation subsystem exhibits the emergence of complexity and non-classicality. These findings could be experimentally tested in several condensed matter scenarios – for example, diamond-NV centers and superconductor qubits in confined radiation environments.

¹Facultad de Ciencias Research Funds, Universidad de los Andes.

K1.00295 Exploring the Nitrogen-Vacancy center as a high resolution magnetometer¹, ABDELGHANI LARAOUI, CARLOS MERILES, Department of Physics, City College of New York - CUNY — New schemes that exploit the unique properties of NV centers in diamond are presently being explored as a platform to high resolution magnetic sensing [1, 2]. First we focus on the ability of a NV center to monitor a set of adjacent nuclear spins. For this purpose, we conduct comparative experiments where the NV spin evolves under the influence of surrounding ¹³C nuclei or, alternatively, in the presence of asynchronous AC fields engineered to emulate bath fluctuations [3]. Our study reveals substantial differences that underscore the limitations of the semi-classical picture when interpreting and predicting the outcome of experiments designed to probe small nuclear spin ensembles. In particular, our study sheds light on the role of bath fluctuations in the response of NV centers to common pulse sequences, and explores a detection protocol designed to probe time correlations within the random nuclear spin dynamics. Further, we show that the presence of macroscopic nuclear spin order is key to the emergence of traditional spin magnetometry. [1] J. R. Maze, et al., Nature 455, 644 (2008). [2] A. Laraoui, J.S. Hodges, C.A. Meriles, Appl. Phys. Lett. 97, 143104 (2010). [3] A. Laraoui, J. S. Hodges, C. A. Ryan, and C. A. Meriles, Phys. Rev.B 84, 104301 (2011).

¹We acknowledge support from Research Corporation and from the National Science Foundation.

K1.00296 High dynamic range diamond magnetometry for time dependent magnetic fields¹, M. UMMAL MOMEEN, N.M. NUSRAN, M.V. GURUDEV DUTT, Department of Physics and Astronomy, University of Pittsburgh — Nitrogen-Vacancy (NV) centers in diamond have become a topic of great interest in recent years due to their promising applications in high resolution nanoscale magnetometry and quantum information processing devices at ambient conditions. We will present our recent progress on implementing novel phase estimation algorithms with a single electron spin qubit associated with the NV center, in combination with dynamical decoupling techniques, to improve the dynamic range and sensitivity of magnetometry with time-varying magnetic fields.

¹This work is supported by NSF, DOE and the Alfred P. Sloan Research Fellowship.

K1.00297 Optical Control of Nuclear Spin Ensembles in Diamond, JONATHAN KING, JEFFREY REIMER, University of California, Berkeley — We present new results on the hyperpolarization of ¹³C nuclear spins in diamond through optically-oriented nitrogen vacancy (NV-) defects. Optical illumination of high NV- concentration diamonds at cryogenic temperatures and 9.4 Tesla results in a negative nuclear spin temperature with measured bulk-average polarization over 5%, although local polarization may be higher. The negative spin-temperature is attributed to a population inversion within the dipolar energy levels of the NV- spin ensemble. In our quantitative model, nuclei near defects equilibrate with the NV- dipolar energy reservoir and polarization is transported to the bulk material via spin diffusion. This model is tested by investigating a series of samples with varied defect density. We also investigate the nuclear hyperpolarization of NV- containing diamond nanocrystals. Such materials may be useful for surface transfer of polarization to target molecules for enhanced NMR sensitivity. Additionally, we investigate the dynamics and decoherence of the hyperpolarized nuclear spin ensemble and its interaction with electronic defect spins. Such phenomena are of fundamental interest to the use of diamond for quantum information applications.

K1.00298 Thwarting the Photon Number Splitting Attack with Entanglement Enhanced BB84 Quantum Key Distribution, CHRIS RICHARDSON, CARL SABOTTKE, Louisiana State University, ULVI YURTSEVER, MathSense Analytics, ANTIA LAMAS, National University of Singapore, JONATHAN DOWLING, Louisiana State University, PETR ANISIMOV, Stony Brook University — We develop an improvement to the weak laser pulse BB84 scheme for quantum key distribution, which utilizes entanglement to improve the security of the scheme and enhance its resilience to the photon number splitting attack. This protocol relies on the non-commutation of photon phase and number to detect an eavesdropper performing quantum non-demolition measurement on number. The potential advantages and disadvantages of this scheme are compared to the coherent decoy state solution. Most entanglement based quantum key distribution schemes rely on violations of Bell's inequalities to ensure security. However, this is not the strategy that our entanglement enhanced (EE) BB84 employs here. Instead, we detect Eve by introducing an entangled quantum state into the system that is sensitive to Eve's QND measurements. This allows for a recovery of an approximately linear dependence on transmittivity for the key rate. EE BB84 shares this advantage with coherent decoy state protocols as well as schemes that utilize strong phase reference pulses to eliminate Eve's ability to send Bob vacuum signals.

K1.00299 Efficient quantum communication under collective noise¹, MICHAEL SKOTINIOTIS, University of Calgary, BARBARA KRAUS, WOLFGANG DÜR, University of Innsbruck — We propose a novel communication protocol for the transmission of quantum information via quantum channels subject to collective noise. Our protocol makes use of decoherence-free subspaces in such a way that an optimal asymptotic rate of transmission is achieved, while at the same time encoding and decoding operations can be implemented efficiently. In particular, for a quantum channel whose collective noise is associated with a discrete group, G , i.e. with a discrete number, $|G|$, of possible noise operators, our protocol achieves perfect transmission at a rate of $m/(m+r)$, where r is a finite number of auxiliary systems that depends solely on the channel in question. In the case where the collective noise of the channel is associated with a continuous group, such as a collective phase noise channel, our protocol leads to efficient, approximate transmission of quantum data with arbitrarily high fidelity and optimal transmission rate. The coding and decoding circuit of our protocol requires a number of elementary gates that scale linearly with the number of transmitted qudits, m , in contrast to the best known protocols utilizing a decoherence-free subspace.

¹Austrian Science Fund, European Union, NSERC Canada, EU-Canada exchange, and USARO

K1.00300 Continuous-Variable Quantum Key Distribution using Thermal States, CHRISTIAN WEED-BROOK, University of Toronto, STEFANO PIRANDOLA, University of York, TIM RALPH, University of Queensland — We consider the security of continuous-variable quantum key distribution using thermal (or noisy) Gaussian resource states. Specifically, we analyze this against collective Gaussian attacks using direct and reverse reconciliation where both protocols use either homodyne or heterodyne detection. We show that in the case of direct reconciliation with heterodyne detection, an improved robustness to channel noise is achieved when large amounts of preparation noise is added, as compared to the case when no preparation noise is added. We also consider the theoretical limit of infinite preparation noise and show a secure key can still be achieved in this limit provided the channel noise is less than the preparation noise. Finally, we consider the security of quantum key distribution at various electromagnetic wavelengths and derive an upper bound related to an entanglement-breaking eavesdropping attack and discuss the feasibility of microwave quantum key distribution.

K1.00301 Interaction Free Measurement of Quantum Systems, ONOFRIO RUSSO, Department of Physics, New Jersey Institute of Technology, LIANG JIANG, Institute for Quantum Information, Caltech — A measurement of the state of a physical system always causes some degree of disturbance in the system. When the scaling consists of nano or smaller quantities, measurements can cause severe changes in the information contained in the system. Noteworthy are the quantum computing elements, or qubits, used operationally and as memory. The main and foremost concern for the quantum computing elements is decoherence which is exacerbated by the measuring process. We propose to overcome these obstacles using an intriguing quantum mechanical interaction free measurement (IFM) method. High-efficiency IFM has been demonstrated by combining quantum interference and the quantum Zeno effect [P. G. Kwiat, et al., Phys. Rev. Lett. 83, 4725 (1999)]. In addition, IFM can be useful for quantum information processing, because it eliminates photon absorbing/scattering processes, which often are responsible for undesired information loss and decoherence in neighboring atoms. This is manifested in optical lattices, dephasing of proximal nuclear spins of nitrogen-vacancy centers in diamond, etc. We further propose and investigate using IFM to replace conventional optical readouts for specific quantum systems with the advantage of elimination of undesired decoherence.

K1.00302 Spatial entanglement in two-electron atomic systems¹, YEW KAM HO, Y.-C. LIN, Institute of Atomic and Molecular Sciences — Recently, there have been considerable interests to investigate quantum entanglement in two-electron model atoms [1, 2]. Here we investigate quantum entanglement for the ground and excited states of two-electron atomic systems using correlated wave functions, concentrating on the particle-particle entanglement coming from the continuous spatial degrees of freedom. We use the two-electron wave functions constructed by employing B -spline basis to calculate the linear entropy of the reduced density matrix $L = 1 - \text{Tr}_A(\rho_A^2)$ as a measure of the spatial entanglement. Here $\rho_A = \text{Tr}_B(|\varphi\rangle_{AB} \langle \varphi|)$ is the one-electron reduced density matrix obtained after tracing the two-electron density matrix over the degrees of freedom of the other electron. Here, we investigate spatial entanglement for two-electron systems with $Z=1$ to $Z=10$. When Z is decreased from $Z=1.0$ to about $Z \leq 0.911$, the H^- ion becomes unbound. This would lead in a situation of one electron bound by the nucleus with the other electron being free. Such a wave function would be expected to have a spatial entanglement of $L=1/2$. Numerical results will be presented at the meeting.

[1] J. P. Coe and I. D'Amico, *J. Phys.: Conf. Ser.* **254**, 012010 (2010)

[2] D. Manzano *et. al.*, *J. Phys. A: Math. Theor.* **43**, 275301 (2010)

¹Supported by NSC of Taiwan

K1.00303 Delayed Choice with Haunted Quantum Entanglement for Choosing at a Distance an Overall Distribution Exhibiting Either Which-Way Information or Interference, DOUGLAS SNYDER, None — Particles 1 and 2 are entangled at one of two possible locations (providing which-way info). The entangled particles physically separate from each other where one particle [P1] preserves the ww information that accompanied entanglement and the other particle's motion [P2] supports interference in P2's overall distribution due to the device setup. With this step, P1 now supplies which-way info to P2 due to their entanglement. Next, there is a delayed choice at a distance. Choice A: P1 and the ww info it carries are essentially lost by releasing many other particles of similar character to P1 into the container with P1 before P2 is detected and before ww info for P1 becomes available to the environment or an irreversible ww measurement is made on P1. (The entanglement is then lost and so is the ww info supplied by P1 to P2.) Choice B: P1 that carries ww info is not lost. (The entanglement is not lost and neither is the ww info P1 has supplied to P2.) Repeat runs of method with choice A 100 times consecutively to develop an overall interference distribution pattern for P2, or instead repeat runs of method with choice B 100 times consecutively to develop an overall ww distribution pattern for P2.

K1.00304 Full counting statistics and entanglement in a disordered free fermion system¹, MICHAEL BANTEGUI, JOSEPH BURG, GREGORY LEVINE, Hofstra University — The Full Counting Statistics (FCS) is studied for a one-dimensional system of non-interacting fermions with and without disorder. For two L site translationally invariant lattices connected at time $t = 0$, the charge variance increases logarithmically in t , following the universal expression $\langle \delta N^2 \rangle \approx \frac{1}{\pi^2} \log t$, for t much shorter than the ballistic time to encounter the boundary, $t_b \sim L$. Since the static charge variance for a length L region is given by $\langle \delta N^2 \rangle \approx \frac{1}{\pi^2} \log L$, this result reflects the underlying relativistic or conformal invariance and dynamical exponent $z = 1$. With disorder and strongly localized fermions, the variance is also found to increase logarithmically in time, but saturates at times $t \approx t_d \propto L^2$, a diffusive time scale. Despite the fact that 1-d fermions are fully localized for any disorder strength, the entanglement responsible for charge fluctuations appears to propagate with dynamical exponent $z = 2$.

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K1.00305 Excitation and entanglement dynamics of light harvesting complex II B850 ring, SHU-HAO YEH, JING ZHU, SABRE KAIS, Department of Chemistry, Purdue University, West Lafayette, IN 47907 — The electronic excitation and the entanglement dynamics between the chromophores of photosynthetic harvesting complex II (LHCII) B850 ring have been studied and analyzed theoretically. Since the coupling energy between the adjacent chromophore electronic excitation is comparable to the bath organization energy, the modified scaled hierarchical equation of motion (HEOM) approach is implemented to treat the whole system in an intermediate coupling regime. Comparing our results to the well-studied Fenna-Matthews-Olson (FMO) protein, we found that quantum coherence of electronic excitation between chromophores also exist in this system at the same temperature level (77K), which also suggests that the excitation energy transfer coherently through the B850 ring instead of incoherent hopping. The calculation of bipartite entanglement between chromophore electronic excitation shows the existence of a long-lived entanglement in this system, illustrates that this kind of quantum effect could survive even in such a noisy environment.

K1.00306 Tuning the entanglement for a two-dimensional magnetic system with anisotropic coupling and impurities, QING XU, SABRE KAIS, Purdue University — We study a set of localized spins coupled through exchange interaction and subject to an external magnetic field. For such a class of two-dimensional magnetic systems, we introduce two impurities, and treat as the source, while the rest as the environment bath. It is demonstrated that entanglement can be controlled and tuned by varying the anisotropy parameter γ , the ratio of magnetic field h and exchange interaction J in the Hamiltonian and three different exchange interaction strengths: J (between environment spins), J' (impurity - impurity) and JJ' (between impurities and environment), respectively.

K1.00307 Decoherence and Quantum Walks under the regime of weak measurements and weak values, DEBABRATA GHOSHAL, George Mason University, MARCO LANZAGORTA, ITT Corporation, SALVADOR VENEGAS-ANDRACA, Tecnológico de Monterrey Campus Estado de México — Our research on Quantum Walks under the regime of quantum weak measurements and weak values (QWWM) is being continued from the perspective of quantum algorithms. Previously we investigated several statistical measures of a QWWM on an infinite line, and did some comparative study of such results with corresponding classical and quantum walks position probability distributions and statistical measures. Now we are interested to show the entanglement and decoherence effects of QWWM. We show preliminary results with respect to how the performance of Grover's algorithm is affected by entangled qubits when decoherence happens due to temperature difference. Furthermore, we provide a physical interpretation of such decoherence of the QWWM so that our results could have some useful applications in the area of quantum information.

K1.00308 Perfect mixed state quantum transport in correlated spin networks, ASHOK AJOY, PAOLA CAPPELLARO, Massachusetts Institute of Technology — Spin-based quantum networks form an attractive physical setting for quantum information processing and simulation. We consider the transport of quantum states in arbitrarily large and complex spin networks, with applications to distributed quantum computing. Specifically, we consider transport through spin networks in the mixed-state, since they are the least experimentally demanding to produce in high-temperature laboratory settings. We analyze conditions on the interaction and propagators that allow perfect state transfer in such networks. We show that when there is more than one possible transport path through the network, it is necessary to phase correlate the transport processes occurring along each path. We provide a modified isotropic XY-Hamiltonian that achieves this correlation, and use it to derive engineered couplings for perfect transport in complicated network topologies. Finally, we show that this Hamiltonian can perfectly transfer mixed states, even in arbitrary networks, as long as the spins between which the transport occurs are weakly coupled to the remaining spins.

K1.00309 APL simulation of Grover's algorithm , SAMIR LIPOVACA, None — Grover's algorithm is a fast quantum search algorithm. Classically, to solve the search problem for a search space of size N we need approximately N operations. Grover's algorithm offers a quadratic speedup. Since present quantum computers are not robust enough for code writing and execution, to experiment with Grover's algorithm, we will simulate it using the APL programming language. The APL programming language is especially suited for this task. For example, to compute Walsh-Hadamard transformation matrix for N quantum states via a tensor product of N Hadamard matrices we need to iterate $N-1$ times only one line of the code. Initial study indicates the quantum mechanical amplitude of the solution is almost independent of the search space size and rapidly reaches 0.999 values with slight variations at higher decimal places.

K1.00310 Non-Markovian finite-temperature two-time correlation functions of system operators of a quantum Brownian motion model , PO-WEN CHEN, YU-AN TASI, HSI-SHENG GOAN, Department of Physics, National Taiwan University, NTU TEAM — We evaluate the non-Markovian two-time correlations (CF's) of system operators of a quantum Brownian motion (QBM) model in two different ways, one by the exactly solvable Heisenberg equation of motion through fluctuation-dissipation theorem and the other by the projection operator technique through the perturbative time-convolutionless non-Markovian effective master equation. In Markovian case, a famous procedure to compute two-time CF's of system operators in open quantum systems is the quantum regression theorem (QRT). However, the QRT is not valid or needs corrections in the non-Markovian domain even in the weak system-bath coupling regime. The calculated non-Markovian two-time CF's up to fourth order in system-environment coupling strength agree well with those obtained from exact evaluation in the weak and mediate coupling regime, which demonstrates the validity of our derived non-Markovian evolution equations. But, the exact analytical two-time CF's for an Ohmic bath presented in the literature are only for the initial time t_2 being in the steady state ($t_2 \rightarrow \infty$), i.e. at equilibrium. Our evolution equations of the non-Markovian two-time CF's are, however, valid for any initial time t_2 . For a finite initial time t_2 , considerable difference in the non-Markovian CF's between the fourth-order system-bath coupling case and its second order counterparts can be observed. These results obtained using our derived non-Markovian evolution equations differ significantly from the Markovian case obtained using the QRT and from the non-Markovian case obtained directly using the QRT.

K1.00311 Combatting decoherence in OAM states due to turbulence , JOSE RAUL GONZALEZ ALONSO, TODD BRUN, University of Southern California — Photons have always been the information carriers of choice in quantum information, with many protocols taking advantage of the polarization degrees of freedom to encode quantum information. Exploiting the photon's orbital angular momentum (OAM) can provide distinctive advantages. The main one is an increased alphabet size for information transmission. Since the Hilbert space of OAM states is infinite dimensional, it can be used to encode more than one bit (or qubit) per photon. However, this potential can only be realized if suitable quantum information can be encoded in the OAM photon states, and if it can be protected from the decohering effect of atmospheric turbulence. In this work, we will numerically simulate the effects of turbulence (using the Kolmogorov model) on photons with a certain value of OAM and how to protect them from the decoherence caused by the atmospheric turbulence.

K1.00312 Average quantum tunneling times for asymmetric potentials , LUIZ MANZONI, BRYCE FRENTZ, Concordia College, Moorhead, MN, JOSE LUNARDI, Universidade Estadual de Ponta Grossa, Brazil — We generalize a recent definition of average quantum tunneling times, using the Salecker-Wigner-Peres (SWP) clock, to be applicable to the tunneling of a localized wave packet through asymmetric potentials. We investigate the properties of the average transmission and reflection times, including their interpretation in the framework of the weak measurement theory, and compare them with other standard average times. Finally, we discuss the advantages of the definition of average tunneling times as prescribed by the SWP clock (such as the non-saturation of the transmission time for opaque barriers).

K1.00313 A Modified Special Relativity Theory in the Light of Breaking the Speed of Light , AZZAM ALMOSALLAMI, Malaya University — In the OPERA experiment the neutrino broke the speed of light. It moved with speed greater than the highest speed in the universe (the speed of light in vacuum) according to the special relativity [32]. This experiment if it is confirmed will contradict the main basis that the special relativity built on which is the constancy of speed of light, and no particle or electromagnetic wave can exceed this speed [37]. Quantum tunneling experiments have shown that the signal moving superluminal [1-9]. In this work (the modified special relativity theory), we will unify the special relativity theory and quantum theory (Copenhagen school) in concepts, principles and laws. While this new theory is in agreement with the concepts, principles and laws of the quantum theory (Copenhagen school), and it introduces some changes in the concepts, principles and laws of quantum to be descriptive, and imaginative. Quantum theory was applied to the micro world, while the macro world was controlled by the laws of classical physics. In my paper I believe that the theory that controls the micro and macro worlds are the same.

K1.00314 Relativistic tunneling times for Gaussian wave packets , BRENT PERREAULT, LUIZ MANZONI, Concordia College, Moorhead, MN, JOSE LUNARDI, Universidade Estadual de Ponta Grossa, Brazil — We investigated an average tunneling time, as suggested by the Salecker-Wigner-Peres clock, for a localized particle described by the Dirac equation. Then we evaluate this average transmission time for a Gaussian wave packet incident on a square barrier. It was found that the time does not saturate for large barriers, that is, the average time doesn't suffer from the Hartmann effect. We also consider the contribution of the negative energy components of the localized wave packet for the average time.

K1.00315 Wheeler thought experiment with delayed choice , JEFFREY BOYD, Retired — This is an alternative interpretation of Jacques, et. al. (2007), Wheeler's thought experiment with delayed choice. The researchers find that the choice of observables changes the previous behavior of the photon inside the interferometer. Stepping outside the QM box, we propose that elementary waves from the detectors travel backwards through the interferometer, and the photon is following such a ray in the reverse direction. Thus a change in observables changes the behavior of the photon for the simple reason that the observable is transmitting information to the photon and the photon is able to change its polarization mid-stream in response to a change in that information. According to this explanation there is no delayed choice. It is an illusion.

K1.00316 PHYSICS OF BEAMS —

K1.00317 Measurement of the Depression of the Velocity of Focused Beams of Light with a Gouy-Phase Interferometer , ANDREW MADEY¹, University of Oregon — An apparatus is demonstrated that was constructed to show the depression in group velocity v_g of a focused Gaussian (HeNe laser) beam, and arguments presented for the effects of this demonstration on the theoretical basis of Special Relativity. An exploration is conducted of Einstein's theoretical underpinnings for Special Relativity, that light pulses travel at a fixed group velocity $v_g = c$. This is accompanied by theoretical proof that v_g for a focused Gaussian beam is depressed upon focusing, if the beam has a frequency-independent radius, related to the Gouy phase shift. An account of the operation of the apparatus is presented, and data from the operations related, verifying the change in v_g . This contradiction of Einstein's assumption, without effect on the experimental validity of Special Relativity, is reconciled by referring to Poincaré's derivation of Special Relativity's equations, which assumes simply that Maxwell's equations retain their form across inertial reference frames.

¹Andrew Madey is an Undergraduate Physics student at the University of Oregon

K1.00318 POLYMERS AND SOFT MATTER PHYSICS —

K1.00319 Amphiphilic Peptide-Polymer Conjugates with Side-Conjugation, NIKHIL DUBE, University of California, Berkeley, ANDREW PRESLEY, JESSICA SHU, TING XU, Department of Materials Science and Engineering, University of California, Berkeley — As an emerging family of soft matter, peptide-polymer conjugates are highly promising for the design of functional materials. The fundamental understanding of the effect of the interaction between peptides and polymers on the structural and functional properties of these materials is crucial for their development into technologically relevant materials. We have designed a family of amphiphilic materials based on polymer conjugates of coiled-coil helix bundle and characterized their self assembly in surfactant containing aqueous solution. Conjugation of two hydrophobic polymers, PS and PMMA to the exterior of bundle led to unfolding of helix and the extent of structural retention was dependant on polymer hydrophobicity. However, the deleterious effects of hydrophobic polymers on the peptide structures can be eliminated on adding organic solvent to solubilize the hydrophobic polymers. To understand the importance of polymer hydrophobicity, conjugates of the peptide with PNIPAM, which exhibits temperature controlled hydrophobicity, have been studied and the results underscore the significance of the hydrophobic interaction between the polymer and the peptide on the structural retention of peptide. These fundamental studies signify the importance of maintaining the balance between different competitive intermolecular interactions on the peptide structure in these hybrid materials.

K1.00320 POST-DEADLINE ABSTRACTS —

K1.00321 Carbon nanotubes synthesized by pulsed laser deposition for light harvesting devices, JIN CHU, University of Puerto Rico, BOQIAN YANG, University of Massachusetts Amherst, PETER FENG, University of Puerto Rico — A large-area vertically aligned carbon nanotubes (CNTs) have been fabricated by catalyst-assisted pulsed laser deposition techniques on indium tin oxide (ITO) glass substrates. The CNTs have a uniform shape and length, aligned vertically on the surface of the ITO substrates and the average diameter is about 8 nm. The long-term field emission current stability of the CNTs has also been investigated. No obvious current density decay was observed after 15 days continuous experiments, indicating the super stability of the sample. A highly stable, cheap and nontoxic material which can be used as electrodes in dye-sensitized solar cells was obtained.

K1.00322 Thermodynamic curvature measures interactions, GEORGE RUPPEINER, New College of Florida — Thermodynamic fluctuation theory originated with Einstein who inverted the relation $S = k_B \ln \Omega$ to express the number of states in terms of entropy: $\Omega = \exp(S/k_B)$. The theory's Gaussian approximation is discussed in most statistical mechanics texts. I review work showing how to go beyond the Gaussian approximation by adding covariance, conservation, and consistency. This generalization leads to a fundamentally new object: the thermodynamic Riemannian curvature scalar R , a thermodynamic invariant. I argue that $|R|$ is a thermodynamic measure of the correlation length and suggest that the sign of R corresponds to whether the interparticle interactions are effectively attractive or repulsive. These ideas have been tested in a number of model systems. They are also significant in real fluids near the critical point, along the coexistence curve, and near the triple point. Also interesting are results for black hole thermodynamics, for which a foundation in terms of an underlying microscopic system is so far absent.

K1.00323 Numerical method of the quasiclassical theory for mesoscopic superconductors, YUKI NAGAI, CCSE, Japan Atomic Energy Agency, K. TANAKA, Department of Physics and Engineering Physics, University of Saskatchewan, NOBUHIKO HAYASHI, N2RC, Osaka Prefecture University — We propose a numerical method for describing mesoscopic superconductors in terms of the quasiclassical theory of superconductivity. Our method releases us from the problems as to how to determine initial values in a system that does not have a bulk solution. To examine the efficiency of our method, we calculate the local density of states of a circular d -wave island sustaining a single vortex. We find that the vortex shadow effect strongly depends on the quasiparticle energy in the circular mesoscopic island.

K1.00324 Discontinuous percolation transition with full step order parameter jump, HYUN KEUN LEE, University of Seoul, HYUNGGYU PARK, Korea Institute for Advanced Study, JAE DONG NOH, University of Seoul, PARK COLLABORATION, NOH COLLABORATION — We demonstrate that there is a class of discontinuous percolation that is characterized by full step jump in order parameter at threshold $p_c = 1$. Such a percolation takes place in the infinite dimension if the critical exponent τ , the decay exponent of the cluster number density distribution in critical regime, holds $1 < \tau \leq 2$. The scaling relations of $\sigma = 2 - \tau$ and $\gamma = 1/\sigma$ are derived for the critical exponents σ and γ associated with the characteristic cluster size and with the susceptibility, respectively. We also show that the cluster number density distribution is compact and can be widened up to $\sim \sqrt{N}$ for system size N .

K1.00325 Three Dimensional Morphology of Lamellae-forming Block Copolymer Thin Films between Two Chemically Nanopatterned Surfaces, GUOLIANG LIU, ABELARDO RAMIREZ-HERNANDEZ, PAUL F. NEALEY, JUAN J. DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA — Previous work has demonstrated the directed assembly of block copolymers on one chemically patterned surface into desired two dimensional and three dimensional structures. Here, we report on the structures formed by block copolymer thin film equilibrated between two chemically patterned surfaces with orthogonal stripes. The patterned stripes have a width of $L_0/2$ and a period of L_0 , where L_0 is the natural period of the block copolymer. Our experiments and simulations reveal that the block copolymer domains are continuous through the film and the interface between domains resembles the Scherk's first minimal surface. Different from that in the bulk, the interface between the domains is at equilibrium in the presence of the defined boundary conditions, and has a remarkable level of perfection over the patterned areas in centimeter scale. The impact of chemical patterns on block copolymer morphologies and the underlying physics gives insight into the nanofabrication of complex nanostructures with directed self-assembly using two engineered boundary conditions, as opposed to only one.

K1.00326 Initial condition dependence of the probability density function of the injected power in the Langevin equation, JAE SUNG LEE, Korea Institute for Advanced Study, CHULAN KWON, Department of Physics, Myongji University, HYUNGGYU PARK, School of Physics, Korea Institute for Advanced Study — We study the diffusive dynamics of a Brownian particle described by the Langevin's equation with time varying heat bath temperature. Initially (when time $t < 0$) the heat bath temperature is T_{init} and the particle equilibrates with the heat bath. At time $t = 0$, the temperature abruptly changes from T_{init} to T , where their ratio is denoted by $\alpha = T/T_{\text{init}}$. Then the particle follows the Langevin dynamics with the temperature T for $t > 0$. Using the path integral method, we compute the probability density function (PDF) of the injection power (injected energy per unit time into the Brownian particle by the random noise, see J. Stat. Phys. 107, 314 (2002)). We find that the PDF or the corresponding large deviation function depends on the initial temperature T_{init} even in the $t \rightarrow \infty$ limit. In addition, we show that “phase transition” of the large deviation function occurs at $\alpha = 1/4$.

K1.00327 Mechanical detection of flux quanta as a candidate for small force standard, JAE-HYUK CHOI, HEON-HWA CHOI, YUN WON KIM, Korea Research Institute of Standards and Science, SOON-GUL LEE, Dep. of Display and Semiconductor Physics, Korea University, MAHN-SOO CHOI, Dep. of Physics, Korea University — Ultra-small force measurement with a micro-cantilever is a novel and powerful tool to probe micro- and nano-scale physical quantities, such as persistent current in mesoscopic metal rings, with unprecedented sensitivity. However, the precision of such small force is often limited by uncertainty of cantilevers spring constant, partly because of absence of small force standard. In this talk, I will introduce our metrological project for developing a small force standard based on superconducting flux quantum, from its concept to experimental progress. Our experimental results will cover the device fabrication, optical cooling effect, and mechanical detection of magnetic flux quantization and relaxation in a well-defined Nb micro-annulus at a temperature of 4 K.

K1.00328 Exploring Photocarrier Generation and Recombination in a Smectic Semiconductor *via* Transport Simulations, SANJOY PAUL, Department of Physics, Kent State University, JARROD WILLIAMS, ROBERT TWIEG, Department of Chemistry, Kent State University, BRETT ELLMAN, Department of Physics, Kent State University — Photocarrier generation and charge transport in the smectic B phase of the liquid crystalline semiconductor 2-(4'-octylphenyl)-6-dodecyloxynaphthalene (8PNPO12) have been investigated by using the time of flight (TOF) technique as a function of light intensity, electric field, and wavelength. The results probe both the low-intensity and space-charge perturbed regimes. The sharply different hole and electron TOF transients are quantitatively analyzed using comprehensive transport simulations to explore exciton dynamics, exciton decay, and bimolecular recombination.

K1.00329 Charge density waves and superconductivity in a minimal tight-binding model¹, JASON W. SADOWSKI², K. TANAKA, Department of Physics and Engineering Physics, University of Saskatchewan, YUKI NAGAI, CCSE, Japan Atomic Energy Agency — Charge density waves (CDW) and superconductivity (SC) are observed in a variety of materials such as layered transition-metal dichalcogenides, high-temperature cuprates, organic compounds, and other novel superconductors. The question as to whether CDW cooperate or compete with SC in those materials is under hot debate. In this work, we study possible mechanisms of CDW and its interplay with SC within an extended Hubbard model. In particular, CDW states caused by van Hove singularities as due to the mechanism proposed by Rice and Scott [1] are examined in detail.

[1] T. M. Rice and G. K. Scott, Phys. Rev. Lett. **35**, 120 (1975).

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K1.00330 Evidence of anisotropic Kondo coupling in nanostructured devices¹, LUIZ N. OLIVEIRA, KRISSIA ZAWADZKI, Instituto Fisica Sao Carlos, University of Sao Paulo — In spite of recent advances, the theory of electrical conductance through semiconducting nanodevices has fallen short of quantitative agreement with experiment. Consider, in particular, the single-electron transistor, a quantum dot bridging two otherwise independent two-dimensional electron gases. One would expect the universal function $G_u(T/T_K)$ describing the zero-bias conductance for the symmetric spin-degenerate Anderson model as a function of the temperature scaled by the Kondo temperature T_K to match experimental data. In practice, however, attempts to fit measurements with G_u have had to rely on *ad hoc* offset adjustments and, even then, obtained only fair agreement. Here, we extend a freshly-derived mapping between the function $G_u(T/T_K)$ and the conductance for the (generally asymmetric) Anderson model to allow for partial screening of the dot moment at high temperatures and show the mapping to fit the zero-bias conductances reported by Grobis et al., Phys. Rev. Lett. **100**, 246601 (2008) within experimental error. While other sources of partial screening cannot be ruled out, our results suggest the Kondo coupling between the dot moment and the electron spins in the adjacent gases to be anisotropic.

¹Supported by the CNPq and FAPESP

K1.00331 Interactive Learning Solid State with Quantum Mechanical programs, SABINA RUIZ-CHAVARRIA, PABLO DE LA MORA, Fac. de Ciencias, Universidad Nacional Autonoma de Mexico — Nowadays Solid State can be learnt interactively with Quantum Mechanical programs. Here we present four systems Na, graphite, diamond and MgB₂. With these programs their properties, charge density, band structure, density of states can be obtained and with the help of plotting programs their particular characteristics can be studied; type of bond (covalent, ionic, metallic, van der Waals), electrical properties (conductivity, anisotropy). In this form the student can interactively learn to ask questions and obtain answers about the properties of crystalline solids.

K1.00332 Observation of All-Optical Berezinskii-Kosterlitz-Thouless Transition¹, GUOHAI SITU, JASON W. FLEISCHER, Princeton University — The Berezinskii-Kosterlitz-Thouless (BKT) transition is a two-dimensional dynamic phase transition in which vortex creation competes with entropy production. Each factor is logarithmic in energy, with attempts at long-range order restricted by both geometry and thermal fluctuations. The BKT transition has been observed in a variety of quantum systems, including superfluid films, superconductors, and trapped atomic gases, but it is at root a classical process. Here, we demonstrate a classical BKT transition by observing the 2+1D propagation of an optical beam in a photonic lattice. In this system, there is a one-to-one mapping between the discrete nonlinear Schrödinger equation for paraxial propagation and the traditional XY model of condensed matter physics, with thermodynamic averaging replaced by ensemble averaging over initial random phases. We show experimentally that both the number of vortices produced and the universal jump in correlations agree with predictions from mean-field theory. The results give new confirmation of BKT theory, in a purely classical context, and reinforce the use of photonic systems as an experimental testbed for statistical physics.

¹This work was supported by the AFOSR.

K1.00333 Study of the ionic conductivity in Ce_{1/3}NbO₃, JOSE FRANCISCO GOMEZ GARCIA, GUSTAVO TAVIZON, Fac. de Quimica, PABLO DE LA MORA, Fac. de Ciencias, Universidad Nacional Autonoma de Mexico — Ce_{1/3}NbO₃ was synthesized using stoichiometric quantities of CeO₂ and Nb₂O₅ and heated for 48h at 1350°C in air. The electric conductivity was measured in the 25°C-1000°C interval. A small gap of 0.25-0.78eV was found. To study the origin of the transport DFT calculations were carried out; the results show a 0.4eV gap, but since the gaps are not correctly predicted with DFT, a further calculation with a modified Becke-Johnson (mBJ) potential was carried out obtaining a gap of 2eV, but a Ce 4f peak was found at the Fermi energy (E_F). When an intra-atomic repulsion term was added (LDA+U) the Ce 4f peak moved down and a 2.4eV gap was found. The calculations show that the conductivity does not have electronic origin but ionic. Atomistic calculations rule out that the transport is due to the Ce ions; on the other hand, these calculations agree very well with oxygen ions as charge carriers in this material.

K1.00334 Sensitive imaging of electromagnetic fields with cold polar molecules, SERGEY ALYABYSHEV, University of British Columbia, MIKHAIL LEMESHKO, Institute for Theoretical Atomic, Molecular, and Optical Physics Harvard-Smithsonian Center for Astrophysics, ROMAN KREMS, University of British Columbia — Detection of electromagnetic fields from rf to infrared frequency range is required for numerous applications ranging from test of fundamental symmetries to bioimaging. We propose to use polar paramagnetic molecules, such as SrF, CaH and NH, for sensitive parallel detection of electromagnetic fields. We discuss several methods of detection of both electric and magnetic field components in a wide range of detectable frequencies up to a few THz with high sensitivity and μm spatial resolution. Our calculations show that, using a gas of SrF molecules, it is possible to achieve sensitivity to ac fields that is two orders of magnitude higher than with ultracold Rb atoms [1]. Various applications are discussed.

[1] P.Bohi, M.F.Riedel, T.W.Hansch, and P.Treutlein, Appl. Phys. Lett. **97**, 051101 (2010).

K1.00335 Resistively Detected NMR and phonon-assisted dynamical nuclear polarization, GERSON J. FERREIRA, J. CARLOS EGUES, IFSC, USP, Brazil, W.A. COISH, McGill University, Canada — The resistively detected NMR (RDNMR) is used to detect the nuclear spin polarization and relaxation rates via magnetotransport in the quantum Hall regime. The diagonal term of the hyperfine coupling act on the electrons as an effective magnetic field B_n (Overhauser effect) proportional to the nuclear spin polarization. An oscillatory magnetic field with RF frequency in resonance with the nuclear spin splitting destroys the nuclear spin polarization, and thus the effective magnetic B_n . This induces a measurable change in the longitudinal resistance. Here we show that a finite current dynamically enhances the nuclear spin polarization via two processes: (i) near Landau level crossings a first order hyperfine spin-flip dominates, while (ii) away from crossings a second order phonon-assisted hyperfine spin-flip dominates. Our model show quantitative agreement with recent experiments [Zhang et al., PRL 98, 246802 (2007); Dean et. al., PRB, 80, 153301 (2009); Guo et al., PRB 81, 041306 (2010)]. See also [Ferreira et al., PRL 104, 066803 (2010)].

K1.00336 Crystal structure and electronic properties of the oxygen deficient $\text{Sr}_3\text{Ru}_2\text{O}_{7-y}$ ($0 \leq y \leq 0.5$) ruthenate, OLIVER MARTINEZ-ANAYA, GUSTAVO TAVIZON, Facultad de Química, PABLO DE LA MORA, Facultad de Ciencias, ROBERTO ESCUDERO, Instituto de Investigación en Materiales, Universidad Nacional Autónoma de México — In this work a study of the structural properties of the new non-stoichiometric Ruddlesden-Popper type $\text{Sr}_3\text{Ru}_2\text{O}_{7-y}$ compounds is presented. $\text{Sr}_3\text{Ru}_2\text{O}_{7-y}$ ($y = 0.17, 0.23, 0.28, 0.40$ and 0.47) were synthesized by hydrogen reduction of the parent $\text{Sr}_3\text{Ru}_2\text{O}_7$ ruthenate. Rietveld structure refinements were performed to determine the crystal structure of the reduced compounds. Oxygen content of the samples was studied by redox chemical titration and ESR spectra confirmed the presence of Ru^{3+} . Removal of oxygen atoms from the parent compound results in shrinkage of the c and growing of the a lattice parameters, which we related to the Ru^{4+} to Ru^{3+} partial reduction in $\text{Sr}_3\text{Ru}_2\text{O}_7$. On basis of DFT calculations, with WIEN2k code, we compared the electronic properties of reduced and stoichiometric compounds.

K1.00337 Dielectrophoretic Tweezers as a Platform for Single Molecular Force Spectroscopy in a Highly Parallel Format, PENG CHENG, MICHAEL BARRETT, PIERCEN OLIVER, DMITRI VEZENOV, Chemistry Department, Lehigh University — Miniaturization has driven down the cost of tools used in bioanalysis and diagnostics, with single molecules becoming the ultimate detection limit. I will describe how one can exploit mechanical properties of individual biomolecules to determine changes in their state or structure. Our aim is to build a force-spectroscopy-on-a-chip device that can detect and manipulate many (millions) single molecules in parallel. A critical element of this approach is the design of materials properties of molecular handles or probes. By tuning interactions of these probes with electric fields which generate by a simple electrode geometry, we are able to apply piconewton forces to individual DNA molecules and record their response with a single base sensitivity. I will present how we determined the approximate crossover frequency between negative and positive DEP using plain electrodes instead of conventional micro-structures. The technique is attractive not only for conducting single molecule force spectroscopy but also for label-free single cell detection. I will discuss potential applications of this approach to high throughput analyses such as genome sequencing and HIV detection.

K1.00338 New structural phase transitions in PbMBO_4 complex oxides: Raman spectroscopy and x-ray diffraction studies¹, PATRICIA KALITA, ANDREW CORNELIUS, Dept. of Physics and Astronomy, University of Nevada Las Vegas, Las Vegas, NV, USA, KRISTINA LIPINSKA, OLIVER HEMMERS, Harry Reid Center for Environmental Studies, University of Nevada Las Vegas, NV, USA, STANISLAV SINOGEIKIN, Geophysical Lab., Carnegie Institution of Washington, Washington, DC, USA, M. MANGIR MURSHED, THORSTEN GESING, Chemische Kristallographie fester Stoffe, Universität Bremen, Bremen, Germany, HARTMUT SCHNEIDER, Inst. of Crystallography, University of Köln, Köln, Germany — Complex oxides with the mullite crystal structure belong to the most important phase in both traditional and advanced ceramics. Mullites are built of infinite chains of edge-sharing MO_6 octahedra, bridged by various oxide groups. Interest in metal borates stems from their useful nonlinear optical properties. New complex oxides in the mullite family PbMBO_4 ($M = \text{Fe}, \text{Mn}, \text{Al}$) were synthesized and characterized. Using Raman spectroscopy and synchrotron x-ray diffraction at elevated pressure we demonstrate new structural phase transitions.

¹DOE-NNSA DE-FC08-01NV14049. DOE-BES, DOE-NNSA, NSF, DOD TACOM, the W.M. Keck Found. DOE-BES, W-31-109-ENG-38

K1.00339 Spin-orbit coupling in GaN/AlGaN wurtzite quantum wells¹, POLIANA H. PENTEADO, J.Y. FU, ESIMERINDO BERNARDES, J. CARLOS EGUES, University of São Paulo — We investigate the spin-orbit coupling for electrons in wurtzite quantum wells with two subbands [1]. By folding down the 8×8 Kane model, accounting for the s-pz orbital mixing [2, 3] absent in zincblende structures, we derive an effective 2×2 Hamiltonian for the conduction electrons. In this derivation we consider the renormalization of the spinor component of the conduction band wave function, which is crucial to properly obtain the corresponding spin-orbit couplings. In addition to the Rashba-type term arising from the bulk inversion asymmetry of the wurtzite lattice, we obtain the usual linear in momentum Rashba term induced by the structural inversion asymmetry of the well and; interestingly, we also find a new Rashba-like contribution. The spin-orbit coupling parameters are obtained via a self-consistent calculation. For completeness, the Dresselhaus term is also included in our calculation.

[1] Rafael S. Calsaverini, Esmerindo Bernardes, J. Carlos Egues, and Daniel Loss, Phys. Rev. B 78, 155313 (2008).

[2] L. C. Lew Yan Voon, M. Willatzen, and M. Cardona, Phys. Rev. B 53, 10703 (1996).

[3] J. Y. Fu and M. W. Wu, J. Appl. Phys 104, 093712 (2008).

¹The authors acknowledge financial support from FAPESP, CNPq, and CAPES.

K1.00340 Decoherence Times of Rabi Oscillations in Micro-Plasmas¹, DMITRI ROMANOV, GEORGE HECK, ALEX FILIN, ROBERT LEVIS, Center for Advanced Photonics Research, Temple University — We study the broadband Rabi oscillations supported by excited states of oxygen atoms in a microplasma. The contrast of characteristic fringe patterns of spectral interference in dynamic Rabi sidebands is determined by decoherence phenomena in a nonequilibrium underdense microplasma channel formed in atmospheric-pressure oxygen gas via interaction with a femtosecond pump pulse. We have established the decoherence rate as a function of the pump pulse intensity, and we have traced the evolution of the decoherence rate as the microplasma evolved toward equilibrium. The rate increases with the pump laser intensity and decreases with the delay with corresponding decoherence times in the range of 750 fs to 3 ps, in good agreement with theory revealing that electron scattering dominates the dynamics for the subnanosecond relaxation processes. The results provide insight into both the behavior of the transient effective two-state systems and the evolution of the characteristics of the laser-generated microplasma.

¹We gratefully acknowledge financial support through the AFOSR MURI grant FA9550-10-1-0561

K1.00341 Formation of Alkaline Earth Template Layers for Oxide Epitaxy on Semiconductors: Surface Alloying and Self-Organization, BORIS LUKANOV, KEVIN GARRITY, JAMES REINER, FRED WALKER, SOHRAB ISMAIL-BEIGI, ERIC ALTMAN, Yale University — The finding that Sr and Ba titanates can be grown epitaxially on Si and Ge (100) surfaces without oxidizing the semiconductor and with atomically abrupt interfaces, has spurred research into exploiting these materials for high-k gate dielectrics and for integrating new functionality into traditional semiconductor devices. To date, all successful oxide epitaxy on Si and Ge (100) surfaces has required the initial formation of a sub-monolayer of an alkaline earth metal. To understand how this layer promotes oxide epitaxy, we have been using scanning tunneling microscopy complemented by electron diffraction and density functional theory to characterize the formation of the template layer on the atomic scale. The results reveal a complex series of phase transitions as Sr is deposited onto Ge(100). Interestingly, each phase transition is accompanied by drastic changes in the surface morphology that can only be explained by formation of an alloy surface. Through comparison of atomic-resolution STM images with DFT predictions, structural models of two of the surface alloy phases have been deduced. Incorporation of the larger alkaline earth atoms into the surface creates strain that is ultimately relieved by the formation of remarkably well-ordered arrays of stripes and trenches. The alloy formation leads to double-height steps on the surface, resulting in unidirectional trenches and nanowires extending for thousands of Angstroms.

K1.00342 Photothermal Therapy of Cancer Cells mediated by Blue Hydrogel Nanoparticles, TAEYJUANA CURRY, Department of Physics, University of Michigan, Ann Arbor, MI, USA 48109, TAMIR EPSTEIN, H. Lee Moffitt Cancer Center & Research Institute, Tampa, FL, USA 33612, RAOUL KOPELMAN, Department of Chemistry, University of Michigan, Ann Arbor, MI, USA 48109 — Coomassie Blue dye has been covalently linked into a polyacrylamide nanoparticle matrix, so as to form nontoxic, biologically compatible, biodegradable and cell-specific targetable nanoparticles for photothermal therapy (PTT) of cancer. The nanoparticles were found to be approximately 80-95 nm in diameter, with an absorbance value of 0.52. Using an inexpensive, low intensity LED array light source (590nm, 25mW/cm²), with 20 minute excitation times, at 37°, PTT induced hyperthermia/thermolysis in HeLa cells, in vitro, resulting in virtually complete cell death when observed 3 hours after exposure. These multifunctional particles have been previously used in cancer delineation, for surgery, and in photoacoustic imaging studies; the addition of the PTT function now enables a multi-pronged medical approach to cancer.

K1.00343 Entangled Photon Fluorescence with Organic Conjugated Dendrimers, LESLIE UPTON, THEODORE GOODSON, University of Michigan — The use of entangled photons for spectroscopy is a novel technique with several potential applications in entangled two-photon excited fluorescence microscopy, quantum imaging and remote sensing. Classical TPA depends quadratically on the input photon flux, whereas, non-classical entangled two-photon absorption (ETPA) has a linear dependence on input flux rate. The total TPA rate measured using an entangled photon source is given by the summation of the ETPA rate and the random TPA rate. This work focuses on the entangled two-photon absorption cross-section and the entangled two-photon fluorescence efficiency of a G1 Dendrimer. From these results, it is shown that the entangled two-photon excited fluorescence of the G1 Dendrimer has a linear dependence at low input photon fluxes. This result has great impact on spectroscopy where the need for small numbers of photons is great, such as microscopy and sensing.

Tuesday, February 28, 2012 2:30PM - 5:30PM –

Session L1 DMP GIMS: Focus Session: Imaging and Modifying Materials at the Limits of Space and Time Resolution 203

2:30PM L1.00001 In-Situ Transmission Electron Microscopy with Nanosecond Temporal Resolution¹, NIGEL BROWNING, Pacific Northwest National Laboratory — The dynamic transmission electron microscope (DTEM) can obtain both high spatial (~1nm or better) and high temporal (~1μs or faster) resolution. The high temporal resolution is achieved by using a short pulse laser to create the pulse of electrons through photo-emission. This pulse of electrons is propagated down the microscope column in the same way as in a conventional high-resolution TEM. The only difference is that the spatial resolution is limited by the electron-electron interactions in the pulse (a typical 10ns pulse contains ~10⁹ electrons). To synchronize this pulse of electrons with a particular dynamic event, a second laser is used to “drive” the sample a defined time interval prior to the arrival of the laser pulse. The important aspect of the DTEM is that one pulse of electrons is used to form the whole image, allowing irreversible transitions and cumulative phenomena such as nucleation and growth, to be studied directly in the microscope. The use of the drive laser for fast heating of the specimen presents differences and several advantages over conventional resistive heating *in-situ* TEM – such as the ability to drive the sample into non-equilibrium states. So far, the drive laser has been used for *in-situ* processing of nanoscale materials, rapid and high temperature phase transformations, and controlled thermal activation of materials. In this presentation, a summary of the development of the DTEM and *in-situ* stages to control the environment around the specimen will be described. Particular attention will be paid to the potential for gas stages to study catalytic processes and liquid stages to study biological specimens in their live hydrated states. The future potential improvements in spatial and temporal resolution that can be expected through the implementation of upgrades to the lasers, electron optics and detectors will also be discussed.

¹Pacific Northwest National Laboratory is operated by Battelle Memorial Institute for the U.S. Department of Energy under Contract No. DE-AC05-76RL01830.

3:06PM L1.00002 Design and performance of a Near Ultra High Vacuum Helium Ion Microscope, BENE POELSEMA, RAOUL VAN GASTEL, GREGOR HLAWACEK, HAROLD J.W. ZANDVLIET, Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, P.O.Box 217, 7500 AE Enschede — The advent of He Ion Microscopy (HIM) as a new nanoscopic technique to image materials has enabled a new look at materials that is based on the interaction of swift light ions with matter. Initial HIM instruments have demonstrated high-resolution imaging, combined with great surface sensitivity, the ability to neutralize charge very efficiently, and with enhanced materials contrast when ion induced secondary electrons are used for imaging. To achieve ultimate performance, the chamber vacuum of the existing platform may be improved. For instance, carbon deposits due to beam interaction are readily seen due to the surface sensitivity of the technique. At high current densities the sharply focused beam may very efficiently decompose residual hydrocarbons. Not only can this obscure a clear view of the sample, thereby negating the benefits of the small spot size, it also limits the available acquisition time. This has proven extremely useful for nanopatterning for sensors, and other device fabrication applications at the sub-10nm level. However, it is undesirable when the instrument is used for materials characterization. We will discuss the basic considerations that went into the design of a Near-UHV He Ion Microscope [1]. First applications that the instrument was used for will be highlighted and its impact in surface physics and other research areas that require increased imaging sensitivity will be discussed.

[1] R.van Gastel et al, *Microscopy and Microanalysis* **17**, 928-929 (2011)

3:18PM L1.00003 Instrumentation Development for Dynamic Atom Probe Tomography¹, BRIAN GORMAN, DAVID DIERCKS, Colorado School of Mines — Atom probe tomography (APT) is a materials characterization technique widely recognized as having the highest combined spatial (sub-nm) and chemical (less than 10^{17} atoms / cm^3) resolution. This imaging time of flight mass spectrometry technique typically utilizes laser pulsed field emission in semiconductors and dielectrics. Laser pulsed field emission is widely considered to be a thermal effect, with specimen temperatures from 100 K to greater than 1500 K observed. Following the thermal spike, specimens typically cool to their base temperature in less than 5 ns, depending upon their thermal transport and geometry. Combining the laser pulsed atom probe experiment with pulsed transmission electron diffraction will enable thermal annealing and quenching experiments at atomic resolution with nanosecond temporal resolution. The combined instrument, titled a Dynamic Atom Probe, will be used to monitor solid state processes including solute drag effects on grain boundary motion, atomic scale kinetics of crystallization in amorphous semiconductors and oxides, atomic scale nucleation and spinodal decomposition kinetics in oxides, and phase transformations in metallic alloys. This discussion will include the specifics of the instrumentation currently under development as well as proof of principle first experiments.

¹Funding provided by NSF-DMR under award # 1040456.

3:30PM L1.00004 Simulation of ultrashort photoelectron pulses as a guide for developing reliable ultrafast electron diffraction systems¹, JENNI PORTMAN, HE ZHANG, ZHENSHENG TAO, CHONG-YU RUAN, MARTIN BERZ, PHILLIP DUXBURY, Michigan State University — The development of a reliable experimental ultrafast electron diffraction and imaging system requires a theoretical understanding of the underlying physical phenomena and an accurate modeling of the optical elements present in the beam column. To achieve this goal, we have developed two types of computer simulations: a mean-field Gaussian approximation, in which the linear effects of realistic optical elements are incorporated. Due to the limitations inherent in the theory, it fails to capture the intricate behavior of a real system but it is computationally very inexpensive and offers valuable information on the relevant parameter ranges. The second type of simulation considered is an explicit N particle model which uses a O(N) method for calculating the space charge effects, enabling simulations of over one million electrons in a pulse. While being computationally very expensive, it offers the advantage of incorporating realistic descriptions for the electromagnetic fields of the optical elements, along with their linear and non-linear contributions. The results of this work show the limits of the validity of the mean-field approach and offer a detailed and highly accurate physical description of the beam dynamics under different operational regimes.

¹This work was supported by the National Science Foundation under Grant No. NSF-DMR 1126343

3:42PM L1.00005 Charged nanoparticle dynamics in water induced by scanning transmission electron microscopy¹, E.R. WHITE, MATTHEW MECKLENBURG, BRIAN SHEVITSKI, S.B. SINGER, B.C. REGAN, UCLA Department of Physics and Astronomy & CNSI — Using scanning transmission electron microscopy we image ~ 4 nm platinum nanoparticles deposited on an insulating membrane, where the membrane is one of two electron-transparent windows separating an aqueous environment from the microscope's high vacuum. Upon receiving a relatively moderate dose of $\sim 10^4 e^-/\text{nm}^2$, initially immobile nanoparticles begin to move along trajectories that are directed radially outward from the center of the field of view. As the dose rate is increased the particle motion becomes increasingly dramatic. These observations demonstrate that even under mild imaging conditions, the *in situ* electron microscopy of aqueous environments can produce charging effects that dominate the dynamics of nanoparticles under observation. Such effects provide a new tool for modifying *in vitro* environments such as those used for TEM studies of wet biological systems.

¹Supported by the ACS Petroleum Research Fund, NSF CAREER Award 0748880, and the EICN at UCLA.

3:54PM L1.00006 Coherent X-ray microscopy of real materials at 10nm resolution, ANDREAS MENZEL, Paul Scherrer Institut — Coherent X-ray microscopy replaces image-forming optics by mathematical algorithms to “reconstruct” the micrograph from the distribution of scattered light. In case of X-rays, its popularity is largely based on its ability to alleviate limitations of resolution and efficiency of available optics. Various methodologies have been developed, and high resolving power could be demonstrated. Yet, stringent constraints on sample preparation and data quality had to be addressed before the technique could advance from proof of principle studies to application. About a decade after the first demonstration using X-rays [J.W. Miao et al., Nature 400 (1999) 342] coherent diffractive imaging (CDI) seems to have matured into a microscopy technique that proves useful in real-life scientific investigations. The major coherent diffractive imaging methods will be reviewed, i.e., its original implementation using plane waves, the so-called Fresnel CDI that exploits curvature in the illuminating wavefront, and ptychographic CDI, which is a scanning microscopy method using multiple exposures. Being fully compatible with spectroscopic contrast channels makes quantitative structural, chemical, and magnetic information accessible, and the penetration power of X-rays can be exploited by tomographic or ab initio reconstruction methods in order to yield three-dimensional reconstructions with high resolution, high specificity, and high dose efficiency. These recent advances have turned coherent X-ray microscopy into a reliable and robust method that is attractive for scientists independent on how (un-)familiar they are with X-ray microscopy. Applications from the materials and life sciences will be discussed.

4:30PM L1.00007 Time-Resolved Near-Edge Coherent Diffractive Imaging, FABIAN WEISE, DANIEL NEUMARK¹, STEPHEN R. LEONE², OLIVER GESSNER, Ultrafast X-ray Science Laboratory, Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA — Coherent diffractive imaging (CDI) with x-rays is a well-established technique that provides structural information beyond the limitations of optical microscopy. Free electron lasers provide ultrashort x-ray pulses with sufficiently high peak brightness to facilitate single-shot imaging and the extension of CDI into the time-domain. Recent progress in the generation of spatially coherent ultrashort x-ray pulses by high harmonic generation (HHG) using tabletop lasers lead to the emergence of a new field of laboratory-based CDI. While a relatively low photon flux and limited photon energies result in lower imaging resolution compared to x-ray studies at large-scale facilities, the significantly greater availability makes laboratory-based experiments well suited for developing new CDI techniques. We present a new apparatus for CDI, which provides ultrashort XUV pulses with tunable photon energies. By implementing a monochromator in a HHG-based CDI setup, the photon energy can be tuned to the inner-shell absorption edges of different elements in the sample. The wavelength-dependence of the x-ray optical constants close to the resonances facilitates to exploit the element selectivity and chemical sensitivity of x-ray transitions in time-domain CDI experiments.

¹and Department of Chemistry, University of California, Berkeley

²and Departments of Chemistry and Physics, University of California, Berkeley

4:42PM L1.00008 In-situ proton radiography of solidification in Sn-Bi, Al-Cu, Al-In and Bi-Ga melts¹, JASON COOLEY, AMY CLARKE, CHRISTOPHER MORRIS, BRIAN HOLLANDER, TIM TUCKER, Los Alamos National Laboratory, THOMAS OTT, Florida State University, ROBERT FIELD, DAVID KORZEKWA, DUNCAN HAMMON, KESTER CLARKE, PATRICK KENNEDY, FRANK MERILL, FESSAHA MARIAM, Los Alamos National Laboratory, MARTHA BARKER, New Mexico Institute of Mining and Technology, JAMES FOLEY, ROBERT AIKIN, JOSHUA HILL, DAN THOMA, Los Alamos National Laboratory, FINIAN O'NEILL, Boston College, MEGAN EMIGH, New Mexico Institute of Mining and Technology, BO FOLKS, Los Alamos National Laboratory — In-situ observation of the solidification phenomena in metals can lead to better understanding and control of microstructure evolution. Proton radiography offers the ability to image thick samples of high z material. Recently, in-situ proton radiography was used to directly observe dynamic processes during melting and solidification in bulk binary alloy systems. The spatial resolution was ~65 microns for a 44 x 44 mm² field of view. The time scale of each experiment was 2 to 6 hours. The data collected allowed for the determination of solidification front velocities, captured the changes in solid/liquid densities and showed evidence of convective fluid flow in the melt. Microstructural features larger than approximately 100 microns in the solid phase were observed.

¹Work at Los Alamos supported by NNSA and the Department of Energy

4:54PM L1.00009 True Attosecond Imaging of Inhomogeneous Systems with Standing-Wave Inelastic X-Ray Scattering¹, YU GAN, PETER ABBAMONTE, University of Illinois at Urbana-Champaign — Inelastic X-ray scattering (IXS) has recently been used to image electron dynamics at the attosecond scale, but it has been shown that these images are spatially averaged. The problem is that the existing technique can only access the “diagonal” ($k_1 = -k_2$) elements of the electron density response $\chi(k_1, k_2, \omega)$. It has been shown, however, that inelastic X-ray scattering at the Bragg position is sensitive to the entire response $\chi(k_1, k_2, \omega)$. With this method, a standing wave field is established in the sample by exciting a Bragg condition, allowing access to all the off-diagonal ($k_1 \neq -k_2$) elements of χ . In this talk I will present a simple model demonstrating that, in principle, this approach can be used to map the entire density response. In particular, I show that a one-dimensional system is experimentally impossible to probe, a two-dimensional system is experimentally accessible but typically difficult to measure in practice, and a three-dimensional system is experimentally both plausible and practicable. Finally, I propose possible experimental realizations of this technique.

¹This work was supported by DOE grants DE-FG02-07ER46453 and DE-AC02-06CH11357

5:06PM L1.00010 Sub-Picosecond Dynamics of Displacement Cascades¹, BENNETT LARSON, JON TISCHLER, ROGER STOLLER, YURI OSETSKIY, Oak Ridge National Laboratory, CHRISTIAN DAVID, Paul Scherrer Institute — Sub-picosecond x-ray pulses produced by the Linac Coherent Light Source (LCLS) now enable real time experimental measurements of atomic displacement cascade structure and dynamics on sub-picosecond time scales. Such measurements will make possible the first direct experimental test of molecular dynamics (MD) displacement cascade simulations. Here we will discuss the potential to use single, seeded, 100-fs LCLS hard x-ray pulses focused to ~100 nm diameter by diamond-based Fresnel zone plate optics to make real-time diffuse scattering measurements on 50 keV Ar-ion-induced cascades in thin single-crystal samples. We will present x-ray Bragg diffuse scattering calculations based on ~4M atom, 25 keV primary knock-on energy MD cascade simulations demonstrating that temporally-random, 100 fs LCLS x-ray pulse measurements of diffuse scattering near low index Bragg reflections can be time-ordered from sub-picoseconds to a few picoseconds. Time ordering is made possible in this regime by the distinct nature of diffuse scattering profiles as a function of time that are produced by shock-induced pressure waves according to MD cascade simulations in Fe. The expected results and the experimental challenges anticipated to perform such measurements will be discussed.

¹Research at ORNL supported as part of the Center for Defect Physics, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science.

5:18PM L1.00011 Nanostructure Formation on Sb₂Te₃ Thin Films Induced by Femtosecond Laser Irradiation¹, YUWEI LI, VLADIMIR A. STOICA, LYNN ENDICOTT, GUOYU WANG, Dept. of Physics, Univ. of Michigan, HUARUI SUN, KEVIN. P. PIPE, Dept. of Mechanical Engineering, Univ. of Michigan, CTIRAD UHER, ROY CLARKE, Dept. of Physics, Univ. of Michigan — Sb₂Te₃ has applications in thermoelectrics, phase-change memory devices and topological insulators. In the case of thermoelectricity, nanostructure formation in this type of material has been predicted to enhance its figure of merit for thermal energy conversion. Here, we present our results on modification of the surface morphology of Sb₂Te₃ thin films after femtosecond laser irradiation. Under a narrow range of laser fluence and irradiation time, long and highly-aligned nanotracks were formed in the plane of the film, having a periodicity 10 times smaller than the irradiation laser wavelength. The laser fluence and irradiation time can result in different surface nanostructure morphologies with varying degrees of order. Finally, using an optical pump-probe technique, we find that the laser-irradiated nanostructured areas of the film have a lower thermal conductivity compared to that of the reference smooth areas not irradiated by the laser. Such Sb₂Te₃ nanostructures can be important for thermoelectric applications as well as for further studies of femtosecond laser interaction with opaque materials.

¹This work is supported as part of the Center for Solar and Thermal Energy Conversion, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award No. De-SC00000957

Tuesday, February 28, 2012 2:30PM - 5:30PM – Session L2 DPB FIP: Invited Session: Andrei Sakharov Prize Session 204AB

2:30PM L2.00001 A. Sakharov and Fusion Research¹, BRUNO COPPI, MIT — In the landmark paper by Tamm and Sakharov [1], a controlled nuclear fusion reactor based on an axisymmetric magnetic confinement configuration whose principles remain valid to this day, was proposed. In the light of present understanding of plasma physics the virtues (e.g. that of considering the D-D reaction) and the shortcomings of this paper are pointed out. In fact, relatively recent results of theoretical plasma physics (e.g. discovery of the so called second stability region) and advances in high field magnet technology have made it possible to identify the parameters of meaningful experiments capable of exploring D-D and D-³He burn conditions. At the same time an experimental program (IGNIR) has been undertaken through a (funded) collaboration between Italy and Russia to investigate D-T plasmas close to ignition conditions based on an advanced high field toroidal confinement configuration. A. Sakharov envisioned a bolder approach to fusion research than that advocated by some of his contemporaries. The time taken to design and decide to fabricate the first experiment capable of reaching ignition conditions is due in part to the problem of gaining an adequate understanding the expected physics of fusion burning plasmas. However, most of the relevant financial effort has gone in the pursuit of slow and indirect enterprises complying with the “playing it safe” tendencies of large organizations or motivated by the purpose to develop technologies or maintain a high level of expertise in plasma physics to the expected benefit of other kinds of endeavors. The creativity demonstrated by A. Sakharov in dealing with civil rights and disarmament issues is needed, while maintaining our concerns for energy and the environment on a global scale, to orient the funding for fusion research toward a direct and well based scientific effort on concepts for which a variety of developments can be envisioned. These can span from uncovering new physics relevant, for instance, to high energy astrophysics to the feasibility of new neutron sources.

[1] A. Sakharov, Collected Scientific Works (Publ. Marcel Dekkes, Inc., New York, N.Y., 1982).

¹Sponsored in part by the US Department of Energy.

3:06PM L2.00002 CP Violation and the Matter Anti-Matter Asymmetry of the Universe¹

ROBERT CAHN, Lawrence Berkeley National Laboratory — There is no scientific question more fundamental than “Why are we here?” or as we physicists might phrase it “Why is there more matter than anti-matter?” Because, as Andrei Sakharov first showed, CP violation is necessary to any explanation of the matter anti-matter asymmetry, CP violation is the focus of much of the international experimental program in particle physics. CP conservation was what could be salvaged after parity was overthrown in 1956, but it survived only until 1964 when K mesons were found not to respect it. While parity violation was a large effect in weak interactions, CP violation seemed small and confined to the kaons. When the Standard Model of particle physics emerged in early 1970's, Kobayashi and Maskawa observed that if there were three families of quarks, CP violation would arise quite naturally. The Standard Model suggested that CP violation could be large in decays of B mesons. Nonetheless, no matter what parameters are used in the Standard Model, CP violation among quarks cannot be large enough to explain the matter anti-matter asymmetry. Major experiments in the U.S. and Japan were undertaken to explore CP violation in B mesons to search for signs of CP violation outside the Standard Model, which might explain the dominance of matter over anti-matter. Neither experiment found such a discrepancy, but new programs will continue this search with much higher statistics. While the three families of leptons are in many ways analogous to the three families of quarks, the neutrinos have a unique character. As neutral particles, it is possible that they are their own antiparticles. If this is so, there may be additional, very heavy, neutrinos beyond those we know already. If they violate CP they may be the source of the matter anti-matter asymmetry. But do neutrinos experience CP violation? Experiments around the world are just now setting out to answer this question.

¹Supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231

3:42PM L2.00003 Sakharov and his Times , TATIANA YANKELEVICH, Harvard — No abstract available.

4:18PM L2.00004 Sakharov Prize Lecture , RICHARD WILSON, Harvard University — No abstract available.

4:54PM L2.00005 Scientists and Human Rights , YOUSEF MAKDISI, Brookhaven National Laboratory — The American Physical Society has a long history of involvement in defense of human rights. The Committee on International Freedom of Scientists was formed in the mid seventies as a subcommittee within the Panel On Public Affairs “to deal with matters of an international nature that endangers the abilities of scientists to function as scientists” and by 1980 it was established as an independent committee. In this presentation I will describe some aspects of the early history and the impetus that led to such an advocacy, the methods employed then and how they evolved to the present CIFS responsibility “for monitoring concerns regarding human rights for scientists throughout the world”. I will also describe the current approach and some sample cases the committee has pursued recently, the interaction with other human rights organizations, and touch upon some venues through which the community can engage to help in this noble cause.

Tuesday, February 28, 2012 2:30PM - 5:30PM –

Session L3 DCMP: Invited Session: Fermiology of Electron and Hole Doped Cuprates - A Guide to High Temperature Superconductivity 205AB

2:30PM L3.00001 Hidden Fermi Liquid: Self-Consistent Theory for the Normal State of High-Tc Superconductors , PHILIP ANDERSON, Princeton Univ — No abstract available.

3:06PM L3.00002 Quantum oscillations and nodal pockets from Fermi surface reconstruction in the underdoped cuprates , NEIL HARRISON¹, Los Alamos National Laboratory — Fermiology in the underdoped high T_c cuprates presents us with unique challenges, requiring experimentalists to look deeper into the data than is normally required for clues. Recent measurements of an oscillatory chemical potential affecting the oscillations at high magnetic fields provide a strong indication of a single type of carrier pocket. When considered in conjunction with photoemission and specific heat measurements, a Fermi surface comprised almost entirely of nodal pockets is suggested. The mystery of the Fermi surface is deepened, however, by a near doping-independent Fermi surface cross-sectional area and negative Hall and Seebeck coefficients. We explore ways in which these findings can be reconciled, taking an important hint from the diverging effective mass yielded by quantum oscillations at low dopings. The author wishes to thank Suchitra Sebastian, Moaz Atarawneh, Doug Bonn, Walter Hardy, Ruixing Liang, Charles Mielke and Gilbert Lonzarich who have contributed to this work. The work is supported by the NSF through the NHMFL and by the DOE project “Science at 100 tesla.”

¹NHMFL

3:42PM L3.00003 Phase competition in trisected superconducting dome , INNA VISHIK, Stanford University — The momentum-resolved nature of angle-resolved photoemission spectroscopy (ARPES) has made it a key probe of emergent phases in the cuprates, such as superconductivity and the pseudogap, which have anisotropic momentum-space structure. ARPES can be used to infer the origin of spectral gaps from their distinct phenomenology—temperature, doping, and momentum dependence, and this principle has been used to argue that the pseudogap is a distinct phase from superconductivity, rather than a precursor [1]. We have studied $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (Bi-2212) using laser-ARPES, and our data give evidence for three distinct quantum phases comprising the superconducting ground state, accompanied by abrupt changes at $p \sim 0.076$ and $p \sim 0.19$ in the doping-and-temperature dependence of the gaps near the bond-diagonal (nodal) direction [2]. The latter doping likely marks the quantum critical point of the pseudogap, while the former represents a distinct competing phase at the edge of the superconducting dome. Additionally, we find that the pseudogap advances closer towards the node when superconductivity is weak, just below T_c or at low doping, and retreats towards the antinode well below T_c and at higher doping. This phase competition picture together with the two critical doping are synthesized into our proposed phase diagram, which also reconciles conflicting phase diagrams commonly used in the field. Our results underscore the importance of quantum critical phenomena to cuprate superconductivity, provide a microscopic picture of phase competition in momentum space, and predict the existence of phase boundaries inside the superconducting dome which are different from simple extrapolations from outside the dome.

[1] I. M. Vishik, W. S. Lee, R.-H. He, M. Hashimoto, Z. Hussain, T. P. Devereaux, and Z.-X. Shen. *New J. Phys.* **12**, 105008 (2010).

[2] I. M. Vishik, M. Hashimoto, R.-H. He, W. S. Lee, F. Schmitt, D. H. Lu, R.G. Moore, C. Zhang, W. Meevasana, T. Sasagawa, S. Uchida, K. Fujita, S. Ishida, M. Ishikado, Y. Yoshida, H. Eisaki, Z. Hussain, T. P. Devereaux, and Z.-X. Shen, *Submitted* (2011).

4:18PM L3.00004 Novel Magnetism in the Pseudogap Phase of the Cuprates¹, MARTIN GREVEN, University of Minnesota — Magnetic correlations might cause the superconductivity in the cuprates and are generally believed to be antiferromagnetic. Following our success in growing sizable crystals of the tetragonal compound $\text{HgBa}_2\text{CuO}_{4+\delta}$ [1], we used polarized neutron diffraction to demonstrate that the unusual magnetic order previously observed in $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$ [2] is a universal property of the pseudogap phase [3]. Subsequent inelastic neutron scattering experiments revealed several accompanying, weakly-dispersive magnetic excitation branches in $\text{HgBa}_2\text{CuO}_{4+\delta}$ [4]. Unlike antiferromagnetism, the novel magnetic order does not break the lattice translational symmetry. Nevertheless, the excitations mix with conventional antiferromagnetic fluctuations. Our results point toward the need for a multi-band description of the cuprates, and they are consistent with the notion that the phase diagram is controlled by an underlying quantum critical point [5]. The neutron scattering results will be discussed together with new dc resistivity data for the pseudogap phase of $\text{HgBa}_2\text{CuO}_{4+\delta}$ [6].

[1] X. Zhao *et al.*, Adv. Mat. **18**, 3243 (2006).

[2] B. Fauque *et al.*, Phys. Rev. Lett. **96**, 197001 (2006).

[3] Y. Li *et al.*, Nature **455**, 372 (2008).

[4] Y. Li *et al.*, Nature **468**, 283 (2010), and unpublished results.

[5] C. Varma, Nature **468**, 184 (2010).

[6] N. Barisic *et al.*, unpublished results.

¹Work supported by DOE BES.

4:54PM L3.00005 From Spin Liquid to High T_c Superconductors, PATRICK A. LEE, MIT — The discovery of high T_c superconductors has revived interest in Anderson's resonating valence bond theory (RVB) of a quantum spin liquid, first proposed in 1973. In the past few years, several examples of quantum spin liquids have been discovered experimentally. The organic spin liquid has been studied most thoroughly and shows strong evidence for emergent fermionic spinons. I shall review some of the data and argue that theories based on slave particles and gauge fields have been successful in accounting for these remarkable data. The question remains as to whether a similar formulation of fermionic spinon and bosonic holes can form the basis for a theory of high T_c superconductors. I shall show that a recent modification¹ of the mean field RVB phase diagram can explain a lot of the phenomenology. I shall also attempt to put this theory in the context of recent discoveries concerning symmetry breaking in the pseudogap phase.

¹T. Senthil and P.A. Lee, Phys. Rev. Lett. **103**, 076402 (2009).

Tuesday, February 28, 2012 2:30PM - 5:18PM –

Session L4 DAMOP: Focus Session: Numerical Methods for Studying Nonequilibrium Many-Body Dynamics; DMRG, DMFT, Truncated Wigner Approximation, Exact Diagonalization 205C

2:30PM L4.00001 Finite temperature DMRG and the Drude weight of spin 1/2 Heisenberg chains, CHRISTOPH KARRASCH, JENS BARDARSON, JOEL MOORE, University of California at Berkeley — We propose an easy-to-implement approach to study time-dependent correlation functions of one dimensional systems at finite temperature T using the density matrix renormalization group (DMRG). If the auxiliary degrees of freedom which purify the statistical operator are time-evolved with the physical Hamiltonian but reversed time, the entanglement blow-up inherent to any time-dependent DMRG calculation is dramatically reduced. The numerical effort of finite temperature DMRG becomes comparable to that at $T = 0$, and thus significantly longer timescales can be reached. We exploit this to investigate current correlation functions of the XXZ spin 1/2 Heisenberg chain. At intermediate to large T , we can explicitly extract the Drude weight D from the long-time asymptotics. For the isotropic chain, D is finite. At low temperatures, we establish an upper bound for the Drude weight.

2:42PM L4.00002 Universal non-equilibrium quantum dynamics in imaginary time, CLAUDIA DE GRANDI, Yale University, ANATOLI POLKOVNIKOV, ANDERS SANDVIK, Boston University — We propose a method to study the dynamical response of a quantum system by evolving it with an imaginary-time dependent Hamiltonian. The leading non-adiabatic response of the system driven to a quantum-critical point is universal and characterized by the same exponents in real and imaginary time. For a linear quench protocol, the fidelity susceptibility and the geometric tensor naturally emerge in the response functions. Beyond linear response we extend the finite-size scaling theory of quantum phase transitions to non-equilibrium setups. Imaginary-time dynamics is also amenable to quantum Monte Carlo simulations, which we apply here to quenches of the transverse-field Ising model to quantum critical points in one and two dimensions.

2:54PM L4.00003 The Approach To Typicality in Many-Body Quantum Systems, SAI VINJANAMPATHY, SHAWN DUBEY, LUCIANO SILVESTRI, KURT JACOBS, University of Massachusetts, Boston — The recent discovery that for large Hilbert spaces, almost all (that is, typical) Hamiltonians have eigenstates that place small subsystems in thermal equilibrium, has shed much light on the origins of irreversibility and thermalization. Here we present numerical evidence that many-body lattice systems generically approach typicality as the number of subsystems is increased, and thus provide further support for the eigenstate thermalization hypothesis. We will present our results that indicate that the deviation of many-body systems from typicality scales as an inverse power of the number of systems, and we compare this with the equivalent scaling for random Hamiltonians.

3:06PM L4.00004 Quantum Dynamics of Population-Imbalanced Fermi Mixture in One-dimensional Optical Lattices¹, BIN WANG, Department of Physics and Astronomy, University of Pittsburgh, ERHAI ZHAO, Department of Physics and Astronomy, George Mason University, W. VINCENT LIU, Department of Physics and Astronomy, University of Pittsburgh — We study the (pseudo-)spin dynamics of two-component Fermi mixture with population imbalance in one-dimensional (1D) optical lattices within the framework of 1D Hubbard model, utilizing the time-evolving block decimation (TEBD) algorithm. We consider the situation in which the center region of the system is initially fully occupied and the left-over fully polarized fermions are initially localized on the wings. It is found that for strong interaction the (pseudo-)spin polarization diffuses throughout the system qualitatively in the same way as the diffusion of non-interacting particles in 1D optical lattices. We further look into the time evolution of correlation functions such as pairing correlation and single particle green functions. According to our simulations, the partially polarized inhomogeneous Fermi gas appears to show no tendency of dynamically developing into a FFLO-type of state, contrary to what might have been expected.

¹We acknowledge the support from DARPA OLE.

3:18PM L4.00005 Non-equilibrium dynamics of the driven Hubbard model , ADRIANO AMARICCI, CNR-IOM, uos SISSA Trieste, Via Bonomea 265, 34125 Italy, CEDRIC WEBER, Cavendish Laboratory, Cambridge University, J.J. Thomson Ave. , Cambridge, UK, MASSIMO CAPONE, CNR-IOM, uos SISSA Trieste, Via Bonomea 265, 34125 Italy/Physics Department, University “Sapienza”, Piazzale A. Moro 2, 00185 Rome, Italy, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — We investigate the dynamics of a two-dimensional Hubbard model in a static electric field in order to identify the conditions to reach a non-equilibrium stationary state. For a generic electric field, the convergence to a stationary state requires the coupling to a thermostating bath absorbing the work done by the external force. Following the real-time dynamics of the system, we show that a non-equilibrium stationary state is reached for essentially any value of the coupling to the bath. We map out a phase diagram in terms of dissipation and electric field strengths and identify the dissipation values in which steady current is largest, and correspondingly a suitable entropy function is smallest, for a given field.

3:30PM L4.00006 Probing Phases and Quantum Criticality using Deviations from the Local Fluctuation-Dissipation Theorem¹ , ERIC DUCHON, The Ohio State University, YASUYUKI KATO, Los Alamos National Laboratory, NAOKI KAWASHIMA, University of Tokyo, NANDINI TRIVEDI, The Ohio State University — One of the major open questions in the study of ultracold atom systems is how to obtain the finite temperature phase diagram of a given Hamiltonian directly from experiments.² Previous work in this direction required quantum Monte Carlo simulations to directly model the experimental situation in order to extract quantitative information, clearly defeating the purpose of an optical lattice emulator. We propose a new method that utilizes deviations from a local fluctuation dissipation theorem to construct a finite temperature phase diagram, for the first time, from local observables accessible by *in situ* experimental observations. Our approach extends the utility of the fluctuation-dissipation theorem from thermometry to the identification of quantum phases, associated energy scales and the quantum critical region. We test our ideas using large-scale quantum Monte Carlo simulations of the two-dimensional Bose Hubbard model.³

¹We acknowledge support from NSF DMR-0907275 (ED), ARO W911NF-08-1-0338 (NT) and the DARPA OLE program.

²Q. Zhou, et al., *Phys. Rev. Lett.* **103**, 085701 (2009).

³Y. Kato, et al., *Nature Physics* **4**, 592 - 593 (2008).

3:42PM L4.00007 A new theoretical method to describe nonequilibrium cold atoms in optical lattices , KARLIS MIKELSONS, JIM FREERICKS, Georgetown University, H. R. KRISHNAMURTHY, Indian Institute of Science, Bangalore — We use perturbation theory in the hopping (strong-coupling expansion) to describe the nonequilibrium dynamics of strongly correlated fermions. Our expansion is a self-consistent expansion for the self-energy which goes beyond the RPA and allows for damping and relaxation effects. We apply this method to solve the homogeneous Fermi - Hubbard model driven by an external field. We investigate the damping of Bloch oscillations (for a uniform dc field) and show results for the current, the nonequilibrium density of states and the momentum distribution. We carefully benchmark the technique using the exact sum rules to determine its accuracy and we discuss regions of parameter space where the method no longer converges. This technique is quite competitive with other methods (such as DMFT) in the regions where it converges.

3:54PM L4.00008 A Slave Spin Impurity Solver for Non Equilibrium Dynamical Mean Field Theory , MARCO SCHIRO, Princeton Center for Theoretical Science and Department of Physics, Joseph Henry Laboratories, Princeton University, Princeton, NJ 08544 — The non equilibrium dynamics of strongly correlated electronic systems represents a challenging theoretical problem in condensed matter physics with applications ranging from pump probe experiments in correlated materials to dynamics in ultracold atomic gases. Dynamical Mean Field Theory (DMFT) has emerged in recent years as a powerful theoretical framework to deal with strong correlations in a non perturbative way. Its extension to the out of equilibrium case requires the solution of an auxiliary quantum impurity model in a non equilibrium bath. Here we present an impurity solver for Non Equilibrium DMFT based on a slave spin representation of the fermionic degrees of freedom. We apply this method to study the quench dynamics in the single band fermionic Hubbard model and compare the results with the time dependent Gutzwiller method.

4:06PM L4.00009 A multi-site mean-field theory for cold bosonic atoms in optical lattices¹ , PAWEL PISARSKI, THOMAS MCINTOSH, ROBERT GOODING, EUGENE ZAREMBA, Queen's University — Mean-field theory is one of the most commonly used approximate methods in condensed matter physics. As applied to the Bose-Hubbard model it provides a simple, qualitative explanation of the Mott insulator – superfluid transition. In its usual form, one invokes a superfluid order parameter to decouple the Bose-Hubbard Hamiltonian into a sum of independent site Hamiltonians. Within this single-site mean-field theory (SSMFT) the equilibrium state is determined by minimizing the grand potential with respect to the order parameter. To improve on this procedure we have developed a multi-site mean-field theory (MSMFT), whereby the lattice is partitioned into small clusters which are decoupled by means of the usual mean-field method. The most general decoupling procedure necessitates the assignment of site-dependent order parameters to the sites bounding the cluster. This leads to a non-trivial topology of the grand potential and one finds, in general, that the equilibrium state is a saddle point. As a result, one cannot use a variational principle to locate the equilibrium states of interest. In this talk, we outline the MSMFT we have developed and give an example of its application.

¹Supported by NSERC of Canada

4:18PM L4.00010 Feynman diagrams versus Feynman quantum emulator , KRIS VAN HOUCKE, Ghent University, FÉLIX WERNER, Laboratoire Kastler Brossel, Ecole Normale Supérieure, EVGENY KOZIK, ETH, Zürich, NIKOLAY PROKOF'EV, BORIS SVISTUNOV, University of Massachusetts, Amherst, MARK KU, ARIEL SOMMER, LAWRENCE CHEUK, Massachusetts Institute of Technology, ANDRÉ SCHIROTZEK, Advanced Light Source, Lawrence Berkeley National Laboratory, MARTIN ZWIERLEIN, Massachusetts Institute of Technology — Precise understanding of strongly interacting fermions, from electrons in modern materials to nuclear matter, presents a major goal in modern physics. However, the theoretical description of interacting Fermi systems is usually plagued by the intricate quantum statistics at play. Here we present a cross-validation between a new theoretical approach, Bold Diagrammatic Monte Carlo (BDMC), and precision experiments on ultra-cold atoms. Specifically, we compute and measure with unprecedented accuracy the normal-state equation of state of the unitary gas, a prototypical example of a strongly correlated fermionic system. Excellent agreement demonstrates that a series of Feynman diagrams can be controllably resummed in a non-perturbative regime using BDMC. This opens the door to the solution of some of the most challenging problems across many areas of physics.

4:30PM L4.00011 Non-equilibrium dynamics, heating, and thermalization of cold atoms in optical lattices, ANDREW DALEY, University of Pittsburgh — In recent years, out of equilibrium many-body dynamics have become accessible in a controlled way in experiments with ultracold quantum gases. Time-dependent processes in these systems are not only intrinsically interesting, but also extremely important for understanding many-body state preparation, heating, and thermalization as they arise in experiments. They also offer new connections to phenomena studied in solid-state systems. This interest has been complemented by the development of a range of numerical methods, including time-dependent density matrix renormalization group (t-DMRG) methods and matrix product state approaches, which have been applied to study dynamics in 1D lattice systems and spin chains. We have extended and applied these methods to study the non-equilibrium dynamics of cold atoms in optical lattices arising from different heating mechanisms, especially due to spontaneous emissions from incoherent scattering of the lattice light, or via classical noise on the optical potential. Understanding how these heating mechanisms affect the properties of different many-body states is crucial in addressing current experimental challenges in the preparation of interesting quantum phases at low temperatures. The resulting non-equilibrium dynamics typically depend strongly on the properties of the many-body state, with different states being more or less sensitive to different heating mechanisms. Moreover, there is often a separation of timescales between some excitations that thermalize rapidly, and some that do not properly thermalize in the duration of an experimental run, which can strongly modify, and even reduce the overall effects of the heating processes. Part of this work involves the treatment of open many-body quantum systems, where we derive many-body master equations to describe the dynamics and solve these numerically by combining t-DMRG methods with quantum trajectory techniques from quantum optics.

5:06PM L4.00012 Pattern formation in time-of-flight images of heavy-light mixtures of atoms undergoing Bloch oscillations¹, JAMES FREERICKS, Department of Physics, Georgetown University — Nonequilibrium dynamical mean-field theory is employed to solve for the response of a light-heavy Fermi-Fermi mixture of atoms to the presence of a uniform electric field (via “pulling” the lattice through the cloud of atoms). When we express the (momentum-dependent) light atom distribution functions as functions of the band energy and the projection of the velocity along the direction of the artificial electric field, the system develops characteristic spiral patterns that become more complex as the system evolves, but remain stable for a long period of time. These patterns typically show a contrast of about 10-20% fluctuations about the mean density, so they are challenging but possible to observe in a time-of-flight measurement. We also show a characteristic change of character of the system between small fields and large fields. The best candidate system for examining these patterns is a $\text{Li}^6\text{-K}^{40}$ mixture on a two-dimensional optical lattice. We expect similar results should occur for light Fermi-heavy Bose mixtures as well, but it is likely this behavior will not be seen in Bose-Bose mixtures.

¹Supported by the NSF under grant No. DMR-1006605 and by the McDevitt bequest at Georgetown.

Tuesday, February 28, 2012 2:30PM - 5:30PM – Session L5 DMP: Focus Session: Interfaces in Complex Oxides - Nickelates 206A

2:30PM L5.00001 Exchange Bias in LaNiO_3 -based heterostructures, MARTA GIBERT, RAOUL SCHERWITZL, PAVLO ZUBKO, DPMC, University of Geneva, JORGE IÑIGUEZ, ICMAB-CSIC, JEAN-MARC TRISCONE, DPMC, University of Geneva — The wide spectrum of exotic properties exhibited by transition-metal based oxides is triggered by the interplay between the spin, charge, orbital and lattice degrees of freedom. In this context, interface engineering in complex oxide heterostructures enables not only further tuning of the exceptional properties of these materials, but also gives access to hidden phases and emergent physical phenomena. Here, we show how interface engineering can induce a complex magnetic structure in a non-magnetic material. We specifically show that exchange bias phenomenon can unexpectedly emerge in (111)-oriented heterostructures involving materials a priori non-candidates for the development of such behavior, namely paramagnetic LaNiO_3 (LNO) and ferromagnetic LaMnO_3 (LMO). The observation of the exchange bias in LNO/LMO superlattices not only implies the development of interface-induced magnetism in the paramagnetic LNO layers, but also provides us with a very subtle tool for probing the interfacial coupling between the LNO and the LMO layers. First-principles calculations indicate that this interfacial interaction may give rise to an unusual spin order resembling a spin density wave within the LNO layers. Other possible magnetic orders are also discussed.

2:42PM L5.00002 Resonant x-ray reflectivity study of interface reconstructions in LaCoO_3 and other transition-metal-oxide heterostructures, VLADIMIR HINKOV, Max-Planck-UBC Centre for Quantum Materials and University of British Columbia, Canada, WOO-SEOK CHOI, Oakridge National Laboratory, U.S.A., JORGE HAMANN-BORRERO, IFW Dresden, Germany and University of British Columbia, Canada, GEORGE A. SAWATZKY, Department of Physics and Astronomy, University of British Columbia, Canada, HO-NYUNG LEE, Oakridge National Laboratory, U.S.A., SEBASTIAN MACKE, Max-Planck-Institut, FKF, Germany and Max-Planck-UBC Centre for Quantum Materials, ABDULLAH RAD, Department of Chemistry, University of British Columbia, Canada — Transition-metal-oxide (TMO) heterostructures offer the opportunity to combine the study of unconventional physical properties with the design of novel functionalities, which are not observed in simple semiconductor or metal heterostructures. In my talk I will concentrate on electronic and chemical reconstructions observed at the interfaces of heterostructures based on LaCoO_3 and other correlated oxides. After briefly summarizing the properties of the novel resonant x-ray technique of orbital reflectometry which we recently used to study the orbital reconstruction in LaNiO_3 heterostructures (Benckiser et al., Nature Materials 10, 189, (2010)), I will discuss the application of this technique, and of usual resonant x-ray reflectometry, to study the electronic and orbital properties at the interfaces and at the surface of LaCoO_3 / LaAlO_3 heterostructures. Finally, I will offer an outlook to the application of orbital reflectometry to other systems.

2:54PM L5.00003 Quantum confinement of correlated e_g^1 electrons in rare earth nickelate heterostructures, JIAN LIU¹, Department of Physics, University of Arkansas, M. VAN VEENENDAAL, Argonne National Lab, S. OKAMOTO, Oak Ridge National Lab, M. KAREEV, B. GRAY, Department of Physics, University of Arkansas, P. RYAN, J.W. FREELAND, Argonne National Lab, J. CHAKHALIAN, Department of Physics, University of Arkansas — Complex oxide heterostructures have emerged as a new playground for controlling the mutually coupled charge, spin, orbital and lattice degrees of freedom, and a promising route to stabilize unusual phases not existing in the bulk. In particular, quantum well structures have recently attracted attention due to the potential in creating novel two-dimensional systems with confined correlated electrons. To this end, we have studied the e_g^1 system based on the $3d^7$ low-spin state in perovskite rare earth nickelates which are artificially confined by wide-gap dielectrics LaAlO_3 . The combination of transport measurements and dynamical-mean-field calculations indicate that, a Mott-type metal-insulator transition can be induced by confinement via dimensionality-control. X-ray absorption spectroscopy reveals that the electronic modification in proximity to the confining interfaces is caused by modulated covalency, which is in good agreement with cluster calculations. J.C. was supported by DOD-ARO under the Contract No. 0402-17291 and NSF Contract No. DMR-0747808.

¹also affiliated with Lawrence Berkeley National Lab

3:06PM L5.00004 Epitaxial Stabilization of Ultrathin Rare-Earth Nickelates¹, D.J. MEYERS, E.J. MOON, M. KAREEV, University of Arkansas, I.C. TUNG, Northwestern University, B.A. GRAY, JIAN LIU, University of Arkansas, M.J. BEDZYK, Northwestern University, J.W. FREELAND, Advanced Photon Source, Argonne National Laboratory, J. CHAKHALIAN, University of Arkansas — The nickelate family of perovskite materials has attracted great attention in recent years due to the interesting range of properties they exhibit. In this talk we report on the successful synthesis of EuNiO_3 , YNiO_3 , and PrNiO_3 films grown by interrupted pulse laser epitaxy on various substrates. Investigation of the phase space of nickelate thin film epitaxy revealed a linear trend between the optimized growth temperature and the Goldschmidt tolerance factor. This correlation is explained through epitaxial stabilization and the increase of the lattice energy via distortion of the ideal perovskite cell. This explanation offers the additional benefit of not being restricted only to the nickelate perovskite family, giving it possible applicability for a wide range of perovskite-structured materials.

¹JC was funded by grants from majority DOD-ARO (W911NF-11-1-0200) and partially NSF (DMR-0747808). Work at the Advanced Photon Source is supported by the U.S. Department of Energy, Office of Science under grant No. DEAC02-06CH11357.

3:18PM L5.00005 Unipolar Field-Effect Diode Based on a Complex Oxide¹, WENG LEE LIM, SERGEI URAZHIN, Department of Physics, Emory University, Atlanta, EUN JU MOON, MICHAEL KAREEV, DEREK MEYERS, JAK CHAKHALIAN, Department of Physics, University of Arkansas, Fayetteville, JOHN FREELAND, Argonne National Laboratory, Argonne — We demonstrate rectifying behavior in a field-effect device structure fabricated from thin NdNiO_3 films grown on SrTiO_3 substrates by the pulsed laser deposition technique. In contrast to the conventional three-terminal field effect devices, the device has only two terminals with the field gate electrode connected to one of the terminal electrodes. The active device area is a $10\mu\text{m} \times 10\mu\text{m}$ square with a $\text{Au}/\text{Al}_2\text{O}_3/\text{NdNiO}_3/\text{SrTiO}_3$ structure, where Au and Al_2O_3 are the gate and the gate insulator, respectively. At small bias voltages, the device exhibits a metal-insulator transition near $T=150\text{K}$, similar to extended NdNiO_3 films. I-V measurements reveal a strong dependence of device characteristics on temperature, applied bias, and both thermal and applied bias histories. We analyze the IV characteristics by using a modified charge-control model based on accumulation of charges in the channel near the gate oxide interface. We deduce the temperature dependence of the effective zero-field charge carrier mobility for the channel by including a field-dependence mobility. The observed hysteretic effects can be utilized in complex oxide devices that combine together both the diode and the memory functionalities.

¹This work is supported by ONR grant 10-001-SA1002031.

3:30PM L5.00006 Asymmetric Orbital-Lattice Interactions in Ultrathin Correlated Oxide Films¹, JAK CHAKHALIAN, Physics Department, University of Arkansas — Epitaxial control of strongly correlated electrons offers opportunities to push beyond the bulk phase diagram and access new ground states. Using resonant x-ray spectroscopies combined with density functional calculations, we report the discovery of an asymmetric biaxial strain-induced 3d-orbital response in ultrathin films of the correlated metal LaNiO_3 that are not accessible in the bulk [J. Chakhalian et al., PRL, 107, 116805 (2011)]. Compressive strain results in an orbital polarization due to structural induced changes in the crystal field, but tensile strain shows no orbital response. This is accompanied by a strong change in the oxygen hole states due a systematic change of the charge transfer energy as a function of strain. We suggest that knowledge of this asymmetric orbital-lattice interaction is fundamental to the rational design of quantum materials with exotic correlated phases and enhanced critical temperatures.

¹J.C. was supported by DOD-ARO under the Contract No. W911NF-11-1-0200 and NSF Contract No. DMR-0747808.

3:42PM L5.00007 ABSTRACT WITHDRAWN —

3:54PM L5.00008 *in situ* studied correlated oxide LaNiO_3 ultra thin film by angle resolved photoemission spectroscopy, H.K. YOO, Seoul National University, Y.J. CHANG, Advanced Light Source (ALS), LBNL & Fritz-Haber-Institut, K.S. KIM, L. MORESCHINI, Advanced Light Source (ALS), LBNL, D.W. JEONG, Y.S. KIM, Seoul National University, A. BOSTWICK, E. ROTENBERG, Advanced Light Source (ALS), LBNL, T.W. NOH, Seoul National University — Recently, RNiO_3 (R : rare earth) attracted increasing attention due to the possible realization of the electronic band structure similar to the high-temperature superconductor cuprates. Among them, LaNiO_3 based heterostructures have shown various fascinating physical properties such as dimensionality controlled electronic phase transitions. Theoretical works on confined LaNiO_3 through heterostructuring predicted cuprate-like band structure and magnetic properties. Here, we reports *in-situ* angle resolved photoemission spectroscopy results on the LaNiO_3 films grown by pulsed laser deposition method. We carefully controlled the thickness of LaNiO_3 films from one to 30 unit cells and measured the thickness dependent band dispersions. First, we will discuss the strong electronic correlation effect in bulk-like band structure of thick LaNiO_3 films comparing to the previously reported LDA+DMFT calculation. Moreover, we will discuss the thickness dependent band structure. As decreasing the film thickness, we observed the charge redistribution of two $\text{Ni } e_g$ orbitals at the Fermi surface. The origins of thickness dependent electronic structure will be discussed.

4:06PM L5.00009 Influence of Symmetry on the Octahedral Rotations of Epitaxial RNiO_3 Thin Films, I.C. TUNG, Department of Materials Science and Engineering, Northwestern University; Advanced Photon Source, Argonne National Laboratory, JIAN LIU, B. GRAY, J. CHAKHALIAN, Department of Physics, University of Arkansas, J.M. RONDINELLI, E.A. KARAPETROVA, J.H. LEE, Advanced Photon Source, Argonne National Laboratory, M.J. BEDZYK, Department of Materials Science and Engineering, Northwestern University, J.W. FREELAND, Advanced Photon Source, Argonne National Laboratory — Understanding the structural and electronic behavior of ABO_3 thin films subjected to confinement, lattice misfit and broken symmetry at the interface in the ultra-thin limit is fundamentally important for the rational design of new materials [1]. However, the epitaxial strain will not only due to a change the in-plane lattice constants but also the octahedral rotations connected to bond angles and crystallographic symmetry. Here we present a study of the effect of the bulk lattice symmetry on octahedral rotations under epitaxial strain in thin films of RNiO_3 ($R=\text{La, Pr, Nd}$) grown on various substrates by pulsed laser deposition. A combination of high-resolution x-ray diffraction, polarization-dependent soft x-ray absorption spectroscopy, and first-principles density functional calculations has been applied to elucidate structural and electronic properties of the samples. Work at the Advanced Photon Source, Argonne is supported by the U.S. Department of Energy, Office of Science under Contract No. DE-AC02-06CH11357.

[1] J. Chakhalian et al., Phys. Rev. Lett., 107, 116805 (2011).

4:18PM L5.00010 Probing the Nickelate Ground State in NdNiO_3 Superlattices, ANKIT DISA, DIVINE KUMAR, JOSEPH NGAI, FRED WALKER, CHARLES AHN, Center for Research on Interface Structures and Phenomena and Department of Applied Physics, Yale University — The rare-earth nickelates of the type RNiO_3 exhibit tunable, sharp metal-insulator transitions as a function of R size, film thickness, and external fields. The nature of these transitions has been the subject of much study, including examination of the insulating ground state. NdNiO_3 has garnered particular interest due to a concomitant magnetic crossover to an antiferromagnetic state occurring at the metal-insulator transition temperature. Several previous studies have focused on thin films; in this work, we examine NdNiO_3 layers confined in heterostructures. The metal-insulator transition temperature can be manipulated based on the thickness of the NdNiO_3 layers within the heterostructure, and a suppression of the high-temperature metallic phase leads to a crossover to localization related to a change in dimensionality. The electronic structure of these phases probed using x-ray absorption spectroscopy enables us to elucidate the link between potential charge ordering and dimensionality in the ground state of this system.

4:30PM L5.00011 Electrostatic control of the metal-insulator transition of ultrathin NdNiO₃ films, JUNWOO SON, BHARAT JALAN, ADAM P. KAJDOS, Materials, UCSB, LEON BALENTS, S. JAMES ALLEN, Physics, UCSB, SUSANNE STEMMER, Materials, UCSB — Rare earth nickelates (RNiO₃) exhibit a first order metal insulator transition upon cooling. Bulk studies on chemical doping indicated that both divalent and quaternary ions were effective in shifting T_{MIT} to lower temperatures by ~ 50 to 25 K for 1 % hole and electron doping, respectively. However, separating the influence of structural distortions from band filling is particularly important for the nickelates. Here we present a new approach to control the band-filling in nanoscale NdNiO₃ thin films by modulation doping. NdNiO₃ is remotely doped by interfacing it with a degenerately doped conventional band insulator, La-doped SrTiO₃. We show that the remote doping approach allows for purely electronic modulation of a carrier density in the absence of other structural changes. The proposed approach is experimentally tested using ultrathin (2.5 nm) NdNiO₃ films grown on La-doped SrTiO₃ films with different carrier concentrations. We show that remote doping systematically changes the charge carrier density in the NdNiO₃ film and causes a moderate shift (~ 20 K) in the metal-insulator transition temperature. These results will be discussed in the context of theoretical models of the materials exhibiting a metal-insulator transition.

4:42PM L5.00012 Tuning Electronic Conductivity in Nickelate Heterostructures, DIVINE KUMAR, JOSEPH NGAI, HANGHUI CHEN, ANKIT DISA, Center for Research on Interface Structure and Phenomena and Department of Applied Physics, Yale University, KARYN LEHUR, Department of Physics Yale University, SOHRAB ISMAIL-BEIGI, CHARLES AHN, FREDRICK WALKER, Center for Research on Interface Structure and Phenomena and Department of Applied Physics, Yale University — Bulk LaNiO₃ (LNO) is a metallic material, but for thin films below a critical thickness of about 5-6 unit cells of LNO, a transition occurs from metallic to insulating transport behavior. This transition is suppressed in superlattice structures with LaAlO₃ (LAO) spacers which are found to be metallic down to 3 unit cell thick LNO. To understand the differences between thin film and superlattices, we have identified structural differences in thin films and superlattice structures of LNO and LAO using a combination of first principles theory and synchrotron x-ray diffraction. Distortions are observed in the Ni-O-Ni bond angle in LNO epilayers grown on LAO resulting from relaxations at the vacuum-LNO interface. These distortions are suppressed in superlattice structures. Based on our observations, we propose that the electronic properties of nickelate superlattices can be designed by carefully selecting spacer layers that result in specific structural distortions in the LNO conducting layers. By tuning the observed distortions in this fashion, we identify a new pathway for controlling the electronic properties of rare earth nickelate compounds.

4:54PM L5.00013 Composition spread studies of (RE)NiO₃-LaNiO₃ thin films¹, RICHARD SUCHOSKI, ICHIRO TAKEUCHI, University of Maryland, College Park - MSE, CNAM, KUI JIN, RICHARD GREENE, University of Maryland, College Park - Physics, CNAM — Epitaxial thin films of La_xNd_{1-x}NiO₃ and La_xPr_{1-x}NiO₃ were grown via pulsed laser deposition on SrTiO₃ (001) with an automated moving shutter system to create 100 nm thick composition spreads. These films have the advantage of providing a continuous spectrum of doping compositions at the same deposition conditions, such as temperature and oxygen pressure, without the need to prepare different stoichiometric targets or perform different depositions for desired compositions. Composition evolution is verified via wavelength dispersive spectroscopy, and x-ray diffraction mapping shows that the lattice constant of the film varies continuously from LaNiO₃ to NdNiO₃. Simultaneous measurements of resistance versus temperature down to 4.2 K across the spreads show evolution in transport behavior. The details will be discussed.

¹Funding provided by AFO SR MURI Grant #FA95500910603 and NSF MRSEC @ UMD (DMR 0520471).

5:06PM L5.00014 Conduction mechanisms in epitaxial and polycrystalline SmNiO₃ thin films, SIEU D. HA, SHRIRAM RAMANATHAN, Harvard University, School of Engineering and Applied Sciences — Correlated oxides that exhibit metal-insulator phase transitions are emerging as potential candidates for switching devices and their fundamental physical properties are of interest. One such material is SmNiO₃, which has a transition temperature above room temperature (~ 400 K in bulk crystals). We present temperature- and bias-dependent conduction mechanisms in epitaxial and polycrystalline SmNiO₃ thin films. In both cases, at low electric field we observe thermally assisted hopping conduction through defect states. At high electric field the conduction transitions to a space-charge limited regime controlled by an exponential trap distribution. The trap decay parameter in epitaxial films does not have the expected $1/T$ temperature dependence, which may be a signature of band gap narrowing at high temperature due to the insulator to metal transition. The role of defects in affecting charge transport parameters will be discussed.

5:18PM L5.00015 Many-body effects in the capacitance of multilayers composed of Mott insulators, SIMON HALE, JIM FREERICKS, Georgetown University — Inhomogeneous dynamical mean-field theory is employed to investigate the non-linearity of the capacitance of multilayer nanostructures. The multilayer nanostructures are constructed with semi-infinite metallic leads coupled via a strongly correlated (Mott insulating) dielectric barrier. Results on the effects of varying barrier thickness, temperature, potential difference, screening length, and chemical potential will be presented. In addition, we also intend to examine phase separation effects which have been experimentally measured to enhance the many-body capacitance over the geometric capacitance.

Tuesday, February 28, 2012 2:30PM - 5:18PM —

Session L6 DMP: Focus Session: van der Waals Bonding in Advanced Materials - Metal Oxide Frameworks & Active Materials 206B

2:30PM L6.00001 Trends in CO₂-MOF Binding from First Principles: Implications for Gas Separations¹, JOSHUA HOWE, Department of Chemical and Biomolecular Engineering, UC Berkeley; The Molecular Foundry, LBNL, BEREND SMIT, Department of Chemical and Biomolecular Engineering, UC Berkeley, JEFFREY NEATON, Molecular Foundry, LBNL — Metal-organic frameworks (MOFs) are a class of highly ordered, highly customizable nanoporous materials that are attractive for use in energy-relevant gas separations. MOF-253 Al(OH)(bpydc) can be post-synthetically modified by introduction of metal cations and charge-stabilizing anions [1]. These post-synthetically modified MOF-253 samples have been shown to exhibit enhanced CO₂-N₂ selectivity over the unmodified framework [1]. Here we use van der Waals-corrected density functional theory (DFT) to study CO₂ binding energy trends in this series of modified frameworks. Particular focus is paid to examining the predictive power of our calculations on modified bipyridine fragments as a proxy for the full framework, as well as the suitability of binding energy trends to predict measured gas selectivity trends [1]. We focus on the following series of 10 post-synthetic modifications: CoCl₂, CuCl₂, FeCl₂, NiCl₂, PdCl₂, Co(BF₄)₂, Cu(BF₄)₂, Fe(BF₄)₂, Ni(BF₄)₂, Pd(BF₄)₂. [1] E. Bloch, et. al, J. Am. Chem. Soc., 132, 14382-14384, 2010.

¹We acknowledge support from DOE and computational resources from NERSC.

2:42PM L6.00002 Ligand-Assisted Enhancement of CO₂ Capture in Tunable MOFs: Balancing Electrostatic and van der Waals Interactions¹, ROBERTA POLONI, Molecular Foundry, LBNL and UC Berkeley, BEREND SMIT, UC Berkeley, JEFFREY B. NEATON, Molecular Foundry, LBNL — Metal-organic frameworks (MOFs) are promising nanoporous materials for CO₂ separation technologies. Here, we use first-principles van der Waals (vdW)-corrected calculations to identify and understand how CO₂ binds to a novel “BTT-type” MOF [1] featuring open metal centers. Our study indicates that CO₂ binds to the open metal cation sites, but with an adsorption energy that can be enhanced by more than a factor of two depending on the choice of the bridging ligand. Judicious choices for metal cations and bridging ligands are shown to lead to a maximum binding energy of 0.67 eV for MgBTT. In all cases, the binding can be attributed to a combination of electrostatics and dispersion, both critically sensitive to the local environment, and contributing nearly equally to the overall binding strength. The possibility to independently tailor these energetics in a manner optimal for CO₂ capture is discussed in the context of recent experiments.

¹We acknowledge DOE-BES for support, and NERSC for computational resources

2:54PM L6.00003 Simulations of physical adsorption of gases in IRMOFs, OSARO HARRIOTT, SILVINA GATICA, Howard University — We performed grand canonical Monte Carlo simulations to study the adsorption of noble gases, H₂ and CO₂ in IRMOF-1. The IRMOF is modeled as a simple structure where a cubic lattice is composed of adsorption centers that reproduce the strength of the metallic corners and organic linkers in the real structure. From the adsorption isotherms obtained in our simulations we calculated the isosteric heat of adsorption and compare with available experimental results. Research supported by NSF and ACS, PRF.

3:06PM L6.00004 Graphene Oxide Derived Carbons (GODC); High-Surface Area NanoPorous Materials for Hydrogen Storage and Carbon Capture¹, TANER YILDIRIM, NIST, Gaithersburg, MD 20899 and UPENN/Philadelphia, PA 19104 — Even though there has been extensive research on gas adsorption properties of various carbon materials based on activated carbon and nanotubes, there has been little work done on the gas adsorption properties of graphite oxide (GO). In this study [1], we show that one-and-a-half-century-old graphite oxide can be easily turned into a potentially useful gas storage material. In order to create high-surface nanoporous materials from GO, we used two different approaches. In the first approach, we have successfully synthesized graphene-oxide framework materials (GOFs) by interlinking GO layers by diboric acids. The resulting GOF materials have well defined pore size and BET surface area up to 500 m²/g with twice larger heat of adsorption of H₂ and CO₂ than those found in other physisorption materials such as MOF5. In the second approach, we synthesized a range of high surface area GO derived carbons (GODC) and studied their applications toward H₂, CO₂ and CH₄ gas storage. The GODCs, with wide range of pore structure, have been prepared by chemical activation with potassium hydroxide (KOH). We obtain largely increased surface areas up to nearly 1900 m²/g for GODC samples from 10 m²/g for initial GO. A detailed experimental study of high pressure excess sorption isotherms on GODCs reveal an increase in both CO₂ and CH₄ storage capacities compared to other high surface area activated carbons. Finally, we compared the gas sorption properties of our GO-based materials with other systems such as MOFs, ZIFs, and COFs.

[1] See <http://www.ncnr.nist.gov/staff/taner> for references and more information.

¹The work was done in close collaboration with G. Srinivas, J. Bures, J. Ford, J. Simmons, and W. Zhou. The work is supported by DOE BES DE-FG02-08ER46522.

3:42PM L6.00005 Isosteric heat of adsorption of CO₂ in bundles of carbon nanotubes., MAMADOU MBAYE, SIDI MAIGA, SILVINA GATICA, Howard University — Using the grand canonical Monte Carlo method, we have evaluated the adsorption isotherms of CO₂ on the exterior of a bundle of carbon nanotubes. The isosteric heat is a property of the adsorbate that can be calculated from experimental or simulation data, and gives hints of the energy of adsorption and the structure of the adsorbate. From the simulated adsorption isotherms we calculated the isosteric heat of CO₂, Ar and CH₄ and compare with existing experimental data. Research supported by NSF and ACS, PRF.

3:54PM L6.00006 Gas Adsorption and Selectivity in Zeolitic Imidazolate Frameworks from First Principles Calculations, KEITH RAY, UC Berkeley Department of Physics, DAVID OLMSTED, UC Berkeley Department of Materials Science and Engineering, NING HE, University of Kansas Department of Chemistry, YAO HOUNDONOUGBO, Eastern Washington University Department of Chemistry and Biochemistry, BRIAN LAIRD, University of Kansas Department of Chemistry, MARK ASTA, UC Berkeley Department of Materials Science and Engineering — Zeolitic Imidazolate Framework (ZIFs) are excellent candidate materials for carbon capture and gas separation. Here we employ the van der Waals density functional (vdW-DF) [1] in an analysis of the binding energetics for CO₂, CH₄ and N₂ molecules in a set of ZIFs featuring different chemical functionalizations. We investigate multiple low-energy binding sites, which differ in their positions relative to functional groups on the imidazole linkers. In all cases an accurate treatment of van der Waals forces appears essential to provide reasonable binding energy magnitudes. We report results obtained from different parameterizations of the vdW-DF, providing comparisons between calculations and experimental values of the heat of adsorption [2]. This research is supported by the Energy Frontier Research Center “Molecularly Engineered Energy Materials,” funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001342. [1] M. Dion, H. Rydberg, E. Schroder, D. C. Langreth, B. I. Lundqvist, Phys. Rev. Lett. 92, 246401 (2004) [2] W. Morris, B. Leung, H. Furukawa, O. K. Yaghi, N. He, H. Hayashi, Y. Houndonougbo, M. Asta, B. B. Laird, O. M. Yaghi, J. AM. CHEM. SOC. 2010, 132, 11006-11008

4:06PM L6.00007 A theoretical study of the hydrogen-storage potential of (H₂)₄CH₄ in nanotubes and MOFs, TIMO THONHAUSER, QI LI, Wake Forest University — The material (H₂)₄CH₄, also called H4M, has exceptional hydrogen-storage potential of up to 33.3 mass%, not including the hydrogen in CH₄.¹ But, unfortunately, H4M is not stable under ambient conditions. For hydrogen storage near ambient pressure, it needs to be cooled to 65 K, and ambient temperature requires a pressure of 5–6 GPa.² In this study we use *ab initio* methods based on van der Waals DFT^{3,4} to investigate the possibility of creating such pressures through external agents such as metal organic framework (MOF) materials and carbon nanotubes. We find that MOFs can create considerable pressure for H4M in their cavities, but not the required 5–6 GPa, and therefore moderate cooling is still necessary. On the other hand, carbon nanotubes can create these high pressures for H4M, but the fact that this pressure exists only inside the nanotubes—and not in-between tubes in e.g. a bundle—lowers the volumetric storage density and makes this option less favorable for practical applications.

¹W.L. Mao et al., Physics Today **60**, 42 (2007).

²W.L. Mao et al., Chem. Phys. Lett. **402**, 66 (2005).

³M. Dion et al., Phys. Rev. Lett. **92**, 246401 (2004).

⁴T. Thonhauser et al., Phys. Rev. B **76**, 125112 (2007).

4:18PM L6.00008 The Role of Many-Body Dispersion Interactions in Molecular Crystal Polymorphism, LESLIE LEISEROWITZ, Weizmann Institute of Science, Rehovoth, Israel, NOA MAROM, Institute for Computational Engineering and Sciences, The University of Texas at Austin, ROBERT A. DISTASIO, JR., Department of Chemistry, Princeton University, NJ, VIKTOR ATALLA, SERGEY LEVCHENKO, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, SERGEY KAPISHNIKOV, Weizmann Institute of Science, Rehovoth, Israel, JAMES R. CHELIKOWSKY, Institute for Computational Engineering and Sciences, The University of Texas at Austin, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — Molecular crystals often have several polymorphs that are close in energy (few meV per molecule), but possess very different physical and chemical properties. Treating polymorphism from first principles has been a long standing problem because conventional density-functional theory (DFT) lacks a proper description of long-range dispersion interactions that govern the structure and energetics of molecular crystals. Here we assess the effect of the many-body dispersion (MBD) energy on the structure and relative energies of the polymorphs of benchmark molecular crystals: glycine, alanine, and para-diiodobenzene. This is accomplished by using the recently developed first-principles DFT+MBD method [A. Tkatchenko, R.A. DiStasio Jr., R. Car, M. Scheffler, submitted], based on the earlier Tkatchenko-Scheffler (TS) dispersion correction [PRL 102, 073005 (2009)]. We show that the non-additive MBD energy plays a crucial role in making qualitatively and quantitatively accurate predictions for the structure and relative energies of polymorphs.

4:30PM L6.00009 Interaction of endohedral molecular hydrogen with C₆₀: infrared study¹, TOOMAS RÖÖM, MIN GE, D. HÜVONEN, U. NAGEL, NICPB, Tallinn, Estonia, S. MAMONE, M.H. LEVITT, M. CARRAVETTA, Southampton Uni., UK, Y. MURATA, K. KOMATSU, Kyoto Uni., Japan, XUEGONG LEI, N.J. TURRO, Columbia Uni., New York — We report on the dynamics of isotopically different hydrogen molecules, H₂, D₂ and HD, trapped in the molecular cages of a fullerene C₆₀ [Min Ge et al., J. Chem. Phys. **134**, 054507 (2011), **135**, 114511 (2011)]. The infrared spectra were measured at temperatures from 5K to 300K and analyzed using a model of a vibrating rotor trapped in a spherical potential. The interaction potential was determined in the ground and in the first excited vibrational state of a hydrogen molecule. The isotropic part of the potential is similar for all three molecules studied. In HD@C₆₀ we observe the mixing of rotational states and an interference effect of the dipole moment terms due to the displacement of the HD rotation center from the fullerene cage center. A three-site Lennard-Jones potential in the pairwise additive five-dimensional potential energy surface reproduces the hydrogen IR spectrum with great accuracy [M. Xu et al., J. Chem. Phys. **130**, 224306 (2009)].

¹We acknowledge support by the Estonian Ministry of Education and Research grant SF0690029s09, Estonian Science Foundation grants ETF7011, ETF8170, JD187, and EPSRC (UK) and the Royal Society (UK).

4:42PM L6.00010 ABSTRACT HAS BEEN MOVED TO D28.00007 —

4:54PM L6.00011 The role of dispersion interactions in the formation of near-surface oxygen defects in CeO₂(111): Comparing DFT+*U* with HF/DFT hybrid functionals using plane-waves as a basis set¹, JOACHIM PAIER, CHRISTOPHER PENSCHKE, JOACHIM SAUER, Humboldt-University, Unter den Linden 6, 10099 Berlin, Germany — Cerium oxide is of paramount importance in the field of heterogeneous catalysis and in solid oxide fuel cells. Its ability to easily release and store oxygen goes together with the distinct facility to form and heal oxygen vacancies. Upon its formation, the electrons left need to localize, but conventional semilocal density functionals (LDA, GGA) are known to fail here. Viable solutions to this problem are the DFT+*U* approach and hybrid Hartree-Fock/DFT functionals being computationally more demanding [1]. However, common implementations of aforementioned approaches do not incorporate long-range dispersion interactions. Given that relaxation effects upon defect formation lead to more open structures and given the relatively high polarizability of Ce-atoms, dispersion interactions are supposed to be non-negligible. We apply Grimme's dispersion correction [2] and carefully cross-check results. Furthermore, we will give thorough estimates on dynamic effects and try to shed some light on the effects induced by the defect concentration. [1] M. V. Ganduglia-Pirovano, J. L. F. Da Silva, and J. Sauer, Phys. Rev. Lett. **102**, 026101 (2009). [2] S. Grimme, J. Comput. Chem. **27**, 1787 (2006).

¹Grants for computing time from HLRN Hannover/Berlin and the Juelich Supercomputing Centre (JSC) are gratefully acknowledged.

5:06PM L6.00012 Interaction of W(CO)₆ with SiO₂ Surfaces, JUAN SHEN, KALIAPPAN MUTHUKUMAR, HARALD O. JESCHKE, ROSER VALENTI, Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, 60438 Frankfurt Germany — The interaction of tungsten hexacarbonyl W(CO)₆ precursor molecules with SiO₂ substrates is investigated by means of density functional theory calculations with and without inclusion of long range van der Waals interactions. We consider two different surface models, a fully hydroxylated and a partially hydroxylated SiO₂ surface, corresponding to substrates under different experimental conditions. For the fully hydroxylated surface we observe only a weak interaction between the precursor molecule and the substrate with physisorption of W(CO)₆. Inclusion of van der Waals corrections results in a stabilization of the molecules on this surface. In contrast, we find a spontaneous dissociation of the precursor molecule on the partially hydroxylated SiO₂ surface where chemisorption of a W(CO)₅ fragment is observed upon removal of one of the CO ligands from the precursor molecule. Irrespective of the hydroxylation, the precursor molecule prefers binding of more than one of its CO ligands. In the light of these results, implications for the initial growth stage of tungsten nano-deposits on SiO₂ in an electron beam induced deposition process are discussed. [1] K. Muthukumar et al. Phys. Rev. B (in press) (2011)

Tuesday, February 28, 2012 2:30PM - 5:18PM —

Session L7 DMP: Carbon Nanotube Hybrid Structures - Properties, Synthesis, Characterization

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2:30PM L7.00001 Self-assembly and electrostatic interactions of carbon nanotubes in nonpolar dielectric liquids, LUCIANA OLIVEIRA, RAMAKRISHNA PODILA, Clemson University, JAY GAILLARD, STEVEN SERKIZ, Savannah River National Laboratory, APPARAO RAO, Clemson University, SAVANNAH RIVER NATIONAL LABORATORY COLLABORATION — We report on the self-assembly of carbon nanotubes (CNTs) in nonpolar dielectric liquids under the influence of DC-generated electric fields. This process gives rise to electrostatic and hydrodynamic interactions of the CNTs in insulating nonpolar solvents. While some studies of the self-assembly of carbon nanotubes in response to a DC-field have been carried out in conductive solvents, the analysis of the self-assembly process is complicated by the current flow temporally affecting the particle charge and an assembly timescale of tenths to hundredths of seconds. In contrast, experiments in insulating liquids allow for the investigation of self-assembly processes where: the particle charge is not expected to change as a function of time and at a timescale of seconds this allows for an investigation of the transient states of the assembly process. In the presence of an electric-field, CNTs present in the solution experience an electrophoretic force due to their surface charges. When a DC field is applied across the electrodes, CNT bundles move according to their electrophoretic mobility. We find that the threshold voltage, above which the insulator-to-conductor transition occurs, varies sensitively as a function of zeta potential and hydrodynamic particle size. In addition, a percolation power law supports the observed threshold voltage as a function of CNT concentration and zeta potential.

2:42PM L7.00002 A Group Theoretic Approach to Nonlinear and Gradient Elastic Terms for Graphene and Carbon Nanotubes, ALEXANDER ALEMI, JAMES SETHNA, Cornell — Nonlinear and gradient corrections to the elastic theory of graphene and carbon nanotubes are important for determining the thermal conductivity, mechanical properties under large deformations, dissipation in nanotube oscillators and other mechanical properties. By applying group theory, we can systematically and efficiently work out all nonlinear elastic terms that can appear in a Ginzburg-Landau formulation of the elastic free energy in terms of the material displacement gradient tensor. Graphene serves as a perfect example material, having an interesting hexagonal symmetry and being a material in which nonlinear elastic terms are important. This approach allows us to demonstrate the usual cubic corrections. Additionally, we find higher order strain corrections which correspond to bending and rolling the graphene sheet, as well as gradient terms which are important for describing the long wavelength phonon dispersion. We will enumerate the most important contributions to the free energy, and measure the corresponding elastic constants with simulation.

2:54PM L7.00003 A Signature of Spatial Correlations between rare earth ions and single-wall nanotubes wrapped with DNA in their mixed solution, TETYANA IGNATOVA, SLAVA V. ROTKIN, Lehigh University, Physics Department — We propose that the fluorescence resonance energy transfer (FRET) between the rare earth ions (REI) and single-wall nanotubes (SWNT) can be used to measure their Coulomb correlation in solution. As a calibration experiment the FRET between two different REIs, being the energy donor and the acceptor, in their mixed solution has been used. From the photoluminescence decay time we were able to extract the characteristic distance between unlike REIs. Our study revealed negative correlation (the repulsion) for Tb-Eu solution. In the case of the solution containing the REI and the SWNTs wrapped with DNA we observed a significant positive correlation (the attraction and the complex formation). The data is in a good agreement with the theoretical estimates and allows to propose REIs and their FRET as a sensitive tool for detecting kinetics of interaction of SWNTs in aqueous solutions.

3:06PM L7.00004 Computational Modeling of Cancer Treatment Using Carbon Nanotubes, FENG GONG, HONGYAN ZHANG, JIN WEN TAN, National University of Singapore, DIMITRIOS V. PAPAVALASSILIOU, University of Oklahoma, USA, VINCENT B.C. TAN, SWEE HIN TEOH, HAI MINH DUONG, National University of Singapore — Laser thermal therapy selectively kills cancer cells without harming surrounding cells due to the high-energy absorbance of the functionalized carbon nanotubes (CNTs). However, the technique application is still very limited due to lack of experimental and computational works to understand how to kill cancer cells effectively and how the CNTs are heated by the external laser. The goal of this work is to present integrated computer models to capture changes in CNT heat transfer characteristics due to variations in the properties of CNTs and tissues during laser surgery. Numerical results show that the models are able to characterize variations of tissue properties for laser surgical procedures (by three dimensional finite element models) and predict anisotropic temperature fields within the CNTs (by finite different models). The current model is made more realistic and accurate than previous models by taking into account the anisotropic properties of CNTs and the energy loss from the CNT surface. The effects of the CNT concentration, morphology, orientations, and the power and heating duration of the laser are also investigated. The developed models help experimentalists to understand cancer treatment mechanisms and optimize operating conditions of the laser thermal therapy.

3:18PM L7.00005 Synthesis and Electronic Properties of Silicon-Nitrogen Hetero-doped Single Walled Carbon Nanotubes, MARTHA AUDIFFRED, Universidad de Guanajuato, Mexico, ANA LAURA ELIAS, HUMBERTO R. GUTIERREZ, PSU, FLORENTINO LOPEZ-URIAS, IPICYT, HUMBERTO TERRONES, PSU, MAURICIO TERRONES, PSU, Shinshu University, GABRIEL MERINO, Universidad de Guanajuato, Mexico — We investigated the stability and electronic properties of hetero-doped carbon nanotubes using first-principles density functional theory. Silicon, silicon-nitrogen, and silicon-oxygen were incorporated within the lattice of different types of single-walled carbon nanotubes. The structural stability, electronic density of states, doping energy, band structure, HOMO and LUMO were analyzed. When silicon and nitrogen are bonded and inserted in the nanotube lattice, non-dispersive bands appear around the Fermi level. The Nitrogen arranged in a pyridine-like fashion together with a silicon atom placed inside the vacancy was also studied. The latter configuration becomes more stable than the substitutional nitrogen embedded in the (9,0) and (5,5) nanotubes. We have also succeeded in the synthesis of Si and SiN-doped single-walled carbon nanotubes (CSixNy-SWNTs) by chemical vapor deposition. We carried out Raman spectroscopy, high-resolution electron microscopy, electron energy loss spectroscopy, energy-dispersive X-Ray spectroscopy, Auger spectroscopy and X-Ray photoelectron spectroscopy, in order to identify the presence of both dopants within the nanotube lattice.

3:30PM L7.00006 Magneto-photoluminescence in lanthanide-bearing endohedral metallofullerenes with various cage symmetries¹, TRAVIS MERRITT, HARRY DORN, GITI A. KHODAPARAST, Virginia Tech, STEVE MCGILL, National High Magnetic Field Laboratory — Taken as a family, endohedral metallofullerenes (EMF) nanomaterials provide opportunities for exquisite functional tunability at the nanoscale, enabling a wide range of synthetic nanoparticles with diverse sizes, symmetries, electronic, optical and, especially, magnetic properties. In particular, metallofullerenes incarcerating lanthanide ions will permit endohedral luminescence due to the 4f optically-active electrons being uninvolved in the stabilizing charge transfer between the endohedral guest and cage. In addition, if those lanthanide ions possess optical transitions beyond the absorption onset of the cage, a well-defined optical spectrum may be observed for the metallofullerene system. In this talk, several magneto-optical and time-resolved studies at high magnetic fields on lanthanide-based EMFs with different cage symmetries will be presented, where the residual magnetic degeneracies in the lanthanide ion energy levels are lifted and observed in the optical spectrum with magnetic field strengths in excess of 10 T.

¹Supported by: NSF-Career Award DMR-0846834

3:42PM L7.00007 Exploring the Fundamental Properties of Carbon Nanotubes using Electro-mechanical Resonators, MEHMET AYKOL, WILLIAM BRANHAM, SHUN-WEN CHANG, ROHAN DHALL, STEPHEN B. CRONIN, University of Southern California — By monitoring the nanoelectromechanical (NEM) response of suspended individual carbon nanotubes (CNT), we measure the expansion coefficient of individual suspended single-walled CNTs. Here, the temperature dependence of the mechanical resonance frequency of NEM CNT resonator is used to determine the change in tension on the device caused by the expansion on the nanotube. We also measured the effects of gas adsorption on the CNT surface, by measuring change in conductivity and its response to gate doping. By monitoring the mass loading on the surface of the resonator we calculate the adsorption energy of the specific gasses on the surface of the nanotube.

3:54PM L7.00008 Fano Resonances in Mid-Infrared Spectra of Single-Walled Carbon Nanotubes, FRANÇOIS LAPOINTE, ÉTIENNE GAUFRÈS, ISABELLE TREMBLAY, NATHALIE TANG, Université de Montreal, PATRICK DESJARDINS, Ecole Polytechnique de Montreal, RICHARD MARTEL, Université de Montreal, REGROUPEMENT QUÉBÉCOIS SUR LES MATÉRIAUX DE POINTE (RQMP) TEAM — We show that optical phonon modes in single-walled carbon nanotubes (SWNTs) become observable in mid-infrared (MIR) spectroscopy by the means of Fano resonances. The scattering of a low energy electronic continuum over phonon discrete states yields anti-resonances that are recognizable in the spectra by their characteristic asymmetric line shape. Experimentally, we control the charge carrier density in SWNTs by p doping with different molecular oxidizers at saturation and compare the spectra of doped and intrinsic samples. The only measurable feature in the intrinsic state is a kink at $\sim 865 \text{ cm}^{-1}$. Kinks at ~ 1600 and $\sim 1250 \text{ cm}^{-1}$ appear upon doping. We find no significant differences between the dopants; hence the bands belong to the SWNTs. Fitting of the band at $\sim 1600 \text{ cm}^{-1}$ yields good agreement with a phenomenological Fano resonance model. Finally, SWNTs mats are functionalized with bromophenyls, which are known to increase the number of defects. We find that upon p doping, the Fano resonances' cross sections of damaged SWNTs increase compared to that of p doped pristine SWNTs. Hence, we conclude that defects lower the symmetry of the lattice and activate optical phonon modes in MIR spectroscopy.

4:06PM L7.00009 Computational modeling of electron transfer in hydrogenase and carbon material complexes, KWISEON KIM, HAI LONG, National Renewable Energy Laboratory — In biohybrid and biomimetic devices for energy conversion, the electron transfer between the enzyme and the electrode plays a central role. We use hydrogenase and carbon material as model systems and investigate the binding and electron transfer configurations between hydrogenase and carbon materials, including single-wall carbon nanotubes and graphene surfaces. We use Brownian dynamics simulations to sample the hydrogenase/carbon material phase-space. The results provide an atomistic picture of how enzyme interacts with the electrode materials. We find that the optimal enzyme/electrode binding configurations are not optimal for electronic transfer.

4:18PM L7.00010 ABSTRACT WITHDRAWN —

4:30PM L7.00011 Theory of coherent phonons in carbon nanoribbons¹, GARY SANDERS, CHRIS STANTON, University of Florida — We have developed a microscopic theory for the generation and detection of coherent phonons in armchair and zigzag carbon nanoribbons using an extended tight-binding model for electrons and a valence force field model for the phonons. Coherent phonons are generated through the electron-phonon deformation potential interaction and we use Heisenberg's equation to obtain a driven oscillator equation for the coherent phonon amplitudes. We find that the driving function depends explicitly on the time-dependent photoexcited carrier distribution functions. We simulate the generation and detection of coherent phonons in coherent phonon spectroscopy experiments. We consider coherent phonon oscillations of the lowest lying radial breathing like mode (RBLM) in zigzag and armchair nanoribbons as a function of ribbon width and pump/probe polarization angle.

¹Supported by NSF through grants OISE-0968405 and DMR-1105437.

4:42PM L7.00012 Biomimetic Carbon Nanotube for Catalytic Hydrolysis of CO₂: First Principles Investigation of Role of Oxidation State and Metal Substitution, DONGHWA LEE, Lawrence Livermore National Laboratory, YOSUKE KANAI, University of North Carolina — Reducing the amount of carbon dioxide (CO₂) in the atmosphere is one of the most important challenges we face in this century. Metallo-enzyme, carbonic anhydrase (CA), is known for its catalytic activity of CO₂ hydrolysis, and a number of research groups have been experimentally working to mimic this activity in small molecules for the CO₂ collection processes. Using accurate first principles electronic structure calculations, we investigate how the catalytic hydrolysis reaction of CA can be mimicked in a metal-porphyrin carbon nanotube system. Our work shows that the two-step catalytic process can be improved remarkably by controlling the oxidation state and also through the metal substitution in the porphyrin unit. Our work shows the feasibility of CO₂ hydrolysis in the metal-porphyrin carbon nanotube and also how the catalytic activity could be improved. This work is Prepared by LLNL under Contract DE-AC52-07NA27344.

4:54PM L7.00013 Coupling of carbon nanotubes and graphene nanoribbons by the titanium and vanadium nanowires: First-principles study¹, CHI-HSUAN LEE, CHIH-KAI YANG, Graduate Institute of Applied Physics, National Chengchi University — We investigate the combined structure of a carbon nanotube (CNT) and graphene nanoribbon (GNR) through the adsorption of a titanium or vanadium nanowire (NW), using first-principles calculations. The binding energy depends upon the stacked configuration and is much larger than that between the two subsystems without the nanowire. The band structure reveals strong hybridization between d orbitals of the transition metal and p orbitals of the carbon atoms. Furthermore, if the CNT is deposited near the border of GNR, structural stability is enhanced and magnetic moments of the edge atoms are reduced. The result points to possible application for synthesizing nanowires in nanoelectronic devices.

¹This work was supported in part by the National Center for High-performance Computing, the National Center for Theoretical Sciences, and the National Science Council of Taiwan, the Republic of China under Grant number NSC 98-2112-M-004-003-MY3

5:06PM L7.00014 Synthesis and phase behavior of AgI atomicwires in carbon nanotubes, SHIN-ICHI ITO, RYO KITAUURA, YASUMITSU MIYATA, HISANORI SHINOHARA, Nagoya University, HIROSHI KITAGAWA COLLABORATION, KUNIO AWAGA COLLABORATION — α -phase silver iodide (α -AgI) has been well-known as a solid state ionic conductor due to its superionic conductivity and is one of the promising candidates for solid-state electrolytes for various electrochemical devices. Below 420 K, α -AgI undergoes a phase transition into the poorly conducting β - and γ -polymorphs, thereby limiting their applications. Recently, we have found that AgI nanowires with a diameter of 10 nm can retain α -phase even at 313 K where size and morphology of AgI presumably plays a great role in this α -AgI stabilization [1]. To investigate the effect further, we have focused on low dimensional nanostructure of AgI with a diameter of 5 - 10 nm. For this purpose, one-dimensional (1D) nanospace of carbon nanotubes (CNTs) has been utilized. CNTs have unique 1D nanospace ranging in diameter from 0.4 to 50 nm, which can stabilize otherwise unstable nanomaterials. We have synthesized AgI@CNTs by the sublimation method already reported [2]. In the presentation, we will discuss detailed characterization of structure and properties based on electron beam diffraction and HR-TEM.

[1] R. Makiura et al., Nature.Mater.8, 476 (2009).

[2] R. Kitaura, et al., Nano Res.1, 152 (2008).

Tuesday, February 28, 2012 2:30PM - 5:30PM —
Session L8 DMP GMAG: Focus Session: Frustrated Magnetism - 1D 208

2:30PM L8.00001 Magnon pairing in Quantum Spin Nematic, MIKE ZHITOMIRSKY, SPSMS, CEA-Grenoble — The phenomenon of the Bose-Einstein condensation is inherent not only to superfluid He-4 and cold atomic gases but also describes in a unified way a variety of field-induced transitions in quantum magnets. In this talk we discuss a novel example of the Bose-Einstein condensation of bound magnon pairs. The binding mechanism is based on a competition between ferro- and antiferromagnetic exchange bonds in a frustrated quantum spin system. As a result bound magnon pairs are formed in the fully polarized magnetic state at high fields. Upon decreasing field magnon pairs undergo a condensation into a state which is bosonic analog of a BCS superconductor [1]. The magnon-pair condensate lacks a conventional transverse magnetic order and is described instead by a quadrupolar or spin-nematic order parameter. We consider in detail magnon-pairing mechanism for two spin models: frustrated chains weakly coupled by interchain interactions and frustrated square-lattice antiferromagnet, which exhibit high-field spin-nematic states. Our theory predicts existence of the long-range spin-nematic phase in the frustrated chain material LiCuVO₄. We also review recent experimental evidences, which support presence of a new phase in this material. Work done in collaboration with H. Tsunetsugu (ISSP, University of Tokyo)

[1] M. E. Zhitomirsky and H. Tsunetsugu, Europhys. Lett. 92, 37001 (2010).

3:06PM L8.00002 Competition between Spin Nematic and Spin Density Wave Orders in Spatially Anisotropic Frustrated Magnets in Magnetic Fields, MASAHIRO SATO, Department of Physics and Mathematics, Aoyama Gakuin University, Japan, TOSHIYA HIKIHARA, Faculty of Engineering, Gunma University, Japan, TSUTOMU MOMOI, Condensed Matter Theory Laboratory, RIKEN, Japan — Magnetic multipolar order including spin nematic order is one of the current topics in frustrated magnetism. Recently, frustrated spin chains with ferromagnetic nearest-neighbor coupling J_1 and antiferromagnetic next-nearest-neighbor one J_2 have been theoretically shown to exhibit multipolar quasi long-range orders in the wide region of J_1/J_2 as an external magnetic field is applied. In addition, it is known that several kinds of quasi one-dimensional cuprates can be described by this J_1 - J_2 spin chain. Particularly, a recent experiment shows that LiCuVO_4 , one of the cuprates, possesses a new phase near saturation and it is expected to be a spin nematic ordered phase. Motivated by these results, we have completed the field-temperature phase diagram for spatially anisotropic magnets consisting of weakly coupled J_1 - J_2 spin chains, by making use of accurate results of the single J_1 - J_2 spin chain. The phase diagram contains spin nematic and spin-density-wave ordered phases, and these two orders compete with each other. We will discuss some universal features of the phase diagram and the relevance of our result to LiCuVO_4 .

3:18PM L8.00003 Unusual interchain coupling effects in frustrated edge-shared chain cuprates with ferromagnetic NN in-chain coupling, STEFAN-LUDWIG DRECHSLER, SATOSHI NISHIMOTO, JEROEN VAN DEN BRINK, JIRI MALEK, IFW-Dresden, Institute of Theoretical Solid State Physics, Dresden, Germany, ROMAN KUZIAN, Institute of Material Sciences NASU, Ukraine, Kiev, JOHANNES RICHTER, University of Magdeburg, Germany, MIRIAM SCHMITT, HELGE ROSNER, MPI-CPFS, Dresden, Germany, KUZIAN COLLABORATION, RICHTER COLLABORATION, ROSNER COLLABORATION — We consider the effect of weak antiferromagnetic interchain coupling (AFM IC) on the saturation field, the magnetization curve, the phase diagram of multipolar phases at high magnetic fields, the dynamical magnetic structure factor, as well as the pitch angle at ambient fields applying the DMRG-technique to clusters of coupled long chains and the hard-core boson method to quasi-1D spin nematics at $T=0$. The critical AFM IC couplings for various multipolar phases and types of IC are determined. The results are applied to Li_2CuO_2 , LiVCuO_4 , $\text{Ca}_2\text{Y}_2\text{Cu}_5\text{O}_{10}$, as well as to linarite. The multipolar phases can be stabilized by easy-axis spin anisotropy. Linarite and LiVCuO_4 , are found to be good candidates for the detection of multipolar phases. Microscopic considerations based on the extended five-band Hubbard model and $L(S)\text{DA}+U$ calculations provide exchange integrals which support the empirically found values for the main exchange integrals. We discuss the applicability of spin-wave theory and the role of quantum fluctuations for a correct description of magnetic excitations. Cases when a weak IC coupling dominates solely or predominantly the saturation field and/or the pitch angle are emphasized.

3:30PM L8.00004 Frustrated 1D Spin-S chain Below Saturation Magnetization¹, TEIMURAZ VEKUA², Leibniz University of Hannover, ALEXEI KOLEZHUK, University of Kiev, FABIAN HEIDRICH-MEISNER, University of Muenchen, SEBASTIAN GRESCHNER, Leibniz University of Hannover, MARCELO ARLEGO, GERARDO ROSSINI, University of La Plata, ANDREAS HONECKER, University of Goettingen — Ground states of frustrated spin-S chains in strong magnetic field in the immediate vicinity of saturation are mapped out. For ferromagnetic nearest-neighbor and frustrating antiferromagnetic next-nearest-neighbor exchange interactions generic feature is metamagnetic behavior under the influence of an external magnetic field for small S, in the form of a first-order transition to the fully polarized state. The magnetization jump increases gradually starting from an S-dependent critical value of exchange couplings and takes a maximum in the vicinity of a ferromagnetic Lifshitz point. The metamagnetism results from resonances in the dilute magnon gas caused by an interplay between quantum fluctuations and frustration. For antiferromagnetic nearest neighbour interactions generic feature is emergence of two-component Luttinger liquid phase and series of phase transitions between that phase and chiral phase.

¹Cluster of excellence QUEST

²Institute of Theoretical Physics, Cluster of Excellence Quantum Information and Space Time Research (QUEST)

3:42PM L8.00005 Quasi-one-dimensional antiferromagnetism and multiferroicity in CuCrO_4 ¹, REINHARD K. KREMER, J.M. LAW, P. REUVEKAMP, MPI for Solid State Research, Stuttgart, Germany, R. GLAUM, Institut fuer Anorganische Chemie, Universitaet Bonn, Bonn, Germany, C. LEE, J. KANG, M.-H. WHANGBO, Department of Chemistry, North Carolina State University, Raleigh, North Carolina 27695-8204, U.S.A — The bulk magnetic properties of the new quasi-one-dimensional Heisenberg antiferromagnet, CuCrO_4 , were characterized by magnetic susceptibility, heat capacity, optical spectroscopy, EPR and dielectric capacitance measurements and density functional evaluations of the intra- and interchain spin exchange interactions. We found type-II multiferroicity below the Néel temperature of 8.2(5) K, arising from competing antiferromagnetic nearest-neighbor (J_{nn}) and next-nearest-neighbor (J_{nnn}) intra-chain spin exchange interactions. Experimental and theoretical results indicate that the ratio J_{nn}/J_{nnn} is close to 2, putting CuCrO_4 in the vicinity of the Majumdar-Ghosh point. First low-temperature neutron powder diffraction data are consistent with a canted magnetic structure below ~ 8 K.

¹Work at NCSU by the Office of Basic Energy Sciences, Division of Materials Sciences, U. S. Department of Energy, under Grant DE-FG02-86ER45259, and also by the computing resources of the NERSC center and the HPC center of NCSU.

3:54PM L8.00006 Magnetic field induced ferroelectric transition of quantum spin chain system $\text{Rb}_2\text{Cu}_2\text{Mo}_3\text{O}_{12}$, YUKIO YASUI, YUDAI YANAGISAWA, RYUJI OKAZAKI, ICHIRO TERASAKI, Department of Physics, Nagoya University, YASUHIRO YAMAGUCHI, TSUYOSHI KIMURA, Graduate School of Engineering Science, Osaka University — Dielectric and magnetic properties have been studied for $\text{Rb}_2\text{Cu}_2\text{Mo}_3\text{O}_{12}$, which includes quasi one-dimensional spin 1/2 chains formed of edge-sharing CuO_4 square planes called CuO_2 ribbon chains. The system does not exhibit a magnetic transition above temperature $T > 2\text{K}$ owing to quantum fluctuation and low dimensionality. We have observed anomalous increase of dielectric constant ϵ with decreasing T below ~ 50 K, which is originated from growing a short range ordering of a helical magnetic structure. For an external magnetic field $H > 0.5\text{T}$, a peak structure is observed in the $\epsilon - T$ curves at $T_c \sim 8\text{K}$ and the ferroelectric polarization has been observed below T_c . However, the magnetic susceptibility and specific heat do not have anomaly at T_c for $H > 0.5\text{T}$. The anomalous increase of ϵ and field-induced ferroelectric transition are found to be suppressed by impurity doping such as Zn and Ni atoms to the Cu sites. These results indicate that the ferroelectric transition is found to be induced by applying field without magnetic transition which strongly suggests a new type of ferroelectric transition triggered by the magnetism of frustrated quantum spin systems.

4:06PM L8.00007 On the onset of incommensurate behavior in the J_1 - J_2 -chain with an odd number of sites, ANDREAS DESCHNER, ERIK S. SORENSEN, McMaster University — The anti-ferromagnetic spin-1/2- J_1 - J_2 -chain is one of the most researched spin-systems. For a chain with an even number of sites the ground-state is analytically known at $J_2/J_1 = 0.5$ and at $J_2/J_1 > 0.5$ spin-spin-correlations become incommensurate. Very little is known about how this incommensurability is manifested in chains with an odd number of sites. In this presentation we show results of variational calculations for J_1 - J_2 -chains with an odd number of sites and open boundary conditions in this incommensurate regime. The results indicate that the system becomes gapless at $J_2/J_1 \approx 0.53$. We show results for the on-site magnetization, the entanglement as well as correlation functions and discuss how the incommensurability dramatically affects them. In particular we show how the usual well defined single soliton excitation breaks up at $J_2/J_1 \approx 0.53$.

4:18PM L8.00008 Broken vector spin chirality in biatomic Fe chains on Ir(001)¹, S. BLUGEL, Y. MOKROUSOV, Peter Grunberg Institut and Institute for Advanced Simulation, Forschungszentrum Juelich and JARA, 52425 Juelich, Germany, M. MENZEL, R. WIESER, K. VON BERGMANN, E. VEDMEDENKO, A. KUBETZKA, R. WIESENDANGER, Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany, S. HEINZE, Institut für Theoretische Physik und Astrophysik, Christian-Albrecht-Universität zu Kiel, 24098 Kiel, Germany — We investigate from *ab initio* the magnetism of biatomic Fe chains, which form due to self-organization on the (5×1)-reconstructed Ir(001) surface [1,2]. Using the FLEUR code [3], we calculate the magnetic properties and exchange interactions in this system, finding a very small Heisenberg exchange along the chain of the order of 10 meV/Fe-atom. Upon including spin-orbit coupling we obtain the contribution from the Dzyaloshinskii-Moriya interaction and find that it leads to a 120° spin-spiral ground state of the Fe chains with a unique rotational sense. The results of the Monte-Carlo simulations based on the parameters from *ab initio* are in a very good agreement to STM experiments on the system. Moreover, simulations indicate a robustness of the spin chiral order parameter, which decays with temperature much slower than the scalar spin correlation, in analogy to a vector spin chiral liquid state. We discuss possible applications of the magnetism in these chains with respect to the transfer of information on the nanoscale.
[1] L. Hammer *et al.*, Phys. Rev. B **67**, 125422 (2003). [2] Y. Mokrousov *et al.*, Phys. Rev. B **80**, 195420 (2009). [3] www.flapw.de

¹We acknowledge funding under HGF-YIG Programme VH-NG-513.

4:30PM L8.00009 Highly frustrated quantum magnetism in the mineral azurite: multi-step approach from first-principles computations to experimental data, HARALD O. JESCHKE, INGO OPAHLE, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany, HENA DAS, TANUSRI SAHA-DASGUPTA, Satyandranath Bose National Centre for Basic Sciences, Kolkata 700098, India, MICHAEL LANG, Physikalisches Institut, Goethe-Universität Frankfurt am Main, 60438 Frankfurt, Germany, SHIJIE HU, XIAOQUN WANG, Department of Physics, Renmin University of China, Beijing 100872, China, ROBERT PETERS, Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan, ANDREAS HONECKER, Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — The natural mineral azurite $\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$ is a frustrated magnet displaying unusual and controversially discussed magnetic behavior. We perform a theoretical study based on density functional theory as well as state-of-the-art numerical many-body calculations [1]. We propose an effective generalized spin-1/2 diamond chain model which provides a consistent description of experiments: low-temperature magnetization, inelastic neutron scattering, nuclear magnetic resonance measurements, magnetic susceptibility as well as new specific heat measurements. With this study we demonstrate that the balanced combination of first principles with powerful many-body methods successfully describes the behavior of this frustrated material.
[1] H. O. Jeschke *et al.*, Phys. Rev. Lett. **106**, 217201 (2011)

4:42PM L8.00010 Magnetic anisotropy in the frustrated spin-ladder system BiCu_2PO_6 from magnetostriction in pulsed fields, ATSUKO UCHIDA, YOSHIMITSU KOHAMA, MPA-CMMS, Los Alamos National Laboratory, USA, SHUANG WANG, Laboratory for Quantum Magnetism, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland Laboratory for Developments and Methods, Pau, MARCELO JAIME, MPA-CMMS, Los Alamos National Laboratory, USA, CHRISTIAN RÜEGG, Laboratory for Neutron Scattering, Paul Scherrer Institute, CH-5232 Villigen, Switzerland — The spin interactions in BiCu_2PO_6 have been studied by inelastic neutron scattering, magnetic susceptibility, and numerical calculation. There is strong frustration between magnetic interactions along the ladder leg, J_{leg} and J_{NNN} , and it has been pointed out that a spin gap persists in this frustrated system. Both J_{leg} and J_{NNN} are intra-ladder and two-leg ladder is always gapped. Longitudinal magnetostriction (MS) measurements were performed using a fiber optic strain gauge in a 60 T pulsed magnet [1]. Specific heat (C_p) and magnetocaloric effect (MCE) measurements were performed in a 35 T DC magnet. C_p vs T was obtained using both a thermal relaxation time and dual slope techniques. We have in this way determined the (H,T) phase diagram of BiCu_2PO_6 up to 45 T. The 3D character of phase transitions is suggested by the observation of sharp anomalies in CM and $\Delta L/L$. Our MCE and MS data provides direct evidence of first-order phase transitions for H//c, while phase transitions for H//a and H//b are characterized as second-order phase transitions. The anisotropic and complex phase boundaries will be discussed.
[1] Daou R *et al.*, Rev. Sci. Instrum. **81**, 033909 (2010).

4:54PM L8.00011 Magnetism of a Frustrated Four-Spin-Tube¹, WOLFRAM BRENIG, Technical University Braunschweig, Germany, MARCELO ARLEGO, Universidad Nacional de La Plata, Argentina — We report on the magnetism of a frustrated four-leg spin-1/2 tube (FFST) [1]. Using a combination of series expansion, based on the continuous unitary transformation method and density-matrix renormalization group we analyze the ground-state correlations, and the one-, and the two-particle excitations in the regime of strong rung-coupling. We find that frustration destabilizes the spin-gapped quadrumer singlet-phase of the FFST, leading to first order quantum phase transitions. Apart from the well-know triplon branch of two-leg spin-ladders, the FFST is shown to sustain additional elementary excitations, including a singlon, and additional triplons. Finally, in the two-particle sector the FFST exhibits several collective (anti)bound states. Frustration has significant impact on the FFST leading to a flattening of the ground-state energy landscape, a mass-enhancement of the excitations, and a relative enhancement of the (anti)binding strength.
[1] Marcelo Arlego and Wolfram Brenig Phys. Rev. B **84**, 134426 (2011).

¹Work supported in part by DFG 444 ARG-113/10/0-1, CONICET Coop. Int. R.2049/09 and PIP 1691, ANPCyT PICT 1426, and NSF PHY05-51164.

5:06PM L8.00012 Pursuit of a spin Bose-metal phase in Hubbard-type models on the two-leg triangular strip, RYAN V. MISHMASH, UCSB, IVAN GONZALEZ, CESGA, ROGER MELKO, University of Waterloo, OLEXEI I. MOTRUNICH, Caltech, MATTHEW P.A. FISHER, UCSB — Motivated by recent experiments on the organic materials $\kappa\text{-(ET)}_2\text{Cu}_2(\text{CN})_3$ and $\text{EtMe}_3\text{Sb}[\text{Pd}(\text{dmit})_2]_2$, we numerically investigate the Mott metal-insulator transition in a system of interacting, itinerant electrons at half-filling on the two-leg triangular strip (i.e., zigzag chain). Previous work [1] has revealed that an exotic “spin Bose-metal” (SBM) phase with three gapless modes is stabilized on the zigzag strip in a pure spin model of Heisenberg exchange supplemented with four-site cyclic ring exchange, a model appropriate for describing weak Mott insulators near the Mott transition. Indeed, a physically appealing picture of the realized SBM phase is to view it as a particular Mott insulating instability out of a two-band metal of interacting electrons. Guided by this idea, we perform large-scale DMRG calculations across the Mott transition in various Hubbard-type models (e.g., with on-site repulsion, longer-ranged repulsion, and/or explicit spin exchange terms). We focus on the successes and failures of describing the insulating phase near the transition within the SBM framework. Finally, the implications of our findings to the full 2D triangular lattice will be discussed.
[1] D. N. Sheng *et al.*, PRB **79**, 250112 (2009).

5:18PM L8.00013 Symmetry protected topological phases for 1-dimensional spin-1 antiferromagnets, ZHENG-XIN LIU, Tsinghua university, XIE CHEN, XIAO-GANG WEN, Massachusetts Institute of Technology — Symmetry protected topological phases for 1-dimensional $S=1$ antiferromagnets respecting D_2+T symmetry (D_2 is a point group and T is the time reversal symmetry) are studied. There are 15 different nontrivial topological phases, all of them are non-symmetry-breaking. One of these phases is the usual Haldane phase, and the others are new. We find that four of the nontrivial SPT phases can be realized in spin-1 chains and the rest can be realized in spin-1 ladders. We propose experimental methods to distinguish all of these phases.

Tuesday, February 28, 2012 2:30PM - 5:30PM –

Session L9 DMP GMAG: Focus Session: Complex Bulk Oxides: Theoretical techniques for oxides 209

2:30PM L9.00001 Thermodynamics of Ferrotoroidic Materials, AVADH SAXENA, Los Alamos National Lab., TERESA CASTAN, ANTONI PLANES, University of Barcelona — The three primary ferroics, namely ferromagnets, ferroelectrics and ferroelastics exhibit corresponding large (or even giant) magnetocaloric, electrocaloric and elastocaloric effects when a phase transition is induced by the application of an appropriate external field (E , H and stress). Recently the suite of primary ferroics has been extended to include ferrotoroidic materials in which there is an ordering of toroidic moments in the form of magnetic vortex-like structures, examples being $\text{LiCo(PO}_4)_3$ and $\text{Ba}_2\text{CoGe}_2\text{O}_7$. We formulate the thermodynamics of ferrotoroidic materials. Within a Landau free energy framework we calculate the toroidocaloric effect by quantifying isothermal entropy change (or adiabatic temperature change) in the presence of an applied toroidic field ($G = E \times H$) when usual magnetization and polarization may also be present simultaneously.

2:42PM L9.00002 Theory of K-edge Resonant Inelastic X-ray Scattering for Perovskite Manganites¹, TSEZAR F. SEMAN, New Jersey Institute of Technology, XUERONG LIU², JOHN P. HILL³, Brookhaven National Laboratory, MICHEL VAN VEENENDAAL, Argonne National Laboratory and Northern Illinois University, KEUN HYUK AHN, New Jersey Institute of Technology — We present calculations of K-edge resonant inelastic x-ray scattering (RIXS) spectrum for layered and three dimensional perovskite manganites with charge, orbital, and spin orderings. We extend the approach in Ref. [1] to the tight binding model for the manganites, calculate RIXS intensity in momentum and energy space, and compare with experiment data. The results show strong dependence of the RIXS intensity on momentum, which agrees well with experimental observation. We discuss its implications on the material properties and the RIXS process.

[1] K. H. Ahn, A. J. Fedro, and M. van Veenendaal, Phys. Rev. B 79, 045103 (2009).

¹Work at NJIT and ANL was supported by the DOE CMCSN under Contract No. DEFG02-08ER46540. Work performed at BNL supported by US DOE DMSE, under contract No. DE-AC02-98CH10886.

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2:54PM L9.00003 Nonreciprocal Directional Dichroism and Toroidalmagnons in Helical Magnets, SHIN MIYAHARA, ERATO-MF, JST, NOUBO FURUKAWA, Aoyama Gakuin Univ. — We investigate a dynamical magnetoelectric effect owing to a magnetic resonance in helical spin structures through a coupling between magnetization and electric polarization via a spin current mechanism [1]. We show that the magnon has a dynamical magnetic moment dM and an electric moment dP which is perpendicular to dM , simultaneously, i.e., a dynamical toroidal moment $T^d = dM \times dP$ under the external magnetic fields, and thus named it as a toroidalmagnon. The toroidalmagnon exists in most conical spin structures due to generality of the spin current mechanism. In absorption of electromagnetic wave, the toroidalmagnon excitation process generally induces nonreciprocal directional dichroism as a consequence of the interference of the magnetic and the electric responses. The nonreciprocal directional dichroism should be experimentally observed in various cycloidal multiferroic materials, e.g. RMnO_3 . [1] H. Katsura, A.V. Balatsky, and N. Nagaosa: Phys. Rev. Lett. **98** 027203 (2007)

3:06PM L9.00004 First-principles Wannier function based methods for disordered materials and applications to studies of oxides and Fe-superconductors¹, WEI KU, CMPMSD, Brookhaven National Laboratory — This talk will discuss recently developed first-principles methods for materials with disordered impurities, and their applications to case studies of correlated oxides and Fe-based superconductors containing vacancies, substitutions and intercallants. Simplified via the use of Wannier functions, the first method [1] is to unfold the one-particle spectral function from the reduced Brillouin zone of a broken symmetry state back to the regular Brillouin zone of the normal state. This unfolding not only allows a clearer visualization of the physical effects of the broken translational symmetry, but also connects directly to the experimental spectral weight of angular resolved photo emission spectroscopy. The second method [2] is to reduce the computational expense of configuration-averaged spectral function of disordered materials by orders of magnitude, to allow inclusion of large length scale required for weakly localized states and short-range orders. This Wannier function based method is systematically improvable, beyond-mean-field, and not perturbation limited. Case studies to be discussed include dilute magnetic semiconductors [3], transition metal oxides[1,2], and Fe-based superconductors [4,5].

[1] Wei Ku et al, PRL 104, 216401 (2010)

[2] T. Berlijn et al, PRL 106, 077005 (2011)

[3] T. S. Herng et al, PRL 105, 207201 (2010)

[4] C.-C. Lee et al, PRL 103, 267001 (2009)

[5] C.-H. Lin et al, arXiv:1107.1485

¹Work supported by DOE DE-AC02-98CH10886 and DOE CMCSN

3:42PM L9.00005 Incommensurate spin excitations stabilized multiferroic phase in CuO, LIXIN HE, University of Science and Technology of China — Cupric oxide is a unique magnetoferroelectrics with transition temperature way above the boiling point of liquid nitrogen. However, the mechanism of high T_c multiferroicity in CuO is still puzzling. In this paper, we clarify the mechanism of high T_c multiferroicity in CuO using combined first-principles calculations and an effective Hamiltonian model. We find that CuO contains two magnetic sublattices, with strong intra-sublattice interactions and weakly frustrated inter-sublattice interactions, which might be one of the main reasons that the compound has a high ordering temperature. The weak spin frustration leads to incommensurate spin excitations that dramatically enhances the entropy of the multiferroic phase, and eventually stabilize the multiferroic phase in CuO.

3:54PM L9.00006 Pressure-driven high-spin to low-spin and orbital-selective insulator to metal transition in cubic CoO, LI HUANG, XI DAI, YILIN WANG, The Institute of Physics, Chinese Academy of Sciences — We studied the magnetic and spectral properties for cubic para-magnetic phases of CoO under high pressures by using *ab initio* many-body method which combining local density approximation with dynamical mean-field theory. Experimentally observed metal-insulator transition at high pressure is successfully reproduced in calculations. Our calculation predicts CoO as a Mott insulator at ambient pressure and metal at extreme high pressure. In the intermediate pressure regime, our results indicate that there is an orbital selective Mott phase with t_{2g} orbitals being metallic and e_g orbitals being insulating. In contrast with MnO and Fe_2O_3 (d^5 configuration) where metal-insulator transition is accompanied by a high-spin to low-spin transition, we found that the local moment of CoO (d^7 configuration) decreases gradually from 2.8 ($S = 3$ states) to 1.4 ($S = 1$ states) with increasing pressure, which is in agreement with experimental data.

4:06PM L9.00007 Mott physics in multi-band Hubbard model with strong spin-orbit interaction, LIANG DU, LI HUANG, XI DAI, Institute of Physics, The Chinese Academy of Sciences — Spin-orbit coupling and electron correlation both play very crucial roles in the Mott physics of $4d$ and $5d$ transition-metal oxides. By studying three band Hubbard model with full Hund's rule coupling and spin-orbit coupling, we show that spin-orbit coupling intends to strongly enhance the Mott transition. By means of generalized Gutzwiller variational method and dynamical mean field (DMFT) with continuous time quantum Monte Carlo (CTQMC) as impurity solver, we obtain the complete phase diagram for this problem, which can be divided into metal, Mott insulator and band insulator phases. At mean while, we have also studied the effect of the Coulomb interaction on the strength of the spin-orbital coupling in the metallic phase. Our conclusion is that the correlation effect on the spin-orbital coupling is far beyond the mean field treatment even in the intermediate coupling regime.

4:18PM L9.00008 Covalency, Excitons, Double Counting and the Metal-Insulator Transition in Transition Metal Oxides, XIN WANG, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park — We present single-site dynamical mean-field studies of realistic models of transition metal oxides, including the cuprate superconductors and rare earth nickelates (in bulk and superlattice form). We include orbital multiplet effects and hybridization to ligands. We explicitly calculate the d-d exciton spectra for cuprates, finding sharp exciton lines in both metallic and insulating phases, which should be visible in experiments. We also find that the additional $d_{3z^2-r^2}$ orbital does not contribute to an additional Fermi surface at any reasonable doping, in contradiction to previous slave-boson studies. The hybridization to ligands is shown to have crucial effects, for example suppressing the ferro-orbital order previously found in Hubbard model studies of nickelates. Hybridization to ligands is shown to be most naturally parametrized by the d-orbital occupancy. For cuprates and nickelates, insulating behavior is found to be present only for a very narrow range of d-occupancy, irrespective of the Coulomb repulsion. The d-occupancy predicted by standard band calculations is found to be very far from the values required to obtain an insulating phase, calling into question the interpretation of these materials as charge transfer insulators.

This work is done in collaboration with A.J. Millis, M.J. Han, C.A. Marianetti, L. de' Medici, and H.T. Dang, and is supported by NSF-DMR-1006282, the Army Office of Scientific Research, and the Condensed Matter Theory Center and CNAM at University of Maryland.

[1] X. Wang, H. T. Dang, and A. J. Millis, Phys. Rev. B 84, 014530 (2011).

[2] X. Wang, M. J. Han, L. de' Medici, C. A. Marianetti, and A. J. Millis, arXiv:1110.2782.

[3] M. J. Han, X. Wang, C. A. Marianetti, and A. J. Millis, Phys. Rev. Lett. 107, 206804 (2011).

4:54PM L9.00009 Ab initio study of the anti-ferromagnetic, non-collinear CuB_2O_4 crystal¹, YIING-REI CHEN, Physics Department, National Taiwan Normal University, Taipei, Taiwan 116, P.-R. LEE, J.-Y. LIN, Institute of Physics, National Chiao Tung University, Hsinchu, Taiwan 300, J.-M. CHEN, National Synchrotron Radiation Research Center (NSRRC), Hsinchu, Taiwan 300, A.N. VASILIEV, Department of Low temperature Physics, Moscow State University, Moscow 119992, Russia — The spiky features in the crystal absorption spectrum, and the distinct differences in the directional oxygen K-edge absorption spectroscopy of the non-collinear anti-ferromagnetic, incommensurate CuB_2O_4 , had led us to this LDA+U study of the crystal, although in the commensurate phase, due to the instrumental limitation. The calculated band structure matches the spiky features in the absorption spectrum, while the orbital analyzed DOS data explain the differences in the directional oxygen K-edge absorption spectroscopy. The two groups of dispersion-less bands, immediately above the gap, come from different groups of plaquettes, of Cu(A) and Cu(B), and are responsible for the spiky features observed experimentally.

¹This study is supported by grant NSC 99-2112-M-003-012-MY2.

5:06PM L9.00010 Exact results on magnon-mediated pairing of spin-polarons¹, MIRKO MOELLER, MONA BERCIU, University of British Columbia — The motion of a charged particle in a magnetically ordered background determines the electronic behavior of weakly doped, magnetically ordered insulators and semiconductors. This problem can be solved exactly for a single charge carrier in a ferromagnetic background at zero-temperature. The solution is a spin-polaron, i.e. a dressed quasiparticle consisting of a charge carrier and a bound magnon which is dynamically emitted and reabsorbed by the charge carrier. If the exchange interaction between the charged particle and the ferromagnetic background is antiferromagnetic, then the spin polaron describes the low-energy states. We generalized the exact solution to the case of two charge carriers. This allows us to characterize the conditions (what ranges of parameters and for what types of lattices) under which magnon-mediated pairing occurs, so that spin-bipolarons describe the low-energy states.

¹NSERC, PROMOS fellowship of the DAAD

5:18PM L9.00011 Understanding the interplay between crystal structures and magnetic states of RCO_2 (R = heavy rare earths)¹, DURGA PAUDYAL, Y. MUDRYK, The Ames Laboratory, U. S. Department of Energy, V.K. PECHARSKY, K.A. GSCHNEIDNER, JR., The Ames Laboratory, U. S. Department of Energy and Department of Materials Science and Engineering, Iowa State University, Ames, IA — The RCO_2 compounds with R = heavy lanthanides are well known model systems for both experimentalists and theorists because of the complex nature of the magnetism of these materials. Better understanding of the magnetism can be achieved from parameter-free first principles calculations as well as carefully executed experiments. From first principles calculations we show that the indirect $4f$ - $4f$ exchange polarizes the $5d$ spins and the spin up $5d$ and spin down $3d$ hybridization gives rise to ferrimagnetism, i.e. antiparallel $5d$ and $3d$ itinerant magnetic moments at low temperature. The itinerant electron metamagnetism is known to support first order phase transformations in some of the RCO_2 compounds. However the clear understanding of this mechanism is lacking and, therefore, we clarify this mechanism from first principles calculations and experimentally confirm the nature of phase transformation of TbCo_2 . The interrelation between the crystal structure and the magnetic states has also been investigated considering TbCo_2 as an example.

¹This work is supported by the Office of Basic Energy Sciences, Materials Science and Engineering Division of the Office of Science. The Ames Laboratory is operated by Iowa State University of Science and Technology for the U.S. Department of Energy.

Tuesday, February 28, 2012 2:30PM - 5:30PM –
Session L10 DLS: Invited Session: Quantum Optics in Condensed Matter 210A

2:30PM L10.00001 Two-photon interference from quantum dot and parametric-down conversion single photons, GLENN SOLOMON, Joint Quantum Institute, NIST & Univ. Maryland — No abstract available.

3:06PM L10.00002 Quantum spectroscopy of semiconductors with Schrödinger's cat states, MACKILLO KIRA, Department of Physics, Philipps-University Marburg, Germany — Quantum investigations on simple systems — such as atoms or quantized light modes — have reached a level where one can read and write information directly onto the density matrix itself. Currently, the same level of quantum-information control seems inconceivable in condensed-matter systems simply because the many-body states involved are unimaginably complicated. In this talk, I will present the first steps in realizing targeted access of many-body states within condensed-matter systems by combining quantum-optics and many-body theory [1] with classical high-precision laser spectroscopy. The light-matter interaction has an inherent capability to directly excite targeted many-body states through the light source's quantum fluctuations [2]. The related quantum-optical responses can be projected from the classical data set by applying the cluster-expansion transformation [3] (CET). As a proof of principle, we CET project the measured nonlinear absorption of semiconductor quantum wells [4] into the quantum absorption generated by Schrödinger's cat-state sources. The results expose a completely new level of many-body physics that remains otherwise hidden. Especially, the investigations reveal an anomalous reduction of Coulomb scattering of excitons, the excitation-induced narrowing of the exciton-molecule resonance, and the formation of electron-hole complexes (multi-exciton clusters) [5].

[1] M. Kira and S.W. Koch, *Semiconductor quantum optics*, (Cambridge University Press, 2011).

[2] M. Kira and S.W. Koch, *Phys. Rev. A* **73**, 013813 (2006); S.W. Koch, M. Kira, G. Khitrova, and H.M. Gibbs, *Nature Mat.* **5**, 523 (2006); M. Kira and S.W. Koch, *Prog. Quantum Electr.* **30**, 155 (2006).

[3] M. Kira and S.W. Koch, *Phys. Rev. A* **78**, 022102 (2008).

[4] R.P. Smith *et al.*, *Phys. Rev. Lett.* **104**, 247401 (2010).

[5] M. Kira *et al.*, *Nature Physics* **7**, 799-804 (2011).

3:42PM L10.00003 Quantum optics with solid-state atom-like systems, MIKHAIL LUKIN, Harvard Univ — No abstract available.

4:18PM L10.00004 Quantum Dot Spins and Photons, METE ATATUR, University of Cambridge — Self-assembled semiconductor quantum dots are interesting and rich physical systems. Their inherently mesoscopic nature leads to a multitude of interesting interaction mechanisms of confined spins with the solid state environment of spins, charges and phonons. In parallel, the relatively clean spin-dependent optical transitions make quantum dots strong candidates for stationary and flying qubits within the context of spin-based quantum information science. The recently observed quantum dot resonance fluorescence has become a key enabler for further progress in this context. I will first discuss the real-time optical detection (or single-shot readout) of quantum dot spins, and then I will discuss how resonance fluorescence allows coherent generation of single photons suitable (and tailored) for linear-optics quantum computation and for establishing a high-efficiency spin-photon quantum interface within a distributed quantum network.

4:54PM L10.00005 Dynamics of vortices in polariton quantum fluids : From full vortices, to half vortices and vortex pairs¹, BENOIT DEVEAUD-PLÉDRAN, EPFL, Lausanne, Switzerland — Polariton quantum fluids may be created both spontaneously through a standard phase transition towards a Bose Einstein condensate, or may be resonantly driven with a well-defined speed. Thanks to the photonic component of polaritons, the properties of the quantum fluid may be accessed rather directly with in particular the possibility of detained interferometric studies. Here, I will detail the dynamics of vortices, obtained with a picosecond time resolution, in different configurations, with in particular their phase dynamics. I will show in particular the dynamics of spontaneous creation of a vortex, the dissociation of a full vortex into two half vortices as well as the dynamics of the dissociation of a dark soliton line into a street of pairs of vortices. Work done at EPFL by a dream team of Postdocs PhD students and collaborators: K. Lagoudakis, G. Nardin, T. Paraiso, G. Grosso, F. Manni, Y Léger, M. Portella Oberli, F. Morier-Genoud and the help of our friend theorists V. Savona, M. Vouters and T. Liew.

¹SNSF funding through Quantum Photonics NCCR is deeply acknowledged

Tuesday, February 28, 2012 2:30PM - 5:30PM –
Session L11 DMP: Focus Session: Graphene Structure, Stacking, Interactions: Magnetism and Interactions 210B

2:30PM L11.00001 Kondo Effect in Bilayer Graphene¹, DIEGO MASTROGIUSEPPE, SERGIO ULLOA, NANCY SANDLER, Ohio University — Because of the linear dependence of the density of states (near Dirac points), the physics of localized magnetic moments on graphene exhibits unique characteristics [1]. From the experiments by Mattos *et al* [2], where a possible observation of the 2-channel Kondo effect was reported, to recent studies on vacancies [3], the role of local moments on graphene remains poorly understood. The technical difficulties to determine the nature of the origin of the local moment add to the complexity of the problem. To gain insight into this problem, we have undertaken a study of a bilayer graphene system with Bernal stacking and an intercalated magnetic impurity. We model the system with a multiband Anderson impurity model and obtain the effective Kondo Hamiltonian via a Schrieffer-Wolff transformation. Although several conducting channels couple to the impurity, the standard 1-channel Kondo regime is recovered at low temperatures. The effective Kondo exchange couplings depend on the interlayer hopping giving rise to tunable Kondo temperatures.

[1] P. S. Cornglia *et al.*, *PRL* **102**, 046801 (2009); B. Uchoa *et al.*, *PRL* **106**, 016801 (2011)

[2] L. Mattos *et al.* (unpublished)

[3] J. -H. Chen *et al.*, *Nature Phys.* **7**, 535(2011); M. M. Ugeda *et al.*, *PRL* **104**, 096804 (2010).

¹Supported by NSF-PIRE and NSF-MWN/CIAM.

2:42PM L11.00002 Mid-gap states and Kondo effect in disordered graphene, CAIO LEWENKOPF, VLADIMIR MIRANDA, Universidade Federal Fluminense, LUIS DIAS DA SILVA, Universidade de São Paulo — Recent experiments on graphene flakes with short range scattering defects have strengthen the interest on Kondo physics in graphene systems. The experimental data show a temperature dependence of the resistivity consistent with the low-temperature Kondo screening of local magnetic moments. While the linear dispersion in the density of states in graphene justify a pseudogap Kondo model showing a rich variety of quantum critical behavior as a function of the gate-controlled chemical potential, the presence of disorder can alter this effect in favor of the "standard" Kondo model, with a Fermi-liquid ground state. We study these effects with different numerical methods. Tight-binding calculations for diluted scattering defects show the appearance of quasi-localized midgap states in the local density of states at the vicinity of the charge neutrality point. This leads to the formulation a Anderson-like model of localized states within the graphene matrix, which may lead to a Kondo screening consistent with the experiments. To verify this hypothesis, we perform numerical renormalization group (NRG) calculations to study the gate-dependence of the Kondo temperature and the transport properties of this model.

2:54PM L11.00003 Dynamic RKKY interaction in graphene, MAURO FERREIRA, STEPHEN POWER, School of Physics, Trinity College Dublin, Ireland, FILIPE GUIMARAES, Department of Physics and Astronomy, University of California, Irvine, ANTONIO COSTA, ROBERTO MUNIZ, Instituto de Física, Universidade Federal Fluminense, Brazil — The growing interest in carbon-based spintronics has stimulated a number of recent theoretical studies on the RKKY interaction in graphene, based on which the energetically favourable alignment between magnetic moments embedded in this material can be calculated. The general consensus is that the strength of the RKKY interaction in graphene decays as $1/D^3$ or faster, where D is the separation between magnetic moments. Such an unusually fast decay for a 2-dimensional system suggests that the RKKY interaction may be too short ranged to be experimentally observed in graphene. Here we show in a mathematically transparent form that a far more long ranged interaction arises when the magnetic moments are taken out of their equilibrium positions and set in motion. We not only show that this dynamic version of the RKKY interaction in graphene decays far more slowly but also propose how it can be observed with currently available experimental methods.

3:06PM L11.00004 Formation of Localized Magnetic States on Adatoms in Uniaxially Strained Graphene, ANAND SHARMA, VALERI KOTOV, University of Vermont, Burlington — We investigate the effect of applied uniaxial strain on the formation of localized magnetic states on adatoms in graphene. In the framework of the single impurity Anderson model, we systematically analyze the interplay between the anisotropic (strain-induced) nature of the Dirac fermions and the on-site Hubbard interaction. We numerically calculate the polarization of the electrons in the localized orbital within the mean-field self-consistent scheme. A phase diagram is obtained, containing non-magnetic as well as large magnetic regions, which can find prospective applications in the field of carbon-based spintronics.

3:18PM L11.00005 Spin and band ferromagnetism in trilayer graphene, RALPH VAN GELDEREN, Utrecht University, LIH-KING LIM, LPS Orsay, Université Paris-Sud, CRISTIANE MORAIS SMITH, Utrecht University — We study the ground state properties of an ABA-stacked trilayer graphene. The low energy band structure can be described by a combination of both a linear and a quadratic particle-hole symmetric dispersion, reminiscent of monolayer- and bilayer-graphene, respectively. The multi-band structure offers more channels for instability towards ferromagnetism when the Coulomb interaction is taken into account. Indeed, if one associates a subband-index degree of freedom to the bands (parabolic/linear), it is possible to realize also a band-ferromagnetic state, where there is a shift in the energy bands, since they fill up differently. By using a variational procedure, we compute the exchange energies for all possible variational ground states and identify the parameter space for the occurrence of spin- and band-ferromagnetic instabilities as a function of doping and interaction strength.

3:30PM L11.00006 Magnetic order in graphene with broken inversion symmetry, J. FERNANDEZ-ROSSIER, International Iberian Nanotechnology Laboratory, Braga, Portugal, D. SORIANO, Institut Català de Nanotecnologia (ICN), Barcelona, Spain — We study the effect of sublattice symmetry breaking on the magnetic and transport properties of two dimensional graphene as well as zigzag terminated one dimensional graphene nanostructures. The systems are described with the Hubbard model within the collinear mean field approximation. In the case of 2D and zigzag ribbons we compute the phase diagram, at half-filling, defined by the normalized interaction strength U/t and the sublattice potential V/t , where t is the first neighbor hopping. In the case of 2D graphene we find that the system is always insulating, except at the transition between the antiferromagnetic (AF) and the non-magnetic (NM) phase where the system is half-metallic. In the case of zigzag ribbons, at finite V we find that the system undergoes a phase transition from non-magnetic insulator for $U < U_c(V)$ to a phase with ferromagnetic order in the edges and antiferromagnetic inter-edge coupling. The conduction properties of the magnetic phase depend on V and can be insulating, conducting and even half-metallic, yet the total magnetic moment in the system is zero. In the latter case, we find a strong spin filter effect.

3:42PM L11.00007 Magnetic Properties of Rhombohedral Graphene Thin Films¹, THANH CUONG NGUYEN, MINORU OTANI, NRI-AIST, Tsukuba, Japan, SUSUMU OKADA, University of Tsukuba, Tsukuba, Japan — Ever since the fabrication of single and few layers graphene, the graphene thin films have been attracting so much attention in the field not only of low-dimensional sciences but also of nano-scale technologies due to their perfect two-dimensional network. One of fascinating issues in this carbon allotrope is the intrinsic magnetism that is inherent in their topological properties. We have demonstrated that the (0001) surfaces of graphene thin film with rhombohedral-stacked arrangement exhibit ferrimagnetic spin ordering induced by flat dispersion band associated with the peculiar surface localized electron states classified as the “edge state” [1]. In this work, we systematically investigate how the electronic and magnetic properties of the rhombohedral-stacked graphene thin films depend on the number of graphene layers, BN substrate, and uniaxial pressure using first-principles total-energy calculations in the framework of density functional theory [2].

[1] M. Otani, M. Koshino, Y. Takagi, and S. Okada, Phys. Rev. B 81 (2010) 161403(R).

[2] N. T. Cuong, M. Otani, and S. Okada, Surf. Sci. (2011), doi:10.1016/j.susc.2011.10.001

¹Work partly supported by CREST-JST.

3:54PM L11.00008 Emergence of atypical magnetic and electronic properties in graphitic nanowiggles, VINCENT MEUNIER, Rensselaer Polytechnic Institute, EDUARDO COSTA-GIRAO, Universidade Federal do Ceará, LIANGBO LIANG, Rensselaer Polytechnic Institute, EDUARDO CRUZ-SILVA, University of Massachusetts, Amherst, ANTONIO GOMES SOUZA FILHO, Universidade Federal do Ceará — Graphitic nanowiggles (GNWs) are periodic repetitions of non-aligned finite-sized graphitic nanoribbon domains seamlessly stitched together without structural defects. These complex nanostructures have been recently fabricated using the self-assembly and subsequent fusion of small aromatic compound (Nature 466, 470 (2010)). The structures are predicted to possess unusual properties, such as tunable bandgaps and versatile magnetic behaviors (Phys. Rev. Lett. 107, 135501 (2011)). First-principles theory was used to highlight the microscopic origin of the emerging electronic and magnetic properties of the main subclasses of GNWs, thereby establishing a road-map for guiding the design and synthesis of specific GNWs with targeted nanoelectronic, optoelectronic, and spintronic properties. We will show the unusual versatility of GNWs' magnetic properties, we will highlight the variation of electronic properties with the details of the structures and how these structures can be used to transport electrons.

4:06PM L11.00009 Chiral superconductivity from repulsive interactions in doped graphene, RAHUL NANDKISHORE, LEONID LEVITOV, Massachusetts Institute of Technology, ANDREY CHUBUKOV, University of Wisconsin-Madison — We present a model wherein repulsive interactions unambiguously lead to superconductivity with enhanced T_c . The superconducting state is the chiral $d + id$ superconducting state, which has no known experimental realizations. Intriguingly, our model has a natural realization in graphene that is doped to the M point of the Brillouin zone. At this doping level, the Fermi surface nesting and the divergent density of states can produce interaction driven instabilities to exotic phases with high energy scales. Analyzing the competition between various ordering tendencies within a renormalisation group framework, we find that the leading instability is to d-wave superconductivity, for any choice of weak repulsive interactions. The instability develops simultaneously in two distinct d-wave channels, which are degenerate by lattice symmetries. Analysis of the pairing below T_c reveals that both orders co-exist to produce $d + id$ superconductivity, with the phase of the order parameter winding by 4π as we go around the Fermi surface.

4:18PM L11.00010 Competing many-body instabilities and unconventional superconductivity in graphene, CHRISTIAN PLATT, MAXIMILIAN KIESEL, WERNER HANKE, Institute for Theoretical Physics, University of Würzburg, DMITRY A. ABANIN, Department of Physics, Harvard University, RONNY THOMALE, Department of Physics, Stanford University — The band structure of graphene exhibits van Hove singularities (VHS) at doping $x = \pm 1/8$ away from the Dirac point. Near the VHS, interactions effects, enhanced due to the large density of states, can give rise to various many-body phases at experimentally accessible temperatures. We study the competition between different many-body instabilities in graphene using functional renormalization group (FRG). We predict a rich phase diagram, which, depending on long range hopping as well as screening strength and absolute scale of the Coulomb interaction, contains a $d + id$ -wave superconducting (SC) phase, or a spin density wave phase at the VHS. The $d + id$ state is expected to exhibit quantized charge and spin Hall response, as well as Majorana modes bound to vortices. In the vicinity of the VHS, we find singlet $d + id$ -wave as well as triplet f -wave SC phases.

[1] arXiv:1109.2953v1

4:30PM L11.00011 Power law Kohn anomaly in graphene induced by Coulomb interactions, FERNANDO DE JUAN, HERBERT A. FERTIG, Indiana University, Bloomington — Phonon dispersions generically display non-analytic points, known as Kohn anomalies, due to electron-phonon interactions. We analyze this phenomenon for a zone boundary phonon in graphene. When electron-electron interactions with coupling constant β are taken into account, one observes behavior demonstrating that the electrons are in a critical phase: the phonon dispersion and lifetime develop power law behavior with β dependent exponents. The observation of this signature would allow experimental access to the critical properties of the electron state, and would provide a measure of its proximity to an excitonic insulating phase.

4:42PM L11.00012 Effect of electron-phonon coupling on energy and density of states renormalizations of dynamically screened graphene, J.P.F. LEBLANC, University of Guelph, J.P. CARBOTTE, McMaster University, E.J. NICOL, University of Guelph — Motivated by recent tunneling and angle-resolved photoemission (ARPES) work [1,2], we explore the combined effect of electron-electron and electron-phonon couplings on the renormalized energy dispersion, the spectral function, and the density of states of doped graphene. We find that the plasmarons seen in ARPES are also observable in the density of states and appear as structures with quadratic dependence on energy about the minima. Further, we illustrate how knowledge of the slopes of both the density of states and the renormalized dispersion near the Fermi level can allow for the separation of momentum and frequency dependent renormalizations to the Fermi velocity. This analysis should allow for the isolation of the renormalization due to the electron-phonon interaction from that of the electron-electron interaction.

[1] Brar et al. Phys. Rev. Lett. 104, 036805 (2010) [2] Bostwick et al. Science 328, p.999 (2010)

4:54PM L11.00013 Screening and electrostatic doping in multilayer graphene systems, MARCELO KURODA, J. TERSOFF, RAZVAN NISTOR, GLENN MARTYNA, IBM TJ Watson Research Center — We study the electrostatic screening in multilayer graphene systems using ab initio calculations and analytical models. First principles calculations reveal that oriented (Bernal) and turbostratic graphene multilayers in contact with a metal slab show only small differences in their charge distribution despite their dissimilar electronic structure. In the turbostratic systems the layer decoupling enables the identification of the Dirac point for each individual layer. We then measure the shift of each Dirac point relative to the Fermi level of the system and compute the charge transfer to each layer. Results are compared with an analytical model considering discrete layers. The model shows that at $T = 0$ charge screening is highly nonlinear due to the vanishing density of states at the Fermi level. More importantly a strong dependence on charge and temperature results in a change of the screening length by more than an order of magnitude depending on the experimental conditions, reconciling the large range of screening lengths previously reported in experiments.

5:06PM L11.00014 Screening in Chiral Multilayer Graphene¹, HONGKI MIN, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea, EUYHEON HWANG, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742, USA — We calculate the static polarization function of multilayer graphene and study the effects of stacking arrangement, carrier density and onsite energy difference. At low densities, the energy spectrum of multilayer graphene is described by a set of chiral two-dimensional electron systems and the associated chiral nature determines the screening properties of multilayer graphene showing very different behavior depending on whether chirality indices are even or odd. As the density increases, the energy spectrum follows that of monolayer graphene thus the polarization function approaches that of monolayer graphene.

¹The work is supported by ONR-MURI and NRI-SWAN.

5:18PM L11.00015 Unusual electron self-energy in graphene, CHOONGYU HWANG, Lawrence Berkeley National Laboratory, DAVID SIEGEL, University of California, Berkeley, SUNG-KWAN MO, Lawrence Berkeley National Laboratory, WILLIAM REGAN, University of California, Berkeley, ARIEL ISMACH, YUEGANG ZHANG, Lawrence Berkeley National Laboratory, ALEX ZETTL, ALESSANDRA LANZARA, University of California, Berkeley — Electron-Electron interactions bear important information on fundamental electronic properties such as electron effective mass, conductivity, and charge mobility. By using angle-resolved photoemission spectroscopy, we study unusual electron self-energy in graphene induced by the electron-electron interactions, which are distinguished from those of an ordinary Fermi liquid. Our findings provide a new route for two-dimensional electron systems toward device applications.

Tuesday, February 28, 2012 2:30PM - 5:30PM –
Session L12 DMP: Focus Session: Graphene: Growth, Mechanical Exfoliation, and Properties
- Growth on Single Crystals 210C

2:30PM L12.00001 Graphene growth on coinage-metal substrates¹, KEVIN MCCARTY, Sandia National Laboratories, Livermore, CA USA — The low solubility of carbon in Cu and Au gives these coinage metals advantages as substrates for graphene growth. Namely, growth occurs exclusively by surface processes, avoiding the complications of C segregating from the bulk of the metal substrate. However, the relatively weak interactions of Cu and Au with graphene can lead to mosaic films having large ranges of in-plane orientations. This talk will emphasize understanding the relationship between the microstructure of graphene sheets and the mechanisms of island nucleation and growth. We use low-energy electron microscopy (LEEM) to observe growth. We find that bunches of substrate steps on Cu(111) can generate misorientation boundaries in a graphene sheet as it overgrows the steps [1]. Thus, growth on rough Cu(111) leads to large rotational disorder. Optimized growth on smooth Cu(111) and Au(111), however, produces islands all in close registry to a single in-plane orientation. On Cu(100), the most abundant grain orientation of commercial Cu foils, graphene islands align around two equivalent in-plane Cu directions [2]. This inherent source of disorder from symmetry mismatch is further compounded by large spreads of orientation around the equivalent directions. The substrate choice also affects the microscopic growth mechanism. The rate that C diffuses to the graphene islands limits growth on Cu(111) [and likely on Au(111)]. The sheet edges are then morphologically unstable, with dendritic islands at low temperature and six-fold loped islands at higher temperature. In contrast, growth on Cu(100) is limited by the rate of C attaching to the graphene edge. This mechanism, combined with the symmetry mismatch, produces two-fold islands. Finally, the coinage metals will be compared to other transition metal substrates.

[1] Phys. Rev. B 84, p. 155425 (2011).

[2] Nano Lett. 10, p. 4890 (2010).

¹Work joint with S. Nie, E. Starodub, K. Thuermer, N. C. Bartelt (Sandia), J. M. Wofford and O. D. Dubon (U.C. Berkeley/LBL) and was supported by the Office of Basic Energy Sciences, Division of Materials and Engineering Sciences of the US DOE.

3:06PM L12.00002 Growth and Characterization of Graphene on Single Crystal Cu Substrates¹, Z.R. ROBINSON, P. TYAGI, H. GEISLER, C.A. VENTRICE, JR., University at Albany, A.A. BOL, J.B. HANNON, IBM T. J. Watson Research Center — One of the key issues for the use of CVD graphene in device applications is the influence of defects on the transport properties of the graphene. Therefore, it is important to understand the influence of the substrate on the orientation of the graphene. Growth of graphene films on Cu(111) has the potential for producing films with a low defect density because of the hexagonal symmetry of the substrate and relatively small lattice mismatch, whereas growth on Cu(100) is expected to result in multi-domain growth because of its square symmetry. In this study, graphene films were grown on Cu single crystal substrates, and characterized with LEEM, LEED, SEM, AFM, and Raman spectroscopy. The clean Cu substrates were prepared by sputtering and annealing in UHV. For the initial growth studies, the samples were transferred to a tube furnace for graphene growth using a technique optimized for Cu foils. The UHV system has recently been modified with a button heater compatible with the conditions needed for graphene growth to enable in-situ growth and characterization.

¹Support from the NSF (1006350/1006411) is appreciated.

3:18PM L12.00003 Suppression of Grain Boundaries in Graphene Growth on Superstructured Mn-Cu(111) Surface¹, WEI CHEN, Univ. of Tennessee, Univ. of Sci. & Tech. of China, HUA CHEN, Univ. of Tennessee, Univ. of Texas at Austin, HAIPING LAN, PING CUI, Univ. of Sci. & Tech. of China, TIM SCHULZE, Univ. of Tennessee, WENGUANG ZHU, Univ. of Tennessee, Oak Ridge National Lab, ZHENYU ZHANG, Univ. of Sci. & Tech. of China, Harvard University — A standing obstacle in epitaxial graphene growth on metal substrates is the prevalence of undesirable grain boundaries (GB) that severely degrade the electronic, transport and mechanical properties of graphene. Employing density functional theory calculations, we demonstrate that the inherent multi-orientational degeneracy of the graphene islands on Cu(111) is the underlying reason for the prevalence of GB. We propose a possible solution, by invoking a functionalized Cu(111) surface to lift the orientational degeneracy of graphene islands and consequently suppress the creation of GB. We have identified the candidate substrate—a superstructured Mn-Cu(111) alloyed surface, which is experimentally achievable and ensures a single orientation for the graphene islands. The proposed approach promises to drastically improve the quality of epitaxial graphene without compromising on efficiency and yield.

¹Supported by USNSF, DMSE/BES of USDOE, and NNSF of China.

3:30PM L12.00004 Rotational homogeneity in graphene grown on Au(111)¹, JOSEPH WOFFORD, UC Berkeley, Lawrence Berkeley National Lab, ELENA STARODUB, Sandia National Laboratories, ANDREW WALTER, Advanced Light Source, LBNL, and Fritz-Haber-Institut der Max-Planck-Gesellschaft, SHU NIE, Sandia National Laboratories, AARON BOSTWICK, Advanced Light Source, LBNL, NORMAN BARTELT, KONRAD THÜRMER, Sandia National Laboratories, ELI ROTENBERG, Advanced Light Source, LBNL, KEVIN MCCARTY, Sandia National Laboratories, OSCAR DUBON, UC Berkeley, Lawrence Berkeley National Lab — The set of properties offered by the (111) surface of gold makes it intriguing as a platform on which to study the fundamental processes that underpin graphene growth on metals. Among these are the low carbon solubility and an interaction strength with graphene that is predicted to be smaller than most transition metals. We have investigated this synthesis process using low-energy electron microscopy and diffraction to monitor the sample surface in real time, and found that the resulting graphene film possesses a remarkable degree of rotational homogeneity. The dominant orientation of the graphene is aligned with the Au lattice, with a small minority rotated by 30 degrees. The origins of this in-plane structuring are puzzling because angularly resolved photo-emission spectroscopy and scanning tunneling microscopy experiments both suggest only a relatively small interaction between the two materials. Finally, the implications of these findings for the growth of high structural-quality graphene films are discussed.

¹DOE Contracts DE-AC04-94AL85000 and DE-AC02-05CH11231.

3:42PM L12.00005 Fundamental growth mechanisms of graphene on nickel surfaces¹, MATTHIAS BATZILL, University of South Florida — CVD growth of graphene over transition metal surfaces has become a main approach for synthesizing large area graphene wafers. The low carbon solubility in copper makes a good material for monolayer graphene synthesis, while carbon dissolution and re-segregation from the bulk of other transition metals, namely nickel, make these materials more demanding for controlling graphene growth. However, lower growth temperatures and defined graphene orientation relative to the substrate are some benefits for graphene synthesis on nickel compared to copper. Here we thoroughly characterize the fundamental growth processes of graphene on nickel substrate with the aim to find growth procedures that enable controlled graphene synthesis. We also identify defect structures in graphene that are formed as a consequence of the nickel substrate.

¹Funding by Office of Naval Research

4:18PM L12.00006 DFT studies of Graphene on Ni(111) and Surface Nickel Carbide Ni₂C ,

ANDREAS GARHOFER, Vienna University of Vienna, PETER JACOBSEN, Vienna University of Vienna, Tulane University, BERNHARD STÖGER, GARETH S. PARKINSON, MICHAEL SCHMID, Vienna University of Vienna, ROMAN CAUDILLO, Intel Corporation, FLORIAN MITTENDORFER, JOSEF REDINGER, Vienna University of Vienna, ULRIKE DIEBOLD, Vienna University of Vienna, Tulane University — Graphene with its unique transport properties supported on ferromagnetic materials is a promising candidate for the fabrication of spin-filtering devices. In order to study the growth of graphene on metal surfaces, graphene on Ni(111) is a perfect system from a structural point of view. The CVD growth of graphene on Ni(111) was studied with STM. The experiments showed not only perfectly aligned (1x1) structures, but also several moiré patterns are observed. They are due to grain rotations of graphene on both Ni(111) and also surface nickel carbide Ni₂C. During CVD growth carbon atoms segregate into the Ni bulk. With an increasing carbon concentration first the surface carbide and then a graphene layer on top is built. We studied the systems using the DFT program package VASP with the DFT-D2 method of Grimme to include van der Waals interactions. In our theoretical analysis we tried to understand the formation of the graphene and Ni₂C on Ni(111). We calculated the stability of the surface carbide phase and the binding energies of rotated and unrotated graphene on Ni(111) as well as on Ni₂C in order to understand the experimental findings. Graphene and Ni₂C have no epitaxial relationship due to their incommensurate lattices, leading to a spread in grain rotations.

4:30PM L12.00007 Graphene nucleation and growth on the transition metal surfaces: the role of pentagon, metal step and magic carbon clusters , JUNFENG GAO, JIJUN ZHAO, Dalian University of Technology, FENG DING, Hong Kong Polytechnic University — The nucleation behavior of graphene on transition metal surfaces, either on a terrace or near a step edge, is systematically explored using density functional theory calculations. The supported carbon clusters, CN (N=1~24), on the Ni(111) surface are carefully optimized [1,2]. A structural transformation from a C chain to a sp² C network at C₁₂ and the most stable structures of sp² graphene islands contain one to three pentagons. In agreement with experimental observations, our calculations show that graphene nucleation near a metal step edge is superior to that on a terrace. Besides, ground state structures of supported CN (N = 16~26), clusters on four selected transition metal surfaces: (Rh(111), Ru(0001), Ni(111) and Cu(111)) are explored [3]. A core-shell structured of C₂₁ stands out as a magic cluster, which is one of the dominating carbon precursors in graphene CVD growth and has been observed in experimental STM images. The energy barrier of two C₂₁ clusters' coalescence is computed to illustrate their influence on the kinetics of graphene CVD growth at different temperatures.

[1] J. Gao, et al., J. Am. Chem. Soc. 133, 5009 (2011).

[2] J. Gao, et al., J. Phys. Chem. C 115, 17695 (2011).

[3] Q. Yuan, et al., J. Am. Chem. Soc. (accepted).

4:42PM L12.00008 Optimizing Epitaxial Cu and Ni Films on Al₂O₃(0001) for Uniform Graphene Growth ,

DAVID L. MILLER, MARK W. KELLER, ROBERT R. KELLER, JUSTIN M. SHAW, ANN N. CHIARAMONTI, National Institute of Standards and Technology, Boulder, CO — Copper and nickel are the most commonly used substrates for the growth of graphene by chemical vapor deposition. While cold-rolled polycrystalline foils are most often selected for their commercial availability and ability to withstand the high temperatures required for graphene growth, (111) crystal faces have been shown to offer better growth characteristics on both materials. We deposited Cu and Ni films onto single crystal Al₂O₃(0001) using magnetron sputtering at temperatures between 250°C and 700°C. This gave films with pure (111) texture but with two epitaxial in-plane orientations as measured by x-ray diffraction and electron backscatter diffraction. Upon heating to graphene CVD temperatures (900°C to 1000°C), the grain boundaries widen and deepen into trenches that prevent the growth of uniform graphene over large areas. Reactive sputtering of a thin layer of Al₂O₃ before depositing the metal results in a single in-plane orientation over > 90% of the film for Ni. In addition, gradually increasing the temperature during metal deposition suppresses the formation of deep trenches under graphene CVD conditions. We compare CVD graphene grown on the optimized films with that grown on commercial foils.

4:54PM L12.00009 Kinetic Pathways towards Fabrication of Narrow Graphene Nanoribbons on Stepped Metal Surfaces¹ ,

PING CUI, JIN-HO CHOI, Univ. of Sci. and Tech. of China, HUA CHEN, Univ. of Tennessee, Univ. of Texas at Austin, WEI CHEN, Univ. of Tennessee, WENGUANG ZHU, Univ. of Tennessee, Oak Ridge National Lab, CHANGGAN ZENG, Univ. of Sci. and Tech. of China, ZHENYU ZHANG, Univ. of Sci. and Tech. of China, Harvard University — Graphene nanoribbons (GNRs) are predicted to exhibit intriguing electronic transport properties that strongly depend on their widths. To this end, one standing challenge is controlled fabrication of narrow GNRs with sizeable band gaps. In this study, we use first-principles approaches to explore the possibility of growing narrow GNRs along the step edges of catalytic metal surfaces. By minimizing the lattice mismatches of the growing graphene islands, optimizing their adsorption geometries, and exploiting the diffusion anisotropy of selective precursor monomers on the stepped surfaces, we identify the growth conditions under which the precursor monomers can be nucleated at the steps and then grow along the steps. Our studies point to kinetic pathways towards controlled fabrication of some of the narrowest GNRs with zigzag or armchair edges, and are expected to stimulate experimental efforts to realize these predictions.

¹Supported by NNSF of China, USNSF, and DMSE/BES of USDOE.

5:06PM L12.00010 Molecular Beam Epitaxy of graphene nanocrystals¹ ,

JORGE M GARCIA², ULRICH WURSTBAUER, THEANNE SCHIROS, Columbia University, NY, NY, ANNETTE S. PLAUT, University of Exeter, UK, LOREN N. PFEIFFER, Princeton University, NJ, ANTONIO LEVY, Columbia University, NY, NY, CHERNO JAYE , DANIEL FISHER , National Institute of Standards and Technology, Gaithersburg, USA, ABHAY PASUPATHY, Columbia University, NY, N, ARON PINCZUK, Columbia University, NY, NY — The ability to produce large-area graphene films on commonly used dielectric substrates can lead to many technological applications. We demonstrate the fabrication of large area conducting graphene nanocrystalline films on arbitrary dielectric substrates by MBE (molecular beam epitaxy) using a solid carbon source that can offer the integration of capable graphene production with high flexibility and variety in ultra-high vacuum environment together with state of the art thin film technology. Synchrotron x-ray and Raman spectroscopies show that the films consist on graphene nanocrystals oriented parallel to the sample surface. The growth rate is a key parameter that determines the bonding environment. Careful control of the growth conditions results in the production of predominantly sp²-bonded carbon thin films on arbitrary substrates, with the potential of growing large graphene grains on epitaxial substrates.

¹Acknowledgments: ONR (N000140610138 and Graphene Muri), NSF (CHE-0117752 and CHE-0641523), NYSTAR, CSIC-PIF (200950I154), Spanish CAM (S2009ESP-1503), Numancia 2 (S2009/ENE-1477) and MICINN (MAT2011-26534, TEC2011-29120-C05-04)

²IMM-CNM, CSIC, Spain

5:18PM L12.00011 ABSTRACT WITHDRAWN —

Tuesday, February 28, 2012 2:30PM - 5:30PM —

Session L13 DMP GMAG: Focus Session: Low-Dimensional and Molecular Magnetism - 1D Magnetism/Single-Chain Magnets - Experiment 211

2:30PM L13.00001 Magnetic Order in the Spin Chain Antiferromagnet $\text{Ca}_3\text{Co}_2\text{O}_6$, MARTIN LEES, Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom, O.A. PETRENKO, C.L. FLECK, Department of Physics, University of Warwick, Coventry, United Kingdom, S. AGRESTINI, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, C. MAZZOLI, Dip.to di Fisica, Politecnico di Milano, Milano, Italy, A. BOMBARDI, Diamond Ltd, Chilton, Oxford, United Kingdom, L.C. CHAPON¹, Institut Laue-Langevin, Grenoble, France — We have used powder neutron diffraction to investigate the magnetic structure of the Ising spin chain compound $\text{Ca}_3\text{Co}_2\text{O}_6$. Our investigation focuses on the low-temperature regime ($T < 14 \text{ K} \ll T_N = 25 \text{ K}$) where previous neutron diffraction studies have shown that there is an increasing instability in the spin density wave (SDW) order within this material. The results of this work reveal that there is an order-order transition from the SDW structure to a new commensurate antiferromagnetic phase. The extraordinary time dependence of the magnetic reflections demonstrates that this transition occurs via a very slow transformation process. As the temperature is reduced the characteristic time of the transition process increases rapidly and at low temperatures the magnetic states become frozen. We have also investigated the stability of the low-temperature commensurate phase in an applied magnetic field.

¹ISIS, Science and Technology Facilities Council, Rutherford Appleton Laboratory, Didcot, United Kingdom

2:42PM L13.00002 Density functional calculation of the electronic and magnetic properties of $\alpha\text{-CoV}_2\text{O}_6$, ANDRES SAUL, CINaM/CNRS, GUILLAUME RADTKE, IM2NP — In this work, the magnetic properties of the low dimensional $\alpha\text{-CoV}_2\text{O}_6$ system have been investigated using density-functional calculations. This system is constituted of CoO_6 octahedra connected by the edges and forming one dimensional linear chains. The experimental magnetization curves recorded at very low temperature show a surprising magnetization plateau at one-third of the saturation magnetization and a strong anisotropy. The estimated Co magnetic moment is large reaching a value of $4.5 \mu_B$ suggesting a large orbital contribution. Our calculations show that three different magnetic configurations for the Co are possible, the lowest energy one being a high spin configuration in agreement with the $S=3/2$ character of the Co^{2+} ion observed in this compound. Spin-orbit interactions have been included in order to calculate the magnetic anisotropy and the orbital contribution to the magnetic moment. The results are discussed in terms of crystal field splitting of the $3d$ orbital and a tight-binding Hamiltonian. Using a broken-symmetry formalism we have evaluated the effective exchange interactions of the Heisenberg Hamiltonian. They allow us to propose the magnetic structures corresponding to the ground state and to the observed magnetization plateaus.

2:54PM L13.00003 Heat capacity and magnetization of CoNb_2O_6 near quantum critical point¹, TIAN LIANG, Department of Physics, Princeton University, SEYED KOOHPAYEH, Institute for Quantum Matter, Johns Hopkins University, JASON KRIZAN, SIAN DUTTON, Department of Chemistry, Princeton University, TYREL MCQUEEN, Department of Physics and Astronomy, Johns Hopkins University, ROBERT CAVA, Department of Chemistry, Princeton University, N. PHUAN ONG, Department of Physics, Princeton University — CoNb_2O_6 is a quasi-1D quantum magnet in which magnetic Co^{2+} ions are ferromagnetically arranged into nearly isolated chains along the c axis with the magnetic moment confined in the ac -plane. By applying transverse magnetic field along b -axis, quantum phase transition from magnetically ordered phase to paramagnetic phase occurs. Evidence for emergent E_8 symmetry was recently obtained by neutron scattering near the quantum critical point (QCP) in an applied transverse magnetic field of 5.5 T. We will report on experiments to investigate the behavior of the heat capacity and torque magnetization in the vicinity of the QCP and discuss their implications.

¹Supported by NSF-DMR Grant 0819860 and the Office of Basic Energy Sciences (DOE) under Award DE-FG02-08ER46544

3:06PM L13.00004 Terahertz excitations in the 1D Ising chain quantum magnet CoNb_2O_6 ¹, CHRISTOPHER M. MORRIS, R. VALDÉS AGUILAR, S. KOOPAYEH, C. BROHOLM, N.P. ARMITAGE, The Institute for Quantum Matter, Department of Physics & Astronomy, The Johns Hopkins University — The one-dimensional magnet CoNb_2O_6 was recently demonstrated to be an excellent realization of a one-dimensional quantum Ising spin chain. It has been shown to undergo a quantum phase transition in a magnetic field oriented transverse to its ferromagnetically aligned spin chains. Low energy spin-flip excitations in the chains were recently observed via inelastic neutron scattering.² The energy spectrum of these excitations was shown to have an interesting energy scaling governed by symmetries of the E_8 exceptional Lie group. Here, time-domain terahertz spectroscopy (TDTS) is used to investigate optically active low energy excitations in CoNb_2O_6 . We take advantage of the polarization sensitivity of this technique to characterize both electric and magnetic dipole active excitations in this compound. A connection is made from the $q = 0$ response observed here to the excitations observed by neutron scattering. In addition, we will show preliminary data on the terahertz spectra of this material as it undergoes the magnetic field-tuned quantum phase transition.

¹Work supported by The Institute of Quantum Matter under DOE grant DE-FG02-08ER46544 and by the Gordon and Betty Moore Foundation.

²R. Coldea, *et al*, Science **327**, 177 (2010)

3:18PM L13.00005 Thermal Transport in CuSb_2O_6 single crystals¹, NARAYAN PRASAI, JOSHUA L. COHN, University of Miami, MICHAEL G. SMITH, ALWYN REBELLO, JOHN J. NEUMEIER, Montana State University — CuSb_2O_6 behaves as a uniform, one-dimensional (1D) $S = 1/2$ Heisenberg spin chain with long-range, antiferromagnetic ordering below $T_N \simeq 8.5 \text{ K}$.² Unusual for cuprates, the Cu^{2+} ions lie within quite regular CuO_6 octahedra and 1D magnetism appears to arise from orbital ordering driven by correlation effects.³ We will report the results of thermal conductivity measurements on single crystals over the temperature range $5 \text{ K} \leq T \leq 330 \text{ K}$.

¹This material is based upon work supported by an award from Research Corporation (Univ. Miami) and the National Science Foundation under grant DMR-0907036 (Mont. St. Univ.).

²A. Nakua *et al.*, J. Solid State Chem. **91**, 105 (1991); B. J. Gibson *et al.*, J. Magn. Magn. Mater. **272-276**, 927 (2004).

³Deepa Kasinathan, Klaus Koepernik, and Helge Rosner, Phys. Rev. Lett. **100**, 237202 (2008).

3:30PM L13.00006 Static and dynamic properties of Single-Chain Magnets with broad domain walls, ALESSANDRO VINDIGNI, THOMAS MICHAELS, Laboratory for Solid State Physics, ETH Zurich, Switzerland, ORLANDO BILLONI, Universidad Nacional de Cordoba, Argentina, DANILO PESCIA, Laboratory for Solid State Physics, ETH Zurich, Switzerland — It is well-known that long-range order cannot occur in 1d magnetic systems with short-range interactions. Remanent magnetization may, however, be observed in anisotropic spin chains due to slow dynamics. The physics of such systems – called Single-Chain Magnets (SCMs) – is mainly dictated by the temperature dependence of the relaxation time (τ) and the correlation length (ξ). The behavior of τ and ξ is, in turn, determined by domain-wall (DW) excitations. Both statics and dynamics are dependent on whether DWs extend over more than one lattice distance (*broad*) or not (*sharp*). The transition from one regime to the other is controlled by the strength of the magnetic anisotropy energy with respect to the exchange interaction. For broad domain walls, we found that the interplay between localized excitations and spin waves turns crucial at finite temperatures. Moreover, all the relevant quantities display universal behaviour, provided that temperature is measured in units of DW energy and distance in units of DW widths. These facts allowed us to explain the experimental behavior of a class of Mn-based SCMs with broad DWs and may also be relevant to the study of metallic nanowires.

3:42PM L13.00007 Light induced kickoff of magnetic domain walls in Ising chains¹, LAPO BOGANI,

1. Physikalisches Institut, Universität Stuttgart — Controlling the speed at which systems evolve is a challenge shared by all disciplines, and otherwise unrelated areas use common theoretical frameworks towards this goal. A particularly widespread model is Glauber dynamics, which describes the time evolution of the Ising model and can be applied to any binary system. Here we show, using molecular nanowires under irradiation, that Glauber dynamics can be controlled by a novel domain-wall kickoff mechanism. Contrary to known processes, the kickoff has unambiguous fingerprints, slowing down the spin-flip attempt rate by several orders of magnitude, and following a scaling law. The required irradiation power is very low, a substantial improvement over present methods of magneto-optical switching: in our experimental demonstration we switched molecular nanowires with light, using powers thousands of times lower than in previous optical switching methods. This manipulation of stochastic dynamic processes is extremely clean, leading to fingerprint signatures and scaling laws. These observations can be used, in material science, to better study domain-wall displacements and solitons in discrete lattices. These results provide a new way to control and study stochastic dynamic processes. Being general for Glauber dynamics, they can be extended to different kinds of magnetic nanowires and to a myriad of fields, ranging from social evolution to neural networks and chemical reactivity. For nanoelectronics and molecular spintronics the kickoff affords external control of molecular spin-valves and a magnetic fingerprint in single molecule measurements. It can also be applied to the dynamics of mechanical switches and the related study of phasons and order-disorder transitions.

¹We thank the Sofja Kovalevskaja award of the Humboldt Stiftung and German DFG for support.

4:18PM L13.00008 On-Surface Design and Characterization of Magnetic Macromolecules, SHIH-

HSIN CHANG, Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan, ANDREW DILULLO, KENDAL CLARK, Department of Physics and Astronomy, Ohio University, Athens OH 45701, USA, JAN-PETER KLOECKNER, MARC-HEINRICH PROSENC, Institute of Inorganic Chemistry, University of Hamburg, Germany, ROLAND WIESENDANGER, GERMAR HOFFMANN, Institute of Applied Physics, University of Hamburg, Germany, SAW-WAI HLA, Department of Physics and Astronomy, Ohio University, Athens OH 45701, USA — The formation of molecular chains from basic magnetic molecular building blocks is addressed on various surfaces. Via a surface catalyzed reaction multi-spin macromolecules are synthesized in ultra-high vacuum and then investigated by scanning tunneling microscopy (STM) at low temperatures. In my presentation, I will discuss the impact of the surface on the catalytic step and present a systematic comparison between Cu(111), Cu(100), NaCl/Cu(111), Co/Cu(111), and Au(111) surfaces. Depending on the substrate system, either unwanted sideproducts or spin-active macromolecules are created. In the latter case, scanning tunneling spectroscopy measurements are performed revealing an intermolecular spin-spin interaction through the analysis of the Kondo resonance. Our approach sheds new light on molecular magnetism where magnetically coupled complexes will be synthesized from basic units on surfaces for future spintronic applications.

4:30PM L13.00009 NMR Study of the Spin-Peierls transition in TiPO_4 ¹, RAIVO STERN, IVO HEINMAA,

ENNO JOON, NICPB, Tallinn, JOSEPH LAW, REINHARD KREMER, Max Planck Institut für Festkörperforschung, Stuttgart, ROBERT GLAUM, Institut für Anorganische Chemie, Universität Bonn — We investigated the magnetic and structural properties of the quasi-one dimensional $3d^1$ -quantum chain system TiPO_4 ($J \sim 965$ K) by NMR measurements. TiPO_4 undergoes two magnetostructural phase transitions, one at 111 K and the other at 74 K. Below 74 K, NMR detects two different ^{31}P signals and the magnetic susceptibility vanishes, while DFT calculations evidence a bond alternation of the $\text{Ti} \dots \text{Ti}$ distances within each chain. Thus, the 74 K phase transition is a spin-Peierls transition which evolves from an incommensurate phase existing between 111 K and 74 K.

¹Work in Tallinn was supported by Estonian Science Foundation

4:42PM L13.00010 Magnetic exchange studies of one-dimensional Co(II) molecular chains

, ASMA AMJAD, University of Central Florida, Orlando, G.M. ESPALLARGAS, J.M. CLEMENTE-JUAN, Instituto de Ciencia Molecular, Universidad de Valencia, Spain, R. KLEMM, E. DEL BARCO, University of Central Florida, Orlando, E. CORANADO, Instituto de Ciencia Molecular, Universidad de Valencia, Spain, M. EVANGELISTI, ICMA, Universidad de Zaragoza, Spain — We present a detailed experimental and theoretical study of a 1D spin $1/2$ Co-based molecular chain, $\text{trans}[\text{CoCl}_2(3,5\text{-Br}_2\text{py})_2]$. Our results show distinct features that are associated to both intra-molecular interactions (along the chain) and inter-molecular interactions (perpendicular to the direction of chains). The hysteresis observed at low temperature (230mK), indicate presence of 3D ordering attributed to the exchange interactions between the chains. Measurements done at different angles from the chains axial direction (c-axis), restricted within the a-c and b-c planes, reveal uniaxial anisotropy along the c-axis. The experimental data are explained using the mean field approximation, focusing on the behavior of inter-chain interactions and g-tensor anisotropy at the Co sites in the presence of a static magnetic field. A transition between two different relaxation regimes encountered for variable sweep rates will also be discussed.

4:54PM L13.00011 Magnetic structure and stability of 1D Co/Fe wires, JESSICA BICKEL, MATTHIAS

MENZEL, KIRSTEN VON BERGMANN, ANDRE KUBETZKA, ROLAND WIESENDANGER, Institute of Applied Physics, University of Hamburg — As device scales continue to decrease low dimensional structures are needed to take the place of wires and thick films. Particularly in the field of spintronics, it is important to develop 1D structures that can transmit information via the spin. This work realizes one method of spin transport via mixed Co/Fe 1D chains on Ir(001). Pure chains and mixed chains were examined by spin-polarized scanning tunneling microscopy (SPSTM) and spectroscopy. Both Fe and Co self-assemble into bi-atomic chains on the Ir(001)-(5x1) surface reconstruction. The Fe deposits as a single stacking chain while the Co exhibits two different stackings. When co-deposited, the materials can be differentiated from one another by spectroscopy due to differences in the local density of states. Spin-resolved measurements of pure Fe chains show a periodic spin-spiral along the entire length of the chain which is stabilized in an applied field but fluctuates at a speed greater than the time resolution of the STM in zero applied field. The Co, however, exhibits a ferromagnetic ground state that is stable at 8K. When the materials are co-deposited on the surface, the Co stabilizes the Fe spin-spiral and information about the magnetic state of the Co can be transmitted via the Fe spin-spiral.

5:06PM L13.00012 Magnetic diamond chains of Cu_3O_4 ¹, BRIGITTE LERIDON, WILLEM RISCHAU, PHILIPPE MONOD,

LPHEM-CNRS/ESPCI ParisTech - 10 rue Vauquelin - 75005 Paris - France, DOROTHÉE COLSON, SPEC - DSM/DRECAM - CEA Saclay - 91191 Gif-Sur-Yvette Cedex - France — We present magnetization measurements on a satellite phase of $\text{YBa}_2\text{Cu}_3\text{O}_x$ namely BaCu_3O_4 . This two-dimensional material is composed of alternate layers of Ba and Cu_3O_4 . In the latter, the Cu and O atoms are one-dimensionally ordered in diamond-shaped chains of formula unit Cu_3O_4 . We will show that this material encounters a magnetic phase transition at around 336 K which is due to intra-ordering through superexchange coupling of the spins born by the Cu atoms in these diamond chains. We will discuss the possibility of either ferrimagnetic or antiferromagnetic inter-ordering of these weakly coupled one-dimensional objects and the possible role of Dzyaloshinskii-Moriya interactions.

¹This work was supported through SESAME grants from Région Ile-de-France.

5:18PM L13.00013 Competing ^1H Spin Relaxation Mechanisms in Low-Dimensional $\text{Per}_2\text{Pt}[\text{mnt}]_2$, ELIZABETH GREEN, J.S. BROOKS, P.L. KUHN, A.P. REYES, NHMFL, J.A. WRIGHT, S.E. BROWN, UCLA, M. ALMEIDA, ITN, M.J. MATOS, R.T. HENRIQUES, Lisboa, NHMFL TEAM¹, UCLA TEAM², ITN TEAM³, LISBOA TEAM⁴ — $\text{Per}_2[\text{Pt}(\text{mnt})_2]$ is a low-dimensional organic conductor consisting of parallel conducting (*perylene*) and magnetic chains ($\text{Pt}[\text{mnt}]_2$) which undergo a charge density wave (CDW) and spin-Peierls (SP)-transition, respectively. The conducting chain has been studied extensively, however fundamental questions about the spin-dynamics of the magnetic chain in the SP-state remained. By using ^1H NMR, we discovered the low temperature nuclear relaxation rates (T_1^{-1}) display an anomalous upturn at the SP-transition which differs from classical SP-systems. This “bump” is suppressed by magnetic field and coincides with the Curie tail, seen in susceptibility measurements. The field-dependent activation energies, extracted from NMR and susceptibility, reveal two distinct behaviors evidencing coexisting spin systems. At low fields, the spin relaxation mechanism derived from a paramagnetic contribution, possibly unpaired Pt spins, is dominant, but is suppressed above 10T. Hence, the intrinsic SP behavior is recovered for high fields. Furthermore, spectra in the field induced (FICDW) state, up to 33T, reveal an increase in the electronic spin polarization. *DMR-NSF-1005293*

¹NHMFL and Florida State University, Tallahassee FL 32310, USA

²University of California Los Angeles, Los Angeles CA 90095, USA

³Instituto Tecnológico e Nuclear, P-2686 Sacavém Codex, Portugal

⁴Instituto de Telecomunicações, Polo de Lisboa, P1049-001, Portugal

Tuesday, February 28, 2012 2:30PM - 5:30PM –
Session L14 GMAG DMP FIAP: Focus Session: Spins in Semiconductors - Magnetic Semiconductors II 212

2:30PM L14.00001 The intra-gap electromagnetic response of gated GaMnAs in an electric double-layer field effect, BRIAN CHAPLER, T.W. ELSON, University of California San Diego, S. MACK, D.D. AWSCHALOM, University of California Santa Barbara, E. NAMMAS, University of Queensland, J. YUEN, A.J. HEEGER, University of California Santa Barbara, L. JU, F. WANG, University of California Berkeley, D.N. BASOV, University of California San Diego — We have fabricated field effect transistors (FETs) utilizing an electrolyte oxide gate insulator for monitoring electrostatic doping in GaMnAs via infrared (IR) spectroscopy. Previous studies of gated GaMnAs have been confined primarily to transport measurements. IR experiments are able to probe the electric field induced changes to the optical conductivity spectrum, providing direct insight into the electronic structure of GaMnAs. The IR spectra show an enhancement of the Drude response and mid-IR resonance of GaMnAs upon hole accumulation, with symmetric decrease in these features in the depletion mode. A sum rule analysis of the IR spectra, combined with charge accumulation/depletion information from transport measurements for the same gated structures, enables accurate evaluation of the effective masses of mobile holes without any underlying assumptions about the level of compensation and/or disorder in the films. The low bound for the effective mass is several m_e , where m_e is the free electron mass. We therefore conclude that electronic states in the vicinity of the Fermi energy retain significant impurity band character.

2:42PM L14.00002 Effect of As vacancies on the binding energy and exchange splitting of Mn impurities on a GaAs surface, M.R. K. MAHANI, C.M. CANALI, Linnaeus University, Kalmar, Sweden, A.H. MACDONALD, University of Texas at Austin — State-of-the-art STM spectroscopy is nowadays able to manipulate and probe the magnetic properties of individual magnetic impurities located near the surface of a semiconductor. A recent advance of these techniques employs the electric field generated by a As vacancy in GaAs to affect the environment surrounding substitutional Mn impurities in the host material [1]. Here we calculate the binding energy of a single Mn dopant in the presence of nearby As vacancies, by using a recently-introduced tight-binding method [2] that is able to capture the salient features of Mn impurities near the (110) GaAs surface. The As vacancies, modeled by the repulsive potential they produce, are expected to decrease the acceptor binding energy in agreement with experiment [1]. Within this theoretical model, we investigate the possible enhancement of the exchange splitting for a pair of ferromagnetically ordered Mn impurities, observed experimentally when As vacancies are present [3]. We also calculate the response of the Mn-impurity—As-vacancy complex to an external magnetic field.

[1] H. Lee and J. A. Gupta, *Science*, 1807-1810, (2010).

[2] T. O. Strandberg, C. M. Canali, A. H. MacDonald, *Phys. Rev. B* 80, 024425, (2009).

[3] J.A. Gupta, private communication.

2:54PM L14.00003 Observation of a Sharp Band Edge Response in GaMnAs Using Nonlinear Spectroscopy¹, TRISTAN DE BOER, ANGELA GAMOURAS, SAM MARCH, Dalhousie University, VIT NOVAK, Institute of Physics AS CR, Czech Republic, KIMBERLEY HALL, Dalhousie University — Diluted magnetic semiconductors (DMS) have gained considerable interest over the last decade owing to their potential use in magneto-sensitive electrical and optical devices, in which the carrier-mediated nature of the ferromagnetism allows the magnetic properties to be controlled using optical or electrical gating techniques. The position of the Fermi level, which may lie within the valence band or within an impurity band, plays a critical role in current theories of ferromagnetism in DMS and has been the subject of intense controversy in recent years. Linear spectroscopy techniques are unable to address this issue due to strong band tailing in the vicinity of the fundamental band gap. Here we present results of time- and spectrally-resolved differential reflection measurements on GaMnAs, as well as low-temperature-grown GaAs and semi-insulating GaAs. Our results indicate a sharp band edge response due to the diminished contributions of band tail states in the nonlinear optical regime. We observe a blue shift of the band gap in GaMnAs, supporting a valence band model of ferromagnetism in DMS. Numerical simulations of the measured nonlinear response using an effective mass model support our conclusions.

¹Supported by CFI, NSERC, Lockheed Martin Corporation, the Canada Research Chairs Program, and the Czech Republic Grants LC510 and KAN400100652

3:06PM L14.00004 Tuning the magnetic interaction between Mn dopants in GaAs, DAVID GOHLKE, JAY GUPTA, Ohio State University, Department of Physics — Manganese can be used as a dopant in gallium arsenide to create a ferromagnetic semiconductor. We use low-temperature scanning tunneling microscopy to study these magnetic properties. The magnetic coupling between Mn dopants in GaAs(110) changes between ferromagnetic and antiferromagnetic depending on the orientation of the acceptors due to the zincblende crystal structure of the surface [Kitchen et al, *Nature*, 2006]. We have recently reported tuning of the resonance energy for a single Mn acceptor by moving charged atomic point defects [Lee and Gupta, *Science*, 2010]. Here, we tune the magnetic interaction between surface-layer Mn atoms in the same way. Funding for this research was provided by the Center for Emergent Materials at the Ohio State University, an NSF MRSEC (Award Number DMR-0820414). <http://www.physics.ohio-state.edu/~jgupta/>

3:18PM L14.00005 Spin-Seebeck Effect in III-V Based Semiconductors, CHRISTOPHER M. JAWORSKI, ROBERTO C. MYERS, JOSEPH P. HEREMANS, The Ohio State University — The spin-Seebeck effect has now been observed in metals¹ (NiFe), semiconductors² (GaMnAs), and insulators³ (YIG). It consists of a thermally generated spin distribution that is phonon driven. Here we extend our measurements of the spin-Seebeck effect to other group III-V based magnetic semiconductors and present measurements of conventional thermomagnetic and galvanomagnetic properties as well as the spin-Seebeck effect. Work supported by the National Science Foundation, NSF-CBET-1133589 1. K. Uchida, et al., *Nature* **455** 778 (2008) 2. C.M. Jaworski et al., *Nature Materials* **8** 898 (2010), *Phys. Rev. Lett.* **106** 186601 (2011) 3. K. Uchida, et al., *Nature Materials* **8** 893 (2010)

3:30PM L14.00006 High Resolution Magneto-Optic Measurements in GaAs using a Sagnac Interferometer, ALEXANDER FRIED, AHARON KAPITULNIK, Stanford University — The Sagnac Interferometer is a tool which measures the Polar Kerr effect—a direct indicator of magnetism. Using 820 nm light from a superluminescent diode, we probe GaAs structures and measure the Kerr angle with sub-microradian resolution. By utilizing diffraction limited optics and a piezoelectric scanner, we also achieve high spatial resolution. Our measurements are performed at cryogenic temperatures and offer a way to measure the Spin Hall Effect in the DC regime along with other forms of magnetic order.

3:42PM L14.00007 All-optical four-state magnetization reversal in (Ga,Mn)As ferromagnetic semiconductors, MYRON KAPETANAKIS¹, ILIAS PERAKIS, Physics Department, University of Crete, Greece, JINGANG WANG, Department of Physics and Astronomy, Iowa State University, and Ames Laboratory US-DOE, CARLO PIERMAROCCHI, Department of Physics and Astronomy, Michigan State University — The emerging field of femtomagnetism has revealed the central role of non-equilibrium interactions and transient optical coherence in determining photoinduced spin dynamics. However the many-body theory of such effects remains controversial. A microscopic theory that engages the elements of coherence, correlation and nonlinearity on an equal footing is needed. We propose here such a theory, based on density matrix equations of motion and a tight-binding band calculation. We prepare the system within 100fs, via coherent nonlinear photoexcitation close to the strong peak of the density of states for interband transitions along the eight equivalent directions {111} of the GaAs BZ in the vicinity of 3eV. It then selectively relaxes to one of the four local minima of the magnetic free energy with biaxial anisotropy. We thus propose a non-thermal mechanism for all-optical switching between four metastable magnetic states, initiated non-thermally within 100fs and completed within 100ps. Our predicted switching comes from magnetic nonlinearities triggered by a femtosecond magnetization tilt that is sensitive to un-adiabatic light-induced spin interactions and controlled via the optical and the external magnetic field.

¹Current address: Vanderbilt University, Nashville, TN, and Oak Ridge National Laboratory.

3:54PM L14.00008 First-Principle Calculation of The Effective Hamiltonian for (Ga,Mn)As and (Ga,Mn)N, RYKY NELSON, ANH NGO, Louisiana State University, WEI KU, Brookhaven National Laboratory, JUANA MORENO, MARK JARRELL, Louisiana State University — Most of the models used to study (Ga,Mn)As have failed to explain the experimental results of (Ga,Mn)N especially its ferromagnetic critical temperature T_C . The need for a consistent and comprehensive model for the dilute magnetic semiconductors (DMS) motivates our study. We obtain the effective Hamiltonian for (Ga,Mn)As and (Ga,Mn)N using a Wannier function based first-principles method. We use density functional theory to calculate the band structure of a range of disordered supercell configurations of (Ga,Mn)As and (Ga,Mn)N and Wannier functions to obtain downfolded Hamiltonians. Those are then disorder averaged to get an effective Hamiltonian. We solved this effective model using the dynamical mean field approximation.

4:06PM L14.00009 Polaronic trapping in magnetic semiconductors¹, HANNES RAEBIGER, Yokohama National University, Yokohama, Japan — GaN doped with iron is an interesting candidate material for magnetic semiconductors, as p-d coupling between the localized Fe-d and extended N-p hole states is expected to facilitate long-range ferromagnetic alignment of the Fe spins [1]. This picture of extended states in GaN:Fe, however, falls apart due to a polaronic localization of the hole carriers nearby the Fe impurities. To elucidate the carrier localization in GaN:Fe and related iron doped III-V semiconductors, I present a systematic study using self-interaction corrected density-functional calculations [2]. These calculations predict three distinct scenarios. (i) Some systems do sustain extended host-like hole states, (ii) some exhibit polaronic trapping, (iii) and some exhibit carrier trapping at Fe-d orbitals. These behaviors are described in detail to give an insight as to how to distinguish them experimentally. I thank T. Fujita, C. Echeverria-Arrondo, and A. Ayuela for their collaboration.

[1] T. Dietl et al, *Science*, **287**, 1019 (2000).

[2] S. Lany and A. Zunger, *Phys. Rev. B*, **80**, 085202 (2009).

¹Funded by JSPS Grant-in-Aid for Young Scientists (A) No. 21686003.

4:18PM L14.00010 Magnetoresistance in antiferromagnet-based spin tunnel junctions, TOMAS JUNGWIRTH, Institute of Physics ASCR, Prague and University of Nottingham — To date spintronics research and applications of magnetically ordered systems have focused on ferromagnets (FMs). There are, however, fundamental physical limitations for FM materials which may make them impractical to realize the full potential of spintronics. Metal FMs offer high temperature operation but the large magnetic stray fields make them unfavorable for high-density integration and metals are unsuitable for transistor and information processing applications. FM semiconductors on the other hand do not allow for high-temperature operation. We present a concept in which these limitations are circumvented in spintronics based on antiferromagnets. The concept is based on relativistic magnetic and magneto-transport anisotropy effects in nanodevices whose common characteristics is that they are an even function of the microscopic magnetic moment vector, i.e., can be equally strong in AFMs as in FMs. As a demonstration we present our experimental observation of >100% tunneling anisotropic magnetoresistance in a device with an IrMn AFM tunnel electrode [1]. We will also discuss candidate materials for high-temperature AFM semiconductor spintronics [2].

[1] B. G. Park, J.Wunderlich, X.Marti, V.Holy, Y.Kurosaki, M.Yamada, H.Yamamoto, A.Nishide, J.Hayakawa, H.Takahashi, A.B.Shick, T.Jungwirth, *Nature Mat.* **10**, 347 (2011).

[2] T.Jungwirth, V.Novák, X.Marti, M.Cukr, F.Máca, A.B. Shick, J.Mašek, P.Horodyská, P.Němec, V.Holý, et al., *Phys. Rev. B* **83**, 035321 (2011).

4:54PM L14.00011 Numerical studies of non-Drude ac-conductivity and infrared magneto-optics in $(\text{Ga}_{1-x}\text{Mn}_x)\text{As}$, HUAWEI GAO, JAIRO SINOVA, Texas A&M University — Optical absorption experiments on (III,Mn)V diluted magnetic semiconductors (DMS's) show that the ac-conductivity has non-Drude behavior at low frequency. The numerical simulation of this problem has been done previously using the effective Hamiltonian model with various treatments of the disorder effects. We are re-examining the previous works with a similar numerical method to establish the nature of the transitions in the low to the high doped regime. We use the effective Hamiltonian k.p model to describe the holes introduced by Mn impurities and treat the Mn impurities exactly using the envelope function approximation. With this technique we are able in principle to analyze spectrally the origin of the mid-infrared absorption peak, its trends, and the nature of the states near the Fermi energy as well as the excitation states. We will also report on numerical results of the magneto-optical response with this more accurate treatment of the effect of disorder.

5:06PM L14.00012 Electric field manipulation of room temperature ferromagnetism in anatase $\text{Ti}_{1-x}\text{Co}_x\text{O}_{2-\delta}$, YOSHINORI YAMADA, Tohoku University, KAZUNORI UENO, TOMOTERU FUKUMURA, HONGTAO YUAN, University of Tokyo, HIDEKAZU SHIMOTANI, Tohoku University, YOSHIHIRO IWASA, University of Tokyo, LIN GU, SUSUMU TSUKIMOTO, Tohoku University, YUICHI IKUHARA, MASASHI KAWASAKI, University of Tokyo — Ferromagnetic semiconductor is one of the most attractive materials for semiconductor spintronics because of the controllability of both charge and spin degrees of freedom. Electric field effect of magnetism in the ferromagnetic semiconductors such as (Ga,Mn)As has been demonstrated only at low temperature due to their low Curie temperatures. In this study, we report the electric field manipulation of ferromagnetism in a ferromagnetic semiconductor $\text{Ti}_{1-x}\text{Co}_x\text{O}_{2-\delta}$ at room temperature [1]. Anatase $\text{Ti}_{1-x}\text{Co}_x\text{O}_{2-\delta}$ (001) epitaxial film was deposited on TiO_2 buffer 5 nm / LaAlO_3 (100) substrate in various oxygen pressures in order to vary an electron density by pulsed laser deposition method. An electric double layer transistor was fabricated on a paramagnetic film with an electron density of $1 \times 10^{19} \text{ cm}^{-3}$. With increasing gate voltage, the electron density was increased to $7 \times 10^{19} \text{ cm}^{-3}$. Ferromagnetic hysteresis loop was observed for V_G above 3.0 V in an anomalous Hall resistivity, which is proportional to a magnetization of the film. This result represents that the ferromagnetism was induced at room temperature by an electrostatic charge accumulation, indicating that the ferromagnetism in this compound is mediated by the electron carriers.

[1] Y. Yamada et al., Science **332**, 1065 (2011).

5:18PM L14.00013 BaMn_2Sb_2 : A New Semiconducting Ferromagnet¹, JIANNENG LI, S. STADLER, A. KARKI, Y. XIONG, R. JIN, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803 — We have grown high-quality single crystals of BaMn_2Sb_2 , which possesses the ThCr_2Si_2 structure as determined by X-ray powder diffraction technique. Magnetization measurements indicate that BaMn_2Fe_2 is ferromagnetic below $T_C = 580\text{K}$. On the other hand, the temperature dependence of electrical resistivity shows semiconducting behavior, which can be described by thermally-activated resistivity formula with thermal activation energy about 0.25 eV. While the Hall coefficient has positive sign between 2 and 300 K, the Seebeck Coefficient undergoes sign change from positive at high temperatures to negative at low temperatures, reaching $-260 \mu\text{V/K}$ at 70 K. The implication will be discussed.

¹Supported by NSF No.DMR-1002622

Tuesday, February 28, 2012 2:30PM - 5:30PM —
Session L15 DMP FIAP GMAG: Focus Session: Spins in Metals - Resonance Phenomena I, Spin Wave Excitation and Spin Torque Oscillators 213

2:30PM L15.00001 Spin-torque excited spin waves revealed by micro-focused Brillouin light scattering¹, MARCO MADAMI, CNISM, Unità di Perugia and Dipartimento di Fisica, Università di Perugia — Since the discovery of the spin transfer torque (STT) effect [1,2] a great effort has been devoted to the realization and study of spin torque oscillators (STOs) because of their potential applications as spin waves injectors in magnonic devices or current-tunable broad-band microwave sources. More recently the possibility to synchronize multiple STOs [3,4] via the emitted spin waves, propagating in the magnetic “free” layer, envisioned a way to overcome their main limitation in the output power. For these reasons it’s now crucial to obtain a detailed knowledge and understanding of the emitted spin waves properties like: their spatial distribution, their propagating or localized character, their decay length, wavelength and group velocity. In the last two years micro-focused Brillouin light scattering (μ -BLS) revealed to be a powerful tool in order to investigate several of these properties [5,6]. In this presentation we discuss the potentialities of μ -BLS to the study of emitted spin waves in STOs systems with particular focus on the results of our latest work [6]. Here we took advantage of our μ -BLS setup in order to study spin waves emitted by an out-of-plane magnetized nano-contact STO. Performing a “wave-vector resolved” μ -BLS experiment we provided the first direct experimental evidence of the *propagating* nature of SWs emitted from an out-of-plane magnetized STO. The decay of the propagating SW intensity up to several microns away from the nano-contact position showed great potential for STT based magnonic devices. We also investigated the STO tunability measuring the emitted SW frequency as a function of both the applied direct current and external field intensities. Micromagnetic simulations provided the theoretical support to quantitatively reproduce the results.

[1] Slonczewski, J. C. J. Magn. Magn. Mater. 159, L1 (1996).

[2] Berger, L. Phys. Rev. B 54, 9353 (1996).

[3] Kaka, S. et al. Nature 437, 389 (2005).

[4] Mancoff, F. B., Rizzo, N. D., Engel, B. N., Tehrani, S. Nature 437, 393 (2005).

[5] Demidov, V. E., Urazhdin, S., and Demokritov, S. O. Nature materials, 9(11), (2010).

[6] Madami, M., Bonetti, S. et al. Nature Nanotechnology, 6, 635 (2011).

¹Support from European Community 7th Framework Programme under G.A. no228673 (MAGNONICS) is gratefully acknowledged.

3:06PM L15.00002 Probing spin wave excitations using magnetic tunnel junction structures¹, XIN FAN, CHONG BI, JOHN XIAO, Department of Physics, University of Delaware, CENTER FOR SPINTRONICS AND BIODETECTION TEAM — We propose a quantitative method based on the use of high tunneling magnetoresistance and small lateral dimension of magnetic tunnel junction (MTJ) to detect spin excitations in magnetic films with promising high spatial resolution and sensitivity. One ferromagnetic (FM) layer of the MTJ is pinned by an antiferromagnetic layer and the other one is free to rotate in response to an external magnetic field. In the presence of microwave magnetic fields, the free layer will precess, leading to the average resistance of MTJ change. By applying a constant dc current bias to the MTJ, a time dependent voltage can be introduced and measured which is related to the time dependent magnetization along the external static field direction. We have demonstrated the usefulness of this method by studying the spin wave excitations in a single elliptical Permalloy thin film ($50 \mu\text{m} \times 30 \mu\text{m} \times 40 \text{nm}$). At low microwave power, a uniform linear ferromagnetic resonance behavior has been observed. Surprisingly, above the spin wave instability threshold, the experimental results show a linear response of the microwave field over a large range, which is followed by a phase limiting behavior. The linear behavior can be described by the theoretical model describing subsidiary resonance.

¹The work is supported by NSF under grant number DMR-0827249 for measurement setup development, DOE under grant number DE-FG02-07ER46374 for measurements and analyses, and NSFC under Grant No. 60721001 and 60425102.

3:18PM L15.00003 Generating Damon-Eshbach Spin Waves in Py using a Conducting Diffraction Grating , J. SKLENAR, Northwestern University, V.S. BHAT, L. DELONG, University of Kentucky, Lexington, J.B. KETTERSON, Northwestern University — We have patterned silver hole arrays directly on top of uniform permalloy (Py) films. Typical Py and Ag film thicknesses are 25nm and 40 nm respectively; the holes in the Ag have a 500nm diameter and are patterned on a 1 micron lattice constant. We have measured resonant modes arising from a quasi-uniform microwave excitation field, applied in the plane of the sample, as a function of the in-plane external field and the in-plane field orientation relative to the principal axes of the array. Measurements were done using our broadband meanderline-based ferromagnetic resonance (FMR) spectrometer.¹ In addition to a uniform FMR mode we observe satellite modes that correspond to the Damon-Eshbach spin waves² with wave vectors having Fourier components of the reciprocal lattice of the silver array. Hence, in an otherwise uniform magnetic film the silver array acts as a *diffraction grating* which excites spin waves with $k \neq 0$ from the dynamic $k \approx 0$ microwave magnetic field. The observed spin wave angular dispersion is in excellent agreement with a magnon dispersion relation for spin waves in a uniform film given by Kriesel et al.³

¹C. C. Tsai, J. Choi, S. Cho, B. K. Sarma, C. Thompson, O. Chernyashevskyy, I. Nevirkovets, and J. B. Ketterson, Rev. of Sci. Instr. **80**, 023904 (2009).

²R. W. Damon and J. R. Eshbach J. Phys. Chem. Solids **19**, 308 (1961).

³A. Kriesel, F. Sauli, L. Bartosch, and P. Kopietz, Eur. Phys. J. B **71**, 59 (2009).

3:30PM L15.00004 Time-dependent spin-wave theory¹ , ANDREAS KREISEL, ANDREAS RÜCKRIEGEL, PETER KOPIETZ, Institute for Theoretical Physics, University of Frankfurt, Germany — We generalize the spin-wave expansion in powers of the inverse spin to time-dependent quantum spin models describing rotating magnets or magnets in time-dependent external fields. We show that in these cases the spin operators should be projected onto properly defined rotating reference frames before the spin components are bosonized using the Holstein-Primakoff transformation. As a first application of our approach, we calculate the re-organization of the magnetic state due to Bose-Einstein condensation of magnons in the magnetic insulator yttrium-iron garnet; we predict a characteristic dip in the magnetization which should be measurable in experiments.

¹With special thanks to DFG for funding within "Transregio 49".

3:42PM L15.00005 Autonomous and driven dynamics of spin torque nano-oscillators¹ , SERGEI URAZHIDIN, Emory University — Understanding the dynamical properties of autonomous spin torque nano-oscillators (STNO) and their response to external perturbations is important for their applications as nanoscale microwave sources. We used spectroscopic measurements to study the dynamical characteristics of nanopillar- and point contact-based STNOs incorporating a microstrip in close proximity to the active magnetic layer. By applying microwave current at frequency f_{ext} to the microstrip, we were able to generate large microwave fields of more than 30 Oe rms at the location of STNO. We demonstrate that for a wide range of f_{ext} , STNO exhibits multiple synchronization regimes with integer and non-integer rational ratios between f_{ext} and the oscillation frequency f . We show that the synchronization ranges are determined by the symmetry of the oscillation orbit and the orientation of the driving field relative to the symmetry axis of the orbit. We observe synchronization hysteresis, i.e. a dependence of the synchronization limits on the dynamical history caused by the nonlinearity of STNO. We also show that the oscillation can be parametrically excited in the subcritical regime of STNO by a microwave field at twice the frequency of the oscillation. By measuring the threshold and the frequency range of parametric excitation, we determine damping, spin-polarization efficiency, and coupling to the microwave signal. In addition, by measuring the frequency range of parametric synchronization in the auto-oscillation regime, we determine the dynamic nonlinearity of the nanomagnet. Thus, analysis of the driven oscillations provides complete information about the dynamical characteristics of STNO. Finally, we discuss several unusual dynamical behaviors of STNO caused by their strong nonlinearity.

¹Supported by NSF DMR-0747609, ECCS-0967195, ECCS-0653901, and the Research Corporation.

4:18PM L15.00006 Improved coherence of a quasi-linear spin-torque nano-oscillator , OUKJAE LEE, VLAD PRIBIAG, DAN RALPH, ROBERT BUHRMAN, Cornell University, CORNELL UNIVERSITY TEAM — We have fabricated tapered nanopillar spin-valve devices, $\sim 50 \times 145$ nm², from a Py(5)/Cu(12)/Py(20) multilayer (thickness in nm) for spin torque nano-oscillator (STNO) studies. When biased with electron flow from the thick layer to the thin layer multiple, high power, but broad ($\Delta f > 50$ MHz), spin torque excitation modes are obtained at hard-axis fields $H_y < 500$ Oe. For $H_y \sim 700$ Oe we obtain much more coherent ST oscillations, $\Delta f < 10$ MHz, close to that predicted for a linear STNO at 300 K. A macrospin model successfully explains the optimum field bias as being where the amplitude-dependent red shift effect due to the demagnetization field is closely balanced by the blue shift effect due to the in-plane anisotropy field. We have also modeled the internal field within the free layer as a function of H_y and conclude that the multiple modes at lower fields originate from the relatively broad spatial distribution of the internal field, or equivalently from the broad natural frequency distribution of the individual magnetic elements. Our results suggest pathways for further enhancements in STNO performance.

4:30PM L15.00007 Time-Domain Measurements of Real-Space Magnetization Trajectories in Spin Torque Oscillators , GRAHAM E. ROWLANDS, JIAN ZHU, Department of Physics and Astronomy, University of California, Irvine, JORDAN A. KATINE, Hitachi Global Storage Technologies, San Jose, CA, JUERGEN LANGER, Singulus Technologies, 63796 Kahl am Main, Germany, PEDRAM KHALILI AMIRI, KANG L. WANG, Department of Electrical Engineering, University of California, Los Angeles, ILYA N. KRIVOROTOV, Department of Physics and Astronomy, University of California, Irvine — We make time-domain measurements of the microwave signal emitted by spin torque nano-oscillators (STNOs) based on magnetic tunnel junctions with Fe-rich free layers. The perpendicular magnetic anisotropy of the free layer nearly cancels its easy-plane shape anisotropy, allowing the magnetization to undergo large amplitude precession. The microwave power emitted by such STNOs reaches values approaching 0.4 μ W. We employ a high-gain low-noise amplifier to further amplify the emitted signal, thereby bringing it to a level (~ 0.5 V rms) far exceeding the noise floor (5mV rms) of a 12 GHz, 40 Gs/s storage oscilloscope used for time-domain measurements. Relying on the assumption that extrema of the measured voltage versus time trace correspond to the magnetization crossing the sample plane, we use these time-domain traces to reconstruct the statistical distributions of the azimuthal angles at which the magnetization vector of the free layer crosses the plane of the sample. We measure the evolution of these crossing angle distributions as a function of current density and compare to theoretical predictions.

4:42PM L15.00008 Network Analyzer Measurements of Spin-Torque Dynamics , LIN XUE, CHEN WANG, YONGTAO CUI, R.A. BUHRMAN, D.C. RALPH, Cornell University — A microwave current flowing through a magnetic tunnel junction (MTJ) produces an oscillating spin torque. This oscillating spin torque is able to excite resonant magnetic dynamics and produce an oscillating resistance. The oscillating resistance combined with an applied DC current can generate a microwave voltage signal at the same frequency as the input microwave signal. We show that a network analyzer measurement of the amplitude and phase of this signal provides a simple way to make a quantitative measurement of the strength and direction of the spin transfer torque vector in MTJs at non-zero biases, the regime of primary interest for applications. Compared with a previous time-domain technique for measuring the spin torque vector, this technique requires no specialized equipment and provides roughly similar sensitivity. Compared to dc-detected spin-torque ferromagnetic resonance, the network-analyzer method is free of artifacts at high bias.

4:54PM L15.00009 Spin-transfer-driven parametric resonance in magnetic nanodomains¹, C. WANG, H. SEINIGE, T. STAUDACHER, M. TSOI, Physics Department, University of Texas at Austin — We study experimentally the parametric excitation of a magnetic nanodomain by spin-transfer-torque (STT). In our experiments, we use a nanoscale point contact to inject high-density ac (microwave frequency) and dc currents into an exchange-biased IrMn/NiFe/Cu/NiFe spin valve (EBSV) and to produce STT [1] on NiFe moments in a small contact region. Here a time-dependent STT associated with the microwave current produces a time-dependent modulation of the effective damping parameter which, in turn, drives the magnetic moments into parametric resonance [2]. The resonance was detected electrically by measuring a small rectified dc voltage which appears across the contact at resonance [3]. We study this resonance signal as a function of frequency and power of the applied microwaves. As expected for parametric excitation, this resonance has an ac threshold and occurs at double the natural frequency of magnetic precession (FMR frequency). We found that both the excitation threshold and the width of the resonance depend on the applied dc bias. Detailed dc bias dependent measurements of the resonance signal provide a means to characterize instability regions in parameter space known as Arnold tongues. The parametric excitation can be potentially used in magnetic memory technology for reducing power and increasing speed of logic and memory devices. [1] J. C. Slonczewski (1996); L. Berger (1996); M. Tsoi et al. (1998). [2] M. Faraday (1831). [3] T. Staudacher and M. Tsoi (2011).

¹This work was supported in part by NSF grant DMR-06-45377

5:06PM L15.00010 Spin-orbit coupling and spin excitations in nanoscopic structures, ANTONIO COSTA, Universidade Federal Fluminense, SAMIR LOUNIS, Forschungszentrum Jülich, ROBERTO MUNIZ, Universidade Federal Fluminense, DOUGLAS MILLS, University of California Irvine — We have developed a formalism to calculate the spectra of spin excitations of structures of nanoscopic dimensions that takes into account spin-orbit coupling. We study structures composed by magnetic units (adatoms, clusters, ultrathin films) deposited on metallic substrates. The reduced symmetry of the magnetic units enhance the effects of spin-orbit coupling and activate mechanisms such as the Dzyaloshinskii-Moriya anti-symmetric exchange coupling. We are also able to predict anisotropic g-factors. In the case of ultrathin films, our formalism can span the entire Brillouin zone, being able to describe within the same framework FMR results and spectra obtained with SPEELS. We can also calculate the spectra that would be obtained by local probes such as inelastic scanning tunneling spectroscopy. We will present results for Fe ultrathin films on W(110) and for several transition metal adatoms on metallic substrates.

5:18PM L15.00011 Spin orbit driven ferromagnetic resonance and torques in single ferromagnetic layers¹, FERRAN MACIÀ, CHARLES PÉPIN, A.D. KENT, New York University, KENT'S GROUP TEAM — The coupling of spin and charge may convert electrical currents into spin currents in non-magnetic metals. In non-magnetic metals with strong spin orbit (SO) interaction in combination with magnetic metals one can also use the effect to excite magnetization dynamics; electrical currents in the non-magnetic metal transform to spin currents and the spin currents diffuse to the magnetic metal interacting with the magnetic moments. The combination of non-magnetic metals and magnetic metals has been recently used to determine spin hall angles. Here we demonstrate that spin currents in a ferromagnetic layer associated with SO interactions can excite ferromagnetic precession in the same layer. We have studied Co—Ni multilayers with both in-plane anisotropy and weak out-of-plane anisotropy. Results show that the samples have strong SO interactions. We have injected microwaves into patterned samples with several geometries and measured the mixed voltage in the same leads. Oscillatory currents drive FMR in the thin-film layer. We show that SO torques are primarily responsible for the magnetic excitations in samples with strong SO interactions, whereas samples with a weaker SO barely respond to the injected microwaves and show asymmetric components from charge current induced Oersted fields.

¹FM thanks support from MC-IOF 253214. Supported by ARO-MURI-Grant #W911NF-08-0317 and NSF-DMR-1006575.

Tuesday, February 28, 2012 2:30PM - 5:30PM — Session L16 DCMP: Heavy Fermions - Theory and Experiment 251

2:30PM L16.00001 $\beta - YbAlB_4$: a critical vortex metal¹, ALINE RAMIRES, PIERS COLEMAN, Rutgers University, ALEXEI TSVELIK, Brookhaven National Laboratory — $\beta - YbAlB_4$ is the first Yb based heavy fermion superconductor and has a non Fermi Liquid behavior in the normal state that develops without external tuning by pressure or doping, making it intrinsically quantum critical [1]. Application of a magnetic field is found to drive the development of a Fermi Liquid in which the Fermi temperature is determined by the Zeeman energy [2]. Here we present a theory for the intrinsic quantum criticality in which the main ingredient is an anisotropic hybridization matrix with line nodes in momentum space that carry a vorticity and resemble topological defects. Our theory predicts that the application of a field induces a novel Lifshitz transition, in which a quasi-two dimensional Fermi Liquid with density of states $N^*(B) \propto 1/\sqrt{B}$ nucleates around the line node in momentum space. We also discuss how the vortex metal picture can account for the ESR anomalies observed in this system [3].

[1] S. Nakatsuji *et al.*, Nature Phys. 4, 603 (2008). [2] Y. Matsumoto *et al.*, Science 21, 316 (2011). [3] L. M. Holanda *et al.*, Phys Rev. Lett. 107, 026402 (2011).

¹Research supported by NSF DMR 0907179 (PC and AR) and US DOE Division of Materials Research contract number DE-AC02-98 CH 10886 (AT).

2:42PM L16.00002 Correlated disorder in Kondo lattice¹, MAXIM DZERO, XINYI HUANG, Kent State University — Motivated by recent experiments on Yb-doped CeCoIn₅, we study the effect of correlated disorder in Kondo lattice. Correlations between the impurities are considered at the two-particle level. We use mean-field theory approximation for the Anderson lattice model to calculate how the emergence of coherence in the Kondo lattice is impacted by correlations between impurities. We show that the rate at which disorder suppresses coherence temperature depends on the length of impurity correlations. As impurity concentration increases, we generally find that the suppression of coherence temperature is significantly reduced. The results are discussed in the context of available experimental data.

¹This work was financially supported by Ohio Board of Regents

2:54PM L16.00003 High-energy dispersion anomalies in actinide compounds, T. DAS, T. DURAKIEWICZ, J.-X. ZHU, J.J. JOYCE, MATTHIAS J. GRAF, Los Alamos National Lab. — The observation of a prominent peak-dip-hump feature in the spectral weight in number of actinide compounds including Pu-115 superconductors and non-superconducting U-115 remains an unsolved problem. We have developed a first-principles intermediate coupling model to show that most aspects of these strong correlation features can be understood from the spin-fluctuation interaction.[1] The results show that a strong peak in the spin-fluctuation dressed self-energy is present around 0.5 eV in all these materials, which is mostly created by spin-orbit split 5f bands. These fluctuations couple to the single-particle spectrum and give rise to a peak-dip-hump feature, characteristic of the coexistence of itinerant and localized electronic states. Results are in quantitative agreement with photoemission spectra. Finally, we show that the studied actinides can be understood within the rigid-band filling approach, in which the spin-fluctuation coupling constant follows the same materials dependence as the superconducting transition temperature T_c . Work is supported by US DOE.

[1] T. Das, J.-X. Zhu, and M. J. Graf, arXiv:1108.0272

3:06PM L16.00004 The Electronic Correlation Strength of Pu¹, R.C. ALBERS, JIAN-XIN ZHU, Los Alamos National Laboratory, A. SVANE, N.E. CHRISTENSEN, Aarhus University, MARK VAN SCHILFGAARDE, Arizona State University — Many materials have strong electron-electron correlation effects that can cause large deviations in electronic structure and materials properties from those predicted by conventional band-structure theory based on the local density approximation. We present a new method or scale to quantify electronic correlations in strongly correlated electron systems and apply it to the different phases of elemental Pu. Using the GW approximation, we show that the f-electron band-width reduction due to correlation effects scales as a function of the initial LDA bandwidth. This relationship is a universal relationship in that it is independent of crystal structure and atomic volume.

¹Supported by the NNSA of the US-DOE at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396, and the Center for Theoretical Natural Science at Aarhus University

3:18PM L16.00005 The Role of the Kondo and Phonon Correlations in the Cerium Volume Collapse¹, PETER REIS, PENG ZHANG, KA MING TAM, JUANA MORENO, MARK JARRELL, Louisiana State University, FAKHER ASSAAD, University of Wuerzburg, ANDY MCMAHAN, Lawrence Livermore National Lab, KONDO VOLUME COLLAPSE COLLABORATION — We review the most recent experimental and theoretical progress of the $\alpha \leftrightarrow \gamma$ volume collapse occurring in the element cerium. We discuss the experimental results which have been important in differentiating the various electronic and phononic properties of the volume collapse of cerium, these experiments illustrate that drastically different electronic and phononic properties exist between the small volume phase α and large volume phase γ of cerium. After interpreting the physical data and realizing that the volume collapse in cerium is primarily the result of different electronic and vibronic correlations in the α and γ phases we set up a Hamiltonian which encompasses the physical properties of the collapse. To model the electronic and phononic properties of the $\alpha \leftrightarrow \gamma$ transition of cerium we use the Periodic Anderson Model (PAM) + Holstein Model, with the aim that the Kondo like electronic correlations of the α phase is encoded in the PAM where the large vibronic physics of the γ phase is encompassed in the Holstein Model which incorporates a conduction electron-phonon mediated interaction.

¹This work was supported by NSF through OISE-0952300 and DMR-0548011.

3:30PM L16.00006 Numerical Study of the Electron-Phonon coupling in the Cerium Volume Collapse, PENG ZHANG, PETE REIS, KA-MING TAM, Department of Physics, Louisiana State University, LA, FAKHER ASSAAD, Department of Physics, University of Wuerzburg, Germany, JUANA MORENO, Department of Physics, Louisiana State University, LA, ANDY MCMAHAN, Lawrence Livermore National Laboratory, CA, MARK JARRELL, Department of Physics, Louisiana State University, LA — Rare earth elements, for example Cerium, will experience a volume collapse with increasing pressure. Researchers have struggled for six decades to discover the mechanism behind this unusual first order phase transition. Although different models have been proposed that provide some qualitatively correct results, there is no theory that completely captures the volume collapse. Notably, some recent experiments show that lattice oscillations play an important role, contrary to the previous consensus that this phase transition is mainly driven by the contributions from spins and electrons. In this talk, we will discuss our study which employs the DMFA method to explore the role of electron-phonon coupling in the Periodic Anderson Model.

3:42PM L16.00007 Lifshitz transition with interactions in high magnetic fields: Application to CeIn₃¹, PEDRO SCHLOTTMANN, Florida State University — The Néel ordered state of CeIn₃ is suppressed by a magnetic field of 61 T at ambient pressure. There is a second transition at ~ 45 T, which has been associated with a Lifshitz transition [1,2]. Skin depth measurements [2] indicate that the transition is discontinuous as $T \rightarrow 0$. Motivated by this transition we study the effects of Landau quantization and interaction among carriers on a Lifshitz transition. The Landau quantization leads to quasi-one-dimensional behavior for the direction parallel to the field. Repulsive Coulomb interactions give rise to a gas of strongly coupled carriers [3]. The density correlation function is calculated for a special long-ranged potential [4]. It is concluded that in CeIn₃ a pocket is being emptied as a function of field in a discontinuous fashion in the ground state. This discontinuity is gradually smeared by the temperature [4] in agreement with the skin depth experiments [2].

[1] S.E. Sebastian *et al.*, PNAS **106**, 7741 (2009).

[2] K.M. Purcell *et al.*, Phys. Rev. B **79**, 214428 (2009).

[3] P. Schlottmann and R. Gerhardt, Z. Phys. B **34**, 363 (1979).

[4] P. Schlottmann, Phys. Rev. B **83**, 115133 (2011); J. Appl. Phys., in print.

¹Work supported by the Department of Energy under grants DE-FG02-98ER45707 and NNSA DE-FG52-10NA29659

3:54PM L16.00008 Coexistence of antiferromagnetism and superconductivity induced by Pauli-paramagnetic pair breaking, KAZUSHI AOYAMA, Young Researcher Development Center, Kyoto University, RYUSUKE IKEDA, Department of Physics, Kyoto University — The heavy-fermion material CeCoIn₅ is a spin singlet d -wave superconductor with a strong Pauli-paramagnetic pair-breaking (PPB) effect. In the case with a magnetic field parallel to the basal plane of this material, there exists a distinct high field and low temperature (HFLT) superconducting (SC) phase in which a Fulde-Ferrell-Larkin-Ovchinnikov vortex lattice may be realized as a result of the strong PPB. Recently, it has been clarified that an antiferromagnetic (AFM) order exists inside the HFLT SC phase in spite of the absence of AFM order in the nonsuperconducting state [1]. Considering that AFM and SC orders are competing with each other in zero field, it is surprising that the AFM ordering is enhanced in the SC state. We theoretically study the stability of an AFM order in a d -wave and paramagnetic superconductor. We show that the PPB enhanced strongly by increasing the magnetic field induces an AFM order inside the SC phase and that, in contrast to the competitive nature of AFM and SC orders, the induced AFM order is not localized in vortex cores but coexistent with the SC order [2]. [1] M. Kenzelmann *et al.*, Science **321**, 1652 (2008). [2] K. Aoyama and R. Ikeda, arXiv:1107.5577.

4:06PM L16.00009 Current-Carrying States in Fulde-Ferrell-Larkin-Ovchinnikov superconductors, JIN AN, CHIN-SEN TING, Texas Center for Superconductivity, University of Houston, CHIA-REN HU, Department of Physics, Texas A&M University — Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) superconducting state is believed to be favorable in Pauli-limited heavy-fermion superconductors such as CeCoIn₅. Based on Bogliubov de-Gennes equations, we present a theoretical study of current-carrying FFLO states, including the stability and characterization of a superconducting order parameter for a current-carrying FFLO state. Inhomogeneous and anisotropic current density distribution and quasi-particle current contribution related to the order parameter modulation and sign change are found in FFLO state, which are expected to provide an easy way to detect the existence of an FFLO state.

4:18PM L16.00010 CeRu₂Al₂B: A new local moment 4f magnet with a complex T-H phase diagram, RYAN E. BAUMBACH, X. LU, K. GOFRYK, F. RONNING, J.D. THOMPSON, Los Alamos National Laboratory, H. CHUDO, HIROSHI YASUOKA, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Ibaraki, JAPAN, C.H. WANG, V.O. GARLEA, A.D. CHRISTIANSON, Oak Ridge National Laboratory, E.D. BAUER, Los Alamos National Laboratory — There is ongoing interest in the study of Ce-based compounds that are derivatives of certain structure types (e.g., ThCr₂Si₂ and PbClF), as they are often associated with correlated electron phenomena. We will report results for a new system that falls into this category, CeRu₂Al₂B. This compound crystallizes in a filled variant of the layered/tetragonal CeMg₂Si₂ structure. Contrary to what is often observed for Ce-based compounds, we find pronounced local moment behavior of the Ce ions, resulting in complicated magnetic ordering at strikingly high temperatures: i.e., antiferromagnetism (AFM) at $T_N = 14.1$ K followed by ferromagnetism (FM) at $T_C = 12.8$ K, which is first order in character. We also find a temperature-magnetic field phase diagram that consists of three distinct ordered phases: (1) AFM, (2) spin reoriented, and (3) FM. Since this type of behavior is unusual for Ce-based compounds, we will discuss prospects for suppressing the ordered state toward $T = 0$ in order to produce a Doniach-like phase diagram, which may provide a route towards a FM quantum critical point.

4:30PM L16.00011 T-P phase diagram for the new local moment 4f ferromagnet CeRu₂Ga₂B, ERIC D. BAUER, R.E. BAUMBACH, X. LU, T. SHANG, F. RONNING, J.D. THOMPSON, Los Alamos National Laboratory, C.H. WANG, V.O. GARLEA, A.D. CHRISTIANSON, Oak Ridge National Laboratory — We will report results for single crystals of a new Ce-based local moment ferromagnet, CeRu₂Ga₂B. Electrical resistivity, magnetization, and magnetic susceptibility measurements reveal ferromagnetism and hysteresis around $T_C = 16.1$ K, while specific heat measurements uncover a huge anomaly at the phase transition, which results in a large discontinuity in the magnetic entropy ($\Delta S_{mag} = 1.7$ J/mol-K). Taken together, these data show that CeRu₂Ga₂B undergoes a first order ferromagnetic phase transition at a surprisingly high temperature. Since this type of behavior is unusual for Ce-based compounds, we additionally undertook an effort to tune the magnetic state using pressure. We will present electrical resistivity measurements under applied pressures and the resulting temperature-pressure phase diagram, with an emphasis on implications for possible nearness to a ferromagnetic quantum critical point.

4:42PM L16.00012 Superconductivity and Magnetic Ordering in RE₂Pt₃Ge₅ (RE = La and Pr) Single Crystals, NAKHEON SUNG, C.J. ROH, B.K. CHO¹, School of Materials Science and Engineering, Gwangju Institute of Science and Technology (GIST), Gwangju 500-712, Korea — Superconductivity and magnetic properties of rare-earth ternary germanide intermetallic compounds, RE₂Pt₃Ge₅ (RE = La and Pr), are investigated. La₂Pt₃Ge₅ and Pr₂Pt₃Ge₅ single crystals were synthesized by high temperature metal flux method with Ge self flux. These two compounds were formed in U₂Co₃Si₅-type orthorhombic structure (space group *Ibam*) and the lattice parameters were determined using XRD of pulverized single crystals. La₂Pt₃Ge₅ exhibits an onset of superconducting phase transition at $T_c = 8.1$ K, which, to the best of our knowledge, is the highest T_c in U₂Co₃Si₅-type superconductors. Pr₂Pt₃Ge₅ shows both superconducting phase transition at $T_c = 7.9$ K and antiferromagnetic transition at $T_N = 4.4$ K. In addition, Pr₂Pt₃Ge₅ reveals strong magnetic anisotropy with an easy magnetic axis perpendicular to the *c*-axis, due to crystalline electric field effect. Including these results, we will discuss the nature of RE₂Pt₃Ge₅ single crystals in detail.

¹ Author to whom correspondence should be addressed. Electronic mail: chobk@gist.ac.kr

4:54PM L16.00013 Multi-orbital Kondo physics of Co in Cu hosts, ALEXANDER LICHTENSTEIN, TIM OLIVER WEHLING, ALJOSCHA WILHELM, 1st Institute for Theoretical Physics, University of Hamburg, Germany, BRIGITTE SURER, MATTHIAS TROYER, PHILIPP WERNER, Theoretische Physik, ETH Zurich, Switzerland, ANDREAS LÄUCHLI, MPI fuer Physik komplexer Systeme, Dresden, Germany — We investigate the electronic structure of cobalt atoms on a copper surface and in a copper host by combining density functional calculations with a numerically exact continuous-time quantum Monte Carlo treatment of the five-orbital impurity problem. In both cases we find low energy resonances in the density of states of all five Co *d*-orbitals. The corresponding self-energies indicate the formation of a Fermi liquid state at low temperatures. Our calculations yield the characteristic energy scale – the Kondo temperature – for both systems in good agreement with experiments. We quantify the charge fluctuations in both geometries and suggest that Co in Cu must be described by an Anderson impurity model rather than by a model assuming frozen impurity valency at low energies. We show that fluctuations of the orbital degrees of freedom are crucial for explaining the Kondo temperatures obtained in our calculations and measured in experiments.

5:06PM L16.00014 Origin of the Heavy-Fermion behavior in Ca_{2-x}Sr_xRuO₄, NAOYA ARAKAWA, MASAO OGATA, Department of Physics, The University of Tokyo — We investigate the electronic states in Ca_{2-x}Sr_xRuO₄ for $0.5 \leq x \leq 2.0$ on the basis of the three-orbital Hubbard model in the Gutzwiller approximation. We take the dominant effects of the Ca-substitution into account as the changes of the hybridizations, whose squares are proportional to the nearest-neighbor hopping integrals of the Ru-*t_{2g}*-orbitals, between the Ru-4*d*- and O-2*p*-orbitals. In this presentation, we show the renormalization factors for the Ru *t_{2g}*-orbitals as a function of the intraorbital Coulomb interaction or an angle of the rotation of RuO₆-octahedra and discuss the origin of the heavy-fermion behavior around $x = 0.5$. Our calculation suggests that moderately strong Coulomb interaction and the orbital-dependent modifications of the electronic structures for the Ru-*t_{2g}*-orbitals due to the Ca-substitution cause the heavy-fermion behavior in Ca_{2-x}Sr_xRuO₄.

5:18PM L16.00015 Far-infrared optical properties of pyrochlore heavy fermion superconductor Cd₂Re₂O₇ in the normal and superconducting states¹, M. REEDYK, M. HAJIALAMDARI², D.A. CRANDLES, F.S. RAZAVI, Dept. Physics, Brock University, R.K. KREMER, Max Planck Institute for Solid State Research — Cd₂Re₂O₇ is a pyrochlore oxide which exhibits superconductivity with a transition temperature T_C near 1 K. The far-infrared optical properties of Cd₂Re₂O₇ will be presented at temperatures above and below T_C . Superconductivity induced changes in the phonon structure are observed. Thermal reflectance spectra show two absorption features, near 9.6 and 19.3 cm⁻¹ which arise in the superconducting state. Optical conductivity spectra reveal a softening (~ 1 cm⁻¹) of the phonon mode at 35 cm⁻¹ in the superconducting state. Analysis of the frequency dependent optical effective mass and scattering rate support the classification of this material as a modest heavy electron system at low temperatures.

¹This work was supported by the Natural Sciences and Engineering Research Council of Canada.

²currently at the University of Waterloo

Tuesday, February 28, 2012 2:30PM - 5:30PM –

Session L17 DMP GERA FIAP: Focus Session: Thermoelectrics - Electronic Structure and Transport 252A

2:30PM L17.00001 Potassium is a resonant level in $\text{Bi}_{1-x}\text{Sb}_x$ alloys¹, JOSEPH P. HEREMANS, The Ohio State University, Department of Mechanical and Aerospace Engineering, and Department of Physics, HYUNGYU JIN, The Ohio State University, Department of Mechanical and Aerospace Engineering, BARTLOMIEJ WIENDLOCHA, AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Krakow, Poland — $\text{Bi}_{1-x}\text{Sb}_x$ alloys are the most promising thermoelectric materials for cryogenic Peltier cooling. Resonant impurity levels are known to increase the thermoelectric power and figure of merit of semiconductors and known examples are Ti:PbTe [1] and $\text{Sn:Bi}_2\text{Te}_3$ [2]. Here we add $\text{K:Bi}_{1-x}\text{Sb}_x$ to that list. Band structure calculations show that substitutional potassium in bismuth can form sharp density of states peaks, suggesting the presence of a resonant level. Single crystal samples were synthesized by a modified horizontal Bridgman-Hor method. Cryogenic thermoelectric transport data will be presented as a function of K and Sb concentrations. At certain concentrations, the addition of potassium has a large effect on the thermopower, and increases the figure of merit to reach $zT = 0.7$ at 100K with $zT > 0.5$ at all temperatures from 50K up to room temperature, numbers are valid along the trigonal axis of single crystals. [1] J. P. Heremans & al. Energy Environ. Sci. DOI:10.1039/C1EE02612G; Science **321**, 554 (2008); [2] C.M. Jaworski & al., Phys. Rev. B **80**, 233201, (2009)

¹AFOSR MURI “Cryogenic Peltier Cooling,” FA9550-10-1-0533.

2:42PM L17.00002 Fermi level pinning in Ti doped PbTe ¹, YI-BIN GAO, Dept of Mechanical and Aeronautical Engineering (MAE), Ohio State University (OSU), JAN KOENIG, Fraunhofer Institute for Physical Measurement Techniques, Germany, MICHELE D. NIELSEN, MAE OSU, BARTLOMIEJ WIENDLOCHA, AGH University of Science and Technology, Poland, HARALD BOETTNER, Fraunhofer Institute for Physical Measurement Techniques, Germany, JOSEPH P. HEREMANS, MAE, Dept of Physics, OSU — The doping of PbTe attracts much interest due to the possible improvement of the thermoelectric properties by forming resonant levels. Here we report on doping of PbTe with Ti by molecular beam epitaxy, and back up the results with band structure calculations that show that Ti is a resonant level in the conduction band of PbTe . Ti is found to be a donor, leading to electron concentrations up to $1 \times 10^{19} \text{cm}^{-3}$, above which it pins the Fermi level at about 52 meV above the conduction band edge, and further increase of Ti shows no effect. At higher Ti contents the concentration of free electrons starts to rise again. However, Ti doping does not enhance the thermopower above that of similarly-doped PbTe , suggesting that the electrons on Ti are localized. We propose a model for Fermi level pinning due to different ionization states of the donor impurity which is similar to a chemical buffer. Further electronic structure calculations for Ti:PbTe confirm existence of the quasi-localized Ti states in the conduction band of PbTe and predict a local magnetic moment on Ti atom of 1.8 Bohr magnetons.

¹Work supported by ZT:Plus, by the joint NSF/DOE program on thermoelectrics NSF-CBET-1048622, and by the Air Force Office of Scientific Research MURI FA9550-10-1-0533.

2:54PM L17.00003 Enhancement of Thermoelectric Figure-of-Merit by Resonant States of Aluminum Doping in Lead Selenide, QINYONG ZHANG, Xihua University, HUI WANG, WEISHU LIU, HENGZHI WANG, BO YU, QIAN ZHANG, Boston College, ZHITING TIAN, GEORGE NI, SANGYEOP LEE, KEIVAN ESFAJANI, GANG CHEN, MIT, ZHIFENG REN, Boston College, XIHUA UNIVERSITY COLLABORATION, BOSTON COLLEGE TEAM, MIT TEAM — By adding aluminium (Al) into lead selenide (PbSe), we successfully prepared n-type PbSe thermoelectric materials with a figure-of-merit (ZT) of 1.3 at 850 K. Such high ZT is achieved by a combination of high Seebeck coefficient caused by very possibly the resonant states in the conduction band created by Al dopant and low thermal conductivity from nanosized phonon scattering centers.

3:06PM L17.00004 Thermoelectric properties of indium-doped PbSe ¹, ERIC EVOLA, The Ohio State University, MICHELE NIELSEN, PhD Student Mentor (OSU), JOSEPH HEREMANS, Advisor (OSU) — P-type [1,2] and n-type [3] PbSe have recently exhibited good thermoelectric properties without using the relatively uncommon element Tellurium. Here we report thermal conductivity, galvanomagnetic and thermomagnetic properties of bulk samples of n-type PbSe doped with indium at varying concentrations within the solid solution solubility range. A figure of merit zT value well in excess of 1 has been achieved. Resonant level effect and changes in the dimensionless figure of merit will be discussed although data indicate that the thermoelectric properties do not lie above the Pisarenko relation.

- [1] D.J. Parker et al, Phys. Rev. B **82**, 035204 (2010)
- [2] H. Wang et al, Adv. Mater. **23** 1366-1370 (2011)
- [3] J. Androulakis et al, Phys. Rev. B **83**, 195209 (2011)

¹This work is supported by NSF-CBET-1048622

3:18PM L17.00005 Study on thermoelectric properties of n-type PbSe doped with B, Ga, and In, QIAN ZHANG, Boston College, QINYONG ZHANG, Xihua University, BO YU, DEZHI WANG, Boston College, GEORGE NI, GANG CHEN, Massachusetts Institute of Technology, ZHIFENG REN, Boston College, BOSTON COLLEGE TEAM, XIHUA UNIVERSITY COLLABORATION, MASSACHUSETTS INSTITUTE OF TECHNOLOGY COLLABORATION — We report here systematic study of the thermoelectric properties of n-type PbSe with B, Ga, and In doping. The comparison of the electrical resistivity, Seebeck coefficient, and thermal conductivity is conducted. Room temperature Hall measurements show the effective increase of carrier concentration by both Ga and In doping to $\sim 10^{20} \text{cm}^{-3}$. The high power factor $\sim 2.4 \times 10^{-3} \text{Wm}^{-1} \text{K}^{-2}$ is obtained when B is doped, however, it is decreased with increasing temperature, which is inverted with the other dopants. No resonant state is found in all these three materials. A figure of merit, $ZT > 1.2$ at 873 K is achieved in 0.5% In doped PbSe .

3:30PM L17.00006 Electronic structure of ferroelectrically distorted PbTe¹, MAL-SOON LEE, Michigan State University, MERCOURI G. KANATZIDIS, Northwestern University, S.D. MAHANTI, Michigan State University — PbTe is one of the most promising thermoelectric materials. The electronic transport properties of the p-doped system are generally explained based on the nearly degenerate pockets near L and along Σ at high temperatures, where the energy at the L point decreases with increasing temperature and approaches the Σ point maxima. Recently, Bozin et al. showed that structure of PbTe is ferroelectrically distorted at high temperatures.² Following this experiment, a lattice dynamics study using first-principle molecular dynamics simulations have shown an increase of the band gap with increased temperature as seen experimentally.³ Motivated from these studies, we have performed electronic structure calculations to investigate the effect of structural distortion and expansion on the band structure. We observe that the ordering of energy levels changes dramatically with distortion. In addition to these results we will also discuss how this can affect the electronic transport properties at high temperatures.

¹This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences as a part of an Energy Frontier Research Center under Award Number DE-SC0001054.

²E. S. Bozin, C. D. Malliakas, P. Souvatzis, T. Proffen, N. A. Spaldin, M. G. Kanatzidis, and S. J. L. Billinge, Science 330, 1660 (2011).

³Y. Zhang, X. Ke, P. R. C. Kent, J. Yang, and C. Chen, Prys. Rev. Lett. 107, 175503 (2011).

3:42PM L17.00007 Potential thermoelectric performance from optimization of hole-doped Bi₂Se₃¹, DAVID PARKER, DAVID SINGH, Oak Ridge National Laboratory — We present an analysis of the potential thermoelectric performance of hole-doped Bi₂Se₃, which is commonly considered to show inferior room temperature performance when compared to Bi₂Te₃. We find that if the lattice thermal conductivity can be reduced by nanostructuring techniques (as have been applied to Bi₂Te₃) the material may show optimized ZT values of unity or more in the 300 - 500 K temperature range and thus be suitable for cooling and moderate temperature waste heat recovery and thermoelectric solar cell applications. Central to this conclusion are the larger band gap and the relatively heavier valence bands of Bi₂Se₃.

¹This research was supported by the U.S. DoE, EERE, Vehicle Technologies, Propulsion Materials Program (DP) and the “Solid State Solar-Thermal Energy Conversion Center (S3 TEC),” an Energy Frontier Research Center funded by the US DOE(DJS)

3:54PM L17.00008 Electronic and Thermoelectric properties of RuIn_{3-x}A_x (A=Sn, Zn) from first principles¹, DEEPA KASINATHAN, MPI CPfS - Dresden, KLAUS KOEPERNIK, IFW Dresden, HELGE ROSNER, MPI CPfS - Dresden — Recently, substitution derivatives of the intermetallic compound RuIn_{3-x}A_x (A = Sn, Zn) have been shown to exhibit relatively high Seebeck coefficients. Substitution by Sn results in n-type behavior while p-type is the norm for substitution of In by Zn. We discuss in detail the electronic structure of the parent compound and the substitution derivatives obtained from density functional theory (DFT) based calculations using the Full Potential Local Orbital (FPLO) code. The substitution effects have been studied using three different approximations: the simple virtual crystal approximation (VCA), the ordered supercell approach and the disordered coherent potential approximation (CPA). Both Sn and Zn prefer different site symmetry positions in the unit cell. While the parent compound RuIn₃ is a semiconductor, the substitution derivatives are not. For small doping concentrations, we observe a rather rigid-band-like behavior due to the parabolic nature of the bands forming the valence band maximum and the conduction band minimum. Transport properties calculated using the semi-classical Boltzmann transport equations (BoltzTraP) based on the constant scattering approximation are consistent with the experiments.

¹Funding from SPP 1386 of the DFG is acknowledged

4:06PM L17.00009 Electronic structure and thermopower of Cu₃SbSe₄¹, DAT DO, Michigan State University, VIDVUDS OZOLINS, University of California, Los Angeles, S.D. MAHANTI, MAL-SOON LEE, Michigan State University, YONGSHENG ZHANG, CHRIS WOLVERTON, Northwestern University — Cu₃SbSe₄ (Se₄), a ternary derivative of the II-VI zincblende semiconductors, is a narrow band gap semiconductor (band gap $\sim 0.1 - 0.4$ eV) and a promising thermoelectric. Recently, Skoug et al. [1] have measured transport properties of pure and doped Se₄ (Ge and Sn substituting for Sb). They find that p-doping by 2% Sn results in optimized value of $ZT=0.72$ at 630 K. To understand the electronic structure and transport properties of Se₄ we have carried out ab initio density functional electronic structure calculations. LDA/GGA/GGA+U approximations do not show that Se₄ is a standard semiconductor. They give a resonance-like peak near the top of the valence band of width ~ 0.5 eV. The Fermi energy for the undoped system lies below the peak, making it a pseudo-gap system, in disagreement with experiment. Non-local exchange with relaxation of Sb-Se bonds lead to the opening of a gap (0.26 eV), its origin being intimately related to the valency of Sb. Transport calculations show that Se₄ is an excellent p-type thermoelectric, in agreement with experiment.

[1] Skoug et al., Sci. Adv. Mater., 3, 602 (2011).

¹This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences as a part of an Energy Frontier Research Center under Award Number DE-SC0001054.

4:18PM L17.00010 Thermoelectric Properties of CoSb₃-xSn_x¹, MICHELE D. NIELSEN, Department of Mechanical Engineering, The Ohio State University, SI HUI, Department of Mechanical Engineering, University of Michigan, CTIRAD UHER, Department of Physics, University of Michigan, JANUSZ TOBOLA, Department of Condensed Matter Physics, AGH University of Science and Technology, Krakow, Poland, JOSEPH P. HEREMANS, Department of Physics, Department of Mechanical Engineering, The Ohio State University — We substitute Sn for Sb in CoSb₃. Band structure calculations predict that Sn should be a resonant level with an energy near the top of the heavy (Co-3d) valence band. This is confirmed experimentally. Indeed, heavily Sn-doped samples show a low-temperature anomaly in their thermopower consistent with this prediction. The hole concentration, however, is too high for this materials to have a high thermopower and figure of merit.

¹This material is based upon work supported by the Department of Energy Award Number DE-PI0000012.

4:30PM L17.00011 Is the high frequency thermopower useful for predicting properties of strongly correlated materials?¹, JESUS CRUZ, JAMES FREERICKS, Georgetown University — Shastry has proposed that the high-frequency thermopower can be used for meaningful predictions of the dc thermopower in many strongly correlated materials. If true, this will make it much easier to screen strongly correlated materials for useful thermoelectric properties because it is much easier to calculate the high-frequency limit. By solving this problem exactly for the Falicov-Kimball model using dynamical mean-field theory, we find that this approach often does not work. We also compare with usual approximations for the thermopower, we find that the Heikes formula gives a good description of the high frequency thermopower while the Kelvin formula is equivalent at high temperature. Unfortunately, the only accurate way to find the dc thermopower is with the conventional Kubo formula.

¹Work supported by the National Science Foundation grant DMR-1006605

4:42PM L17.00012 Electrical and thermal transport properties of the substituted defect manganese silicides $\text{Mn}_{1-x-y}\text{Cr}_x\text{Ru}_y\text{Si}_{\delta\sim 1.74}$ ¹, VIJAYABARATHI PONNAMBALAM, DONALD T. MORELLI, Department of Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI- 48824 — Crystallizing in the TiSi_2 structure with considerable amount of random vacancies at the Si site, defect manganese silicides MnSi_{δ} ($\delta \sim 1.72\text{--}1.74$) are unusual in many respects. One of them is their structural stability which is determined by the electron concentration. In addition, MnSi_{δ} is known for unusually low thermal conductivity $\sim 3\text{--}3.5\text{ W/m K}$ at 300 K. We have substituted MnSi_{δ} with Cr and Ru simultaneously and studied the electrical and thermal transport properties of the resulting alloys. Both resistivity and Seebeck coefficient are less sensitive to substitutions and maintain robust values as high as that of $\text{MnSi}_{\sim 1.74}$. Hall measurements indicate that the carrier concentration remains high around $10^{21}/\text{cm}^3$ and more or less same for all compositions. Thermal conductivity is decreased further and interestingly increases with T reaching values $\sim 2.5\text{ W/m K}$ at 300 K. These results will be presented and discussed.

¹This work was supported as part of the Center for Revolutionary Materials for Solid State Energy Conversion, an Energy Frontier Research Center funded by the U.S. DoE, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001054.

4:54PM L17.00013 Transport in Old and New Thermoelectric Materials¹, DAVID SINGH, Oak Ridge National Laboratory — There is increasing interest in thermoelectric materials motivated in part by recent progress and in part by the potential of these materials in various energy technologies. Thermoelectric performance is a multiply contra-indicated property of matter. For example, it requires (1) high thermopower and high electrical conductivity, (2) high electrical conductivity and low thermal conductivity and (3) low thermal conductivity and high melting point. The key is finding an optimal balance. In this talk, I discuss some of the issues involved in the context of recent results. These include the surprising doping dependence of the thermopower in PbTe and PbSe , and the interplay between acoustic and optical phonons in PbTe . The potential of some new materials is discussed. This work was done in collaboration with David Parker, Olivier Delaire and Mao-Hua Du.

¹Work supported by DOE, BES through the S3TEC Energy Frontier Research Center (phonons) and EERE, Vehicle Technologies Propulsion Materials Program (electronic transport)

Tuesday, February 28, 2012 2:30PM - 5:18PM –
Session L18 DMP: Focus Session: Electron, Ion, and Exciton Transport in Nanostructures - Quantum Dots and Related Structures 252B

2:30PM L18.00001 The Role of Surface Ligands in Electronic Charge Transport in Semiconductor Nanocrystal Arrays, CHERIE KAGAN, University of Pennsylvania — The long, insulating ligands commonly used in the synthesis of colloidal semiconductor nanocrystals (NCs) inhibit strong interparticle coupling and charge transport once NCs are assembled in the solid state into NC arrays. We introduce ammonium thiocyanate (NH_4SCN) and its derivatives, ammonium selenocyanate and selenourea to exchange the long, insulating ligands commonly used in the synthesis of colloidal semiconductor NCs. NCs may be exchanged with the new ligand in solution to form dispersions from which NC arrays are deposited or NC arrays with the long, insulating ligands may be exchanged in the solid state with the new ligands. The new compact ligands enhance interparticle coupling and charge transport in thin film, NC arrays as seen by red-shifts in the optical absorption and concomitant increases in carrier mobilities. Thiocyanate-capped CdSe thin film, NC arrays form sensitive photodetectors and n-type field-effect transistors with electron mobilities of $\sim 10\text{ cm}^2/\text{Vs}$ and current modulation of $>10^6$, while preserving NC quantum confinement. Temperature-dependent transport measurements reveal band-like transport in NC arrays, overcoming carrier hopping that has typified transport in NC arrays until recently. The non-caustic, chemically benign nature of the ammonium thiocyanate treatment enables the fabrication of NC thin film devices and circuits on flexible plastics.

3:06PM L18.00002 n and p Type HgTe Colloidal Quantum Dot Film¹, HENG LIU, SEAN KEULEYAN, PHILIPPE GUYOT-SIONNEST, James Franck Institute, The University of Chicago — HgTe colloidal quantum dots (CQDs) are a new system that can be stably charged n- and p-type by electrochemistry and it exhibits carrier-dependent photoresponse and magneto-resistance. For both electron or hole injection, interband bleach and intraband absorption confirm that the charges can be injected in the delocalized quantum states. Both carrier types lead to conductivity and show similar mobilities ($\sim 0.1\text{ cm}^2/\text{Vs}$). However p-type films show good photoresponse and long photocurrent lifetime of hundreds of microseconds, while n-type films show 100 times shorter lifetimes and little or no photoresponse. With these samples, p-type will therefore be better for photovoltaic response. The magneto-resistance of n-type films is also found to be large while that of p-type films is negligible. This is consistent with the heavier hole mass compared to electrons in HgTe . The HgTe CQDs share similar features with the II-VI CdSe but with the advantage of allowing both n- and p-type charging. While this property is shared with the narrow gap IV-VI PbSe , HgTe has a simpler electronic structure and better stability in ambient conditions. The stability of the HgTe CQDs for n- and p-type charging opens many further investigations.

¹DOE:DE-FG02- 06ER46326; NSF MRSEC: DMR-0820054

3:18PM L18.00003 Tailoring Quantum Dot Assemblies to Extend Exciton Coherence Times and Improve Exciton Transport¹, KENTON SEWARD, ZHIBIN LIN, MARK LUSK, Department of Physics, Colorado School of Mines — The motion of excitons through nanostructured assemblies plays a central role in a wide range of physical phenomena including quantum computing, molecular electronics, photosynthetic processes, excitonic transistors and light emitting diodes. All of these technologies are severely handicapped, though, by quasi-particle lifetimes on the order of a nanosecond. The movement of excitons must therefore be as efficient as possible in order to move excitons meaningful distances. This is problematic for assemblies of small Si quantum dots (QDs), where excitons quickly localize and entangle with dot phonon modes. Ensuing exciton transport is then characterized by a classical random walk reduced to very short distances because of efficient recombination. We use a combination of master equation (Haken-Strobl) formalism and density functional theory to estimate the rate of decoherence in Si QD assemblies and its impact on exciton mobility. Exciton-phonon coupling and Coulomb interactions are calculated as a function of dot size, spacing and termination to minimize the rate of intra-dot phonon entanglement. This extends the time over which more efficient exciton transport, characterized by partial coherence, can be maintained.

¹Renewable Energy Materials Research Science and Engineering Center (NSF Grant No. DMR-0820518) at the Colorado School of Mines and the National Renewable Energy Laboratory

3:30PM L18.00004 Efficient Exciton Transport Between Strongly Quantum-Confined Silicon Quantum Dots¹, MARK LUSK, ZHIBIN LIN, Department of Physics, Colorado School of Mines, ALBERTO FRANCESCHETTI, National Renewable Energy Laboratory — First-order perturbation theory and many-body Green function analysis are used to quantify the influence of size, surface reconstruction and surface treatment on exciton transport between small silicon quantum dots. Competing radiative processes are also considered in order to determine how exciton transport efficiency is influenced. The analysis shows that quantum confinement causes small (~ 1 nm) Si quantum dots to exhibit exciton transport efficiencies far exceeding that of their larger counterparts. We also find that surface reconstruction significantly influences the absorption cross-section and leads to a large reduction in both transport rate and efficiency. Exciton transport efficiency is higher for hydrogen-passivated dots as compared with those terminated with more electronegative ligands. This is because such ligands delocalize electron wave functions towards the surface and result in a lower dipole moment. This work [1] is a first step in the development of a framework for the design of quantum dot assemblies with improved exciton transfer efficiency.

[1] Z. Lin, A. Franceschetti and M. T. Lusk, arXiv:1110.6456v1 [cond-mat.mes-hall]

¹Renewable Energy Materials Research Science and Engineering Center (NSF Grant No. DMR-0820518) at the Colorado School of Mines and the National Renewable Energy Laboratory

3:42PM L18.00005 Finite Element Modeling of Current-Induced Filaments in Nanocrystalline Silicon, SEAN FISCHER, CHRISTIAN OSORIO, NICHOLAS WILLIAMS, HELENA SILVA, ALI GOKIRMAK, University of Connecticut — Rapid, heat induced phase transitions in a mixed phase semiconductor may lead to current percolation along a highly conductive preferred path, or filament. In this study, we use 2-D, finite element simulations to model the time dependent evolution of current-induced filaments in nanocrystalline silicon (nc-Si) wires. nc-Si wires are modeled as isolated crystalline silicon (c-Si) circles randomly distributed in an amorphous silicon (a-Si) wire 500 nm in length and 75 nm in width. Simulations include temperature dependent material parameters for electrical conductivity, thermal conductivity, heat capacity, and account for latent heat of fusion during phase transition from solid to liquid silicon. Field dependent material parameters are neglected to improve simulation convergence. Voltage pulses of amplitude 300 V and rise time less than 1 ns produce molten filaments ~ 5 nm in width extending the length of the wire. The resistance of each wire decreases by four orders of magnitude during formation and filament current density exceeds 500 MA/cm².

3:54PM L18.00006 Ultrashort channel length quantum-dot photodetectors, FERRY PRINS, Kavli Institute of Nanoscience, Delft University of Technology — We present an efficient photodetector based on a one-dimensional array of parallel contacted PbSe quantum dots. In this device-architecture, the electrodes act as optical nano-antennae which concentrate incident light into the nanoparticle junction where they are converted into electron-hole pairs. The excitons are extracted with high efficiency due to the fact that the quantum dots are in direct contact with both source and drain electrodes, in contrast to previous studies which employed assemblies of quantum dots.

4:06PM L18.00007 The Influence of Phonons and Surface Termination on Optical Transitions in Small Silicon Quantum Dots and Implications for Exciton Transport¹, ZHIBIN LIN, Department of Physics, Colorado School of Mines, ALBERTO FRANCESCHETTI, National Renewable Energy Laboratory, MARK LUSK, Department of Physics, Colorado School of Mines — Bulk silicon is an indirect-gap semiconductor, and radiative recombination can proceed only through phonon assistance. Recent experiments suggest, though, that fast, zero-phonon, pseudo-direct transitions occur in silicon quantum dots (Si QDs) as a result of quantum confinement. On the other hand, previous theoretical studies based on tight-binding and effective mass methodologies yield contradictory conclusions on the degree to which phonons play a role in radiative recombination within Si QDs. The resolution of this issue has important repercussions for ways in which Si QDs can be incorporated into future photovoltaic designs. This also has implications as to how QD size, phonons, and surface ligands collectively influence exciton transport. Density functional theory, in concert with a phonon-corrected version of Fermi's Golden Rule, is used to investigate the degree to which phonons influence the rate of optical transitions in Si QDs and to elucidate how the role of phonons changes with dot size and surface termination (H, CH₃, and OH). The results are compared with available experimental data and those of previous calculations. In addition, the implications for phonon-assisted exciton transport dynamics within Si QD assemblies will be discussed.

¹Renewable Energy Materials Research Science and Engineering Center (NSF Grant No. DMR-0820518) at CSM and NREL

4:18PM L18.00008 Dual MOSFET Charge Sensing in PbS Nanocrystal Quantum Dots, NIRAT RAY, TAMAR MENTZEL, KENNETH MACLEAN, DARCY WANGER, MOUNGI BAWENDI, MARC KASTNER, Massachusetts Institute of Technology — We use nanoscale metal-oxide-semiconductor field-effect transistors (MOSFETs) as charge sensors for measuring transport in a nearby nanocrystal array. While our technique enables a high resistance measurement, and enables us to probe a wide range of conductance, the main limitations of using single MOSFET charge sensors is the step-like switching of the current caused by electrons tunneling into and out of traps, presumably in the oxide. This makes it difficult to distinguish events that originate in the film from those that originate in the MOSFETs. We use two MOSFETs as simultaneous charge sensors to perform a correlation analysis and distinguish these events. We pattern a 80 nm wide ordered array of PbS nanocrystals, approximately 50 nm away from each sensor, to maximize the signal in the MOSFETs from charge fluctuations in the nanocrystal film. This configuration then enables us to probe electron transport in the nanocrystal array.

4:30PM L18.00009 Measuring electron transport in nano-patterned films of PbS nanocrystals using a charge sensor, TAMAR MENTZEL, Massachusetts Institute of Technology, Department of Physics, DARCY WANGER, Massachusetts Institute of Technology, Department of Chemistry, NIRAT RAY, Massachusetts Institute of Technology, Department of Physics, BRIAN WALKER, MOUNGI BAWENDI, Massachusetts Institute of Technology, Department of Chemistry, MARC KASTNER, Massachusetts Institute of Technology, Department of Physics — The ability to form nanoscale patterns of semiconductor nanocrystal films and to align those patterns to a substrate with nanoscale precision opens the possibility of novel electronic measurements and optoelectronic devices. We demonstrate a novel method for patterning nanoscopic films of semiconductor nanocrystals with electron-beam lithography. The resulting films are ordered and do not suffer from the cracking that arises when annealing or exchanging the capping ligand of the film. The patterning method is effective for a wide range of nanocrystal materials and capping ligands. We pattern a film of PbS nanocrystals approximately 80 nm wide, and position it within 100 nm of charge sensors made from nanoscale metal-oxide-semiconductor field-effect transistors (MOSFETs). The charge sensors, which can measure the fluctuations of individual electrons in the nearby electrostatic environment, are used to measure electron transport in the films as a function of temperature and applied field.

4:42PM L18.00010 Photoinduced modification of surface states in nanoporous InP observed by terahertz spectroscopy, JAMES LLOYD-HUGHES, University of Oxford, Department of Physics, SUSANNE MUELLER, GIACOMO SCALARI, ETH Zurich, Institute for Quantum Electronics, HUGH BISHOP, ALISON CROSSLEY, University of Oxford, Department of Materials, MIHAI ENACHI, LILIAN SIRBU, ION TIGINYANU, Technical University of Moldova — A precise control of the surface properties of semiconductor nanomaterials is vital for their functionality and use in many opto-electronic applications. Terahertz time-domain spectroscopy allows the non-contact investigation of electron transport in semiconductor nanomaterials, without the complication of contact fabrication. The technique allows the photoconductivity to be determined on picosecond timescales, under the assumption that the material's properties are not permanently altered by photoexcitation. Here we demonstrate that this assumption is not always valid. We report an investigation of nanoporous honeycombs of n-type InP using terahertz time-domain and X-ray photoemission spectroscopies. After photoexcitation the dark conductivity was found to increase quasi-irreversibly, recovering only after several hours in air. The calculated electron density for different surface pinning energies suggests that photoexcitation may reduce the density of surface states. The photoinduced modification of porous semiconductors may be useful in material processing as it is a clean, dry, and area-selective method to increase the conductivity.

4:54PM L18.00011 Delayed photoluminescence in three-dimensional silicon/silicon germanium nanostructures, LEONID TSYBESKOV, NIKHIL MODI, SELINA MALA, New Jersey Institute of Technology, J.-M BARIBEAU, X WU, D. J. LOCKWOOD, Institute for Microstructural Sciences, National Research Council of Canada — In three-dimensional (3D), SiGe nano-island multi-layers separated by nanometer-thick Si layers with the enhanced local strain field visualized by transmission electron microscopy (TEM), we find unusual low temperature photoluminescence (PL) dynamics. The PL detected at 1350 nm rises practically instantly and decays with a lifetime faster than 20 nanoseconds. In contrast, the PL detected at 1550 nm has a rise time of longer than 3-4 microseconds, and it decays with a characteristic lifetime which changes from 10 microseconds to milliseconds. The proposed model considers recombination of excitons bound to SiGe/Si interface as a mechanism responsible for the fast PL at 1350 nm. The observed slow rising PL with a peak near 1550 nm is associated with Auger ionization of SiGe clusters and separation of electrons and holes followed by carrier/exciton diffusion within Si layers toward a longer wavelength luminescence sites. These sites are associated with SiGe cluster areas containing a higher Ge concentration, and they are detected by analytical TEM.

5:06PM L18.00012 Transport of exciton-polariton condensation in semiconductor microcavity at BEC-BCS crossover, JUNG-JUNG SU, YOSHIHISA YAMAMOTO, National Institute of Informatics, Japan; E. Ginzton Laboratory, Stanford University — We study the transport properties of exciton-polariton condensation in the microcavity at the BEC-BCS crossover. Exciton-polariton (EP) is the quasiparticle of exciton and photon that can condense at a temperature as high as room temperature due to its extreme lightness. So far intense studies of this intriguing condensation have been limited to the photoluminescence (PL) measurement, mostly at the lower density BEC regime. When increasing density, the condensate enters the EP BCS regime in which the fermionic nature of electron and hole inside of exciton becomes important. This electron-hole nature is more prominent in the transport than in the PL measurements. We propose a transport measurement scheme of creating indirect-excitons in semiconductor bilayer which is embedded in the planar microcavity filled with photons. Leads are attached to the two sides of the bilayers to perform transport measurements. We present the different features of tunneling conductance signature for EP condensation in the BCS and in the BEC regime.

Tuesday, February 28, 2012 2:30PM - 5:30PM – Session L19 DCMP GMAG: Invited Session: Spin Liquids with Disorder 253AB

2:30PM L19.00001 The spin liquid ground state of the $S = 1/2$ Heisenberg model on the kagome lattice, STEVEN WHITE, UC Irvine — Condensed matter physicists have long sought a realistic two-dimensional (2D) magnetic system whose ground state is a *spin liquid*—a zero temperature state in which quantum fluctuations have melted away any form of magnetic order. The nearest-neighbor $S = 1/2$ Heisenberg model on the kagome lattice has seemed an ideal candidate, but in recent years some approximate numerical approaches to it have yielded instead a valence bond crystal. We have used the density matrix renormalization group to perform very accurate simulations on numerous cylinders with circumferences up to 12 lattice spacings, finding instead of the valence bond crystal a spin liquid, gapped in both the singlet and triplet sectors, with substantially lower energy. [Simeng Yan, David A. Huse, and Steven R. White, *Science* 332, 1173 (2011). *Cover article*] Our results, through a combination of very low energy, short correlation lengths and corresponding small finite size effects, a new rigorous energy bound, and consistent behavior on many cylinders, provide strong evidence that the 2D ground state of this model is a gapped spin liquid. One key feature of this spin liquid is that the predominant valence bond resonances occur on eight site loops rather than the shortest six site loops. The eight site loops allow a greater fraction of the bonds in the lattice to resonate. Our recent studies including a next nearest neighbor interaction J_2 reveal that the $J_2 = 0$ point is near the edge of a substantial spin liquid phase centered near $J_2 = 0.05 - 0.1$.

3:06PM L19.00002 Structure, disorder, and magnetism in Herbertsmithite, a kagomé Heisenberg antiferromagnet, TYREL MCQUEEN, Johns Hopkins University — Geometric frustration of magnetic ordering on triangle-based lattices is thought to be one avenue to inducing macroscopic quantum states in electron systems. Due to the triangular arrangement of ions, it is impossible to satisfy all nearest-neighbor interactions simultaneously. This “frustration” suppresses classical magnetic long-range order and is thought to be capable of resulting in novel quantum states such as various resonating-valence-bond or “spin-liquid” ground states for a two-dimensional (2D) $S = 1/2$ antiferromagnet. However, “structurally perfect” frustrated materials are rare; frequently, materials undergo a structural distortion at low temperature, relieving the magnetic frustration and giving rise to a classical ground state. In this talk, I will present recent structural and property studies of the 2D candidate spin-liquid material “ $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$.” Using X-ray scattering differences at elemental absorption edges and an improved analysis technique, I will show that there is no Zn occupation of the intralayer Cu sites within the kagomé layer, as previously reported; however there is Cu present on the Zn intersite, leading to a real structural formula of $(\text{Zn}_{0.85}\text{Cu}_{0.15})\text{Cu}_3(\text{OH})_6\text{Cl}_2$. Combined with recent pulsed high field magnetic measurements, the lack of Zn mixing onto the kagomé lattice sites lends support to the idea that the electronic ground state in “ $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$ ” and its relatives is non-trivial.

3:42PM L19.00003 Disorder in a quantum spin liquid: the Kitaev honeycomb model with vacancies, RODERICH MOESSNER¹, MPI-PKS Dresden — We address the effects of disorder in the Kitaev honeycomb model, focussing on the interplay of disorder and strong interactions in a quantum spin liquid. It is shown that nonmagnetic impurities bind a quantum of the emergent gauge flux. We find the formation of a local moment, which leads to a local magnetic response near the impurity which is parametrically larger than in the bulk. The magnetic response of a pair of impurities can be parametrically larger than that of an isolated one, and can in particular dominate the magnetic response of the system. The role of such impurities as diagnostic of the spin liquid state are emphasized – most remarkably, they provide a direct signature of the emergent gauge field.

¹In collaboration with Adam Willans and John Chalker (Oxford University): Phys. Rev. Lett. 104, 237203 (2010); Phys. Rev. B 84, 115146 (2011).

4:18PM L19.00004 Hole doping in frustrated spinels, ZnCr_2O_4 and MgCr_2O_4 , and their two dimensional analogue SCGO, $\text{SrCr}_8\text{Ga}_4\text{O}_{19}$ ¹, SIAN DUTTON, Princeton University — Recent experiments on the complex geometrically frustrated magnet, $\beta\text{-CaCr}_2\text{O}_4$, clearly illustrate the divergent effect of hole and static doping on the magnetic properties [1]. Given the complex parent state of $\beta\text{-CaCr}_2\text{O}_4$ this is not an ideal system for studying perturbations to the magnetic interactions. However, the onset of ferromagnetic fluctuations and ferrimagnetic ordering in $\beta\text{-Ca}_{1-y}\text{Cr}_2\text{O}_4$ suggests that other hole doped $\text{Cr}^{3+/4+}$ systems may be of interest. The extreme sensitivity in the balance of competing magnetic interactions in geometrically frustrated magnets is illustrated clearly in Cr^{3+} spinels, ACr_2O_4 . Antiferromagnetic (AFM) ordering in ACr_2O_4 occurs at a spin-Peierls transition. Both the low temperature magnetic and structural regimes are found to be highly sensitive to the A cation. In the case of ZnCr_2O_4 we find that very fine control of the reaction conditions is necessary to make stoichiometric ZnCr_2O_4 , rather than hole doped $\text{Zn}_{1+x}\text{Cr}_{2-x}\text{O}_4$ ($x \leq 0.04$). From analysis of magnetic measurements, specific heat and neutron diffraction we have probed the nature of the transitions at T_N [2]. How hole doping effects the low temperature properties and the role of the $d^2 \text{Cr}^{4+}$ cations on the isotropic $d^3 \text{Cr}^{3+}$ magnetic lattice will be discussed. Our results on the more robust MgCr_2O_4 spinel will also be presented. A 2D analogue of the 3D pyrochlore magnetic lattice in the ACr_2O_4 spinels is found in SCGO, $\text{SrCr}_8\text{Ga}_4\text{O}_{19}$. In hole doped SCGO, $\text{SrCr}_8\text{M}_x\text{Ga}_{4-x}\text{O}_{19}$ ($\text{M} = \text{Zn, Mg, Cu}$), a larger fraction of the Cr^{3+} can be oxidized. Hole doping is found to have a significant effect on the magnetic fluctuations, how this depends on the nature of the dopant cation will be addressed [3].

[1] S. E. Dutton, C. L. Broholm, and R. J. Cava, *Journal of Solid State Chemistry* **183**, 1798 (2010).

[2] S. E. Dutton *et al.*, *Physical Review B* **83**, 064407 (2011).

[3] S. E. Dutton *et al.*, *Journal of Physics-Condensed Matter* **23**, 386001 (2011).

¹Contributing Authors: E. D. Hanson, Q. Huang, O. Tchernyshyov, C. L. Broholm, and R. J. Cava. Research supported by the DoE, Office of Basic Energy Science, Division of Materials Sciences and Engineering under Award DE-FG02-08ER46544.

4:54PM L19.00005 Impurity Effects in Highly Frustrated Diamond-Lattice Antiferromagnets, LUCILE SAVARY, University of California, Santa Barbara — We consider the effects of local impurities in highly frustrated diamond lattice antiferromagnets, which exhibit large but non-extensive ground state degeneracies. Such models are appropriate to many A-site magnetic spinels. We argue very generally that sufficiently dilute impurities induce an *ordered* magnetic ground state, and provide a mechanism of degeneracy breaking. The states which are selected can be determined by a “swiss cheese model” analysis, which we demonstrate numerically for a particular impurity model in this case. Moreover, we present criteria for estimating the stability of the resulting ordered phase to a competing frozen (spin glass) one. The results may explain the contrasting finding of frozen and ordered ground states in CoAl_2O_4 and MnSc_2S_4 , respectively.

Tuesday, February 28, 2012 2:30PM - 5:30PM –

Session L20 CSWP COM: Invited Session: STEM Outreach to Underrepresented Communities

253C

2:30PM L20.00001 LIGO: Impacting science education through gravity-wave research in the local community and beyond¹, STEPHEN MCGUIRE, Southern University and A&M College — We describe our integration of the science teacher pre-service and in-service education programs at Southern University (SUBR) with the Laser Interferometer Gravitational-wave Observatory (LIGO) Science Education Center (SEC). Inquiry-based interactive exhibits are employed wherein we emphasize classical physics concepts of oscillations, waves, wave propagation, interference, resonance, lasers, light and Newtonian gravity. An aggressive museum docent training program is providing a means for undergraduates to learn how to effectively communicate science concepts within informal learning environments. This local educational partnership will ultimately create a science education continuum of engagement, working at multiple levels and multiple audiences to strengthen science literacy within the targeted STEM African-American community. Following a brief overview of our program of LIGO-related optical materials research, we give a detailed presentation of our K-12 science teacher preparation program with results.

¹Work supported by National Science Foundation Grants No. (s), PHY-011077, PHY-0701652, PHY-030554, and PHY-0917543.

3:06PM L20.00002 STEM Outreach to the African Canadian Community - The Imhotep Legacy Academy¹, KEVIN HEWITT, Dalhousie University — Like the African American community in the US, the African Canadian community is underrepresented in the Science Technology Engineering and Mathematics (STEM) fields. To serve these communities two outreach organizations emerged in Canadian cities where there is a critical mass of learners of African Descent - Toronto and Halifax. I will describe the Imhotep's Legacy Academy, which began in the Physics labs of Dalhousie University in Halifax, Nova Scotia and has grown to a province-wide program serving three-quarters of the school boards in the province with an annual budget that has grown to \$400,000 in 2011-12. It follows the learner from the time they enter grade 7 to the time they graduate from university, through three programs: (a) Weekly After-School science enrichment for junior high learners, (b) Virtual High school tutoring program and (c) Summer student internships and research scholarships for post-secondary students. This year, the program was the beneficiary of funding from TD Bank to establish scholarships for program participants to enter Dalhousie university. Modeled on the Meyerhoff scholarships the program participants are identified at an early stage and are promised a subset of funding as they meet selected criteria during participation in the program. The program enjoys support from the Department of Education and the highest levels of government. A tri-mentoring system exists where faculty of African descent train mentors, who are science students of African descent at associated universities, to deliver hands-on enrichment activities to learners of African Descent. Evidence supporting the success of the program will be highlighted. Project outcomes measured include (i) recruitment; (ii) attendance; (iii) stakeholder relationships; (iv) programming; (v) staff training; (vi) perception of ILASP's value; (vii) academic performance. The end results are new lessons and best practices that are incorporated into a strategic plan for the new project year. Teachers perceived that ILASP had a positive ripple effect on the entire academic and non-academic educational experience of the learners, crediting the project with (i) encouraging self-learning; (ii) assisting in honing learners' science and math skills; (iii) developing core skills that were applicable in learners' schoolwork; (iv) boosting learners' self-esteem; (v) improving school attendance; (vi) boosting learners' motivation to be engaged participants in all other classes.

¹We acknowledge financial support from the Nova Scotia Department of Education - African Canadian Services Division, NSERC, EnCana Corporation, TD Bank, Dalhousie University, CACE, OANSA, NS Labour and Advanced Education and SuperNova.

3:42PM L20.00003 Knowing your Hispanic community to improve outreach effectiveness, CRISTINA TORRES, LIGO Livingston Observatory — “Know your audience,” wise words for properly conveying information. For outreach, this can make the difference between successful connection or failure to connect to the community around us. When the target audience is the Hispanic community knowing your audience can potentially take on unexpected complexity. Like some other minority communities, the Hispanic community's culture is complex dual culture system. I will discuss my own personal observations about how this community interacts with the academic world. I also will discuss how the Hispanic community perceives itself as a member of the broader community we all live in and how non-homogeneous, our broadly defined Hispanic community really is. Discussing the Hispanic community's hidden nuances will bring to light the difficulty in getting to “know your audience,” when it comes to effective outreach in the rapidly growing Hispanic community.

4:18PM L20.00004 Outreach to the Native American community through the Navajo-Hopi program, KEVIN SCHINDLER, Lowell Observatory — No abstract available.

4:54PM L20.00005 Intersections of Gender and Power: Improving the Status of Women in Physics, SAEQA VRTILEK, Harvard-Smithsonian Center for Astrophysics — Numerous problems bedevil the twin goals of increasing the numerical participation in science, technology, engineering, and mathematics (STEM) fields by women and increasing the quality of that participation. The nature of the difficulties is everywhere slightly different, but there are underlying commonalities. A wide portfolio of lessons learned that can be applied to the confluence of cultures, backgrounds, and experiences that shape any given institution have been developed and will be presented. Among these, common and dominant themes are the need for mentoring, management training, and the increased visibility of successful women scientists. These have been identified (Nelson and Rogers 2004; Sonnert and Holton 1995a; Vetter 1996) as some of the key factors in securing the encouragement and increased stability needed for more senior women scientists to thrive to their full potential and provide the example and mentoring needed for a larger and more productive new generation.

Tuesday, February 28, 2012 2:30PM - 5:18PM —
Session L21 DCMP: Superconductivity: Mostly Mesoscopics & Low-d 254A

2:30PM L21.00001 Superconducting and Critical Current Properties of NiBi₃ Microfibers and Thin Films¹, NEEL HALDOLAARACHCHIGE, YIMIN XIONG, PHIL ADAMS, DAVID YOUNG, Louisiana State University — We report the superconducting and critical current properties of thin films of NiBi₃ formed on the surface of carbon microfibers and on sapphire substrates. The NiBi₃ coated C-fibers were prepared by reacting 7- μ m diameter Ni-coated carbon fibers with Bi shot, and the thin films on sapphire were formed by exposing electron-beam deposited Ni films to Bi vapor. The fibers and films show $T_c = 4.25$ K and $T_c = 4.35$ K, respectively, which was slightly higher than that of bulk polycrystalline NiBi₃. The extrapolated upper critical fields of the fibers [$H_{c2}(0) = 12$ T] and films [$H_{c2}(0) = 9$ T] are higher than the reported data on polycrystalline samples. The temperature dependence of the critical current density (J_c) is well described by Ginzburg-Landau theory and gives an extrapolated value of 5.26×10^5 A/cm².

¹NSF DMR Grant #1005764

2:42PM L21.00002 Proximity effect in superconductor exchange spring-superconductor junction, JIYEONG GU, CHRISTOPHER SAFRANSKI, HANMING YUAN, California State University, Long Beach — It is known that in ferromagnet/superconductor hybrid system when the magnetizations of the ferromagnetic layer are inhomogeneous superconductivity is not necessarily suppressed by the ferromagnet due to the presence of the triplet superconducting pairing. In our current work we used exchange spring magnet to produce inhomogeneous noncollinear magnetic configuration in the ferromagnet. Exchange spring trilayer structure, soft/hard/soft, was fabricated between two superconducting Nb layers; Nb/Py/SmFe(SmCo)/Py/Nb. Magnetic property of the structure was characterized using Vibrating Sample Magnetometer and Magneto Optical Kerr Effect (MOKE). MOKE was used to measure the magnetizations of the top Py and the bottom Py separately. Transition temperature of the system was measured as a function of magnitude and direction of the external magnetic field.

2:54PM L21.00003 Results of Resonant Activation and Macroscopic Quantum Tunneling Experiments in Magnesium Diboride Thin Film Josephson Junctions¹, ROBERTO RAMOS, Indiana Wesleyan University, STEVE CARABELLO, JOSEPH LAMBERT, JEROME MLACK, Drexel University, WENQING DAI, YI. SHEN, QI LI, The Pennsylvania State University, DANIEL CUNNANE, C.G. ZHUANG, KE CHEN, X.X. XI, Temple University — The Josephson junction is an experimental testbed widely used to study resonant activation and macroscopic quantum tunneling. These phenomena have been observed in junctions based on conventional low-temperature superconductors such as Nb and Al, and even in high- T_c , intrinsic superconductors. We report results of superconducting-to normal state switching experiments below 1 K using MgB₂-based Josephson heterojunctions with Pb and Nb counter-electrodes. Measurements were made with and without RF excitation. With microwaves, we see evidence of a resonant peak, in addition to the primary escape (from ground state) peak – consistent with resonant activation. We also observe features suggestive of macroscopic quantum tunneling including peaks in the escape rate enhancements and an “elbow” in the graph of calculated escape temperatures T_{esc} versus sample temperature.

¹This research has been supported by a grant-in-aid from Sigma Xi.

3:06PM L21.00004 Carrier Transport in Heterojunction Nanocrystals Under Strain, MARK SWEENEY, JOEL EAVES, Department of Chemistry and Biochemistry, University of Colorado, Boulder — We present a theory for carrier transport in semiconducting nanoscale heterostructures that emphasizes the effects of strain at the interface between two different crystal structures. An exactly solvable model shows that the interface region, or junction, acts as a scattering potential that facilitates charge separation. As a case study, we model a Type-II CdS/ZnSe heterostructure. After advancing a theory similar to that employed in model molecular conductance calculations, we calculate the electron and hole photocurrents and conductances, including non-linear effects, through the junction at steady-state.

3:18PM L21.00005 Progress towards measuring electron-electron interactions in persistent currents, MANUEL A. CASTELLANOS-BELTRAN, DUSTIN Q. NGO, Department of Physics, Yale University, JACK G.E. HARRIS, Department of Physics and Department of Applied Physics, Yale University — The equilibrium persistent current (PC) in normal metal rings have been a challenge for both experimentalists and theorists. Specifically, the magnitude of the average PC's in normal metals has been a long-standing puzzle. Previous measurements of the average current ($\langle I_{h/2e} \rangle$) were larger than theoretical predictions and indicated a diamagnetic sign. A possible explanation for these results is that they arise from the interplay of attractive electron-electron interactions within the metal (leading to the enhanced average PC) and trace magnetic impurities (which suppress the BCS superconductivity that would otherwise result from the attractive interactions). In this talk, I will discuss our progress towards measurements that intend to clarify the role that electron-electron interactions and magnetic impurities play in the persistent current.

3:30PM L21.00006 Tuning effective pairing potential through atomic scale control of super-conductor heterostructures¹, CHENDONG ZHANG, Department of Physics, the University of Texas at Austin; Institute of Physics, Chinese Academy of Sciences, JISUN KIM, JUNGDAE KIM, HYOUNGDO NAM, QIAN NIU, Department of Physics, the University of Texas at Austin, HONGJUN GAO, Institute of Physics, Chinese Academy of Sciences, CHIH-KANG SHIH, Department of Physics, the University of Texas at Austin — Previous experiments showed that superconductivity persists in ultrathin films of conventional superconductors, even in films that are only 1-2 atomic layers thick. However, it has also been implied that the interface and substrate can strongly influence the electronic properties in the quasi two-dimensional regime. In this work, we fabricated a heterostructure with a normal metal layer (Ag here) placed in between a superconducting film (Pb here) and an insulating substrate, and measured its superconductivity with scanning tunneling spectroscopy subsequently. The most striking observation is the requirement of an overlayer (L_{Pb}) to recover the superconductivity, while the recovery thickness is linearly dependent on the underlayer thickness. Considering the renormalization of pairing interaction strength for Cooper pair in the hybrid structure, the “effective attractive potential” model was developed in this work. It could serve as a model with predictive power to describe the general behavior of superconductor heterostructures. Moreover, the physical origin of some discrepancies in the reported transition temperature as a function of film thickness is partly elucidated by this work as well.

¹This work is supported by NSF Grants No. DMR-0906025, CMMI-0928664, Welch Foundation F-1672.

3:42PM L21.00007 Area-dependence of spin-triplet supercurrent in ferromagnetic Josephson junctions¹, YIXING WANG, WILLIAM P. PRATT, JR., NORMAN O. BIRGE, Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824 — Spin-triplet supercurrents in strong ferromagnetic Josephson junctions were reported by several groups in 2010. At the same time, the 0- π current-phase relationship of the spin-triplet supercurrent was predicted to be controllable by the magnetization orientations of different ferromagnetic layers. Our junctions contain a series of ferromagnetic layers consisting of a synthetic antiferromagnet Co/Ru/Co sandwiched between two thin magnetic layers such as PdNi or Ni [1]. When looking along the direction of current flow, one should obtain 0 junctions if the rotation direction of magnetizations is the same from one to the next, and π junctions when the opposite rotation direction is the case. Since our magnetic layers have multiple domains in the virgin state, we should expect 0 and π phases to alternate randomly in different locations in the junctions. The critical current in the virgin state should scale with the square-root of the junction area. After aligning the outer ferromagnetic layers in the same direction with an external field, the current-phase relation should be uniform across the whole junction area and the critical current should be proportional to the junction area. We will present data confirming this expectation for the magnetized state, whereas the situation for the virgin state is presently unclear.

[1] T.S. Khaire, M.A. Khasawneh, W.P. Pratt Jr and N.O. Birge, *Phys. Rev. Lett.* 104 137002 (2010).

¹Supported by the DOE under grant DE-FG02-06ER46341.

3:54PM L21.00008 Magnetic-field dependence of energy levels of superconducting nano-scale metallic grains with strong spin-orbit scattering¹, KONSTANTIN NESTEROV, YORAM ALHASSID, Center for Theoretical Physics, Sloane Physics Laboratory, Yale University, New Haven, CT 06520, USA — We study the Zeeman splitting of discrete energy levels of superconducting nano-scale metallic grains whose single-electron dynamics is chaotic [1]. In the absence of spin-orbit scattering the Zeeman splitting of a single-electron level is trivial; it is the same for all levels and linear in magnetic field. Spin-orbit coupling suppresses this splitting, induces level-to-level fluctuations and non-linear corrections to the energies. We investigate the combined effect of pairing correlations, which lead to superconductivity in the bulk limit, and spin-orbit scattering on the many-electron energy levels in a weak magnetic field. In particular, we focus our studies on the linear (g-factor) and quadratic (zero-field level curvature) corrections and their mesoscopic fluctuations. The single-electron part of the Hamiltonian follows the statistics of the Gaussian symplectic ensemble of random matrix theory, which is applicable in the limit of strong spin-orbit scattering and a large dimensionless Thouless conductance. The interaction is given by a BCS-like pairing term and the magnetic field coupling is described by a Zeeman term. [1] K. Nesterov and Y. Alhassid, to be published.

¹This work was supported in part by U.S. DOE grant No. DE-FG-0291-ER-40608. Computational cycles were provided by the Yale University High Performance Computing Center.

4:06PM L21.00009 Temperature induced epitaxial strain and superconductivity in (Cu,C)Ba₂CuO_{4+ δ} thin films, F.N.U. SHIPRA, University of Cincinnati, Jawaharlal Nehru Centre for Advanced Scientific Research, A. SUNDARESAN, Jawaharlal Nehru Centre for Advanced Scientific Research, SUPERCONDUCTIVITY AND MAGNETISM LAB TEAM — We have studied the effects of substrate temperature in establishing superconductivity in carbon incorporated thin films of Infinite Layered (IL) BaCuO_{2+ δ} . Carbon in the form of CO₃²⁻ group modulates the IL structure into a superstructure with doubled out of plane lattice parameter, ‘c’. The superstructure, (Cu,C)Ba₂CuO_{4+ δ} (Cu-1201) shows superconductivity within a narrow window of ‘c’ lattice parameter varying between 8.28 Å and 8.33 Å. The structural analysis of these thin films using reciprocal space maps (RSMs) shows a pseudomorphic growth with an in-plane lattice parameter, ‘a’, of 3.90 Å, similar to that of the SrTiO₃ substrate. Growth of these films under compressive strain is obtained at substrate temperatures varying between 530 °C and 560 °C. At deposition temperatures less than 500 °C, films with a relaxed in-plane lattice parameter of 4.00 Å were obtained which were non-superconducting. Deviations in the substrate temperature led to the coexistence of strained and relaxed phases. Thus the elongation along c – axis is compensated by the compression along a– axis with increasing substrate temperature. Flexibility of tuning the in-plane mismatch between substrate and film also rule out the use of buffer layers. Such structural changes result in the change of bond lengths and subsequently rearrange the number of charge carriers in the CuO₂ planes. Optimum number of charge carriers lead to superconductivity.

4:18PM L21.00010 Coexistence of a Triplet Nodal Order Parameter and a Singlet Order Parameter at Co / CoO / In contacts, SHAY HACOEN-GOURGY, BOAZ ALMOG, GUY DEUTSCHER, Tel-Aviv University — We present differential conductance measurements of Cobalt / Cobalt-Oxide / Indium planar junctions, 500nm x 500nm in size. The junctions span a wide range of barriers, from very low to a tunnel barrier. The characteristic conductance of all the junctions show a V-shape structure at low bias instead of the U-shape characteristic of a s-wave order parameter. The bias of the conductance peaks is, for all junctions, larger than the gap of indium. Both properties exclude pure s-wave pairing. The data is well fitted by a model that assumes the coexistence of s-wave singlet and equal spin p-wave triplet fluids. We find that the values of the s-wave and p-wave gaps follow the BCS temperature dependence and that the amplitude of the s-wave fluid increases with the barrier strength.

4:30PM L21.00011 Exploring triplet superconductivity by controlling the magnetic non-collinearity, L.Y. ZHU, YAOHUA LIU, MSD, Argonne National Laboratory, F.S. BERGERET, Centro de Física de Materiales, Centro Mixto CSIC-UPV/EHU, Donostia International Physics Center, J.E. PEARSON, S.G.E. TE VELTHUIS, S.D. BADER, J.S. JIANG, MSD, ANL — Recent theories predict spin-triplet superconductivity at the interface between a singlet superconductor (SC) and a ferromagnet (FM) with *inhomogeneous* magnetization [1]. Magnetic non-collinearity is a crucial but not quantitatively controlled parameter in most experiments inferring triplet superconductivity [2]. In this work, we use Nb as the SC, and an epitaxial exchange spring Py/Sm-Co bilayer with in-plane uniaxial anisotropy in Sm-Co layer as the FM. Due to the interfacial exchange coupling, a *tunable* noncollinear spin spiral can be achieved by controlling the external field. At a fixed temperature within the superconducting transition, starting from a collinear magnetic configuration, as the spin spiral winding angle ϕ increases, the superconducting critical current (I_c) first increases. There is an optimized winding angle ϕ_o , which maximizes I_c , after which I_c decreases with increasing ϕ . This *non-monotonic* $I_c(\phi)$ dependence cannot be explained by the short range proximity effect alone and suggests triplet pairing. More importantly, combining micromagnetic simulations with magnetoresistance measurements, we have determined the magnetic non-collinearity and correlated it *quantitatively* with the superconducting transport results. Our findings demonstrate the superconducting proximity effect can be tuned by manipulating the magnetic non-collinearity in a *single* sample.
[1] F. S. Bergeret et al., PRL **86**, 4096. [2] M. Eschrig, Physics Today **64**, 43.

4:42PM L21.00012 The Images of vortex penetration into superconducting MoGe plates observed by scanning SQUID microscope¹, HO THANH HUY, Osaka Prefecture University, MASAHICO HAYASHI, Akita University, TSUTOMU YOTSUYA, TAKEKAZU ISHIDA, Osaka Prefecture University — The amorphous superconducting film is very preferential as a good model in studying nanostructured superconductors because it has weakened pinning centers compared to other superconductors. The MoGe films have been deposited by a DC sputtering apparatus using a Mo₈₀Ge₂₀ target and a number of small MoGe plates were fabricated with the aid of photolithography. The vortex distribution in a MoGe circle has been investigated by means of a scanning SQUID microscope. We found that vortices form different configurations including shell structures, which evolves with the increase in applied magnetic field. Observed results are compared to theoretical studies for vortices in mesoscopic circles.

¹This work was partly supported by a Grant-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology of Japan (Grant Nos. 19206104, 23246173, 23226019).

4:54PM L21.00013 Image processing of scanning SQUID microscope for observing superconducting nanostructures, MASAHICO HAYASHI, Akita University, HO THANH HUY, TAKEKAZU ISHIDA, Osaka Prefecture University — A newly developed image processing technique for the scanning superconducting quantum interference device (SQUID) microscope is presented and its application to several measurements on superconducting nanostructures, including networks and dots, is discussed. This method is based on the detailed analysis of the structures characteristic to the measurement apparatus, such as the shape and position of the pickup coil. We take account of the Meissner effect in the coil body and its influences on the obtained image are carefully removed. The separation between the coil and the sample is also considered. Actually applying this method, we present images of the superconducting networks and dots, which show clear improvement from the raw images. The results are also discussed from physical point of view.

5:06PM L21.00014 Fluctuating pancake vortices revealed by dissipation of Josephson vortex lattice¹, ITSUHIRO KAKEYA, Kyoto University, Japan, ALEXEI KOSHELEV, Materials Science Division, Argonne National Laboratory, IL, ALEXANDER BUZDIN, Institut Universite de France and Universite de Bordeaux, France, TAKASHI YAMAMOTO, KAZUO KADOWAKI, University of Tsukuba, Japan — In strongly anisotropic layered superconductors in tilted magnetic fields the Josephson vortex lattice coexists with the lattice of pancake vortices. Due to the interaction between them, the dissipation of the Josephson-vortex lattice occurs to be very sensitive to the presence of the pancake vortices. If the c-axis magnetic field is smaller than the corresponding lower critical field the pancake stacks are not formed but the individual pancakes may exist in the fluctuational regime either near surface in large-size samples or in the central region for small-size mesas. We calculate the contribution of such fluctuating pancake vortices to the c-axis conductivity of the Josephson vortex lattice and compare the theoretical result with measurements on small mesas fabricated out of Bi₂Sr₂CaCu₂O_{8+δ} crystals. A fingerprint of fluctuating pancakes is characteristic exponential dependence of the c-axis conductivity observed experimentally. Our results provide strong evidence of the existence of the fluctuating pancakes and their influence on the Josephson-vortex-lattice dissipation.

¹I.K. was supported by Sumitomo Foundation and Kakenhi (Grant-in-Aid) No. 23681030. A.E.K. was supported by UChicago Argonne, LLC, operator of Argonne National Laboratory, a U.S. DOE laboratory, operated under contract No. DE-AC02-06CH11357.

Tuesday, February 28, 2012 2:30PM - 5:30PM —

Session L22 DMP DCOMP: Focus Session: Fe-based Superconductors: – Inelastic Neutron Scattering and Magnetic Excitations 254B

2:30PM L22.00001 Interstitial Iron Effects on Magnetic Excitations in Parent Phases Fe_{1+x}Te from Polarized and Inelastic Neutron Scattering, EFRAIN RODRIGUEZ, NIST Center for Neutron Research — One of the simplest systems of the iron-based superconducting family, Fe_{1+x}Ch (where Ch = S, Se, or Te) presents ample opportunity to study the relationship between antiferromagnetism and superconductivity. Several studies have demonstrated how the makeup of the Ch anions changes the electronic properties drastically, but the effect of excess interstitial iron, the x in Fe_{1+x}Ch, is not as well understood. Our previous diffraction experiments on samples varying x from 4 % to 16 % demonstrated how the magnetic ordering changes from collinear antiferromagnetic to helical incommensurate via a spin-density wave state at the special composition of x ≈ 12%. We present inelastic neutron scattering measurements of the phases Fe_{1+x}Te for two amounts of interstitial iron in the lattice, 5% and 14 %. We have combined data from cold neutron triple-axis, thermal neutron triple-axis, and spallation source time-of-flight to provide a full picture of the magnetic excitations in Fe_{1+x}Te for x = 14% from 0.5 meV to 150 meV. In addition, we present polarized inelastic studies on this particular composition to investigate the nature of the spin waves, *i.e.* longitudinal *vs.* transverse. The results are compared with those found in the phase with low amounts of interstitial iron (≈ 5 %), in order to understand the nature of the exchange interactions in this important parent compound.

3:06PM L22.00002 Temperature-enhanced nearly critical magnetic scattering in nearly superconducting $\text{FeTe}_{0.87}\text{S}_{0.13}$ ¹, IGOR ZALIZNYAK, CEDOMIR PETROVIC, RONGWEI HU, Brookhaven National Laboratory, ANDREI SAVICI, KAROL MARTY, MARK LUMSDEN, Oak Ridge National Laboratory — Recent neutron scattering measurements [1] have revealed an unusual temperature-induced enhancement of dynamical magnetism in iron telluride, FeTe , the parent material of the chalcogenide family of iron-based superconductors. Here we report a study of magnetic excitations in the sulfur-doped $\text{FeTe}_{0.87}\text{S}_{0.13}$, where bulk measurements show presence of the filamentary superconductivity [2]. Our neutron measurements probe the bulk of the material, which is nearly critical (filamentary superconductivity emerges in a small volume fraction of the sample, which is supercritical). We observe a peculiar pattern of low-energy magnetic scattering, characteristic of critical magnetic fluctuations, and find that it is also anomalously enhanced with the increasing temperature up to ~ 100 K.

[1] I. A. Zaliznyak, *et. al.*, Z. J. Xu, J. M. Tranquada, G. D. Gu, A. M. Tsvelik, M. B. Stone, Phys. Rev. Lett., in press (2011).

[2] Rongwei Hu, E. S. Bozin, J. B. Warren, C. Petrovic, Phys. Rev. B **80**, 214514 (2009).

¹We acknowledge useful discussions with J. Tranquada. This work was supported by the US DOE under Contract DE-AC02-98CH10886.

3:18PM L22.00003 Friedel-like Oscillations from Interstitial Iron in Superconducting $\text{Fe}_{1+y}\text{Te}_{0.62}\text{Se}_{0.38}$ ¹, VIVEK THAMPY, Johns Hopkins University, J. KANG, Institute for Quantum Matter, Johns Hopkins University, J.A. RODRIGUEZ-RIVERA, NIST Center for Neutron Research, W. BAO, Department of Physics, Renmin University of China, A.T. SAVICI, NSSD, Oak Ridge National Laboratory, J. HU, T. J. LIU, B. QIAN, D. FOBES, Z.Q. MAO, Department of Physics, Tulane University, C.B. FU, Department of Physics, Indiana University, W.C. CHEN, Department of Materials Science and Engineering, University of Maryland, Q. YE, NSSD, Oak Ridge National Laboratory, R.W. ERWIN, NIST Center for Neutron Research, T.R. GENTILE, National Institute of Standards and Technology, Z. TESANOVIC, C. BROHOLM, Institute for Quantum Matter, Johns Hopkins University — Using polarized and unpolarized neutron scattering we show that interstitial Fe in superconducting $\text{Fe}_{1+y}\text{Te}_{1-x}\text{Se}_x$ induces a magnetic Friedel-like oscillation that diffracts at $\mathbf{Q}_{\perp} = (\frac{1}{2}, 0)$ and involves >50 neighboring Fe sites. The interstitial $> 2 \mu_B$ moment is surrounded by compensating ferromagnetic four spin clusters that may seed double stripe ordering in Fe_{1+y}Te . A semi-metallic 5-band model with $(\frac{1}{2}, \frac{1}{2})$ Fermi surface nesting and four fold symmetric super-exchange between interstitial Fe and two in-plane nearest neighbors largely accounts for the observed diffraction.

¹Work at IQM was supported by DoE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-08ER46544

3:30PM L22.00004 Copper-tuned magnetic order and excitations in iron-based superconductors $\text{Fe}_{1+y}\text{Te}_{1-x}\text{Se}_x$ ¹, JINSHENG WEN, University of California at Berkeley, ZHIJUN XU, GUANGYONG XU, Brookhaven Natl Lab, MARK LUMSDEN, MASAAKI MATSUDA, Oak Ridge Natl Lab, PATRICK VALDIVIA, UC Berkeley, EDITH BOURRET, Lawrence Berkeley Lab, DUNGHAI LEE, UC Berkeley, GENDA GU, JOHN TRANQUADA, Brookhaven Natl Lab, ROBERT BIRGENEAU, UC Berkeley — We report neutron scattering results on the Cu-substitution effects in the iron-based superconductors, $\text{Fe}_{1+y}\text{Te}_{1-x}\text{Se}_x$. In the parent compound, it is found that Cu drives the low-temperature magnetic ground state from long-range commensurate antiferromagnetic order in $\text{Fe}_{1.06}\text{TeCu}_{0.04}$ to short-range incommensurate order in $\text{FeTeCu}_{0.1}$. In the former sample, the structural and magnetic ordering temperature is 40 K; in $\text{FeTeCu}_{0.1}$, the structural phase transition is not obvious and a transition to the spin-glass state is found at 22 K. Cu suppresses superconductivity in $\text{FeTe}_{0.5}\text{Se}_{0.5}$ — T_c is reduced to 7 K with a 2% Cu doping, and no superconductivity is found in the 10% Cu-doped sample. In the meantime, the intensity and energy of the resonance mode are suppressed in the 2% Cu-doped sample, while there is no resonance in the non-superconducting sample. Besides, the low-temperature magnetic excitation spectra are distinct for these two samples, with the superconducting one having an “hour-glass” shape and the other one having a “waterfall” shape. Our results provide further insights on the interplay between magnetism and superconductivity in the iron-based superconductors.

¹The work is supported by the U.S. Department of Energy.

3:42PM L22.00005 Neutron Scattering Study of Magnetic Excitation Spectrum on $\text{Fe}_{1-x}(\text{Ni/Cu})_x\text{Te}_{0.5}\text{Se}_{0.5}$, ZHIJUN XU, JINSHENG WEN, GUANGYONG XU, GENDA GU, JOHN TRANQUADA, Brookhaven National Laboratory — We have performed a series of neutron scattering and magnetization measurements on $\text{Fe}_{1-x}(\text{Ni/Cu})_x\text{Te}_{0.5}\text{Se}_{0.5}$ with different Ni/Cu compositions to study the interplay between magnetism and superconductivity. Substituting 2% and 4% of Ni for Fe reduces T_c from 15 K to 12 K and 8 K, while 10% of Cu results in loss of superconductivity. Spin resonance with lower energy are found in all superconducting samples. The overall shape of the low energy magnetic dispersion changes from two incommensurate vertical columns at $T \gg T_c$ to a distinctly different U-shaped dispersion at low temperature in superconducting samples. This spectral reconstruction is apparent for temperature up to $3T_c$. On the other hand, no static order around $(0.5, 0, 0.5)$ was found in any of these samples.

3:54PM L22.00006 Magnetic excitations in $\text{Fe}_{1.01}\text{Te}_{0.7}\text{Se}_{0.3}$, JOOSEOP LEE, University of Virginia, IGOR ZALIZNYAK, Brookhaven National Laboratory, NAOYUKI KATAYAMA, Nagoya University, RYOICHI KAJIMOTO, Japan Proton Accelerator Research Complex, SEUNGHUN LEE, University of Virginia — Recently, there have been intense studies on the magnetism in $\text{FeTe}_{1-x}\text{Se}_x$, which resulted in contradicting observations making the nature of its magnetism controversial. While the Fermi surface nesting picture can well predict the position of magnetic resonance in superconducting region, it clearly fails to predict the magnetic ordering wave vector in the parent compound. To investigate the magnetism in this iron chalcogenide series, we synthesized $\text{Fe}_{1.01}\text{Te}_{0.7}\text{Se}_{0.3}$. At this doping, it resides very close to the superconducting doping region, but is in spin glass phase. By using the Time-of-Flight neutron scattering, we obtained magnetic dispersions in this material at energies up to 257 meV. We find characteristic lines of diffuse scattering in Q-space, which provide the evidence for highly frustrated interactions. These lines of degeneracy persist up to about 10 meV, and start to disperse above it. Based on the shape of this quasi-degenerate manifold in Q-space, we propose a description of spin excitations using the J1-J2-J3 Heisenberg model on square lattice model near the limit of maximum frustration with weak extrinsic perturbation.

4:06PM L22.00007 Temperature Dependence of Magnetic Correlations in Fe-based Parents, LELAND HARRIGER, University of Tennessee at Knoxville, HUIQIAN LUO, Beijing National Laboratory for Condensed Matter Physics, MENGSHU LIU, University of Tennessee at Knoxville, CHRISTOPHER FROST, ISIS Facility, Rutherford Appleton Laboratory, PENGCHENG DAI, University of Tennessee at Knoxville — Key results from time of flight (TOF) neutron scattering measurements of BaFe_2As_2 and Fe_2Te_2 will be reviewed. These measurements were carried out over temperatures directly above and below T_N as well as base temperature measurements deep inside the order state and intermediate temperatures between T_N and room temperature where loosely correlated spin fluctuations persist. The large (TOF) data sets provide enough coverage of $(\mathbf{Q}, \omega)$ space to integrate out the correlated fluctuating moment, dispersion softening, and correlation length of the excitations as a function of temperature. Taken together, these results provide a systematic accounting of how the magnetic excitations in these parents evolve as they transition from long range ordered magnets to paramagnets.

4:18PM L22.00008 Effect of the in-plane magnetic field on the neutron spin resonance in optimally doped FeSe_{0.4}Te_{0.6} and BaFe_{1.9}Ni_{0.1}As₂ superconductors¹, XINGYE LU, SHILIANG LI, MENG WANG, HUIQIAN LUO, Institute of Physics, Chinese Academy of Sciences, Beijing, 100190, China, PENGCHENG DAI², Department of Physics and Astronomy, The University of Tennessee, Knoxville, Tennessee 37996-1200, USA, PANDA, FRM II COLLABORATION³, IN22, ILL COLLABORATION⁴, NIST COLLABORATION⁵ — We use inelastic neutron scattering to study the effect of an in-plane magnetic field on the magnetic resonance in optimally doped superconductors FeSe_{0.4}Te_{0.6} (T_c = 14 K) and BaFe_{1.9}Ni_{0.1}As₂ (T_c = 20 K). While the magnetic field up to 14.5 T does not change the energy of the resonance, it partially suppresses T_c and the corresponding superconductivity-induced intensity gain of the mode. However, we find no direct evidence for the field-induced spin-1 Zeeman splitting of the resonance. Therefore it is still unclear if the resonance is the long-sought singlet-triplet excitation directly coupled to the superconducting electron Cooper pairs.

¹This work was supported by CAS, 973 program and US DOE, BES.

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⁵Deepak Singh, NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA

4:30PM L22.00009 Itinerant Spin Excitations in SrFe₂As₂ Measured by Inelastic Neutron Scattering, RUSSELL EWINGS, TOBY PERRING, ISIS Pulsed Neutron and Muon Source, JACK GILLET, SITIKANTHA DAS, SUCHITRA SEBASTIAN, University of Cambridge, ALICE TAYLOR, University of Oxford, TATIANA GUIDI, ISIS Pulsed Neutron and Muon Source, ANDREW BOOTHROYD, University of Oxford — We have performed inelastic neutron scattering (INS) measurements of the magnetic excitations in SrFe₂As₂, an iron pnictide parent compound [1]. The data extend up to energies of ~ 260 meV. We find that the spectrum calculated from a local-moment J₁-J₂ model fails to describe our data in several key respects. In particular, the data can only be fitted by using different exchange parameters at high and low energies, for which there is no obvious physical justification. In both cases the nearest-neighbor exchange parameters, J_{1a} and J_{1b}, are very different. Also, on warming above the magnetic/structural ordering transition, one would expect J_{1a} → J_{1b} and hence a soft mode at **Q** = (0.5, 0.5), due to frustration in the local-moment model. However we find that the spectrum is largely unaltered. We find that the qualitative features of the INS spectra that cannot be described by the J₁-J₂ model are readily explained by calculations from a 5-band itinerant mean-field model. This also implies that it is not necessary to invoke additional broken symmetry, such as electronic nematic or orbital order, to explain the lack of a soft mode. [1] R. A. Ewings et al, Phys. Rev. B **83**, 214519 (2011)

4:42PM L22.00010 Magnetic resonance from the interplay of frustration and superconductivity, ILYA EREMIN, Institute for Theoretical Physics III, Ruhr-University Bochum, JOHANNES KNOLLE, Max Planck Institute for the Physics of Complex Systems, JOERG SCHMALIAN, Karlsruhe Institute of Technology, Institute for Theory of Condensed Matter, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems — Motivated by iron-based superconductors, we develop a self-consistent electronic theory for the itinerant spin excitations in the regime of coexistence of the antiferromagnetic stripe order with wave vector **Q**₁ = (π, 0) and s[±] superconductivity. The onset of superconductivity leads to the appearance of a magnetic resonance near the wave vector **Q**₂ = (0, π), where magnetic order is absent. This resonance is isotropic in spin space, unlike the excitations near **Q**₁, where the magnetic Goldstone mode resides. We discuss several features which can be observed experimentally.

4:54PM L22.00011 Spin excitations in isovalently doped Ba(Fe_{1-x}Ru_x)₂As₂¹, JUN ZHAO, UC Berkeley, Y. ZHAO, NIST NCR, K. MARTY, ORNL, C. ROTUNDU, LBNL, M. MATSUDA, ORNL, E. BOURRET-COURCHESNE, LBNL, H. YAO, J. WEN, P.N. VALDIVIA, T.R. FORREST, UC Berkeley, J.P. HU, Purdue University, DUNG-HAI LEE, R.J. BIRGENEAU, UC Berkeley — Iron based superconductors exhibit remarkably rich phase diagrams: superconductivity can be obtained through carrier doping, application of external pressure, or isovalent doping. Here we present the elastic and inelastic neutron scattering measurements on the magnetic correlations in isovalently doped Ba(Fe_{1-x}Ru_x)₂As₂. For the underdoped sample the static order moment are partially suppressed and the low energy spin correlation length increases upon entering the superconducting state. The spin excitation intensity is reduced with increasing Ru doping toward the over doped regime. We also studied the transfer of the magnetic spectral weight across T_c in this system.

¹J.Z. is supported by a fellowship from the Miller Institute for Basic Research in Science

5:06PM L22.00012 Polarized Neutron Scattering Study of Over-doped BaFe_{2-x}Ni_xAs₂, MENGSHU LIU, University of Tennessee, CHRIS LESTER, University of Bristol, JIRI KULDA, ILL, France, XINGYE LU, HUIQIAN LUO, Institute of Physics, Beijing, STEPHEN HAYDEN, University of Bristol, PENGCHENG DAI, University of Tennessee — Spin excitations in over-doped superconducting BaFe_{2-x}Ni_xAs₂ (x=0.15) were investigated using polarized neutron scattering. In a previous experiment on the optimally (x=0.1) doped sample, polarization analysis reveals that the magnetic response is highly anisotropic, at energies as high as 10 meV. Since this optimally doped sample is close to the boundary where antiferromagnetism disappears, there are still relatively strong antiferromagnetic correlations presented in the normal state. We will report our results on the over-doped sample, where the correlation is considerably weakened but still superconducting.

5:18PM L22.00013 Neutron scattering studies on LiFeAs and BaFe₂As₂, M. BRADEN, N. QURESHI, J. BRAND, P. STEFFENS, Univ. of Cologne, Germany, A. STUNAU, ILL, Grenoble, France, Y. SIDIS, D. LAMAGO, LLB, Saclay, France, L. HARNAGEA, S. WURMEHL, B. BÜCHNER, IFW, Dresden, Germany — The anisotropy of the magnetic excitations in BaFe₂As₂ was studied by polarization analysis. We find the in-plane polarized transverse magnon to lie at higher energy than the out-of-plane polarized one indicating very strong in-plane single-ion anisotropy. Superconducting LiFeAs exhibits the suppression of local susceptibility expected for spin-singlet pairing. Inelastic correlations appear in LiFeAs at the incommensurate wave vectors, they respond to the opening of the superconducting gap by a transfer of spectral weight.

Tuesday, February 28, 2012 2:30PM - 5:06PM —

Session L23 DMP DCOMP: Focus Session: Fe-based Superconductors - First Principles, Models, and Spectroscopy 255

2:30PM L23.00001 Fe Based Superconductors from first Principles, FRANK ESSENBERGER, PAWEŁ BUCZEK, ARTHUR ERNST, ANTONIO SANNA, LEONID SANDRATSKII, EBERHARD K.U. GROSS, Max-Planck-Institut für Mikrostrukturphysik — Density functional theory (DFT) for superconductors (SCs) is, in principle, exact and contains no adjustable parameters.¹ However, for real calculations an approximation to the pairing potential Δ_{xc} is needed. Many-body perturbation theory can be used to derive approximations to Δ_{xc} . The perturbation series is developed in orders of the screened Coulomb and phonon interactions and truncated at the first order. Unfortunately, this approach fails to predict superconductivity in unconventional SCs, like Fe based compounds.² Hence, an alternative pairing mechanism has to be present in these materials, the leading contender for which is spin fluctuations.³ We present a scheme to extend the current approximation Δ_{xc} to include spin fluctuations, which involves two steps: (1) the fluctuations are calculated with time dependent DFT,⁴ (2) an effective electron interaction mediated by the spin fluctuations is constructed.⁵ We present results for FeSe.

¹ *Phys. Rev. Lett.*, 1988, 60, 2430

² *Phys. Rev. Lett.*, 2008, 101, 026403

³ *Phys. Rev. Lett.*, 2008, 101, 057003

⁴ *Phys. Rev. Lett.*, 2009, 102, 247206

⁵ *Phys. Rev. B*, 1985, 32, 2156

2:42PM L23.00002 First-principles study on electronic structure of Ca-Fe-Pt-As-type iron-based superconductors, HIROKI NAKAMURA, MASHIKO MACHIDA, Japan Atomic Energy Agency — Since the discovery of the iron-based superconductor, LaFeAsO_{1-x}F_x whose T_c reached 26K, various types of iron-based superconductors have been fabricated to attain higher T_c. Recently, new Ca-Fe-Pt-As system of iron-based superconductors was discovered, and the highest T_c in this class becomes 38K. In this system, the crystal structure is different from those of well-known iron-based superconductors. In particular, the blocking layers of some materials in this system are expected to be metallic unlike the other types of iron-based superconductors. We perform first-principles calculations for Ca-Fe-Pt-As system and evaluate their electronic structure.

2:54PM L23.00003 First-principles study of cobalt pnictides: Example compound SrCo₂N₂, ANDREW O'HARA, ALEXANDER DEMKOV, The University of Texas at Austin — Although it has been known for several decades that many materials with chemical form AT₂X₂ (A = alkaline earth element or lanthanide, T = transition metal, X = an element of groups IIIB-VIB) crystallize with the same structure, it was only recently that interest was renewed in these materials with the discovery that BaFe₂As₂ can be made to superconductor at temperatures as high as 38 K. Although the precise mechanism of superconductivity has yet to be determined, there is a growing interest in the study of materials that have similar electronic properties to BaFe₂As₂. In our work, we employ density functional theory in the local density approximation in order to study the isochemically substituted variant, SrCo₂N₂. In this work, we determine both the stability of SrCo₂N₂ as well as how the substitution changes the electronic properties in comparison to BaFe₂As₂.

3:06PM L23.00004 Density functional study on d-orbital characters of the Fe magnetic moment in BaFe₂As₂, HYUNGJU OH, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — There have been many published papers related on the orbital characters of band structures in the iron-based superconductors. However, the orbital characters of the Fe magnetic moment still remain unrevealed. By performing first-principles calculations of the electronic and magnetic properties with constraint on the real space shape of Fe magnetic moments, we study the d-orbital characters of the Fe magnetic moment in BaFe₂As₂. We compare obtained band structures with published angle-resolved photoemission spectroscopy (ARPES) result, and propose that the Fe magnetic moment in BaFe₂As₂ has in-plane d_{xy} character. This work was supported by the NRF of Korea (Grant Nos. 2009-0081204 and 2011-0018306). Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2011-C3-05)

3:18PM L23.00005 Theoretical insight on layered Mn-compounds under pressure, MARIA PEZZOLI, Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY 11794, USA, ZHIPING YIN, Serin Physics Laboratory, Rutgers University, Piscataway, NJ 08854, USA., JACK SIMONSON, Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY 11794, USA, MEIGAN ARONSON, Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY 11794, USA and Brookhaven National Laboratory, Upton, NY, 11973, USA., GABRIEL KOTLIAR, Serin Physics Laboratory, Rutgers University, Piscataway, NJ 08854, USA. — Since the unexpected discovery of Fe-based superconductors, the search for new materials with a higher superconducting T_c has been reinvigorated. Mn based compounds in the ThCr₂Si₂ structure contain square lattice layers of the transition metal atom, like the cuprates and the iron arsenides, but the strong antiferromagnetic correlations typical of these compounds suggest that superconductivity in the manganites is impossible. However new experiments carried under pressure show that some of these layered Mn-compounds go through an electron delocalization transition. Here we study these compounds from a theoretical point of view. Looking at the magnetic properties and the Fermi surfaces close to the electron delocalization transition, we discuss the possibility of superconductivity for these compounds.

3:30PM L23.00006 Renormalization group study up to two-loop order of an effective two-band model for iron-based superconductors¹, HERMANN FREIRE, VANILDO DE CARVALHO, Federal University of Goias — We perform a renormalization group (RG) study up to two-loop order of an effective low-energy two-band model to describe some of the recently discovered iron-based superconductors. Our starting point is the itinerant electronic model proposed by Chubukov *et al.* [*Phys. Rev. B* **78**, 134512 (2008)], which displays two small, almost nested Fermi pockets with one hole pocket centered at (0,0) and one electron pocket centered at **Q** = (π, π) in the folded Brillouin zone. We then proceed to implement a two-loop RG calculation for this model of four-point vertex corrections, quasiparticle weight and several order-parameter susceptibilities in order to evaluate the robustness of one-loop RG results available in the literature with respect to including self-energy effects and higher-order quantum fluctuations.

¹ We acknowledge support from the Brazilian agency CNPq through grant No. 474109/2010-0 for this project.

3:42PM L23.00007 Microscopic derivation of GL theory for magnetism and superconductivity in multiband electronic systems¹, VLADIMIR CVETKOVIC, OSKAR VAJEK, National High Magnetic Field Laboratory, Florida State University — The superconductivity in pnictides arises due to interband scattering between Cooper pairs belonging to hole and particle Fermi surfaces. The amplitude of the scattering, while weak at bare level, is enhanced under RG flow, and competes with the SDW to become the leading instability when the hole and particle FS's are nearly, but not perfectly, nested. This motivates us to construct a GL theory with multiple order parameters from the microscopic action. It allows us to study the two competing orders and their interplay including a possible coexistence. The presence of both attractive and repulsive pairing terms requires a novel approach to the derivation with imaginary terms in the action as one consequence. The construction of the GL theory is a two-step process, with RG flow to an intermediate cut-off scale, determined by the deviations from the nesting, as the first step.

¹ This work was supported in part by the NSF CAREER Award under Grant no. DMR-0955561.

3:54PM L23.00008 Impurity Dimer Scattering as Reflection of Band Reconstruction in Iron Pnictides¹, JIAN KANG, ZLATKO TESANOVIC, Institute for Quantum Matter, Johns Hopkins University — While the impurity induced nanoscale electronic disorder has been extensively reported in the underdoped iron pnictides its microscopic origin remains a theoretical challenge. Recent STM measurements reveal a resonance in the impurity dimer scattering in cobalt-doped iron arsenides. These resonant dimers are randomly distributed but aligned with antiferromagnetic a-axis. We present a theoretical study of the impurity induced quasiparticle interference patterns in these materials, based on the five orbital model. The local density of states oscillates with the “imperfect nesting” wavevector encoded in the reconstructed Fermi pockets, provided one assumes the ordered pocket density wave (PDW) state along the b-axis. This anisotropic oscillation pattern breaks C_4 symmetry and is in agreement with the electronic dimer resonance found in the STM experiments, hinting at the existence of “hidden” PDW order in iron-based superconductors [1]. [1] J. Kang and Z. Tesanovic, Phys. Rev. B 83, 020505(R) (2011).

¹Research supported in part by the DOE under Grant No. DE-FG02-08ER46544.

4:06PM L23.00009 Jump in specific heat at the superconducting transition in iron pnictides¹, MAXIM G. VAVILOV, ANDREY V. CHUBUKOV, University of Wisconsin, ANTON B. VORONTSOV, Montana State University — Experiments reveal that in iron-based superconductors the jump ΔC of the specific heat at the superconducting transition is not proportional to the transition temperature T_c , as expected in the BCS theory. Rather, the ratio $\Delta C/T_c$ varies with T_c , and has a peak near optimal doping and decreases at smaller and larger dopings. We show that this behavior can be naturally explained by the interplay between superconductivity and antiferromagnetism in the underdoped regime. We demonstrate that $\Delta C/T_c$ is indeed peaked at the doping where the coexistence phase with antiferromagnetism develops, and decreases at deviations from this doping in both directions.

¹NSF-DMR 0955500, 0906953, 0954342

4:18PM L23.00010 Beyond anharmonicity: signature of spin-phonon coupling at the surface of BaFe₂As₂¹, CHEN CHEN, JING TENG, YIMIN XIONG, JIANDI ZHANG, RONGYING JIN, E.W. PLUMMER, Louisiana State University — High Resolution Electron Energy Loss Spectroscopy (HREELS) has been used to investigate the temperature dependence of the lattice dynamics of cleaved single crystals of BaFe₂As₂, one of the parent compounds of Fe-based superconductors. Both the phonon frequency as well as phonon linewidth of the intense 32 meV out-of-plane Fe/As mode (A_{2u}) and the 24 meV out-of-plane As vibration mode (A_{1g}) show a dramatic temperature dependence and anomalous behavior below ~ 150 K. The anomalous behavior is associated with the coupled elasto-magnetic transition in the bulk but occurs appreciably higher at the surface than in the bulk (~ 138 K). The anharmonicity at the surface is considerably larger than that in the bulk for the orthorhombic phase, but is significantly less in the tetragonal phase. A detailed discussion is given in terms of the interplay between the spin and lattice in this novel system.

¹Supported by NSF DMR-1002622

4:30PM L23.00011 Low magnetic field microwave absorption and ESR studies of coexisting superconductivity and ferromagnetism in Eu-based pnictides¹, AUSTIN HOWARD, Nanotech Institute, University of Texas at Dallas, TIAN SHANG, JIAOWEN HE, GUANGHAN CAO, HUIQUI YUAN, Zhejiang University, MYRON SALAMON, ANVAR ZAKHIDOV, Nanotech Institute, University of Texas at Dallas — We have studied the coexistence of FM ordering and SC in the doped pnictide EuFe₂(As_{1-x}P_x)₂ system, with doping levels of $x = 0.3$ and 0.27 , by combined ESR and non-resonant low field microwave absorption (LFMA) methods, and magnetization in SQUID. LFMA uses an external magnetic field to create vortices in the material, which are non-resonantly excited by MW radiation. The resulting spectrum's hysteresis shape and form changes with T , revealing transitions around 9 and 20 K, and showing the FM onset and SC T_c . Two types of coexisting LFMA signals have been observed: a) a superconducting hysteretic LFMA loop, appearing below T_c and changing its shape, phase and intensity with T , and b) the non-hysteretic, reversed phase LFMA, above SC T_c , which is assigned to the magnetically ordered ferromagnetic phase, since it does not depend on T . Additionally, in the $x = 0.27$ sample, a reemergence of hysteresis is seen near 18K, corresponding with the reentrant superconductivity observed in transport measurements. LFMA has also been used to determine the position of the irreversibility line and to estimate the critical current density for the two samples.

¹AFOSR grant FA 9550-09-10384

4:42PM L23.00012 ab Plane Point Contact Spectroscopy of Co-doped Iron Pnictide Superconductors, JOHN TIMMERWILKE, J.S. KIM, G.R. STEWART, AMLAN BISWAS, Dept. of Physics, University of Florida — Point contact measurements on iron-based superconductors provide valuable information about these new superconductors, including gap sizes, number of gaps, and gap symmetries. We use a point contact apparatus capable of taking measurements in the abplane using a tungsten wire lowered mechanically onto a superconducting sample. Using this method allows us to measure the variation of superconducting gap(s) with Z, a dimensionless barrier strength parameter. Previous point contact measurements have shown Co-doped iron pnictide superconductors to be a two gapped material. Our measurements confirm the presence of two gaps in single crystal Ba(Fe_{0.926}Co_{0.074})₂As₂ and the Z variation of the measurements imply the gaps are isotropic. Acknowledgments: NSF DMR-0804452, DOE contract # DE-FG02-86ER45268

4:54PM L23.00013 Highly anisotropic Dirac fermions in a Bi square net of SrMnBi₂, JUN SUNG KIM, JOONBUM PARK, Department of Physics, Pohang University of Science and Technology, GEUNSIK LEE, Department of Chemistry, Pohang University of Science and Technology, FREDERIK WOLFF-FABRIS, Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, YOON YOUNG KOH, Institute of Physics and Applied Physics, Yonsei University, MAN JIN EOM, Department of Physics, Pohang University of Science and Technology, YEONGKWAN KIM, Institute of Physics and Applied Physics, Yonsei University, M.A. FARHAN, Department of Chemistry, Pohang University of Science and Technology, YOUNJUNG JO, Department of Physics, Kyungpook National University, CHANGYOUNG KIM, Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Korea, JI HOON SHIM, Department of Chemistry, Pohang University of Science and Technology, Pohang 790-784, Korea — We report the highly anisotropic Dirac fermions in a Bi square net of SrMnBi₂, based on a first principle calculation, angle resolved photoemission spectroscopy, and quantum oscillations for high-quality single crystals. We found that the Dirac dispersion is generally induced in the (SrBi)⁺ layer containing a double-sized Bi square net. In contrast to the commonly observed isotropic Dirac cone, the Dirac cone in SrMnBi₂ is highly anisotropic with a large momentum-dependent disparity of Fermi velocities of ~ 8 . These findings demonstrate that a Bi square net, a common building block of various layered pnictides, provide a new platform that hosts highly anisotropic Dirac fermions.

Tuesday, February 28, 2012 2:30PM - 5:30PM –

Session L24 DMP: Focus Session: Dopants and Defects in Semiconductors - Chalcogenides, Oxides, and Ternaries 256

2:30PM L24.00001 AX centers in II-VI semiconductors: Hybrid functional calculations¹, KOUSHIK BISWAS, MAO-HUA DU, Materials Science and Technology Division, Center for Radiation Detection Materials and Systems, Oak Ridge National Laboratory — Group-V acceptors should be efficient hole producers in II-VI compounds as in ZnTe. However, good *p*-type conductivity remains elusive, for example in ZnO and ZnS. With regard to this low doping efficiency, we will discuss the dopant self-compensation in II-VI semiconductors through the formation of the AX center. These are acceptor-induced defect that acts as a donor to compensate the acceptor itself. We show that the artificially high valence band maximum in Local density approximation and Generalized gradient approximation calculations can lead to incorrect prediction on the stability of the AX center in these semiconductors. The hybrid functional calculations that correct the band gap, significantly stabilize the AX centers for selected group-V acceptor dopants in ZnO, ZnS, and ZnSe. The results on AX centers obtained by hybrid functional calculations agree well with the experimentally observed doping phenomena in ZnS and ZnSe.[1] [1] Koushik Biswas and Mao-Hua Du, Applied Physics Letters 98, 181913 (2011).

¹This work was supported by the U.S. DOE Office of Nonproliferation Research and Development NA22.

2:42PM L24.00002 Magnetic Main Group Impurities in CdS, PEDRO BEDOLLA-VELAZQUEZ, CHRISTOPH GRUBER, PETER MOHN, Vienna University of Technology — With the development of magnetic semiconductors, the role of the magnetism of impurities came again into the focus of research. For *d*- and *f*-electron impurities, the situation seems to be rather clear. A new field appears when one starts to study magnetism produced by vacancies or by atoms, which usually do not carry any magnetic moments in a bulk solid. Starting from the magnetism of carbon vacancies in graphene we will present a study of CdS where S is replaced by main group elements. On the basis of abinitio supercell calculations employing density functional theory (DFT) we investigate the behaviour of impurities (B, N, C, O, F, Al, Si, P, Ga, Ge) in wurtzite (w) and zincblende (zb) CdS lattices. It is found that the impurities prefer the sulfur position and most of them, depending on the concentration exhibit magnetic order. We find that for small concentrations (64zb/72w and 32zb atom supercells) a half metallic ferromagnetic behaviour is found. For a 16 atom supercell for both zb and wstructure partly also unsaturated magnetic moments occur. A field dependence of the magnetic moments in these materials may lead to new technological applications in these magnetic semiconductors as tunable spin injection materials.

2:54PM L24.00003 Mechanisms and Kinetics of Tellurium Precipitation in CdTe-based Materials, VINCENZO LORDI, Lawrence Livermore National Lab — CdTe and related alloys are important materials for solar photovoltaic application as well as for high-resolution room-temperature gamma radiation detectors. However, the performance of devices, particularly in high-energy applications, is limited by various material defects. Among the most important defects are Te precipitates of various sizes caused by non-stoichiometric growth conditions. In this work, we study the kinetics of Te aggregation and precipitation at the atomic scale. Density functional theory is used to compute the energetics, migration rates, and binding energies of point defects involved in Te aggregation, which include various interstitials, vacancies, and anti-site defects. Kinetic Monte Carlo is then used to simulate the aggregation process leading to precipitation nuclei. The mechanisms and kinetics of formation of these Te-rich regions are analyzed for various conditions. Prepared by LLNL under Contract DE-AC52-07NA27344.

3:06PM L24.00004 Luminescence-Based Characterization of Copper Vacancies in Optical Float Zone Refined Cuprous Oxide, N. LASZLO FRAZER, KELVIN CHANG, KENNETH POEPELMEIER, JOHN KETTERSON, Northwestern University — Cuprous oxide (Cu₂O) is ideal for studying Wannier-Mott excitons which have anomalously long lifetimes in this material. However copper vacancies have a deleterious effect on the exciton lifetimes. We have measured the associated luminescence spectra in optically excited single crystals. These crystals were prepared in a radiantly-heated float-zone refiner from thermally oxidized copper rod of purity 0.999. The behavior of the vacancy luminescence can be related to exciton propagation.

3:18PM L24.00005 Ab initio calculations of intrinsic defects in ZnSb, LASSE BJERG, Aarhus University & Massachusetts Institute of Technology, GEORG K.H. MADSEN, Ruhr-Universität Bochum, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology, BO B. IVERSEN, Aarhus University — Thermoelectric materials are capable of interconverting heat and electricity. The most efficient thermoelectric materials are heavily doped semiconductors, and hence they can be either *n*- or *p*-type. ZnSb has recently been predicted by theoretical calculations to be a good *n*-type thermoelectric material. However, synthesis produces *p*-type materials. Intrinsic point defects have been investigated as a possible origin using ab initio calculations. Negatively charged Zn vacancies are found to have a low formation energy, and an intrinsic *p*-type behavior is predicted.

3:30PM L24.00006 First-principles study of defect properties of zinc blende MgTe, JI-HUI YANG, Key Laboratory for Computational Physical Sciences (MOST) and Surface Physics Laboratory, Fudan University, SHIYOU CHEN, HONGJUN XIANG, XINGAO GONG, Key Laboratory for Computational Physical Sciences (MOST) and Surface Physics Laboratory, Fudan University, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, Colorado 80401, USA — We studied the general chemical trends of defect formation in MgTe using first-principles band structure methods. The formation energies and transition energy levels of intrinsic defects and extrinsic impurities and some defect complexes in zinc blende MgTe were calculated systematically using a new hybrid scheme. The limiting factors for *p*- and *n*-type doping in MgTe were investigated. Possible solutions to overcome the doping limitation of MgTe are proposed. The best *p*-type dopant is suggested to be N with nonequilibrium growth process and the best *n*-type dopant is suggested to be I with its doping complex $V_{Mg} + 4I_{Te}$.

3:42PM L24.00007 Charged excitons and biexcitons bound to isoelectronic centers, GABRIEL ETHIER-MAJCHER, STEPHANE MARCET, CLAUDERIC OUELLET-PLAMONDON, PHILIPPE ST-JEAN, Ecole Polytechnique de Montreal, REGIS ANDRE, Institut Neel, CEA/CNRS/Universite Joseph Fourier, Grenoble, France, JOHN F. KLEM, Sandia National Laboratory, Albuquerque, New Mexico, SEBASTIEN FRANCOEUR, Ecole Polytechnique de Montreal — We demonstrate that isoelectronic centers formed from two isoelectronic traps can bind, in addition to the well-studied excitons, various number of positive and negative charges. Two different systems are studied by microphotoluminescence: 1) tellurium dyads in ZnSe forming hole traps and 2) nitrogen dyads in GaAs forming electron traps. By analyzing their emission fine structure, polarization and diamagnetic shifts, we establish that Te and N dyads can bind, respectively, positively and negatively charged excitons. Using the power dependence of the emission intensity, we clearly demonstrate that both systems can also bind biexcitons. This ability to bind various charge configurations, in addition to their very low inhomogeneous broadenings and perfectly defined symmetries, further establishes isoelectronic centers as an interesting alternative to epitaxial quantum dots for a number of applications.

3:54PM L24.00008 New perspective on formation energies and energy levels of point defects in non-metals, HONG ZHU, University of Connecticut, PATRICK RINKE, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, RAMPI RAMPRASAD, University of Connecticut — We propose a powerful scheme to accurately determine the formation energy and thermodynamic charge transition levels of point defects in non-metals. Previously unknown correlations between defect properties and the valence-band width of the defect-free host material are identified allowing for a determination of the former via an accurate knowledge of the latter. These correlations are identified through a series of hybrid density functional theory computations and an unbiased exploration of the parameter space that defines the Hyde-Scuseria-Ernzerhof family of hybrid-functionals. The applicability of this paradigm is demonstrated for point defects in several insulators, including Si, Ge, ZrO₂ and ZnO

4:06PM L24.00009 Hydrogen-related defects in SnO_2 ¹, W. BEALL FOWLER, FIGEN BEKISLI, MICHAEL STAVOLA, Lehigh University — Symmetry arguments along with a mass-and spring analysis of infrared absorption experiments made with polarized light on OH defects in SnO_2 yield significant insights into the possible structures of one- and two-OH defects that have been observed recently [1]. Namely, a two-OH defect must involve symmetry-equivalent OH sites, and the axes of both one- and two-OH defects are only slightly displaced from the perpendicular to the c-axis of the rutile structure. Such results cannot be explained by models involving one or two H trapped at a Sn vacancy. Rather, they are consistent with OH defects associated with either a metal atom substituting for Sn, or an interstitial metal atom (such as Sn). Results of detailed quantum-mechanical calculations [2] using CRYSTAL06 are consistent with OH structures involving a Sn interstitial.

[1] Figen Bekisli *et al.*, Phys. Rev. B **84**, 035213 (2011).

[2] R. Dovesi *et al.*, **Crystal06 User's Manual**, Univ. of Torino, Torino, 2006.

¹Supported in part by NSF grant DMR 0802278.

4:18PM L24.00010 Polarization effect in the Ionic conductor TlBr ¹, CEDRIC ROCHA LEO, VINCENZO LORDI, Lawrence Livermore National Laboratory — TlBr is an ionic crystal that in recent years has been standing out as one of the most promising materials for effective room temperature radiation detection. However, its exceptional performance invariably degrades after operation times that vary from hours to several weeks. This phenomenon, known as polarization, is assigned to the undesirable ionic current that sets in the crystal under an applied bias, leading to the accumulation of oppositely charged Tl^+ and Br^- ions at the electric contacts of the device. This charge build up induces a field that opposes the applied bias, impairing the collection of the photo-induced carriers. In this presentation, we use parameter free quantum mechanical simulations to discuss the possible origins of the polarization effect in TlBr , showing that ionic mobility in the intrinsic material is not enough to account for effects reported by several groups. We then discuss other possible causes for the degradation of biased TlBr and propose ways to prevent its occurrence, via careful co-doping as well as a judicious choice of the metal contacts to be employed.

¹Prepared by LLNL under Contract DE-AC52-07NA27344.

4:30PM L24.00011 Structural diversity and electronic properties of Cu_2SnX_3 (X=S, Se): A first-principles investigation, YINGTENG ZHAI, Key Laboratory for Computational Physical Sciences (MOE) and Surface Physics, Fudan University, Shanghai 200433, China, SHIYOU CHEN, Key Laboratory of Polar Materials and Devices (MOE), East China Normal University, Shanghai 200241, China, JIHUI YANG, HONGJUN XIANG, XINGAO GONG, Key Laboratory for Computational Physical Sciences (MOE) and Surface Physics, Fudan University, Shanghai 200433, China, ARON WALSH, Centre for Sustainable Chemical Technologies and Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom, JOONGOO KANG, SUHUAI WEI, National Renewable Energy Laboratory, Golden, Colorado 80401, USA — The ternary semiconductors Cu_2SnX_3 (X=S, Se) are found frequently as secondary phases in synthesized $\text{Cu}_2\text{ZnSnS}_4$ and $\text{Cu}_2\text{ZnSnSe}_4$ samples, but previous reports on their crystal structures and electronic band gaps are conflicting. Here we report their properties as calculated using a first-principles approach. We find that: (i) the diverse range of crystal structures can all be derived from the zinc-blende structure. (ii) The energy stability of different structures is determined primarily by the local cation coordination around anions, which makes Cu and Sn partially disordered in the cation sublattice. (iii) The direct band gaps of the low energy compounds Cu_2SnS_3 and Cu_2SnSe_3 should be in the range of 0.8-0.9 eV and 0.4 eV respectively.

4:42PM L24.00012 Fe_2MCh_4 (M=Si,Ge, Ch=S,Se): optical, electrical properties and defects, ROBERT KOKENYESI¹, Department of Chemistry, Oregon State University, Corvallis, OR, LIPING YU, STEPHAN LANY, National Renewable Energy Lab, Golden, CO, ALEX ZUNGER, University of Colorado at Boulder, Boulder, CO, DOUGLAS KESZLER, Department of Chemistry, Oregon State University, Corvallis, OR, CENTER FOR INVERSE DESIGN, EFRC COLLABORATION — Fe_2MCh_4 (M=Si,Ge, Ch=S,Se) are proposed as solar absorber materials, as a single phase, stable alternative to FeS_2 pyrite. Native defects have high formation energy in the band gap and no Fermi level pinning is predicted by DFT. External defect calculations, including B,Al,Ga,In, N, P, As, Sb, Bi, O, Se, predict substantial effect on the bulk electronic properties.

¹formerly Robert Kykyneshi

4:54PM L24.00013 Structure, stability, and defect analysis of potential solar absorber Cu_3PSe_4 , DAVID H. FOSTER, JASON M. VIELMA, GUENTER SCHNEIDER, Oregon State University — The semiconductor Cu_3PSe_4 has recently been established to have a direct band gap of 1.4 eV and exhibit p-type conductivity [Applied Physics Letters, 99, 181903 (2011)]. Here we present density functional theory (DFT) and post-DFT results regarding the structure, stability, and dopability of Cu_3PSe_4 . We find a strong coupling between the electronic band gap and the atomic structure, clearly caused by the strong P-Se antibonding character of the conduction band. Using the Heyd-Scuseria-Enzerhof hybrid functional and *GW* approximation methods, we find that structural relaxation using standard DFT is not sufficiently accurate to be used as input to static, post-DFT electronic structure calculations. We use the generalized gradient approximation (GGA) and the GGA+*U* method to show a thermodynamically stable low temperature region. We calculate the formation enthalpies of intrinsic and extrinsic defects in order to understand the observed p-type behavior and to examine n-type doping mechanisms.

5:06PM L24.00014 Effect of Cation Disorder on Electronic Structures and Optical Properties of Magnetoelectric Gallium Ferrite: A First-principles Study, AMRITENDU ROY, IIT Kanpur, SUSHIL AULUCK, NPL Delhi, RAJENDRA PRASAD, ASHISH GARG, IIT Kanpur — Discovery of photovoltaic effects in oxide materials, especially in magnetoelectrics and multiferroics has lead to renewed interests in the optical properties of these materials. Magnetoelectrics with their transition temperature close to room temperature are of particular interest from the perspective of practical applications. Magnetoelectric gallium ferrite (GFO), a material of current interest, exhibits good optical activity and a transition temperature tunable to room temperature and above upon tailoring of cation stoichiometry. Here, we show a detailed first principle study on the electronic structure and optical properties of GFO. We have performed first-principles density functional calculations using GGA+*U* method to compute the electronic band structure and density of states of the ground state structure of GFO having orthorhombic $Pc2_1n$ symmetry and A-type antiferromagnetic spin configuration. The calculations show that GFO possesses a direct band gap of ~ 2.3 eV, making it a rather low band gap oxide. Subsequent calculations of real and imaginary parts of dielectric constants, refractive index (*n*), extinction coefficient (*k*), reflectivity (*R*), etc demonstrate good agreement with experimental spectra which is further improved upon introduction of cationic site disorder into the ground state structure substantiating the presence of cation site disorder in the material. We also show that major optical transitions in GFO involve transitions from valence band O 2p to conduction band Fe 3d states.

5:18PM L24.00015 Radiative defects in thallium chalcogenide semiconductors¹, J.A. PETERS, N.K. CHO, ZHIFU LIU, B.W. WESSELS, Dept. of Materials Science and Engineering, Northwestern University, S. JOHNSEN, S. NGUYEN, M. SEBASTIAN, M.G. KANATZIDIS, Dept. of Chemistry, Northwestern University, Evanston, IL 60208 — Thallium chalcogenides constitute a promising new class of semiconductor compounds for radiation detectors. Due to their wide energy bandgap, high atomic number, and high resistivity, they are being considered as potential replacement for conventional II-VI semiconductor x-ray and γ -ray detectors for room temperature operation. For these applications resistivities of $\sim 10^{10}$ ohm-cm are required. Although defects play a major role in detector response, little is known about their nature and origin in these compounds. We have investigated $\text{Ti}_6\text{I}_4\text{Se}$ and $\text{Ti}_6\text{I}_4\text{S}$ compounds which have bandgaps of 1.86 and 2.03 eV, respectively. Photoluminescence (PL) spectra of single crystals were investigated in the 650-885 nm wavelength region and over a temperature range of 20-100 K. For $\text{Ti}_6\text{I}_4\text{Se}$ we observed PL bands centered at 1.61 eV. A detailed study of the peak, as function of temperature and excitation intensity, indicates that it is due to radiative transitions from donor-acceptor pairs (DAP). The ionization energies of the donor and acceptor levels in $\text{Ti}_6\text{I}_4\text{Se}$ were estimated at 52 and 290 meV, respectively. Similarly DAP emission in $\text{Ti}_6\text{I}_4\text{S}$ with a peak at 1.66 eV was observed. The role of crystalline stoichiometry in DAP formation is currently under study.

¹This work is supported by the Dept. of Homeland Security under grant no. 2010-DN-077-ARI042-02.

Tuesday, February 28, 2012 2:30PM - 5:30PM –
Session L25 DCOMP GSCCM DMP: Focus Session: Simulation of Matter at Extreme Conditions - Warm Dense Matter 257A

2:30PM L25.00001 Simulation of the Correlated Electron Plasma in the Warm Dense Matter Regime by Restricted Path-Integral Molecular Dynamics¹, VIVEK KAPILA, University of Florida, PIERRE DEYMIER, University of Arizona, KEITH RUNGE, University of Florida — Warm dense matter (WDM) can be characterized by electron temperatures of a few eV and densities an order of magnitude or more beyond ambient. This regime currently lacks any adequate highly developed class of simulation methods. Recent developments in orbital-free Density Functional Theory (ofDFT) aim to provide such a simulation method, however, little benchmark information is available on temperature and pressure dependence of simple but realistic models in WDM regime. The present work aims to fill this critical gap using the restricted path-integral molecular dynamics (rPIMD) method. Within the discrete path integral representation, electrons are described as harmonic necklaces, while, quantum exchange takes the form of cross linking between electron necklaces. The fermion sign problem is addressed by restricting the density matrix to positive values and a molecular dynamics algorithm is employed to sample phase space. Here, we focus on the behavior of strongly correlated electron plasmas under WDM conditions. We compute the kinetic and potential energies and compare them to those obtained with the ofDFT method.

¹Work supported under US DoE Grant DE-SC0002139

2:42PM L25.00002 Comparison of Finite Temperature Hartree-Fock and Density Functional Theory for Confined Systems¹, TRAVIS SJOSTROM, S.B. TRICKEY, Quantum Theory Project, University of Florida, FRANK E. HARRIS, Quantum Theory Project, University of Florida and Physics Dept. University of Utah — Warm dense matter (WDM) at elevated temperatures (*e.g.*, $T \approx 1$ to several eV) and densities (*e.g.* one or more orders of magnitude denser than equilibrium) is of growing importance. So far, the most detailed studies of WDM use Born-Oppenheimer molecular dynamics with ground-state density functional theory (DFT) approximations. Little, however, is known about the behavior of the free energy over the temperature and density ranges of interest. In the case of DFT, this deficiency is a barrier to assessing the validity of proposed approximate free-energy functionals. For insight into this problem, we have undertaken systematic numerical study of the thermal Hartree-Fock (THF) approximation. We report progress on application of THF to the problem of eight one-electron atoms at arbitrary positions in a hard-walled box. We discuss the physics which emerges for both high- and low-symmetry ionic arrays, including molecular binding transitions. In addition, we compare the THF results directly with approximate DFT results, including approximate finite-temperature orbital-free kinetic and exchange functionals.

¹Supported in part under US DoE Grant DE-SC0002139.

2:54PM L25.00003 The Korrington-Kohn-Rostoker Method Applied to Warm Dense Matter¹, DANIEL FINKENSTADT, U.S. Naval Academy, Physics Dept., Annapolis, MD, CHARLES E. NEWNAM, U.S. Naval Academy, Aerospace Dept., Annapolis, MD, BRIAN G. WILSON, Lawrence Livermore National Laboratory, Livermore, CA — The electronic structure, EOS and transport properties of warm electrons in an amorphous or disordered configuration of ions is not well described by either solid-state or plasma models. Such warm, dense systems share the characteristic of the solid state that multi-center scattering effects are of paramount importance in forming bands of valence states. Theoretical treatment of the EOS of warm, dense matter therefore requires a way to include significant occupation of higher energy and angular momentum channel continuum states. We are extending the Green's function Kohn-Korrington-Rostoker code *MECCA* as an all-electron (non-pseudo potential) method that treats arbitrary mixtures of atoms on an ab-initio basis over a broad range of conditions, from cold, solid matter up to hot plasmas at extreme (ICF) compression. Specific examples of Aluminum and Boron-Nitride will be discussed.

¹Supported by the Military Academy Research Associates program, LLNL/USNA.

3:06PM L25.00004 Density Functional versus Thermal Hartree-Fock Approximations in Warm Dense Lithium¹, VALENTIN V. KARASIEV, TRAVIS SJOSTROM, S.B. TRICKEY, Quantum Theory Project, Physics Dept. U. Florida — We compare the behaviors of the thermal Hartree-Fock (tHF) model and thermal Density Functional Theory (tDFT) using both ground-state and temperature-dependent approximate functionals. The test system is bcc Li in the temperature-density regime of warm dense matter. In the exchange-only case, we find significant qualitative differences between the exact tHF and the DFT calculations with zero-temperature local density approximation (LDA) exchange. A temperature-dependent LDA functional provides much better agreement with the tHF exchange. An underlying need is for well-characterized, reliable pseudopotentials over demanding temperature and density ranges. Thus we compare pseudopotential and all-electron results for small Li clusters of local bcc symmetry and bond-lengths appropriate to high density bulk Li. We determine the density range over which both standard projector-augmented wave (PAW) and norm-conserving pseudopotentials are reliable. Then we construct small-cutoff-radius PAW data sets (for both the local density and the generalized gradient exchange-correlation approximations) which are valid for lithium densities up to at least 80 g/cm³.

¹Supported in part under US DoE Grant DE-SC0002139.

3:18PM L25.00005 A Different Time-Dependent Variational Principle Approach: Going Beyond Wave Packet Molecular Dynamics, PAUL GRABOWSKI, Los Alamos National Laboratory, ANDREAS MARKMANN, Yale University, MIKE SURH, Lawrence Livermore National Laboratory, MICHAEL MURILLO, Los Alamos National Laboratory, FRANK GRAZIANI, Lawrence Livermore National Laboratory, CIMARRON COLLABORATION — During inertial confinement fusion, matter evolves from a solid condensed matter phase through the warm dense matter (WDM) regime to a hot dense matter. In WDM, quantum mechanical effects are important because of both Fermi-Dirac statistics and the rate of electrons transitioning in and out of bound states is large. The time-dependent temperature and quickly changing local environment require a time-dependent quantum method. A converged dynamical quantum simulation is intractable for more than a few particles. Instead, we take as a feasible goal to match the statistical properties of a warm dense plasma. The time-dependent variational principle gives a framework for producing equations of motion. A commonly used variational form is a Hartree product of isotropic Gaussian wave packets (wave packet molecular dynamics). The resulting dynamics do not produce the right statistics. We therefore introduce a plane wave basis and discuss its advantages and test its ability to reproduce radial distribution functions produced by hyper-netted chain calculations.

3:30PM L25.00006 All-Electron Path Integral Simulations of Warm, Dense Matter: Application to Water and Carbon¹, KEVIN DRIVER, Department of Earth and Planetary Science, University of California, Berkeley, CA 94720, USA, BURKHARD MILITZER, Department of Earth and Planetary Science and Department of Astronomy, University of California, Berkeley, CA 94720, USA — We develop an all-electron path integral Monte Carlo (PIMC) method for warm dense matter and apply it to study water and carbon. PIMC pressures, internal energies, and pair-correlation functions compare well with density functional theory molecular dynamics (DFT-MD) at lower temperatures and enable the construction of a coherent equation of state over a density-temperature range of 3–12 g/cm³ and 10²–10⁹ K. PIMC results converge to the Debye-Huckel limiting law at high-temperatures and illuminate the breakdown of DFT pseudopotentials due to core excitations.

¹Funding provided by the NSF (DMS-1025370). Computational resources provided by the National Center for Atmospheric Research and Lawrence Berkeley National Laboratory.

3:42PM L25.00007 ABSTRACT WITHDRAWN —

3:54PM L25.00008 Non-equilibrium Warm Dense Matter: Electron-Ion Dynamics of Pumped Nanofoils¹, YUAN PING, TADASHI OGITSU, ALFREDO CORREA, ERIC SCHWEGLER, GILBERT COLLINS, LLNL, JUN ZHOU, JIANMING CAO, Florida State University, BYOUNG-ICK CHO, KYLE ENGELHORN, PHILIP HEIMANN, ROGER FALCONE, LBNL/UC Berkeley — In 2006, it was reported that the dielectric function of laser-excited gold nanofoils exhibits a peculiar behavior; the interband transition peak of gold is enhanced and undergoes a clear red shift [PRL **96**, 255003 (2006)]. In 2009, based on ultrafast electron diffraction measurements on pumped gold nanofoils, it was reported that the time evolution of the Debye-Waller factor is too slow to be explained by a two-temperature model that included temperature dependent el-ph coupling. This anomaly has been attributed to a phonon hardening process caused by high electron temperatures (a few eV) [Science **323**, 1033 (2009)]. Later, it was pointed out that at such a high electron temperatures the dielectric function of gold calculated by first-principles DFT simulations does not reproduce the enhanced and red-shifted interband transition peak and an alternative explanation was proposed to reconcile the discrepancies where the effect of ejected electrons was addressed [HEDP **6**, 246 (2010)]. In this talk, we will discuss recent experimental/theoretical efforts to further examine the issues relevant to this problem, el-ph coupling, dynamics of ejected electrons, and ballistic transport of electrons [submitted to HEDP; PRL **106**, 167601(2011)].

¹Prepared by LLNL under Contract DE-AC52-07NA27344.

4:06PM L25.00009 High field terahertz response of materials, DAN DARANCIANG, Department of Chemistry, Stanford University, JOHN GOODFELLOW, Department of Materials Science, Stanford University, ALAN FISHER, Linac Coherent Light Source, SLAC National Accelerator Laboratory, AARON LINDENBERG, Department of Materials Science, Stanford University — We report on studies of the response of materials to intense ultrashort electromagnetic fields at terahertz frequencies. These are generated through coherent transition radiation using femtosecond electron bunches at the Linac Coherent Light Source and correspond to single-cycle pulses with electric field amplitudes $\gtrsim 20$ MV/cm with a frequency centered at 10 THz. Large amplitude nonlinear responses are observed in a range of semiconductor materials associated with field-induced ionization processes, and we show how these processes can be used to carry out nonlinear autocorrelation measurements of the pulse shape. We also discuss recent results probing the response of ferroelectric materials at high fields coupled with ultrafast x-ray probes enabling measurement of their atomic-scale response on sub-picosecond time-scales.

4:18PM L25.00010 An Analytic Screening Potential for Dense, Strongly-Coupled Plasmas¹, LIAM STANTON, LLNL, MICHAEL MURILLO, LANL, FRANK GRAZIANI, LLNL — Characterizing warm dense matter (WDM) has gained renewed interest due to advances in powerful lasers and next generation light sources. Because WDM is strongly coupled and moderately degenerate, we must often rely on simulations of WDM, which are necessarily based on molecular dynamics of ions interacting through a screened potential. Almost always, a Debye- (Yukawa-) like interaction is assumed; however, it is well known that such long wavelength models over-screen. Here, we present a new effective ion-ion interaction, which recovers the exact fermionic linear response in the long-wave limit while retaining a pair-potential functionally similar to that of the Yukawa form. This new potential not only improves the accuracy of screening effects without contributing to the computational complexity of the model, but it also adds physics entirely missing from Yukawa models (such as the onset of Friedel oscillations). Simulations of the ion structure factor are compared to XRTS data for Be and C in the WDM regime.

¹This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-490714

4:30PM L25.00011 Large-Scale Reactive Simulations of Materials in Extreme Conditions, ANDRES JARAMILLO-BOTERO, WILLIAM GODDARD, California Institute of Technology, MSC TEAM — First-principles quantum mechanics methods are inadequate for accurately describing the effects of thermal, mechanical, chemical or radiation excitations that may occur in materials operating under extreme conditions, or impractical to use due to the prohibitive scaling cost of propagating the total Schrodinger equation for a large set of atoms. In the regime of a high number of electronic excitations, the electronic portion of the wave function contains contributions from many stationary states, and the Born-Oppenheimer approximation breaks down. We have been developing a mixed quantum-classical dynamics approach, called the Electron Force Field (eFF), to simulate the non-adiabatic dynamics of materials in extreme conditions. We have demonstrated its application to describe the: thermodynamics of dense hydrogen over 0-100,000 Kelvin; real-time dynamics of Auger fragmentation of diamond nano particles; transient electronic effects in high-strain rate silicon fracture; Coulomb explosion of carbon clusters; dynamics of cascaded valence ionizations in shocked hydrocarbons; and the dynamics of hypervelocity impact of materials. Here, we summarize our recent progress in the theory and application of eFF for modeling and simulation of materials in extreme conditions.

4:42PM L25.00012 ABSTRACT WITHDRAWN —

4:54PM L25.00013 First-principle Calculations of Equation of State for Metals at High Energy Density, DMITRY MINAKOV, PAVEL LEVASHOV, KONSTANTIN KHISHCHENKO, Joint Institute for High Temperatures RAS — In this work, we present quantum molecular dynamics calculations of the shock Hugoniot of solid and porous samples as well as release isentropes and isentropic sound velocity behind the shock front for aluminum. Also we perform similar calculations for nickel and iron. We use the VASP code with ultrasoft and PAW pseudopotentials and GGA exchange-correlation functional. Up to 512 particles have been used in calculations. To calculate Hugoniot we solve the Hugoniot equation numerically. To obtain release isentropes, we use Zel'dovich's approach and integrate an ordinary differential equation for the temperature thus restoring all thermodynamic parameters. Isentropic sound velocity is calculated by differentiation of pressure along isentropes. The results of our calculations are in good agreement with experimental data at densities both higher and lower than the normal one. Thus, quantum molecular dynamics results can be effectively used for verification or calibration of semiempirical equations of state under conditions of lack of experimental information at high energy densities.

5:06PM L25.00014 Color quantum simulations of strongly coupled quark-gluon plasma, VLADIMIR FILINOV¹, VLADIMIR FORTOV, Joint Institute for High Temperatures RAS, Moscow, Russia, MISHAEL BONITZ, Institute for Theoretical Physics and Astrophysics, Kiel, Germany, YURI IVANOV, GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt, Germany, PAVEL LEVASHOV, Joint Institute for High Temperatures RAS, Moscow, Russia — We propose stochastic simulation of thermodynamics and kinetic properties for quark-gluon plasma (QGP) in semi-classical approximation in the wide region of temperature, density and quasi-particles masses. In grand canonical ensemble for finite and zero baryon chemical potential we use the direct quantum path integral Monte Carlo method (PIMC) developed for finite temperature within Feynman formulation of quantum mechanics to do calculations of internal energy, pressure and pair correlation functions. The QGP quasi-particles representing dressed quarks, antiquarks and gluons interact via color quantum Kelbg pseudopotential rigorously derived for Coulomb particles. This method has been successfully applied to strongly coupled electrodynamic plasmas (EMP). A strongly correlated behavior of the QGP is expected to show up in long-ranged spatial correlations of quarks and gluons which, in fact, may give rise to liquid-like and, possibly, solid-like structures. We have done already the first calculation of the QGP equation of state, spatial and color pair distribution functions, diffusion coefficients and shear viscosity.

¹Presenting Author Contact person

5:18PM L25.00015 Proton crystallization and quantum melting of proton crystals in a dense hydrogen plasma, PAVEL LEVASHOV, VLADIMIR FORTOV, VLADIMIR FILINOV, Joint Institute for High Temperatures RAS, Moscow, Russia, HOLGER FEHSKE, Institut für Physik, EMAU Greifswald, Germany, MICHAEL BONITZ, Institute for Theoretical Physics and Astrophysics, Kiel University, — We present extensive new simulation results which allow to predict the temperature and density range for proton crystallization. We simulate a macroscopic spatially homogeneous fully ionized two-component electron-proton plasma in thermodynamic equilibrium from first principles using direct fermionic path integral Monte Carlo simulations. Our results for the phase diagram differ substantially from the previous predictions based on the one-component plasma (OCP) model: In the classical part of the phase diagram the crystal appears to be stabilized compared to the OCP prediction. In contrast, in the quantum part of the phase diagram the crystal appears to be de-stabilized and vanishes at lower densities compared to the OCP prediction. Finally, the maximum temperature for the proton crystal is found to be around 40 000K, slightly below the previous prediction. Our results indicate that the OCP treatment of the liquid-solid transition in a two-component plasma has to be questioned. The OCP-assumption of a homogeneous rigid neutralizing background gives rise to substantial deviations of the critical parameters.

Tuesday, February 28, 2012 2:30PM - 5:18PM —
Session L26 DCOMP GSNP: Focus Session: Friction, Fracture and Deformation Across Length Scales - Dislocations and Fracture 257B

2:30PM L26.00001 How dislocations and grain boundaries control wear at the nanoscale, IZABELA SZLUFARSKA, University of Wisconsin — Ceramics show outstanding mechanical properties such as high strength and high hardness over a wide range of temperatures and are stable in harsh environments. However, the low fracture toughness of ceramics limits their practical utility for instance as wear-resistance coatings. There have been several reports of improving wear resistance of ceramics by reducing the grain sizes and/or the dimension of the cutting tools to the nanometer regime. Using SiC as a model covalent ceramic, we performed molecular dynamics (MD) simulations of wear for both single crystal and nanocrystalline material. We determined the role of dislocations and grain boundary sliding in improving wear resistance of SiC and we have quantified contributions from these mechanisms to friction and wear. We have discovered instabilities that control sliding of the amorphous-like highly disordered grain boundaries in SiC, in analogy to instabilities and deformation mechanisms that occur in bulk amorphous materials. In this talk we will also present our newly developed analytical model for plowing friction in nanoscale contacts, which model has been validated for both ceramics and metals. In order to isolate the contribution from grain boundary sliding to deformation of nanocrystalline materials, we have performed MD simulations of nanoindentation and uniaxial testing on ultrananocrystalline diamond (UNCD). We have shown that in the absence of dislocation plasticity, hardness and yield strength of nanocrystalline materials scale linearly with the grain boundary shear strength, where the latter property can be controlled by grain boundary doping. Our findings explain the experimental observations that hardness and elastic properties of UNCD decrease with an increasing H content.

3:06PM L26.00002 Plastic flow and failure in metallic glass/nanocrystal composites¹, MICHAEL FALK, PENGFEI GUAN, Johns Hopkins University — The exploitation of metallic glasses' high strength in structural applications is limited by their lack of any hardening subsequent to yield. This lack of hardening leads to plastic localization as evidenced by the spontaneous formation of shear bands. One proposed method of forestalling such instabilities is to introduce nanocrystal inclusions to disrupt shear band nucleation and propagation. We have undertaken a series of molecular dynamics simulations of glasses with different morphologies of nanocrystallites. We report the resulting plastic response, and we use various simulations of these types to test the applicability of the shear transformation zone (STZ) constitutive relation for modeling such complex nano-composite materials.

¹Funded by NSF under grant DMR0808704

3:18PM L26.00003 Atomic Origins of Friction Reduction in Metal Alloys, MICHAEL CHANDROSS, SHENGFENG CHENG, Sandia National Laboratories — Gold is a desirable material for use in high performance electrical contacts because it offers low contact resistance, does not corrode or oxidize, and can be easily made into thin sheets. However, gold contacts generally suffer from high adhesion and friction. The tribological issues are mitigated in nanocrystalline gold alloys (with, for example, Ni or Co), which can exhibit both low friction and low contact resistance. The atomic scale mechanisms responsible for the change in frictional response are poorly understood. We will present the results of large scale molecular dynamics simulations which study the tribological response of nanocrystalline films of pure gold and alloys under a variety of sliding conditions. Our results indicate that in pure metals, cold welding and microstructural reorientation lead to the formation of a commensurate sliding interface and high friction resulting from dislocation controlled plasticity. In alloys, however, differing lattice constants suppress the reorientation of grains at the contact point, which leads to grain boundary sliding and lower friction.

3:30PM L26.00004 Deformation Initiation by Non-planar {10-12} Twinning Nucleation in Magnesium Crystal, SUNGHO KIM, HAITHAM KADIRI, MARK HORSTEMEYER, Mississippi State University — The nucleation mechanism of experimentally most commonly observed twinning in Mg crystal initiating deformation process are studied using molecular dynamic simulation. We observed nucleation of radially growing {10-12} twinning under tensile loading in Mg rectangular wire system without artificial creation of an twinning. The twinning nucleation mechanism is very different from the conventional twinning mechanism in that the twin nucleates from a point source rather than the fault plane following the partial dislocation line in FCC crystal. The wire axis is normal to basal plane of Mg crystal. The tensile deformation in c-axis nucleates {10-12} twinning starting at the corner of square of cross section of the wire. The twin boundary is spherical at the beginning and become linear boundaries in {10-12} planes as time goes by.

3:42PM L26.00005 Softening of nanocrystalline materials at small grain size, GEORGIOS KOPIDAKIS, NIKOS GALANIS, IOANNIS REMEDIKIS, Dept. of Materials Science and Technology, University of Crete — We examine the dependence of the mechanical properties of nanocrystalline materials on grain size. Our extensive atomistic simulations for several nanocrystalline solids show a universal softening at grain sizes of less than a few nanometers. The elastic constants decrease as the average grain size becomes smaller, in analogy with the reverse Hall-Petch effect for nanocrystalline metals. This behavior is explained by the increase of the fraction of grain boundary atoms as grain size decreases. We derive simple scaling laws for various mechanical properties as a function of the grain size by decomposing the energy into contributions from atoms in the bulk of grains and from atoms at the interfaces. Our theoretical predictions fit very well our results from atomistic simulations of different nanocrystalline materials, from nanocrystalline metals to ultrananocrystalline diamond. It is therefore argued, and quantitatively explained, that softening at small grain size is a general nanoscale effect.

3:54PM L26.00006 Large scale NEMD simulations of polycrystalline Al sliding interfaces¹, JACQUELINE MILHANS, J.E. HAMMERBERG, R. RAVELO, T.C. GERMANN, B.L. HOLIAN, Los Alamos National Laboratory — We present the results of NonEquilibrium Molecular Dynamics (NEMD) simulations for the frictional force between polycrystalline Al samples. Polycrystalline Al samples of order 26M atoms with grain sizes from 10 - 20 nm at compressions of 15 GPa are considered as a function of sliding velocity. Typical sample dimensions are 58nm in the sliding and transverse directions and 116nm in the direction normal to the sliding interface. A constant temperature (300K) and constant tangential velocity boundary condition is imposed at the boundaries in the direction normal to the sliding plane. We discuss the modes of plastic deformation and polycrystalline deformation which determine the steady state frictional force and compare these results with results for defect free Al single crystals and highly defective Al single crystal samples.

¹This work was performed under the auspices of the U.S. Dept. of Energy under contract DE-AC52-06NA25396.

4:06PM L26.00007 Fracture In Disordered Media: Nucleated, Critical or Percolative?¹, ASHVINI SHEKHAWAT, Cornell University, STEFANO ZAPPERI, CNR - Consiglio Nazionale delle Ricerche, JAMES SETHNA, Cornell University — Fracture is often considered to be an abrupt transition and is modeled by nucleation theory. However, the precursor events leading to macroscopic failure display scaling behavior and are understood in terms of critical phenomena. Further, the universal roughness properties of fracture surfaces have been explained by modeling fracture as a percolative process. We attempt to unify these disparate descriptions of fracture in one comprehensive theory. We study the random fuse network as a typical model of disordered brittle media. We show that in this model fracture can be nucleated, critical or percolative depending on the behavior of the tail of the distribution of fuse strengths. We explore the phase diagram by using numerical simulations as well as theoretical arguments.

¹This research was supported by DOE-BES DE-FG02-07ER-46393

4:18PM L26.00008 Homogeneous Dislocation Nucleation, ASAD HASAN, CRAIG MALONEY, Carnegie Mellon University — We perform atomistic computer simulations to study the mechanism of homogeneous dislocation nucleation (HDN) in a 2D hexagonal crystalline film under circular indentation. The nucleation process is governed by vanishing of energy associated with a single normal mode. For fixed film thickness, L , the spatial extent, ξ , of the critical mode grows with indenter radius, R . For fixed R/L , ξ scales roughly as $\xi \sim L^{0.4}$. We perform a *mesoscale* analysis to determine the lowest energy normal mode for regions of varying radius, r_{meso} , centered on the critical mode's core. The energy of the lowest normal mode $\lambda_{\text{meso}} \rightarrow 0$ rapidly as $r_{\text{meso}} \rightarrow \xi$. The lowest mode shows a spatial extent, ξ_{meso} , which increases sublinearly for $r_{\text{meso}} \leq \xi$ and saturates at $r_{\text{meso}} \approx 1.5 \xi$. We demonstrate that the ξ_{meso}/ξ versus r_{meso}/ξ curve is *universal* (independent of L or R). Hence small regions, $r_{\text{meso}} \leq \xi$, can reveal the presence of incipient instability but give excellent estimates for the critical mode's energy and spatial extent *only* for $r_{\text{meso}} \geq 1.5 \xi$. Thus HDN is a *quasi-local* phenomenon.

4:30PM L26.00009 Fracture Energy Issues of Brittle, Microcrack Brittle, and Dislocation Ductile Materials¹, RAY B. STOUT, RhoBetaSigma Aff, 954 Venus Way, Livermore CA 94550-6346, RHOBETASIGMA AFF COLLABORATION — Somigliana elasticity models(1915) for dislocation-microcrack defect discontinuities in a material form an analog basis to relate dislocation density evolution to microcrack density evolution near an existing idealized crack-tip. Thus, a recent idealized field solution derived for stochastic dislocation density evolution near a crack-tip in a ductile material is also an analog applicable field solution for stochastic microcrack density evolution in a brittle material near a crack-tip. A non-equilibrium thermodynamic functional is derived and integrated to evaluate rates of dislocation and microcrack internal energy evolution due to the singularity terms of these crack-tip solutions in an arbitrary spatial crack-tip neighborhood and during an arbitrary fracture toughness load-up time interval of $[0, t^*]$. At some time greater than t^* , the available inter-atomic lattice(analog recoverable elastic) internal energy at a crack-tip becomes probabilistically sufficient, in an energy transfer-stability sense of Gibbs[1906], Griffith[1920], and Eshelby[Phil Trans Roy Soc, 1951], to be configurationally transported from locally recoverable internal energy at a crack-tip to non-recoverable crack-tip surface energy as a crack-tip propagates.

¹N/A

4:42PM L26.00010 Role of interactions and damage in a cohesive fracture model, JOSEPH GRAN, JOHN RUNDLE, DONALD TURCOTTE, University of California, Davis, WILLIAM KLEIN, Boston University — We study the influences of local and long range interactions in a numerical model of tensile fracture. Our model simulates fracture events on a 2D square lattice plane with a Metropolis algorithm. We chose a Hamiltonian that is written as a function of the crack separation (offset field) and includes contributions from an external field, interactions, as well as a cohesive energy across the crack surfaces. Included in our study is both a ferromagnetic-type (attractive) and antiferromagnetic-type (repulsive) interactions. We test both of these interactions individually as well as a hybrid interaction in which over a short range the interaction is antiferromagnetic and in the long range the interaction becomes ferromagnetic. This dual interaction approximates a Lennard-Jones potential. We also propose a characterization of damage and investigate the increase of damage in time for fractures occurring by a static-load as well as a time-dependent load. Damaged sites do not interact with neighboring sites and cannot hold any load. We compare our damage model to previous studies of fiber-bundle models.

4:54PM L26.00011 Indentation of Graphene Membranes: Non-Linear Response, Nano-Fracture, and Crack Propagation, ROMAIN PERRIOT, YOU LIN, VASILY ZHAKHOVSKY, Department of Physics, University of South Florida, XIANG GU, Department of Applied Physics, Aalto University, IVAN OLEYNIK, Department of Physics, University of South Florida — Recent indentation experiments on graphene have revealed its exceptional strength, making it an excellent candidate for the design of nano- and micro- electromechanical systems. Therefore, it is critical to understand the mechanical properties of graphene, and its response to a wide range of loading pressures beyond the elastic regime. In this work molecular dynamics (MD) simulations of indentation of circular graphene membranes were performed with a newly developed interatomic potential, specifically designed to study graphene under extreme tensile stress. The indentation curves confirmed the experimental observation of a non-linear response at large loads, as well as the brittle failure of the membranes via the generation of nano-cracks. Our MD simulations showed that the fracture process consists of two consecutive stages: an initial bond-breaking event followed by the formation and propagation of cracks. The kinetic theory of bond breaking was applied to determine the breaking strength of graphene and its dependence on the indenter radius, as well as the waiting time for failure. MD simulations were used to provide an atomic-scale description of fracture dynamics.

5:06PM L26.00012 Investigation of Nonlinear Elastic Behavior of Two-Dimensional Molybdenum Disulfide¹, RYAN COOPER, Columbia University, CHANGGU LEE, Sung Kyun Kwan University, CHRISTOPHER MARIANETTI, JAMES HONE, JEFFREY KYSSAR, Columbia University — The present study investigates the nonlinear elastic properties of a single-layer molybdenum disulfide crystal through experiment, finite element modeling, and density functional theory. Suspended single-layer molybdenum disulfide crystals are suspended over circular holes that were etched on a silicon oxide surface. Crystals are loaded at the center with an atomic force microscope until fracture occurs. The load-displacement curve is used to determine the pretension and linear-elastic response of the crystal. The force at which fracture occurs gives insight into the intrinsic strength and higher order elastic constants of the crystal. These experiments provide a platform to validate first-principles derivation of fifth-order elastic constants for in-plane stiffness using density functional theory. The derived higher order elastic constants are used in a finite element model to predict the breaking strength of two-dimensional molybdenum disulfide. The study bridges the gap between density functional theory and finite element analysis with experimental evidence.

¹NSF CMMI grant

Tuesday, February 28, 2012 2:30PM - 5:30PM –
Session L27 DCMP FIAP: Invited Session: Quantum Design of Low-Dimensional Materials Structures for Enhanced Solar Energy Conversion 258AB

2:30PM L27.00001 Use of First-Principles Theory to Identify materials and nano structures for next-generation solar cells¹, ALEX ZUNGER, University of Colorado, Boulder, Colorado 80309 — Three genomic-like material design approaches are explored for finding energy relevant semiconductors: (i) *Search of nanostructure combinations leading to intermediate band solar cells*: Within the ideology of intermediate band solar cells (IBSC) based on quantum dots, it is presently unknown which combination of dot material + matrix material + substrate satisfies the energetic criteria enabling IBSC. Using the modern theory of nano structures (based on atomistic pseudo potentials in plane waves), we examine various combinations, finding that some of the “usual suspect” long believed to be ideal, are, in fact inappropriate. (ii) *Finding new inorganic absorbers with first-principles*: Standard compilations of inorganic compounds reveal thousands of candidate materials that were unexplored for their potential as PV absorbers, among others, because of the absence of a quantifiable “Design Principle” that sorts out various materials. The common Schockley - Queisser criteria gives a universal, gap vs efficiency curve which does not distinguish different types of gaps (direct-allowed vs direct-forbidden vs-indirect) nor does it account for non radiative recombination. A simple treatment, called “Spectroscopically Limited Maximum efficiency” (SLME) accounts for such factors and can be calculated for hundreds of compounds (using the GW approach), providing insight into previously unrecognized candidates, as well as to the mechanisms at work causing absorption enhancement. (iii) *Inverse Band structure search for direct gap Si-Ge nano structures*: Using a genomic approach to pseudo potential configurational search we identify a Si-Ge nano structures that have direct band gaps, solving the long-standing dilemma of crystalline Column IV absorbers. In collaboration with L. Yu, V. Popescu, J.W. Luo and M. Davezac.

¹Funder by DOE Energy Frontier Research Center for Inverse Design, Office of Science, Basic Energy Science.

3:06PM L27.00002 Photovoltaic effect for narrow-gap Mott insulators, EFSTRATIOS MANOUSAKIS, Department of Physics, Florida State University, Tallahassee, Florida, 32306 — Solar cells, based on conventional band-semiconductors, have low efficiency for conversion of solar into electrical energy. The main reason is that the excess energy of the photon absorbed by an electron/hole pair beyond the band-gap becomes heat through electron-phonon scattering and phonon emission; through these processes electrons and holes relax to their band edges within a characteristic time scale of the order of $10^{-12} - 10^{-13}$ secs. We will discuss that a narrow-gap Mott insulator can produce a significant photovoltaic effect and, more importantly, if appropriately chosen it can lead to solar cells of high efficiency. In this case, a single solar photon can produce multiple electron/hole (doublon/hole) pairs, an effect known as impact ionization, faster than other relaxation processes such as relaxation through phonons. It has been proposed previously that this process could lead to an efficient solar cell using band-gap semiconductors; however, the characteristic time-scale for impact ionization is comparable to that for electron-phonon relaxation in band-gap semiconductors. The reason that a Mott insulator can behave differently is that the large Coulomb repulsion present in a Mott insulator leads to a large enhancement of the impact ionization rate. Provided that this enhancement does occur in an appropriately chosen Mott insulator, it can be demonstrated that the efficiency can improve significantly over conventional band-insulators. At present, we are doing calculations on specific transition-metal-oxide based materials believed to be Mott-insulators using extensions of the density functional theory (hybrid functionals) in combination with many-body perturbation theory. Our goal is to determine a promising candidate with suitable band structure and transition matrix elements leading to fast transition rates for impact ionization to occur in a time-scale faster than other relaxation processes.

3:42PM L27.00003 Quantum Dot Solar Cells, VLADIMIR BULOVIC, Massachusetts Institute of Technology —

4:18PM L27.00004 Shaping anomalous molecular electroluminescence by resonant nanocavity plasmons¹, ZHENCHAO DONG, University of Science and Technology of China — Exciton formation and decay of molecules near metallic nanostructures is important for the control of energy conversion at the nanoscale and plasmonic devices. While extensive research has been carried out to such end using photon-excited techniques, complementary insights into the optical transitions and plasmon-exciton coupling can be obtained through electron excitations by a scanning tunneling microscope [1]. In this talk, we shall describe such reversed process of light-to-electricity conversion through single-molecule electroluminescence that demonstrates the critical role of nanocavity plasmons in the generation and decay of molecular excitons. By tuning the resonant interplay between molecular excitons and plasmons in nearby metallic nanostructures, we demonstrate that plasmons can do much more beyond intensity enhancement [2]: the emission band of molecular fluorescence can be effectively tuned by resonant nanocavity plasmons. New optoelectronic effects including resonant hot-electroluminescence and upconversion electroluminescence from higher vibronic levels of singlet excited states have been realized for porphyrin molecules near metals, which breaks the Kasha's rule and conventional Franck-Condon distribution. The highly confined nanocavity plasmons can behave like a strong coherent optical source with tunable frequency, and can be used to actively control the radiative channels of molecular emitters near metals over a wide spectral range. We shall also discuss critical factors that are responsible for the realization of single-molecule electroluminescence [3].

[1] Z.C. Dong, et al., Phys. Rev. Lett. 92, 086801 (2004).

[2] Z.C. Dong, et al., Nat. Photonics 4, 50 (2010).

[3] Y. Zhang, et al., Phys. Rev. Lett. (submitted).

¹This work was supported by National Basic Research Program of China (2011CB921402) and the Natural Science Foundation of China (91021004 and 10974186).

4:54PM L27.00005 Quantum Photocell: Using Quantum Coherence to Reduce Radiative Recombination and Increase Efficiency, MARLAN SCULLY, Texas A&M and Princeton Universities — Laser and photocell quantum heat engines (QHEs) are powered by thermal light and governed by the laws of quantum thermodynamics. We here show how to use quantum coherence (PRL, 104, 207701 (2010)) induced by quantum noise (PNAS, 108, 15097 (2011)) to improve the efficiency of a laser or photocell QHE. Surprisingly, this coherence can be induced by the same noisy (thermal) emission and absorption processes that drive the QHE. Furthermore, this noise-induced coherence can be robust against environmental decoherence. Application of the ideas to photosynthesis (Nature, 446, 782-786 (2007)) will also be discussed.

Tuesday, February 28, 2012 2:30PM - 5:30PM –
Session L28 FIAP GERA DMP: Electricity-to-Light Conversion: Solid State Lighting 258C

2:30PM L28.00001 Auger recombination in gallium arsenide from first principles¹, DANIEL STEIAUF, Materials Department, University of California, Santa Barbara, EMMANOUIL KIOUPAKIS, Materials Department, UC Santa Barbara; Materials Science and Engineering, University of Michigan, Ann Arbor, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — GaAs and its alloys are technologically important materials for solid-state optoelectronic devices such as LEDs and lasers. The internal quantum efficiency of these devices, defined as the fraction of electron-hole pairs converted to photons, is limited by loss mechanisms. Of particular importance at high carrier densities is Auger recombination, a non-radiative process where the energy and momentum of the recombining electron-hole pair is transferred to a third carrier. Here we use density functional theory to study Auger recombination in GaAs from first principles. When considering Auger recombination due to Coulomb interaction only, the calculated rate is too small and cannot account for the experimental observations. However, once additional electron-phonon interactions are included, the theoretical recombination rate increases towards the experimental value. Our work provides insight into the microscopic origins of the loss in III-V LEDs at high injected-carrier densities, and in the mechanisms governing Auger recombination rates in general.

¹This work was supported by DOE.

2:42PM L28.00002 Surface Energies and Cracking in GaN¹, CYRUS E. DREYER, CHRISTIAN CARBOGNO, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — Cracking is one of the biggest limitations to growing thick GaN single crystals and films, caused by the buildup and release of strain energy. Cracking occurs along preferential crystallographic planes in the GaN wurtzite structure, and depends on the tensile stress on the given plane and the energetic balance between the strain energy released from the crack formation versus the cleaved surface area created. It is also well known that the equilibrium shape of a crystal is largely determined by its surface free energy. Therefore, to correctly predict the stresses under which certain planes will crack and aid in understanding crystal growth, knowledge of the absolute surface energy is required. We use first-principles calculations based on density functional theory and a hybrid functional to determine the surface energy for the nonpolar {11-20} *a*- and {10-10} *m*-planes, as well as to explore approximations to the surface energies of the polar {0001}/{000-1} *c*-planes in GaN. The effects of structure relaxations and reconstructions are fully taken into account, and the results are discussed in the light of available experimental observations.

¹This work was supported by NSF and by the UCSB SSLEC.

2:54PM L28.00003 Crystalline Fe films grown on non-polar GaN: theory and experiment, STEVEN ERWIN, Naval Research Laboratory, CUNXU GAO, CLAUDIA RÖDER, JONAS LAEHNEMANN, OLIVER BRANDT, Paul Drude Institute, Berlin — We report an unexpected mechanism by which single crystals of Fe grow epitaxially on *M*-plane GaN substrates despite having a different crystal structure and strongly mismatched lattice constant. A simple model is proposed in which one material tilts out of the interface plane to create a coincidence-site lattice that balances two competing geometrical criteria—low residual strain and short coincidence-lattice period. We apply this model, along with complementary first-principles total energy calculations, to the interface formed by molecular-beam epitaxy of cubic Fe on hexagonal GaN and find excellent agreement between theory and experiment. The success of this model also suggests a strategy for growing non-polar GaN films on a substrate material with a suitably chosen Miller index. One very promising material is Si, which is already in widespread use as a flat substrate for GaN/Si epitaxy despite high dislocation densities. The next talk will present our predictions of the most promising Si(*hkk*) substrates for growing non-polar GaN with high crystalline quality.

3:06PM L28.00004 Crystalline non-polar GaN films grown on vicinal Si: theoretical predictions¹, ALEX KUTANA, STEVEN ERWIN, Naval Research Laboratory, CENTER FOR COMPUTATIONAL MATERIALS SCIENCE TEAM — The ability to grow highly crystalline non-polar GaN films on silicon substrates would be an important advance in optoelectronic device fabrication. We propose a simple strategy to achieve this goal: tilting the Si substrate out of interface plane to provide a good lattice match between the film and substrate. We consider epitaxial interfaces between *M*-plane GaN and arbitrary Si(*hkk*) substrates. Using the model introduced in the previous talk, we downselect these substrates using two geometric criteria—low residual strain and short coincidence-lattice period. We then use density-functional theory to compute the interface formation energies of these selected candidates, which include Si(001), (112), (113), (114), and (223). We find that *M*-plane GaN films have the lowest interface formation energy when grown on the (113) and (112) surfaces. The formation energies are significantly lower than on Si(001) or (111), the substrates most often used for growing GaN. On this basis we predict that Si(113) and (112) substrates will enable growth of non-polar GaN films of higher crystalline quality than can be attained on Si(001) or (111).

¹Part of this work was performed under the ASEE program at NRL.

3:18PM L28.00005 Hybrid functional studies of stability and diffusion of hydrogen in Mg-doped GaN, JI-SANG PARK, K.J. CHANG, Department of Physics, Korea Advanced Institute of Science and Technology — Nitride semiconductors are known to suffer from low p-type doping efficiency due to the high activation energy of Mg acceptors and the compensation of hole carriers. To enhance hole carrier concentration, the hydrogen co-doping method is widely used, in which hydrogen is intentionally doped with Mg dopants and removed by subsequent thermal annealing. In this work, we perform first-principles density functional calculations to study the stability and diffusion of hydrogen in Mg-doped GaN. For the exchange-correlation potential, we employ both the generalized gradient approximation (GGA) proposed by Perdew, Burke, and Ernzerhof and the hybrid density functional of Heyd, Scuseria, and Ernzerhof. We examine the diffusion pathways and dissociation barriers of H from the Mg-H complex using the nudged elastic band and dimer methods. We compare the results of the GGA and hybrid density functional calculations for the stability of various H interstitial configurations and the migration barriers for H diffusion. Finally, using the calculated migration barriers as inputs, we perform kinetic Monte Carlo simulations for the dissociation of the Mg-H complex and find that the Mg acceptors are activated by thermal annealing up to 700-800 °C, in good agreement with experiments.

3:30PM L28.00006 Electroluminescent Schottky Diodes Fabricated Using Plasma Ion Implantation¹, SARAH PURDY, University of Saskatchewan, MARCEL RISCH, Massachusetts Institute of Technology, PHILLIP DESAUTELS, SED Systems, MICHAEL BRADLEY, University of Saskatchewan — Carbon-implanted silicon light-emitting Schottky diodes were produced by Plasma Ion Implantation (PII) in an RF ICP plasma chamber using methane feedstock gas. The electroluminescence spectrum of the devices was fitted with a set of Gaussian peaks corresponding to known emission centers including disordered silicon (broad white background), buried porous silicon and hydrogenated carbon-rich silicon. Some of the emission peaks exhibit a peak intensity at a drive current density of several A/cm², followed by a drop in emission intensity at higher drive current densities. In this presentation we discuss a possible model for this observed drop in electroluminescent intensity.

¹This work was supported by NSERC & the Canada Foundation for Innovation.

3:42PM L28.00007 Sub-250nm room-temperature optical gain from AlGaIn/AlN multiple quantum dot structures, EMANUELE FRANCESCO PECORA, WEI ZHANG, Department of Electrical and Computer Engineering and Photonics Center, Boston University, LIN ZHOU, DAVID J. SMITH, Department of Physics, Arizona State University, JIAN YIN, ROBERTO PAIELLA, LUCA DAL NEGRO, THEODORE D. MOUSTAKAS, Department of Electrical and Computer Engineering and Photonics Center, Boston University — There are many pressing but yet unrealized applications for optoelectronic materials and devices that can function well into the deep-UV. Group-III nitrides, in particular AlGaIn, are particularly suited to cover UV spectral ranges. An intense research effort is targeting the investigation and demonstration of deep-UV lasing from these materials. We developed AlGaIn/AlN MQWs by Molecular Beam Epitaxy under a novel growth mode that introduces band structure potential fluctuations and high-density of nanocluster-like features within the AlGaIn wells. A characterization of this material will be presented. The Variable-Stripe Length technique, a well-established methodology for measuring optical gain coefficient, is applied for a detailed quantification of the gain properties and polarization. We demonstrate optical gain in AlGaIn nanostructures down to 230 nm at room temperature with a maximum net modal gain value of 118 ± 9 cm⁻¹ at the highest excitation fluence of 15 μ J/cm². The optical gain threshold was measured to be 5 ± 1 μ J/cm² from which we estimate the density of optically excited carriers at the threshold to be 1.4×10^{17} cm⁻³, which is two orders of magnitude lower than what currently achieved by quantum well structures. Moreover, we demonstrate that gain is TE-polarized.

3:54PM L28.00008 Room temperature low threshold stimulated emission of electron beam-pumped AlGaIn-based deep UV laser structures emitting below 250 nm, A. NIKIFOROV, W. ZHANG, Boston University, J. WOODWARD, Boston, J. YIN, E. PECORA, Boston University, L. ZHOU, Arizona State University, L. DAL NEGRO, R. PAIELLA, Boston University, D. SMITH, Arizona State University, T. MOUSTAKAS, A. MOLDAWER, Boston University — The development of semiconductor lasers, operating in the deep UV, will find a number of applications such as identification of biological and chemical agents, non-line-of-sight free space communications and point of site medical diagnostics. In this paper we report the growth of QW laser structures in the configuration 6H-SiC / AlN / AlGaIn - AlN MQWs / AlN by PAMBE. A novel growth mode was developed in which arriving active nitrogen species and aluminum atoms dissolve in the excess liquid Ga covering the surface of the growing film and incorporate into the AlGaIn film from the liquid phase. This liquid phase epitaxy (LPE) growth was found to introduce band structure potential fluctuations and high-density of nanocluster-like features within the AlGaIn wells. The structure and microstructure of these devices were investigated by AFM, XRD and TEM and their emission properties were investigated by electron beam pumping at room temperature. The investigated laser structures were found to emit in the 235-250 nm range and stimulated emission was observed at a threshold power of 20-40 KW / cm². This low threshold value is attributed to nanoclusters-like features in the wells.

4:06PM L28.00009 Electronic transport through InGaIn heterojunctions¹, MATHIEU CÉSAR, DONPING LIU, HONG GUO, McGill University — InGaIn nanowires have recently sparked great interest for their high tunability and potential in applications like solid-state lighting (LEDs) and concentrated photovoltaics. Determination of device characteristics from first principles modeling is of great importance. In order to treat quantum transport properties of nanoelectronic devices with atomistic disorder, a non-equilibrium vertex correction (NVC) theory was recently developed and implemented into the Keldysh non-equilibrium Green's function (NEGF) -based density functional theory (DFT). NEGF-DFT-NVC enables the representation of disordered structures such as the InGaIn heterojunction under non-equilibrium conditions. Electronic and transport properties of a InGaIn heterojunction are investigated using this accurate ab initio method.

¹Work supported by NSERC of Canada

4:18PM L28.00010 Effects of Internal Fields on the Optical Emission in Nanostructured III-N LEDs, KRISHNA YALAVARTHI, SASI SUNDARESAN, KY MERRILL, SHAIKH AHMED, Southern Illinois University — Nanostructured optical emitters can accommodate a broader range of lattice mismatch, be used in full-solar-spectrum light emitting diodes, and provide higher temperature stability of the threshold current and the luminescence. However, strong quantum confinement and certain symmetry-lowering mechanisms (caused by various internal fields) lead to pronounced optical polarization anisotropy and strong suppression of interband transitions in these structures. The objective of this work is to study the competing effects of various internal fields on the electronic structure and optical properties of nanostructured III-N LEDs. A multiscale approach has been employed where: 1) the NEMO 3-D tool is used to calculate the atomistic strain distribution and one-particle electronic states within a $sp^3s^*d^5$ tight-binding framework, and 2) the outputs from NEMO 3-D are then coupled to the Synopsys TCAD tool to determine the terminal electrical and optical properties of the device.

4:30PM L28.00011 Accurate first-principles calculation of the rare earth crystal field, FEI ZHOU, VIDVUDS OZOLINS, UCLA — Rare earth (RE) doped wide band-gap semiconductors play an important role in solid state lighting. Many aspects of the performance of these materials are characterized and determined by the f -electron crystal field (CF). However, CF effects are usually rather small for f electron: the CF splitting is at the order of 0.1 eV, compared to several eV for d -electrons. Therefore accurate theoretical description of RE crystal field is challenging. We present a first-principles method of CF calculation based on an improved LDA+U method. By careful cancellation of errors, the method can reach relatively high accuracy for the CF parameters. As a demonstration we calculate the experimentally well-characterized RE:LaF₃ system, which has low point-group symmetry and a large number of CF parameters, representing a stringent test of theory. The predicted CF excitation energies of Ce:LaF₃ agree within about 10 meV with experiment, and within several meV if the errors in the free-ion parameters are excluded. Work is underway to apply the method to other materials for solid-state lighting and laser applications.

4:42PM L28.00012 The role of extended defects in Nitride Semiconductors on the performance of optoelectronic devices, T. MOUSTAKAS, Boston University — The question is why nitride semiconductors, which are plagued by high concentration of extended defects, produce efficient minority carrier optoelectronic devices. The equilibrium phase of these materials is the wurtzite and the metastable phase is the zinc blende. However, since the enthalpy of formation of these two structures differ by only a few meV, the conversion from one to the other can occur easily by the creation of stacking faults on the close packed planes. Thus, stacking faults are one of the most abundant defects in these materials even when they are grown homoepitaxially. Since the basal plane stacking fault is the equivalent of a monolayer of a cubic domain and since the energy band gaps of the wurtzite and their cubic counterparts differ by about 0.2 eV, one expects that stacking faults introduce band structure potential fluctuations. Such fluctuations are beneficial to the performance of lasers and LEDs since they lead to exciton localization and efficient radiative recombination. Other types of abundant defects in heteroepitaxially grown materials are threading dislocations. The insensitivity of the performance of LEDs and lasers to such defects is due to the strong ionicity of these materials as well as to the deep band structure potential fluctuations in the InGaN and AlGaN alloys. Due to the strong ionicity the surface states at free surfaces and dangling bonds in edge dislocations have moved towards the band edges and act as traps rather non-radiative recombination centers.

4:54PM L28.00013 Surface scattering from ceramic phosphors, ALAN LENEFF, JOHN KELSO, CHRISTOPHER PETERS, OSRAM SYLVANIA Inc — Scattering from phosphor converters and epitaxial surfaces is critical for solid state lighting device performance. Volume and surface scattering in solid state lighting devices can play a critical role in efficiency/efficacy, color points, and color angular consistency. Surface scattering in particular has not been well characterized in solid state lighting devices and can be complex to model. Because large angle scattering is important in lighting applications, surface scattering models generally require vector electromagnetic theory to avoid ambiguities often associated with scalar theory at these angles. Furthermore, surface features are often on the order of a few wavelengths, bringing ray tracing approaches into question. In this work, experimental angular scattering measurements are made on ceramic phosphor components where surface scattering dominates. The surface ceramic grain structure is responsible for the scattering. The results are compared to approximate statistical vector theory predictions that use the height autocorrelation functions as input. The autocorrelation measurements were derived from atomic-force microscopy topography measurements. Resulting predictions are in fairly good agreement with measurements.

5:06PM L28.00014 Light emission from electrically stressed ZnO nanorods, LUCA LUCERA, LHACENE ADNANE, KADIR CIL, VENKATA MANTHINA, ALEXANDER AGRIOS, HELENA SILVA, ALI GOKIRMAK, University of Connecticut — Zinc oxide (ZnO) nanorods were grown on various substrates by a chemical growth process based on a ZnO seed solution, and starting from Zinc acetate (ZnAc) material. The nanorods were grown on insulating silicon (low doped) and oxidized silicon substrates, and also over patterned conducting (highly-doped) nanocrystalline silicon microwires. When high voltage is applied directly to the ZnO film using tungsten needles (~ 50 -60 V across ~ 5 -10 μm), high intensity blue and white light emission is observed, both in air and under high vacuum (10^{-4} - 10^{-5} Torr). Blue light appears as broad bright flashes covering a large area whereas white light is more localized and appears to come from individual nanostructures. The results suggest a combination of electroluminescence and photoluminescence processes that take place after an electrical breakdown (possibly across individual ZnO nanorods) that is observed as an exponential increase in current. Percolative conduction and light paths are also observed during the measurements. Measurements of the ZnO films of rods on conducting silicon substrate give more repeatable results, likely due to the higher probability of conducting paths between the two probes. The electrical stress results in significant self-heating and modification of the ZnO nanostructures and the contacts.

[1] Greene L. E. et al. Solution-Grown Zinc oxide nanowires. *Inorganic Chemistry*. Vol 45. 7535-7543. (2006)

5:18PM L28.00015 A First-Principles Analysis of the Crystal Structure, Band Gap Energy, Polarization, and Piezoelectric Properties of ZnO-BeO Solid Solutions, LIANG DONG, S. PAMIR ALPAY, University of Connecticut — The electrical properties, the spontaneous polarization, and the piezoelectric response of ZnO can be tailored by alloying ZnO with BeO for various optoelectronics applications. We present here the results of a study that employs density functional theory to analyze the crystal structure, the band structure, elastic constants, spontaneous polarization, and piezoelectric properties of $\text{Zn}_{1-x}\text{Be}_x\text{O}$ solid solutions. Our findings indicate that $\text{Zn}_{1-x}\text{Be}_x\text{O}$ alloys may have a different crystal structure than the end components ZnO and BeO that crystallize in the prototypical wurtzite structure (P6₃mc). It is shown that orthorhombic lattices with Pmn2₁, Pna2₁, or P2₁ structures may have lower formation energies than the wurtzite lattice at a given Be composition. The band gap energies of $\text{Zn}_{1-x}\text{Be}_x\text{O}$ in the wurtzite and the orthorhombic structures are nearly identical and the bowing of the band gap energy increases with increasing Be concentration. The spontaneous polarization of $\text{Zn}_{1-x}\text{Be}_x\text{O}$ in the orthorhombic lattice is markedly larger compared to the wurtzite structure while the piezoelectric polarization in the wurtzite and orthorhombic structures varies linearly with the Be concentration.

Tuesday, February 28, 2012 2:30PM - 5:30PM —

Session L29 GQI: Focus Session: Semiconductor Qubits - Single and Multi-Qubit Demonstrations 259A

2:30PM L29.00001 Coherent control and detection of spin qubits in semiconductor with magnetic field engineering¹

YASUHIRO TOKURA, NTT Basic Research Laboratories — Electrical control and detection of the spin qubits in semiconductor quantum dots (QDs) are among the major rapidly progressing fields for possible implementation of scalable quantum information processing. Coherent control of one-[1-3] and two-[4,5] spin qubits by electrical means had been demonstrated with various approaches. We have used an engineered magnetic field structure realized with proximal micro-magnets to transduce the spin and charge degrees of freedom and to selectively address one of the two spins [3]. We have demonstrated an all-electrical two-qubit gate consisting of single-spin rotations and interdot spin exchange in double QDs. A partially entangled output state is obtained by the application of the two-qubit gate to an initial, uncorrelated state. Our calculations taking into account of the nuclear spin fluctuation show the degree of entanglement. Non-uniform magnetic field also enables spin selective photon-assisted tunneling in double QDs, which then constitutes non-demolition spin read-out system in combination with a near-by charge detector [6].

In collaboration with R. Brunner, Inst. of Phys., Montanuniversitaet Leoben, 8700, Austria, M. Pioro-Ladrière, Dép. de Phys., Université de Sherbrooke, Sherbrooke, Québec, J1K-2R1, Canada, T. Kubo, Y. -S. Shin, T. Obata, and S. Tarucha, ICORP-JST and Dep. of Appl. Phys., Univ. of Tokyo, Hongo, Bunkyo-ku, Tokyo, 113-8656, Japan.

- [1] F. H. Koppens, et al., Nature 442, 766 (2006).
- [2] K. C. Nowack, et al., Science 318, 1430 (2007).
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- [5] R. Brunner, et al., Phys. Rev. Lett. 107, 146801 (2011).
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¹Part of this work is financially supported by JSPS MEXT Grant-in-Aid for Scientific Research on Innovative Areas (21102003), Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST).

3:06PM L29.00002 Coherent Singlet-Triplet Oscillations in a Silicon-based Double Quantum

Dot, BRETT MAUNE, MATTHEW BORSELLI, BIQIN HUANG, THADDEUS LADD, PETER DEELMAN, KEVIN HOLABIRD, ANDREY KISELEV, IVAN ALVARADO-RODRIGUEZ, RICHARD ROSS, ADELE SCHMITZ, MARKO SOKOLICH, CHRISTOPHER WATSON, MARK GYURE, ANDREW HUNTER, HRL Laboratories LLC — We have performed coherent spin manipulation of a singlet-triplet qubit in a Si/SiGe double quantum-dot device fabricated in an undoped heterostructure. A charge stability diagram showed that the (0,0) charge state was reached and Pauli spin blockade was detected at the (1,1)-(0,2) anticrossing. A singlet-triplet splitting of $\sim 140 \mu\text{eV}$ in the (0,2) charge state provided a read-out window sufficiently wide for singlet-triplet discrimination. We used the S/T₋ spin funnel, Rabi oscillation, and T_2^* pulsing experiments to measure (1,1) exchange energies spanning $\sim 0.6\text{--}700 \text{ neV}$ over a large detuning range and measured a T_2^* of 360 ns, consistent with theoretical expectations for our device. Sponsored by the United States Department of Defense. Approved for Public Release, Distribution Unlimited. The views expressed are those of the author and do not reflect the official policy or position of the Department of Defense or the U.S. Government.

3:18PM L29.00003 Tunable singlet-triplet splitting in a few-electron Si/SiGe quantum dot

ZHAN SHI, University of Wisconsin-Madison, CHRISTIE SIMMONS, Massachusetts Institute of Technology, JONATHAN PRANCE, JOHN GAMBLE, MARK FRIESEN, DONALD SAVAGE, MAX LAGALLY, SUSAN COPPERSMITH, MARK ERIKSSON, University of Wisconsin-Madison — The singlet-triplet energy splitting in a double quantum dot is an important parameter for singlet-triplet qubits, because it determines the energy gap for both initialization and readout. This splitting can also be used to perform gate operations in a newly proposed hybrid qubit [1]. We describe measurements in which we tune the singlet-triplet energy splitting by changing gate voltages on a Si/SiGe double quantum dot [2]. We argue that the energy is changed largely by lateral translation of the dot, which changes the local atomic structure that the electrons experience in the quantum dot, leading to variations in the valley-orbit coupling. We present calculations indicating the experimental results are consistent with the first excited state of the dot having non-zero valley-orbit coupling. [1] Z. Shi, et al., e-print: <http://lanl.arxiv.org/abs/1110.6622>. [2] Z. Shi, et al., e-print: <http://lanl.arxiv.org/abs/1109.0511>.

3:30PM L29.00004 Electric dipole spin resonance measurement of spin-orbit anisotropy in InSb nanowire quantum dots

SERGEY FROLOV, STEVAN NADJ-PERGE, VLAD PRIBIAG, JOHAN VAN DEN BERG, TU Delft, SEBASTIEN PLISSARD, TU Eindhoven, ERIK BAKKERS, LEO KOUWENHOVEN, TU Delft — Indium antimonide nanowires are considered a leading platform for the generation of Majorana fermion bound states, and as hosts of spin-orbit quantum bits based on single electrons. Both efforts are motivated by the strong spin-orbit interaction in the bulk InSb. Here we present measurements of the strength and orientation of the effective spin-orbit magnetic field in InSb nanowire double quantum dots. Spin-orbit interaction induces avoided level crossings between triplet (1,1) and singlet (0,2) double dot states. These avoided crossings are observed in the spectrum of the electric dipole spin resonance performed on strongly-coupled double dots. We find that the spin-orbit field is oriented perpendicular to the nanowire axis, and parallel to the substrate plane. This orientation is consistent with Rashba spin-orbit interaction and is favorable for Majorana experiments. The strength of spin-orbit interaction is characterized by the spin-orbit length which we estimate to be 200 nm. This translates into a temperature scale of 3K for the observation of Majorana states.

3:42PM L29.00005 Coherent manipulation of spin-orbit quantum bits in InSb nanowires

STEVAN NADJ-PERGE, JOHAN VAN DEN BERG, SERGEY FROLOV, VLAD PRIBIAG, TU Delft, SEBASTIEN PLISSARD, TU Eindhoven, ERIK BAKKERS, LEO KOUWENHOVEN, TU Delft — Semiconductor nanowires with strong spin-orbit coupling are becoming an attractive platform for spin-based quantum computation. Here we demonstrate coherent transitions between spin-orbit doublet states of individual electrons in indium antimonide (InSb) nanowire quantum dots induced by gigahertz-frequency electric fields. The spin-orbit doublet states form a qubit which initialization and detection relies on Pauli blockade in the double quantum dot (1,1) configuration. The maximum Rabi frequency exceeds 100 MHz and more than 10 periods of coherent oscillations are observed. We estimate fidelities of single qubit rotations and analyze qubit decoherence times by performing spin echo sequence. The two qubits in a double quantum dot are individually addressable due to different g-factors. The coupling between the qubits can be mediated by exchange interaction. The fidelities of single qubit rotations are sufficiently high to permit the implementation of two-qubit quantum gates such as controlled-not (C-NOT) or controlled-phase (C-Phase).

3:54PM L29.00006 Spin Relaxation and Manipulation in Spin-orbit Qubits¹

MASSOUD BORHANI, Laboratory for Physical Sciences, XUEDONG HU, SUNY at Buffalo — We derive a generalized form of the Electric Dipole Spin Resonance (EDSR) Hamiltonian in the presence of the spin-orbit interaction for single spins in an elliptic quantum dot (QD) subject to an arbitrary (in both direction and magnitude) applied magnetic field. We predict a nonlinear behavior of the Rabi frequency as a function of the magnetic field for sufficiently large Zeeman energies, and present a microscopic expression for the anisotropic electron g-tensor. Similarly, an EDSR Hamiltonian is devised for two spins confined in a double quantum dot (DQD). Finally, we calculate two-electron-spin relaxation rates due to phonon emission, for both in-plane and perpendicular magnetic fields. Our results have immediate applications to current EDSR experiments on nanowire QDs, g-factor optimization of confined carriers, and spin decay measurements in DQD spin-orbit qubits.

¹NSA, ARO, DARPA QuEST

4:06PM L29.00007 Spin coherence in Multi-electron GaAs double dots¹, ANDREW P. HIGGINBOTHAM, FERDINAND KUEMMETH, CHRISTIAN BARTHEL, CHARLES M. MARCUS, Department of Physics, Harvard University, MICAH P. HANSON, ARTHUR C. GOSSARD, Materials Department, University of California, Santa Barbara — Experimental investigation of spin manipulation and readout in multi-electron double quantum dots is reported. For occupations of order 10 electrons, spin blockade in both transport and pulsed-gate measurements is identified. Exchange rotations, dynamical decoupling, S/T+ beamsplitter experiments, and single-shot readout can all be implemented similar to the single-electron case. These demonstrations are relevant for the practical operation and scaling of GaAs spin qubits.

¹Support from IARPA/MQCO, DARPA/QuEST, DOE SCGF, NSF-MWN, and Harvard University is acknowledged.

4:18PM L29.00008 Fast Exchange Oscillations in Quantum Dot Spin Qubits, SHANNON HARVEY, MICHAEL SHULMAN, OLIVER DIAL, Harvard University, HENDRIK BLUHM, RWTH Aachen University, VLADIMIR UMANSKY, Weizmann Institute of Science, AMIR YACOBY, Harvard University — The exchange splitting, J , is an important tool in semiconductor spin qubits, as it can drive both single qubit rotations and two qubit entangling operations. However, qubits operating under exchange can be dephased by electrical noise, as J is a function of the local electrostatic environment. We investigate the exchange interaction in a singlet-triplet qubit created in double quantum dot by measuring exchange oscillations ranging in frequency over three orders of magnitude. In particular, we resolve exchange oscillations at frequencies up to 30GHz, where both electrons occupy the same quantum dot. Here, J saturates to approximately the singlet-triplet splitting, and no longer depends on the electrostatic environment. In this regime exchange oscillations are insensitive to electrical noise. Since semiconductor spin qubits are usually limited by dephasing, these potentially dephasing-free exchange oscillations offer a new regime for studying quantum control in spin qubits.

4:30PM L29.00009 Coherent electrical manipulation of a quantum dot qubit, MATTHEW POOLEY, RAJ PATEL, ANTOINE BOYER DE LA GIRODAY, IAN FARRER, CHRISTINE NICOLL, DAVID RITCHIE, Cavendish Laboratory, Cambridge University, J. J. Thomson Avenue, Cambridge, CB3 0HE, UK, ANTHONY BENNETT, MARK STEVENSON, MARTIN WARD, NIKLAS SKOLD, ANDREW SHIELDS, Toshiba Research Europe Limited, Cambridge Research Laboratory, 208 Science Park, Milton Road, Cambridge, CB4 0GZ, UK — We demonstrate the initialization and coherent manipulation of a spin-based qubit in a InAs quantum dot (QD), implementing a spin-flip gate with a fidelity of 97%. We will discuss new measurements on the effect of fluctuating nuclear magnetic field which have implications on state initialisation, operation fidelity, and qubit storage time. An exciton spin-state is initialised by absorption of an incident polarised photon. The exciton state of QDs has two spin-eigenstates separated by fine-structure splitting (s), which can be manipulated using applied electric field. Superposition spin-states precess around the Bloch-sphere with an angular frequency $|s|/\hbar$. An electric field is used to vary the rate and axis of the spin-state precession, and thus control the time-evolution of the stored qubit. Nuclear magnetic field fluctuations induce additional random variations in s , the effects of which we investigate to understand the ideal initialisation and storage regime. Subsequent radiative decay maps the spin of the exciton onto the polarisation of the emitted photon. These results demonstrate a photon-spin interface, which has potential applications in scalable optical quantum computing schemes.

4:42PM L29.00010 Fabrication and Characterization of Si MOS-Based Triple Quantum Dot Devices, HONG PAN, HONGWEN JIANG, University of California, Los Angeles, RUSKO RUSKOV, CHARLES TAHAN, Laboratory for Physical Sciences, UNIVERSITY OF CALIFORNIA, LOS ANGELES COLLABORATION, LABORATORY FOR PHYSICAL SCIENCES COLLABORATION — We have fabricated electrostatically defined, few electron triple quantum dot (TQD) devices in a silicon metal-oxide-semiconductor structure. The devices show good electrical stability and gate controllability. We have obtained charge stability diagrams for identifying the charging states of the TQD. In this talk, we will describe the technical challenges in the TQD fabrication and present the experimental results of tuning three dots into a resonance. We will also discuss the prospect of these devices to encode a spin qubit that uses exchange interaction alone and possible ways to perform coherent manipulations within the tunable range of inter-dot tunneling of these devices. The work is supported by ARO.

4:54PM L29.00011 Pairwise control of exchange interaction between individual spins in a triple quantum dot, G. GRANGER, SERGEI STUDENIKIN¹, G. AERS, A. KAM, P. ZAWADZKI, L. GAUDREAU, R. WASILEWSKI, National Research Council of Canada, M. PIORO-LADRIERE, University of Sherbrooke, A. SACHRAJDA, National Research Council of Canada — The original spin qubit proposal [1] suggested a linear array of spins for quantum computations and the exchange interaction for 2 qubit operations. An essential component of the proposal was the ability to control pairwise the exchange interaction between neighbouring pairs of spins. In this work we experimentally demonstrate such a pairwise control of the exchange interaction between three spins localized in a triple quantum dot (TQD) device. The TQD potential was formed using electrostatic lateral split-gate technology on a GaAs/GaAlAs heterostructure with a high-mobility two-dimensional electron gas [2]. We employ fast pulsing technique based on the Landau-Zener-Stueckelberg (LZS) approach for creating and manipulating coherent superpositions of three spin quantum states [3]. We show that we are able to maintain coherence when increasing the exchange coupling of one spin with another while simultaneously decreasing its coupling with the third.

[1] D. Loss, and D.P. DiVincenzo, Phys. Rev. A57, 120-126 (1998).

[2] L. Gaudreau, et al., Appl. Phys. Lett. v.95, 193101 (2009)

[3] J.R. Petta, H. Lu, and A.C. Gossard, Science v.327, 669-672 (2010).

¹Presenting this work

5:06PM L29.00012 Entanglement of Two Singlet-Triplet Qubits¹, MICHAEL SHULMAN, OLIVER DIAL, SHANNON HARVEY, Harvard University, HENDRIK BLUHM, RWTH Aachen University, VLADIMIR UMANSKY, Weizmann Institute of Science, AMIR YACOBY, Harvard University — Semiconductor spin qubits are promising candidates for quantum computation because of their potential for scalability. However, their weak interaction with the environment, which leads to long coherence times, makes two-qubit operations challenging. We perform the first two-qubit operation between singlet-triplet qubits. The two qubit operation relies on the capacitive coupling between two adjacent qubits to generate a CPHASE gate. In order to combat low frequency noise we use a dynamically decoupled gate that maintains the two-qubit coupling while decoupling each qubit from its fluctuating environment. Using state tomography we measure the two-qubit density matrix and show that the operation produces the expected state. We extract a concurrence of 0.44 and a Bell state fidelity of 0.72, each providing definitive proof of entanglement.

¹This work is supported by IARPA, the NSA, and HRL.

5:18PM L29.00013 Two-axis Control and Readout of an Exchange-Only Spin Qubit in a GaAs Triple Quantum Dot¹, J. MEDFORD, Harvard University, J.M. TAYLOR, Joint Quantum Institute, NIST, B.D. ARMSTRONG, Harvard University, D.P. DIVINCENZO, RWTH Aachen, C.M. MARCUS, Harvard University, Niels Bohr Institute, University of Copenhagen, H. LU, A.C. GOSSARD, Materials Department, University of California, Santa Barbara — The initialization, full control, and readout of a GaAs triple quantum dot exchange qubit is demonstrated. Appropriate depletion gate design has enabled control and single-shot readout along multiple Bloch sphere axes in a three electron device. Rotations around both non-orthogonal control axes are projected along three separate Bloch sphere axes, and quality factors ($Q \equiv \omega/T_2^*$) of 500 are observed. Finally, we analyze decoherence and dynamical decoupling schemes unique to this system.

¹Support from IARPA MQCO, DARPA QuEST, and NSF Materials World Network.

Tuesday, February 28, 2012 2:30PM - 5:42PM – Session L30 GQI: Focus Session: Topologically Protected Qubits I 259B

2:30PM L30.00001 Non-Abelian Braiding of Lattice Bosons, ELIOT KAPIT, PAUL GINSPARG, ERICH MUELLER, Cornell University — We report on a numerical experiment in which we use time-dependent potentials to braid non-abelian quasiparticles. We consider lattice bosons in a uniform magnetic field within the fractional quantum Hall regime, where ν , the ratio of particles to flux quanta, is near $1/2$, 1 or $3/2$. We introduce time-dependent potentials which move quasiparticle excitations around one another, explicitly simulating a braiding operation which could implement part of a gate in a quantum computation. We find that different braids do not commute for ν near 1 and $3/2$, with Berry matrices respectively consistent with Ising and Fibonacci anyons. Near $\nu = 1/2$, the braids commute.

2:42PM L30.00002 Parafermion braid statistics in quasi-one-dimensional networks, DAVID CLARKE, JASON ALICEA, UC Irvine, KIRILL SHTENGEL, UC Riverside — One dimensional systems with Majorana zero modes at phase boundaries may be thought of as physical realizations of a discrete quantum wire model first put forth by Kitaev [1]. Proposed methods for braiding such Majorana fermions in one-dimensional wire networks [2] have greatly expanded the set of plausible avenues toward topological quantum computation. Recently, a generalization of the Kitaev model to parafermion modes has been developed.[3] Here, we describe the transport of such parafermion modes along the chain by the adiabatic transformation of the Hamiltonian, analogous to the transport of Majorana fermion modes. We determine the (braid) transformations of the ground state sector allowed by the adiabatic exchange of the parafermion modes in wire networks. We show that, as with Majorana fermions, none of the parafermion braid sets are universal for quantum computation. Certain parafermion chain models, unlike Majorana fermion systems, become universal with the addition of measurement operations. We discuss possible physical realizations of the parafermion models.

[1] J Alicea et al., Nature Physics 7, 412-417 (2011)

[2] A. Kitaev, arXiv:cond-mat/0010440v2

[3] P. Fendley, unpublished

2:54PM L30.00003 Ettingshausen effect due to Majorana modes, CHANG-YU HOU, UC Riverside and Caltech, KIRILL SHTENGEL, University of California, Riverside, GIL REFAEL, California Institute of Technology, PAUL GOLDBART, Georgia Institute of Technology — Due to the presence of Majorana fermions (zero mode) at the vortex core of topological superconductor, each vortex carries an extra entropy $s_0 = k_B \ln[2]/2$ that is independent of temperature. Utilizing this special property of Majorana fermions, one can show that the edge states appearing at the edge of a topological superconductor can be cooled (heated) due to the motion of the vortices. We will also discuss possible experimental setups to observe this cooling thermoelectric mechanism tied with the extra entropy carried by the vortex.

3:06PM L30.00004 Quantum information transfer between topological and spin qubit systems, MARTIN LEIJNSE, KARSTEN FLENSBERG, Niels Bohr Institute and Nano-Science Center, University of Copenhagen — In this talk I will introduce a method to coherently transfer quantum information, and to create entanglement, between topological qubits and conventional spin qubits. The transfer method uses gated control to transfer an electron (spin qubit) between a quantum dot and edge Majorana modes in adjacent topological superconductors. Because of the spin polarization of the Majorana modes, the electron transfer translates spin superposition states into superposition states of the Majorana system, and vice versa. Furthermore, I will discuss how a topological superconductor can be used to facilitate long-distance quantum information transfer and entanglement between spatially separated spin qubits.

References:

M. Leijnse, K. Flensberg, PRB 84, 140501(R) (2011)

M. Leijnse, K. Flensberg, PRL, in print, arXiv:1107.5703

3:18PM L30.00005 Braiding anyons and communication between topological and non-topological systems¹, HAITAN XU, JACOB TAYLOR, JQI, University of Maryland-College Park and NIST — Quasi-particles with non-Abelian statistics are intriguing in both fundamental and applied physics. Here we propose a “proof of principle” experimental setup for braiding anyons and observing non-Abelian statistics using nearest-neighbor spin interactions inspired by the Kitaev honeycomb model. We also show an explicit method for teleportation between the topological and non-topological systems.

¹This work is supported by the NSF through the JQI Physics Frontier Center.

3:30PM L30.00006 Electrical manipulation of Majorana Fermions in an interdigitated superconductor-ferromagnet device¹, SHU-PING LEE, California Institute of Technology, JASON ALICEA, University of California, Irvine, GIL REFAEL, California Institute of Technology — We show that a topological phase supporting Majorana fermions can form in a 2DEG adjacent to an interdigitated superconductor-ferromagnet structure. An advantage of this setup is that the 2DEG can inherit the required Zeeman splitting and superconductivity from a single interface, allowing one to utilize a wide class of 2DEG's including the surface states of bulk InAs. We demonstrate that the interdigitated device supports a robust topological phase when the finger spacing λ is smaller than the Fermi wavelength λ_F . In this regime the electrons effectively see a “smeared” Zeeman splitting and pairing field despite the interdigitation. The topological phase survives even in the opposite limit $\lambda < \lambda_F$, though with a reduced bulk gap. We also describe how to electrically generate a vortex in this setup to trap a Majorana mode, which can be detected through edge tunneling spectroscopy.

¹National Science Foundation grant DMR-1055522, and IQIM

3:42PM L30.00007 Interacting topological phases in multiband nanowires¹, ROMAN LUTCHYN, Microsoft Research, Station Q, University of California, Santa Barbara, CA 93106, MATTHEW P.A. FISHER, Department of Physics, University of California, Santa Barbara, California 93106 — We show that semiconductor nanowires coupled to an s-wave superconductor provide a playground to study effects of interactions between different topological superconducting phases supporting Majorana zero-energy modes. We consider quasi-one dimensional system where the topological phases emerge from different transverse subbands in the nanowire. In a certain parameter space, we show that there is a multi-critical point in the phase diagram where the low-energy theory is equivalent to the one describing two coupled Majorana chains. We study effect of interactions as well as symmetry-breaking perturbations on the topological phase diagram in the vicinity of this multi-critical point. Our results shed light on the stability of the topological phase around the multi-critical point and have important implications for the experiments on Majorana nanowires.

¹We acknowledge support from the National Science Foundation through grant DMR-1101912 (M.P.A.F.)

3:54PM L30.00008 Magnetic Control of Majorana Edge Modes in Topological Insulator-Ferromagnet-Superconductor Heterostructures, XIAOTING ZHOU, CHEN FANG, Purdue University, WEI-FENG TSAI, National Sun Yat-sen University, JIANGPING HU, Purdue University — A surface of a strong 3D topological insulator (TI) doped with ferromagnetic atoms can be spin-polarized and similar to a 2D quantum anomalous Hall state. If an s-wave superconductivity can be induced by proximity effect on such a surface, a 2D topological superconducting phase is obtained. If we consider a TI-ferromagnet(FM)-superconductor(SC) heterostructure, a 2D time-reversal symmetry breaking topological superconducting (TSC) phases with Majorana edge mode(s) will be realized. We demonstrate that the existence of the edge modes critically depend on the combination of the directions and magnitudes of spin polarization on all surfaces, and that a model describing the states on only one surface is insufficient. We find that the number, the positions and the chirality of these edge modes corresponding to various TSC phases can be engineered by controlling the ferromagnetism on different surfaces. Our results are obtained by self-consistently solving for the edge modes in a 3D lattice model for topological insulator in contact with an s-wave BCS superconductor. We also offer an analysis to illustrate the underlying physics, using an effective 2D theory for the surface states.

4:06PM L30.00009 Self-consistent Study of Majorana Fermions on a Topological Insulator Surface π Junction, MAHMOUD LABABIDI, ERHAI ZHAO, George Mason University — It has been proposed that a Josephson π junction that resides on the 2D surface of a 3D topological insulator (TI) is host to the Majorana fermion. We present a microscopic study of the π junction TI surface through self-consistent calculations with the Bogoliubov-de Gennes equation. We calculate the order parameter, the singlet correlation function along with the energy spectrum, local density of states, and the spectral function. We also show the evolution of the energy dispersion of Majorana fermion as a function of the TI chemical potential.

4:18PM L30.00010 Unpaired Majorana fermions in a layered topological superconductor¹, BABAK SERADJEH, Indiana University, Bloomington, EYTAN GROSFELD, Ben Gurion University — We study the conditions for the existence of unpaired Majorana modes at the ends of vortex lines or the side edges of a layered topological superconductor. We show that the problem is mapped to that of a general Majorana chain and extend Kitaev's condition for the existence of its nontrivial phase by providing an additional condition when a supercurrent flows in the chain. Unpaired Majorana bound states may exist in a vortex line that threads the layers if the spin-orbit coupling has certain in-layer components but, interestingly, only if a nonzero supercurrent is maintained along the vortex. We discuss the exchange statistics of vortices in the presence of unpaired Majorana modes and comment on their experimental detection.

¹Work supported by and performed at ICMT of UIUC, and published in Phys. Rev. B 83, 174521 (2011).

4:30PM L30.00011 Quantum point contact as a probe of a topological superconductor, MICHAEL WIMMER, ANTON AKHMEROV, JAN DAHLHAUS, CARLO BEENAKKER, Instituut-Lorentz, Universiteit Leiden, The Netherlands — We calculate the conductance of a ballistic point contact to a superconducting wire, produced by the s-wave proximity effect in a semiconductor with spin-orbit coupling in a parallel magnetic field. The conductance G as a function of contact width or Fermi energy shows plateaus at half-integer multiples of $4e^2/h$ if the superconductor is in a topologically nontrivial phase, supporting Majorana fermions. In contrast, the plateaus are at the usual integer multiples in the topologically trivial phase without Majorana fermions. Disorder destroys all plateaus except the first, which remains precisely quantized in the case of a topological superconductor, consistent with previous results for a tunnel contact. The advantage of a ballistic contact over a tunnel contact as a probe of the topological phase is the strongly reduced sensitivity to finite voltage or temperature.

4:42PM L30.00012 Genetic braid optimization for topological quantum computation, R.B. McDONALD, Department of Physics & Astronomy, Texas A&M University, H.G. KATZGRABER, Department of Physics & Astronomy, Texas A&M University, Department of Physics, ETH Zurich — In topologically-protected quantum computation quantum gates can be carried out by adiabatically braiding quasiparticles in two space dimensions, reminiscent of entangled world lines. Bonesteel *et al.* [Phys. Rev. Lett. 95, 140503 (2005)] showed recently how to find braids that yield a universal set of quantum gates. Mathematically, the problem of executing a gate becomes that of finding a product of the matrices in that set that approximates the gate, up to an error. To date efficient methods to compute these gates only strive to optimize for accuracy. We explore the possibility of using evolutionary (genetic) algorithms to efficiently find optimal braids while allowing the user to optimize for the relative utilities of accuracy and length. Furthermore, when optimizing for error only, the method can efficiently produce braids of error $\sim 10^{-6}$ outperforming brute force approaches.

4:54PM L30.00013 Quantum memory on topological spin glass, JEONGWAN HAAH, Institute for Quantum Information and Matter, Caltech, SERGEY BRAVYI, IBM Watson Research Center — We show that any topologically ordered local stabilizer model of spins in three dimensional lattices that lacks string logical operators can be used as a reliable quantum memory against thermal noise. It is shown that any local process creating a topologically charged particle separated from other particles by a distance R must cross an energy barrier of height $c \log R$. This property makes the model glassy. We devise an efficient decoding algorithm that should be used at the final read-out, and prove a lower bound on the memory time until which the fidelity between the outcome of the decoder and the initial state is close to 1. The memory time increases as $L^{c\beta}$ where L is the system size and β the inverse temperature, as long as $L < L^* \sim e^{\beta}$. Hence, the optimal memory time scales as $e^{c\beta^2}$. Our bound applies when the system interacts with thermal bath via a Markovian master equation. We give an example of a strictly local stabilizer code that satisfies all of our assumptions. We numerically verify for this example that our bound is tight up to constants.

5:06PM L30.00014 3D local qubit quantum code without string logical operator, ISAAC KIM, Institute of Quantum Information and Matter — Recently Haah introduced a new class of local quantum error correcting code embedded on a cubic lattice without any string logical operator. We present new codes with similar properties by relaxing the condition on the local particle dimension. The resulting code is well-defined when the local Hilbert space dimension is prime. These codes can be divided into two different classes: the local stabilizer generators are either symmetric or antisymmetric with respect to the inversion operation. We lower bound the number of encoded qudits by computing the commutation relation between the logical operators confined on a plane.

5:18PM L30.00015 Topological Decoding through Artificial Confinement¹, GUILLAUME DUCLOS-CIANCI, DAVID POULIN, Université de Sherbrooke — 2D topological stabilizer codes have attracted a lot of attention in recent years for two main reasons. First, they provide exactly solvable models which exhibit topological order and anyonic excitations. Second, they naturally lead to quantum stabilizer error-correcting codes having macroscopic minimum distance. Although these codes are robust at zero temperature, quasi-particles appear and freely diffuse in the system at any finite temperature. If this diffusion is unchecked, errors will occur. Consequently, active error-correction is needed. We want to propose a cellular automaton that would perform this correction. It would "manually" confine the quasi-particles by simulating artificial attraction between them and moving them accordingly. We obtained encouraging preliminary results for error-correction and hope to generalize them to fault-tolerance.

5:30PM L30.00016 Andreev Bound states in One Dimensional Topological Superconductor with Broken Spatial Inversion Symmetry¹, XIONG-JUN LIU, KAI SUN, SANKAR DAS SARMA², Joint Quantum Institute and Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742 — We study the Andreev bound states (ABSs) at the Josephson junction of one dimensional topological superconductors (SC) when the spatial inversion symmetry (SIS) is broken. While in the absence of inversion symmetry, we show a hidden symmetry for the Bogoliubov de Gennes equations in the case of SC gap much smaller than Fermi energy in addition to the particle-hole symmetry, due to which the ABSs are predicted to carry irrational charge, with the charge value solely depending on the SIS breaking term, regardless of the details of the superconductor order parameter and whether the disorder scattering is present or not. We demonstrate that in the tunneling transport spectroscopy the irrationally charged ABSs are measured by the resonant differential tunneling conductance.

¹This work is supported by funding from JQI, NSF, PFC, Microsoft-Q, DARPA, and QUEST.

²Supervisor

Tuesday, February 28, 2012 2:30PM - 5:30PM –

Session L31 DMP: Focus Session: Topological Insulators: Synthesis and Transport - Magnetism

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2:30PM L31.00001 Thin films of magnetically doped topological insulators, CUI-ZU CHANG, Dept. of Physics, Tsinghua University, China — The interplay between the Dirac surface state and ferromagnetic order in topological insulators can lead to a number of very exotic quantum phenomena. To observe the quantum phenomena such as quantized anomalous Hall (QAH) effect in magnetically doped topological insulators, the materials are required to be in the form of thin film with tunable chemical potential and carrier-independent ferromagnetism. In this talk, I will report our recent progress in molecular beam epitaxy growth, chemical potential tuning and electronic properties of the magnetically doped topological insulator thin films. By Cr doping, we have realized both n-type and p-type conductivity in $(\text{Bi}_x\text{Sb}_{1-x})_2\text{Te}_3$ thin films. Remarkably their ferromagnetism was found independent of the type and concentration of carriers. Moreover, the anomalous Hall effect is significantly enhanced at low carrier concentration regime, with the anomalous Hall angle reaching an unusually large value of 0.2 and the zero field Hall resistance reaching one quarter of the quantum resistance (h/e^2). These findings pave the way to ultimately observing the QAH effect and other quantum effects in magnetic topological insulators.

3:06PM L31.00002 Proximity induced ferromagnetism at the interface between a topological insulator (TI) Bi_2Se_3 and a ferromagnetic insulator (FI)¹, PENG WEI, FERHAT KATMIS, Francis Bitter Magnet Lab, MIT, Cambridge, MA, BADIH ASSAF, DON HEIMAN, Physics Department, Northeastern University, Boston, MA, PABLO JARILLO-HERRERO, Physics Department, MIT, Cambridge, MA, JAGADEESH MOODERA, Francis Bitter Magnet Lab and Physics Department, MIT, Cambridge, MA — The ferromagnetic phase of the surface states of a TI is predicted to carry many exotic properties, for example quantum anomalous Hall effect, magnetic monopole, and magneto-electric effects etc. In our study, we explore this novel phase utilizing the proximity induced exchange splitting to introduce ferromagnetism close to the surface of the Bi_2Se_3 film. High quality Bi_2Se_3 thin films were grown using molecular-beam-epitaxy, and in-situ deposited the ferromagnetic insulator (FI) EuS over this film. Magnetization measurements demonstrated a magnetic moment of more than $7\mu_B$ per Eu^{2+} ion (bulk value), and reaching up to $11\mu_B$ per Eu^{2+} ion for 1nm thick EuS film, showing the unambiguous existence of excess ferromagnetism. The transport studies of these TI/FI bilayers unveiled a clear switching behavior of the magnetoresistance in the Bi_2Se_3 film. There was significant temperature dependence seen in both MR and the coercivity. Due to the near range nature of the exchange interactions, these extra magnetic moments and the MR results are attributed to come from the induced ferromagnetism at the Bi_2Se_3 surface.

¹Work supported by ONR grant N00014-09-1-0177, NSF grant DMR 0504158 and NSF DMR 08-19762 (CMSE - Initiative 2)

3:18PM L31.00003 Possible transport evidence for a surface state gap in a magnetically doped topological insulator, D.M. ZHANG, A. RICHARDELLA, D.W. RENCH, A. KANDALA, T.C. FLANAGAN, P. SCHIFFER, N. SAMARTH, Dept. of Physics, Penn State University, University Park 16802, S.-Y. XU, H. BEIDENKOPF, A. YAZDANI, M.Z. HASAN, Dept. of Physics, Princeton University, Princeton, NJ 08544, A.L. YEATS, B.B. BUCKLEY, P. KLIMOV, D.D. AWSCHALOM, Dept. of Physics, University of California, Santa Barbara CA 93016 — We report magnetoresistance measurements in thin films of a magnetically doped topological insulator $\text{Bi}_{2-x}\text{Mn}_x\text{Se}_3$ synthesized by molecular beam epitaxy. We observe a crossover from positive magnetoresistance to negative magnetoresistance at low temperature ($T \lesssim 15$ K), accompanied by onset of ferromagnetic signatures (hysteresis and anisotropic magnetoresistance). The observations are consistent with the prediction of a transition of diffusive quantum transport from the symplectic to the unitary class due to a magnetically induced surface state gap. This interpretation is supported by the observation of strongly suppressed surface states at the Dirac point in angle-resolved photoemission spectroscopy. We use the magneto-optical Kerr effect, anomalous Hall effect, SQUID magnetometry, electron microscopy and scanning tunneling microscopy to clarify the source of the ferromagnetism in these samples. Supported by DARPA, ONR and NSF-MRSEC.

3:30PM L31.00004 Magnetoconductance crossover and non-linear Hall effect in MBE-grown Cr-doped $\text{Bi}_2\text{Te}_2\text{Se}$ ¹, BADIH A. ASSAF, Physics Dept. Northeastern University, PENG WEI, FERHAT KATMIS, JAGADEESH S. MOODERA, MIT, Francis Bitter Magnet Lab, DON HEIMAN, Physics Dept. Northeastern University — Recent predictions have shown that the magnetoconductance (MC) of a topological insulator should show a crossover from negative MC to positive MC when time-reversal symmetry is broken [1]. Observations of this crossover have been reported in 3 QL thick Cr- Bi_2Se_3 [2] in the quasi-2D regime where surface hybridization is not negligible. We report magneto-transport results on 15 QL thick Cr-doped and undoped $\text{Bi}_2\text{Te}_2\text{Se}$ films grown on Si (111) substrates by MBE. The undoped film exhibits weak anti-localization at low temperatures. In the Cr-doped film, a crossover from negative to positive MC is observed versus temperature at $T=12$ K. SQUID measurements show that the sample is ferromagnetic in this temperature range. In addition, a non-linear Hall voltage is observed despite the large bulk carrier concentration. This paves the way for further experiments on $(\text{Bi,Cr})_2\text{Te}_2\text{Se}$ in our search for the quantum anomalous Hall effect. [1] H.Z. Lu et al. Phys. Rev. Lett. **107**, 076801(2011). [2] M.Liu et al. arXiv 1103.3353(2011).

¹Work supported by NSF-DMR-097007, ONR N00014-09-1-0177 and NSF-DMR-08-19762 (CMSE initiative 2)

3:42PM L31.00005 Ferromagnetism in chromium doped topological insulator thin films and nanoplate crystals¹, ZHIYI CHEN, LUKAS ZHAO, INNA KORZHOVSKA, HAIMING DENG, LIMIN HUANG, City College of New York - CUNY, SIMONE RAOUX, JEAN JORDAN-SWEET, STEPHEN O'BRIEN, IBM Research - Yorktown, LIA KRUSIN-ELBAUM, City College of New York - CUNY — The surface states of topological insulators are protected by time-reversal symmetry. Introducing magnetic impurities should break this symmetry and open a gap in the otherwise gapless surface states. Recent first-principle calculations predict that when topological insulators are doped with transition metal elements, such as Cr or Fe, a *magnetically ordered* insulating state will form – a state that in thin (quasi-2D) samples may support a quantized Hall conductance. Here we report on electrical and magnetic characterization of thin Cr doped topological insulators: Sb₂Te₃ nanoplate crystals and ~ 50 nm thin films of Bi₂Te₃. Electrical contacts to samples were lithographically defined, with *rf* sputtered films grown on pre-patterned substrates. Low-temperature in-plane resistivity, Hall, and magnetization measurements were performed in up to 5 T magnetic fields. For 5 at% Cr content, a distinct ferromagnetic hysteretic response is observed at temperatures below 10 K. Hysteretic loops, also observed in Hall resistivity, indicate low-*T* coercive fields of the order of 0.5 T. Correlation of transport and magnetic measurements indicating anomalous Hall effect, and strong dependence on dopant concentration and sample thickness will be presented.

¹Supported in part by NSF-DMR-1122594.

3:54PM L31.00006 Ferromagnetism in vanadium doped thin films of a topological insulator Bi₂Te₃¹, LUKAS ZHAO, ZHIYI CHEN, INNA KORZHOVSKA, HAIMING DENG, City College of New York - CUNY, SIMONE RAOUX, JEAN JORDAN-SWEET, IBM Research - Yorktown, MYRIAM SARACHIK, LIA KRUSIN-ELBAUM, City College of New York - CUNY — Recent first-principle calculations predict a new class of ferromagnetic systems that are distinctly different from the conventional dilute magnetic semiconductors. A novel ferromagnetic topological insulator (ferro-TI) state can be obtained when topological insulator are doped with certain transition metal elements. In the the quasi-2D limit these ferro-TIs are expected to support a quantized anomalous Hall effect. Here we report on electrical and magnetic characterization of vanadium doped thin (~ 50 nm) films of a topological insulator Bi₂Te₃. Films were grown by *rf* sputtering on S₃N₄/Si substrates with lithographically pre-patterned contact pads. Low-temperature in-plane and Hall resistivity measurements were performed in magnetic fields up to 5 T fields. We find that below 100 K, V-doped films display *negative linear magnetoresistance*, which at lower temperatures becomes hysteretic. Hall resistivity is also hysteretic, suggesting an unusual ferromagnetic ordering below 10 K. Moreover, V-doping turns the *p*-type conduction in as-grown films into *n*-type. The doping and thickness dependence of these effects will be discussed.

¹Supported in part by NSF-DMR-1122594

4:06PM L31.00007 Controllable ferromagnetism of iron doped topological insulator, SHAN QIAO, ZHEN LIU, FUHAO JI, BIN LI, FUCHUN XI, fudan university, K. KURODA, MAO YE, K. MIYAMOTO, A. KIMURA, Hiroshima University — The higher than room temperature ferromagnetism was found in iron doped Bi₂Se₃. Samples generated by different processes have different magnetic characters. The Curie temperature is independent on iron concentration which against all discovered dilute magnetic systems. EXAFS observations show that the local structure of iron in samples with paramagnetic character is complex. On the contrary, that with ferromagnetic character is very simple that the iron atoms make up small single atom, dimer or trimer structures and these structures randomly distributed in Bi₂Se₃ crystal. The ferromagnetism can be enhanced or suppressed by the shift of Fermi edge by co-doping of Mg and Fe to Bi₂Se₃ crystal. The less than 3 atoms small structure cannot have room temperature ferromagnetism, so we believe that the higher than room temperature controllable ferromagnetism is intrinsic character of iron doped topological insulator.

4:18PM L31.00008 In-plane anisotropy of Fe atoms on Bi₂Se₃(111), T. WEHLING, A. LICHTENSTEIN, 1. Institut für Theoretische Physik I, Universität Hamburg, Germany, J. HONOLKA, S. STEPANOW, K. KERN, Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany, V. SESSI, N. BROOKES, ESRF, Grenoble, France, J. MI, B.B. IVERSEN, P. HOFMANN, iNANO, Aarhus University, Denmark, A.A. KHAJETOORIAN, J. WIEBE, T. SCHLENK, R. WIESENDANGER, Institute for Applied Physics, Universität Hamburg, Germany — Topological insulators exhibit a linearly dispersing gapless topological surface state where both the spin and momentum degrees of freedom are locked. The topological nature of this state results in interesting effects such as suppression of back-scattering. Recently, the robustness of these surface states against magnetic order has come under heavy investigation. Here, we explore the magnetic properties of single Fe adatoms on the Bi₂Se₃ surface, in the coverage range < 1%, with combined non-local x-ray magnetic circular dichroism techniques and local low temperature scanning tunneling spectroscopy. We reveal that the adatoms heavily relax into the surface and exhibit a magnetic easy axis within the surface-plane, contrary to recent reports. Furthermore, we demonstrate, using *ab-initio* approaches, how the easy axis can reorient from out-of-plane to in-plane when considering the interplay of Coulomb interactions, spin-orbit coupling, and dynamic hybridization effects.

4:30PM L31.00009 Topological insulators with magnetic impurities in the bulk, GILAD ROSENBERG, MARCEL FRANZ, University of British Columbia — We show that a three dimensional topological insulator with magnetic impurities could have a regime where the surface is magnetically ordered but the bulk is not. This is in contrast to conventional materials where bulk ordered phases are typically more robust than surface ordered phases. This difference originates from the topologically protected gapless surface states characteristic of topological insulators. We study the problem using a mean field approach, using two concrete models that give the same qualitative result, with some interesting differences. This work could help explain recent experimental results showing the emergence of a spectral gap in the surface state of Bi₂Se₃ doped with Mn or Fe atoms, but with no measurable bulk magnetism.

[1] Massive Dirac Fermion on the Surface of a Magnetically Doped Topological Insulator, Y. L. Chen *et al.*, Science **329**, 659-662 (2010).

4:42PM L31.00010 Interface-driven magnetism in topological insulators Bi₂Te₃ and Bi₂Se₃¹, KYUNGWHA PARK, Virginia Tech, Blacksburg, VA 24061 — Topological insulators (TIs) draw great attention due to their unique quantum properties and applications. TIs possess metallic surface states within band gaps induced by spin-orbit coupling (SOC), and they allow only an odd number of Dirac cones in dispersion of the surface states at a given surface. Novel physical phenomena and applications proposed including TIs, critically rely on stability and topological nature of the surface states when TIs are interfaced with other types of materials. Despite many studies on TIs, it still remains unclear how the surface states of TIs behave in contact with other materials. In this talk, we present our study of an effect of interfaces on the surface states of TIs Bi₂Te₃ and Bi₂Se₃, using density-functional theory including SOC self-consistently. We simulate interfaces using adsorption layers on TI films in an asymmetric fashion. We discuss unexpected results on stability and topological nature of the surface states, as well as changes in their spin structure and energy gaps at zero momentum. Our findings reveal importance of interfaces and a possibility of engineering new hybrid TI structures using adsorption layers.

¹Supported by NSF DMR-0804665

4:54PM L31.00011 Magnetic structure of magnetic semiconductor NdBiPt studied by elastic neutron diffraction, ROGER MUELLER, ALEXANDRE DESILETS-BENOIT, ANDREA BIANCHI, LUC LAPOINTE, University of Montreal, ZAHRA YAMANI, Canadian Neutron Beam Centre National Research Council, MICHEL KENZELMANN, Paul Scherrer Institut — We report a study of the magnetic structure of the antiferromagnetic (AFM) half-Heusler NdBiPt via neutron scattering. NdBiPt exhibits an AFM transition at $T_N = 2.2\text{K}$ with an ordered moment of $3.6\mu_B$ per Nd atom, as determined from magnetization measurement. The insulating state of NdBiPt has been proposed to be a new class of a three dimensional topological insulator, which possesses surface states at step edges on facets, with properties that are analogous to those observed in quantum Hall states. However, this would require an orientation of the magnetic moments in the ordered state along the crystallographic direction [001]. Triple-axis neutron diffraction on a single crystal was used to study the magnetic order. We found that in the ordered state consists of a conventional two sublattice antiferromagnet with the spins oriented along [001] with very little fluctuations present close to T_N .

5:06PM L31.00012 Iron impurities on Sb (111) surface and their effects on topological surface state, JINHEE HAN, HYUNJUN LEE, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — We study iron impurities on Sb (111) surface and their effects on topological surface state by using an *ab-initio* pseudopotential density-functional method. We implemented the spin-orbit interaction into the SIESTA in a form of additional fully non-local projectors. To calculate electronic structure of topological surface states, we consider a slab of Sb using a supercell containing 20 atomic layers with experimental bulk Sb lattice parameters. We determine atomic positions of Fe impurities on Sb (111) surface by minimizing the total energy, and calculate surface band structures near the Fermi level. To find effects of the impurity on the surface states of Sb (111) surface, we simulate ARPES spectra as a function of impurity density on the surface. From the results, we find that Fe impurity states are present near Fermi level and they strongly interact with the surface states. This work was supported by the NRF of Korea (Grant Nos. 2009-0081204 and 2011-0018306) and KISTI Supercomputing Center (Project No. KSC-2011-C2-04).

5:18PM L31.00013 Impurities in Bi₂Se₃ topological insulator: *ab initio* calculation, TOME M. SCHMIDT, ROBERTO H. MIWA, Universidade Federal de Uberlândia, ADALBERTO FAZZIO, Universidade de São Paulo — Topological insulators are materials that have a bulk as an ordinary insulator but have protected conducting states on their surface. The surface states with an odd number of Dirac cones are robust against time-reversal invariant perturbation. However the interaction of magnetic impurities with the Dirac fermions can break time reversal symmetry open up a surface band gap. In this work we investigate the magnetic anisotropy and spin-texture of Co impurities embedded at the interlayer vdW spacings and onto the topmost Se network of the topological insulator Bi₂Se₃. The interaction of the magnetic impurity with the surface spin texture break time reversal symmetry, opening up a surface band gap. For Co atom adsorbed onto the surface, the net magnetic moment is aligned perpendicular to the surface plane, with anisotropy energy of $6\sim\text{meV}$. On the other hand for the Co impurity at the vdW interlayers, the net magnetic moment is aligned in-plane. While pristine Bi₂Se₃ presents helical spin-texture in the massless surface Dirac cone and states resonant within the valence band, the presence of Co impurity reduces the planar spin helicity of now massive Dirac fermions. On the other hand O impurities do not break the protected surface Dirac cones, but they move the position of the Dirac crossing upwards. Also we observe that there is an energy barrier for the O₂ molecule when it approximates to the Bi₂Se₃ surface, but atomic O inside the Bi₂Se₃ is more stable than the formation of O₂ molecules.

Tuesday, February 28, 2012 2:30PM - 5:30PM –
Session L32 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides
- Mechanisms of Ferroelectricity 261

2:30PM L32.00001 General Theory for the Ferroelectric Polarization Induced by Spin-Spiral Order, HONGJUN XIANG, Fudan University, ERJUN KAN, Nanjing University of Science and Technology, YUEMEI ZHANG, M.-H. WHANGBO, North Carolina State University, XINGAO GONG, Fudan University — Multiferroics display magnetic, polar and elastic order parameters simultaneously and hence present fascinating fundamental physics and potentially promising applications. The multiferroic phenomenon has been explained by several different models. However, none of them can correctly describe the ferroelectric polarization of triangular-lattice antiferromagnets induced by helical spin-spiral order. To resolve this problem, we develop a general theory for the ferroelectric polarization induced by spin-spiral order on the basis of symmetry considerations and then evaluate the coefficients needed to specify the general theory on the basis of density functional calculations. Our theory not only explains the ferroelectricity of triangular-lattice antiferromagnets driven by helical spin-spiral order, but also incorporates all known models of magnetic-order-driven ferroelectricity as special cases.

2:42PM L32.00002 Modeling functional piezoelectricity in perovskite superlattices with competing instabilities, CHARLES SWARTZ, XIFAN WU, Temple University — Multi-component Perovskite Superlattices (SLs) of the form ABO₃, provide a very promising avenue for the design of materials with multifunctional properties. Furthermore the interfaces of such multi-component SLs are home to competing anti-ferrodistortive and ferroelectric instabilities which can produce unexpected functionalities. However, at present first principles calculations exceeding more than 10 units cells, are particularly costly as they scale with the valence electrons as N^3 . We present a first-principles modeling technique that allows us to accurately model the piezoelectric strains of paraelectric/ferroelectric SLs, BaTiO₃/CaTiO₃ and PbTiO₃/SrTiO₃, under a fixed displacement field. The model is based on a maximally localized Wannier center layer polarization technique, as well as a truncated cluster expansion, that makes use of the fact that such PE/FE SLs have been shown to have highly localized ionic and electronic interface effects. The prediction of the piezoelectricity for a SL of an arbitrary stacking sequence will be demonstrated. We also use our model to conduct a systemic study of the interface effects on piezoelectric response in the above SLs paying special attention to a strong non-linear effect observed in Bulk SrTiO₃.

2:54PM L32.00003 Competing (anti-)ferrodistortive and ferroelectric instabilities in SrTiO₃ and layered La₂Ti₂O₇, ULRICH ASCHAUER, NICOLA SPALDIN, Materials Theory, ETH Zürich — We present first-principles calculations on the competition between antiferrodistortive (AFD) and ferroelectric instabilities in oxides. High temperature cubic SrTiO₃ is well known to undergo an AFD transformation at around 105 K. Further reducing the temperature shows a softening of the ferroelectric polar phonons, however the material remains incipient-ferroelectric with an overall paraelectric behavior. This behavior is believed to be linked to a suppression of the polar instability by the AFD one, the mechanism still being debated. Our calculations show that freezing in the AFD indeed reduces the polar instability. At the theoretical equilibrium angle, the material however still retains a polar instability with a double-well depth of $\sim 0.2\text{ meV}$ per SrTiO₃ unit, inline with the material being incipient-ferroelectric. A change in polar eigenvectors with increasing AFD rotation together with a decomposition of forces into long- and short-range components allows us to propose an underlying mechanism. We will further discuss a similar suppression mechanism observed in layered La₂Ti₂O₇, where conventional ferroelectricity is suppressed by ferrodistortive modes, these modes however still leading to improper ferroelectricity due to the layered structure.

3:06PM L32.00004 First Principles Study of Piezoelectricity in Improper Ferroelectrics, KEVIN GARRITY, KARIN RABE, Rutgers University — Piezoelectric materials are key components of many important technologies, and discovering materials with improved piezoelectric responses is a major goal of materials science. In particular, finding new mechanisms for piezoelectricity which allow for high piezoelectric coefficients, especially in lead-free materials, could have great technological impact. Recently, there has been a renewed interest in improper ferroelectrics, which are materials where a non-zero polarization is induced indirectly by the coupling of the polar distortion to non-polar unstable modes, frequently oxygen octahedral rotations. This mechanism for creating a polarization may also offer the possibility of increased coupling to strain, leading to high piezoelectric coefficients. Here, we use first principles density functional theory to investigate the mechanism of the piezoelectric response of $\text{Ca}_3\text{Ti}_2\text{O}_7$, an improper ferroelectric which we find to have large piezoelectric coefficients.

3:18PM L32.00005 Engineering polar perovskites from centric polyhedra building blocks, JAMES RONDINELLI, Drexel University, CRAIG FENNIE, Cornell University — Increasing demands for electric field-tunable electromagnetic (EM) materials has renewed interests in ferroelectricity and its coupling to EM properties in perovskite oxides. Using density functional computations combined with group theoretical methods, we detail the crystal-chemistry criteria that enable the rational design of new perovskite oxides displaying octahedral rotation-induced ferroelectricity—electric polarizations (P) without second-order Jahn-Teller cations from BO_6 building blocks. We show that interleaving two bulk perovskites to form an ordered and layered arrangement of A-site cations [chemical composition $(A, A')\text{B}_2\text{O}_6$] produces a new trilinear free energy term coupling BO_6 rotations to P . This symmetry rule combined with an energetic condition, describing the lattice dynamical properties of the bulk materials, enables the routine design of synthetic ferroelectric perovskites. We illustrate these guidelines and achieve sizeable electric polarizations in layered gallate and aluminate perovskites, i.e. bulk materials with no tendencies to ferroelectricity. Finally, we argue that this strategy could be exploited for the design of ferroelectricity in a variety of crystal classes exhibiting flexible cation–anion polyhedral frameworks.

3:30PM L32.00006 Crossover between hybrid improper ferroelectricity and proper ferroelectricity in layered perovskites, ANDREW MULDER, NICOLE BENEDEK, CRAIG FENNIE, School of Applied and Engineering Physics, Cornell University — Recent progress in designing materials with unconventional mechanisms of ferroelectricity has shown that nominally non-polar octahedral rotations can induce an electrical polarization in certain layered perovskites, e.g., the $n=2$ Ruddlesden-Popper $\text{Ca}_3\text{Mn}_2\text{O}_7$, and certain A-site ordered $\text{AA}'\text{B}_2\text{O}_6$ double perovskites. In these (what have recently been termed) hybrid improper ferroelectrics, two unstable octahedral rotations of different symmetries couple trilinearly with the polarization. A key question that is still unclear is what the consequences of this coupling are in determining whether these materials exhibit conventional proper ferroelectricity, as in $\text{SrBi}_2\text{Ta}_2\text{O}_9$, or something resembling improper ferroelectricity. In this talk we discuss this question of proper vs improper in $\text{A}_3\text{B}_2\text{O}_7$ layered perovskites. First we develop simple criteria for realizing this novel form of ferroelectricity based solely on the properties of the ABO_3 parent perovskites. Then we explore how composition and epitaxial strain lead to different ferroelectric behaviors arising from the same rotation-polarization coupling. Finally we show how strain can tune a single material between rotation-driven hybrid improper ferroelectricity and conventional proper ferroelectricity.

3:42PM L32.00007 Competition and cooperation between octahedral rotations and ferroelectricity in simple and layered ABX_3 perovskites, NICOLE BENEDEK, School of Applied and Engineering Physics, Cornell University — Researchers have been studying octahedral rotations in perovskites for over half a century. It is now known that such lattice distortions are generally driven by the coordination preferences of the A-site cation. The role of octahedral rotations in modulating the magnetic, electronic and orbital properties of perovskites has been elucidated and a set of empirical rules for rationalizing the structures of known materials and for predicting the structures of as yet unsynthesized materials has been established. Despite this progress, there remains a long-standing problem concerning octahedral rotations and ferroelectricity: there are very few ferroelectric ABX_3 perovskites with octahedral rotations. This has led to the widespread assumption that octahedral rotations compete with and suppress ferroelectricity. In this talk, I will describe our recent work on the interaction between ferroelectricity and octahedral rotations in simple and layered perovskites. Using a combination of Density Functional Theory and simple crystal chemical models, we have shown that in contrast to the common assumption, ferroelectricity and octahedral rotations do not always compete. In particular, I will discuss the manner in which rotations can actually induce ferroelectricity in ABX_3 perovskites and present strategies for designing new functional materials based on this mechanism. In a related direction, I will also discuss the role of layering in inducing hybrid improper ferroelectricity in some Ruddlesden-Popper phases and double perovskites. Our approach provides a chemically intuitive picture – one that combines first-principles lattice dynamics with a local description of bonding – to explain why particular materials adopt particular structures. Such knowledge is at the foundation of the current materials-by-design effort.

4:18PM L32.00008 ABSTRACT WITHDRAWN —

4:30PM L32.00009 A Unified Formalism toward Polarization, Magnetization and the θ -term in a Periodic Insulator, KUANG-TING CHEN, PATRICK LEE, MIT — The traditional perturbative calculation expands in powers of the gauge potential. This procedure proves problematic when a uniform electric or magnetic field is present. Here we provide a perturbative expansion of the electronic Green's functions directly in powers of the fields. On the other hand, the first order correction to the free energy to an insulator with periodic boundary conditions in the presence of the electric field is actually a Berry's phase. To express the Berry's phase in terms of the Green's functions, one is required to extend the Green's function to one extra dimension. With the trick, one can then calculate the effective action to arbitrary order of the electric and magnetic field. One new result we have obtained is that the θ -term is given by the combination of the Green's functions in the extended momentum space, similar to the Wess-Zumino-Witten term, even without time reversal symmetry.

4:42PM L32.00010 Observation and Theory of Intrinsic Ferromagnetism in Ferroelectric Materials, J. LASHLEY, K. GOFRYK, D.J. SAFARIK, J.L. SMITH, Los Alamos National Laboratory, I.E. DZYLASHINSKII, University of California, Irvine — Quantized waves obeying Bose-Einstein statistics will contribute a $T^{3/2}$ term to the specific heat if the dispersion relation goes as q^2 . We measure the magnetic and electric field dependence of the specific heat on the ferroelectric material tri-glycine sulphate (TGS) over the temperature range $0.05 \text{ K} < T < 350 \text{ K}$. We detect a $T^{3/2}$ term in the specific heat in the low-temperature limit, which is taken to be the dielectric analog to magnetic spin wave. Near the Curie temperature ($T_C = 320 \text{ K}$), the shape of the specific-heat anomaly is thermally broadened. However, the anomaly changes to the characteristic sharp lambda-shape expected for a continuous transition with the application of either a magnetic field or electric field, giving the expected entropy change at T_C of $R \ln 2$. These results are explained on the basis that the frequencies of optical dipole oscillations are split by the magnetic field, and the resulting gas of excitations are paramagnetic. Consequently they contribute to the specific heat near T_C , which increases with magnetic field.

4:54PM L32.00011 Dramatic effect of the near-electrode layer configurations on the phase transition characteristics of ferroelectric-paraelectric superstructures¹, BURC MISIRLIOGLU, Asst. Prof., ARKADI LEVANYUK, Professor (Retired) — Ferroelectric-paraelectric superstructures have attracted great interest. A few experimental reports have emphasized the effect of individual layer thickness on the transition temperature of these systems. Here, we theoretically show that the phase transition characteristics of these systems are very sensitive to the structural configuration near the electrodes. The phase transition is homogeneous in the system only if the layers contacting the electrodes are paraelectric layers of 1/2 thickness of other individual layers. If the ferroelectric layer contacts the electrode (and the other electrode is contacted by a paraelectric layer) the phase transition temperature is higher than in the previous structure and the spatial distribution of the polarization at the phase transition is inhomogeneous being maximal near the electrode and disappearing far from it. A striking result is that the transition temperature in one unit bilayer is the same as a system consisting of any number of bilayers. Moreover, the profile of the polarization is unchanged upon addition of new bilayer units to the system. We also discuss general features of the domain structures below the phase transition temperature and transition anomalies.

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5:06PM L32.00012 The phase diagram of $\text{Sr}_{1-x}\text{Eu}_x\text{TiO}_3$: Crossover from displacive to order-disorder dynamics, ZURAB GUGUCHIA¹, HUGO KELLER², Physik Institut der Universität Zürich, ALEXANDER SHENGELAYA³, Department of Physics, Tbilisi State University, JÜRGEN KÖHLER⁴, ANNETTE BUSSMANN-HOLDER⁵, Max-Planck-Institut für Festkörperforschung — The phase diagram of $\text{Sr}_{1-x}\text{Eu}_x\text{TiO}_3$ is determined experimentally by EPR and resistivity measurements and analyzed theoretically in terms of the self-consistent phonon approximation (SPA) as a function of x ($0.0 \leq x \leq 1.0$). It is observed that the oxygen octahedral tilting instability temperature T_S increases nonlinearly with x . The theoretical analysis demonstrates that a crossover from displacive to order-disorder dynamics takes place for $x \geq 0.25$, signaled by a change in the local double-well potential and the soft mode temperature dependence.

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5:18PM L32.00013 Electrocaloric effect in ferroelectric alloys from atomistic simulations¹, SERGEY LISENKOV, INNA PONOMAREVA, University of South Florida — Caloric effects, such as magnetocaloric and electrocaloric effects, have attracted a lot of attention recently in the context of increasing interest in energy conversion and renewable energy materials and devices. Here we develop and use accurate first-principles-based simulations to study electrocaloric effect (ECE) from an atomistic point of view. In particular, we develop a computational technique that allows both direct and indirect simulations of ECE within the *same* atomistic framework. We then use such a tool to provide first systematic comparison between ECE estimates obtained from direct and indirect approach which will allow us to bridge the macroscopic and atomistic description of ECE. The results of our direct atomistic simulations are then used to explore the intrinsic features of ECE in ferroelectrics with multiple transitions.

¹This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under award DE-SC0005245.

Tuesday, February 28, 2012 2:30PM - 5:30PM – Session L33 GSNP DFD: Invited Session: Frontiers of Granular Physics 106

2:30PM L33.00001 Packing Nonspherical Particles: All Shapes Are Not Created Equal¹, SALVATORE TORQUATO, Departments of Chemistry and Physics, and Princeton Center for Theoretical Science, Princeton University, Princeton, NJ 08544 — Over the past decade there has been increasing interest in the effects of particle shape on the characteristics of dense particle packings, since deviations from sphericity can lead to more realistic models of granular media, nanostructured materials, and tissue architecture. It is clear that the broken rotational symmetry of a nonspherical particle is a crucial aspect in determining its resulting packing characteristics, but given the infinite variety of possible shapes (ellipsoids, superballs, regular and irregular polyhedra, etc.) it is desirable to formulate packing organizing principles based the particle shape. Such principles are beginning to be elucidated; see Refs. 1 and 2 and references therein. Depending upon whether the particle has central symmetry, inequivalent principle axes, and smooth or flat surfaces, we can describe the nature of its densest packing (which is typically periodic) as well as its disordered jammed states (which may or may not be isotropic). Changing the shape of a particle can dramatically alter its packing attributes. This tunability capability via particle shape could be used to tailor many-particle systems (e.g., colloids and granular media) to have designed crystal, liquid and glassy states.

[1] S. Torquato and F. H. Stillinger, "Jammed Hard-Particle Packings: From Kepler to Bernal and Beyond," *Rev. Modern Phys.* **82**, 2633 (2010).

[2] Y. Jiao and S. Torquato, Communication: "A Packing of Truncated Tetrahedra That Nearly Fills All of Space and its Melting Properties," *J. Chem. Phys.* **135**, 151101 (2011).

¹This work was supported by the Materials Research Science and Engineering Center (MRSEC) Program of the National Science Foundation under Grant No. DMR-0820341.

3:06PM L33.00002 Network Analysis of Granular Flows, MICHELLE GIRVAN, University of Maryland — The flow of granular materials is important to many natural and industrial processes, yet connecting microscale materials properties of grains to bulk flow behavior has remained a challenging task. Our work leverages tools from complex network theory to study granular flow at multiple scales. By characterizing the statistical properties of time-evolving contact networks using metrics like average path length, giant component size, and modularity, we are able to identify how macroscale system features like the loss of reversibility are connected to micro- and meso- scale rearrangements in the contact network. In addition, we employ a network-based approach to explore the role of rotations in facilitating cooperative rearrangements. For both the reversibility and rotation studies, we apply network analysis to time-dependent contact network data obtained from both experiments and simulations and show that this approach can provide new insights on how bulk system properties are connected to particle-scale motion.

3:42PM L33.00003 Swimming in a granular frictional fluid¹, DANIEL GOLDMAN, School of Physics, Georgia Institute of Technology — X-ray imaging reveals that the sandfish lizard swims within granular media (sand) using axial body undulations to propel itself without the use of limbs. To model the locomotion of the sandfish, we previously developed an empirical resistive force theory (RFT), a numerical sandfish model coupled to an experimentally validated Discrete Element Method (DEM) model of the granular medium, and a physical robot model. The models reveal that only grains close to the swimmer are fluidized, and that the thrust and drag forces are dominated by frictional interactions among grains and the intruder. In this talk I will use these models to discuss principles of swimming within these granular “frictional fluids”. The empirical drag force laws are measured as the steady-state forces on a small cylinder oriented at different angles relative to the displacement direction. Unlike in Newtonian fluids, resistive forces are independent of speed. Drag forces resemble those in viscous fluids while the ratio of thrust to drag forces is always larger in the granular media than in viscous fluids. Using the force laws as inputs, the RFT overestimates swimming speed by approximately 20%. The simulation reveals that this is related to the non-instantaneous increase in force during reversals of body segments. Despite the inaccuracy of the steady-state assumption, we use the force laws and a recently developed geometric mechanics theory to predict optimal gaits for a model system that has been well-studied in Newtonian fluids, the three-link swimmer. The combination of the geometric theory and the force laws allows us to generate a kinematic relationship between the swimmer’s shape and position velocities and to construct connection vector field and constraint curvature function visualizations of the system dynamics. From these we predict optimal gaits for forward, lateral and rotational motion. Experiment and simulation are in accord with the theoretical prediction, and demonstrate that swimming in sand can be viewed as movement in a localized frictional fluid.

¹Work supported by NSF Physics of Living Systems

4:18PM L33.00004 Geometrically Cohesive Granular Materials¹, SCOTT FRANKLIN, Rochester Institute of Technology — Geometrically cohesive granular materials (GCGM) are collections of particles whose individual shape leads to entanglements that resist extension forces, resulting in a non-zero Young’s modulus. Examples include long, thin (anisometric) rods, arcs of varying length, and U-shaped staples. I will report on experimental and computational work that investigates the peculiar rigidity of GCGM. These include canonical stress-strain and vibration-induced melting experiments on U-shaped staples that have revealed a non-monotonic dependence of collective rigidity on particle shape. For concave particles, rigidity appears proportional to an “entanglement number” — the number of neighbors that pass through the area partially bounded by the particle. Computational and analytic work on arcs and staples confirm the non-monotonic behavior of the entanglement number, and simulations that match the experimental conditions are underway to confirm entanglement as the basic mechanism of GCGM’s rigidity.

¹This work funded in part by the National Science Foundation and Donors from the Petroleum Research Fund.

4:54PM L33.00005 Strain-stiffening in random packings of entangled granular chains¹, ERIC BROWN, University of California, Merced — Random packings of granular chains are presented as a model polymer system to investigate the consequences of entanglements in the absence of Brownian motion. The packings are compressed uniaxially and the structure is characterized by x-ray tomography. For short chain lengths, these packings yield when the shear stress exceeds the scale of the confining pressure, similar to packings of spherical particles. In contrast, packings of chains which are long enough to bend into closed loops exhibit strain-stiffening, in which the effective stiffness of the material increases with strain, similar to many polymer materials. The latter packings can sustain stresses orders-of-magnitude greater than the confining pressure, and do not yield until the chain links break. These strain-stiffening packings are found to contain system-spanning clusters of entangled chains.

¹This work was done with Alice Nasto, Athanasios G. Athanassiadis, and Heinrich M. Jaeger at The University of Chicago

Tuesday, February 28, 2012 2:30PM - 4:54PM – Session L34 DCP: Focus Session: Impact of Ultrafast Lasers IV: Applications I 107A

2:30PM L34.00001 Adding a dimension to the infrared spectra of interfaces: 2D SFG spectroscopy via mid-IR pulse shaping, MARTIN ZANNI, University of Wisconsin-Madison — Sum-frequency generation spectroscopy provides an infrared spectrum of interfaces and thus has widespread use in the materials and chemical sciences. In this presentation, I will present our recent work in developing a 2D pulse sequence to generate 2D SFG spectra of interfaces, in analogy to 2D infrared spectra used to measure bulk species. To develop this spectroscopy, we have utilized many of the tricks-of-the-trade developed in the 2D IR and 2D Vis communities in the last decade, including mid-IR pulse shaping. With mid-IR pulse shaping, the 2D pulse sequence is manipulated by computer programming in the desired frequency resolution, rotating frame, and signal pathway. We believe that 2D SFG will become an important tool in the interfacial sciences in an analogous way that 2D IR is now being used in many disciplines.

3:06PM L34.00002 Ultrafast Broadband Infrared Source for Nonlinear Infrared Spectroscopy¹, KRUPA RAMASESHA, ARITRA MANDAL, LUIGI DE MARCO, ANDREI TOKMAKOFF², Massachusetts Institute of Technology — Existing optical parametric amplifiers can generate 200cm⁻¹ to 400 cm⁻¹ of bandwidth at mid-infrared frequencies, which limit the use of these pulses for studying vibrational dynamics. We have developed a new broadband infrared source that can generate pulses with 1000 cm⁻¹ of bandwidth, spanning most of the mid-infrared region of the spectrum. These pulses can allow us to simultaneously probe higher frequency vibrations like the OH stretch and the fingerprint region at lower frequencies. By focusing the first, second and third harmonics of a 25 fs 800 nm pulse in air to create a plasma, we have been able to generate infrared pulses with a broad spectrum ranging from 3 microns to 9 microns and a sub-100 fs pulse duration. This source can thus allow us to study dynamics that involve distinct vibrational transitions on ultrafast timescales. This presentation will discuss our efforts in characterizing the broadband infrared source and the progress we are making towards setting up a pump-probe 2D IR experiment using these broadband infrared pulses.

¹U.S. Department of Energy

²Corresponding Author/P.I

3:18PM L34.00003 Development of a Tunable Ultra-Broadband Mid IR Pulsed Source for Nonlinear Spectroscopy¹, MARK CHENG, ANTHONY REYNOLDS, HEATHER WIDGREN, MUNIRA KHALIL, Department of Chemistry, University of Washington, Seattle, WA 98195 — We generate ultra- broadband mid-IR pulses tunable from 2.5 – 8 μm by focusing 800 nm/400 nm pulses into various gas media. The input 800 nm light is doubled to 400 nm in a type I BBO crystal. The two orthogonally polarized $\omega/2\omega$ pulses encounter a birefringent calcite crystal for time delay compensation and are subsequently focused in various gas media (air, argon, neon and nitrogen) contained within a 1.2 m gas cell using a 1 m focal length silver mirror. The tunability of the broadband mid-IR pulses arises from different gases, pressure of gases and the amount of incident 800 nm/400 nm light focused into the gas cell at a given pressure. We measure IR energies as high as 0.5 μJ /pulse for an input 800 nm energy of 3 mJ/pulse in 900 Torr of Argon. The mid IR pulses exhibit $\sim 2\%$ long term stability. The ultrabroadband IR pulses have a spectral bandwidth of $\sim 2000\text{ cm}^{-1}$ corresponding to a sub-cycle pulse centered at 4.5 μm . We will present our preliminary efforts on using the ultrabroadband IR pulses in nonlinear experiments. The broad spectral content of this novel source affords the possibility of probing multiple vibrations in a coherent manner.

¹This work was supported by the National Science Foundation under CHE-0847790

3:30PM L34.00004 Transient IR Probes of Spinning Molecules in an Optical Centrifuge¹, AMY MULLIN, University of Maryland — A high-power optical centrifuge based on ultrafast laser pulses is used to drive molecules into very high rotational states. The optical centrifuge consists of reversed-chirped laser pulses that generate a linearly polarized electric field that angularly accelerates over the time of the pulse. Molecules trapped in the optical field are spun into high rotor states through sequential Raman transitions. The properties of the spinning molecules and their spatial distribution are interrogated with high-resolution state-resolved IR transient absorption probing.

¹Supported by the University of Maryland and NSF

4:06PM L34.00005 Ultrafast Nonlinear Opto-Electronic Spectroscopy, SHAWN M. PERDUE, JOONHEE LEE, ALEJANDRO RODRIGUEZ PEREZ, V. ARA APKARIAN, Department of Chemistry, University of California, Irvine — Using a single color of light and rf beam tagging, parametric nonlinear optical mixing processes can be read not just in photons, but also in electrons. The scheme allows ultrafast time-resolved opto-electronics, which we demonstrate at a tunneling junction. Acousto-optic modulators are used to frequency tag ultrashort laser pulse trains, whereby carrier beats generated in nonlinear mixing processes are down shifted by sampling at the repetition rate of the laser (80 MHz). The method down converts optical carrier frequencies (PHz) to baseband (kHz), where direct current readout is possible with single electron sensitivity. Various parametric processes can be identified through their one-to-one map in baseband. Illustrative implementations that will be presented include the determination of the temporal profile of field-emitted ultrashort electron packets and characterization of the highly nonlinear dynamics involved in light-induced tunneling emission.

4:18PM L34.00006 Coherence-Modulated Third Harmonic Generation for Second Hyper-Raman Spectroscopy of Molecules at an Interface, KEVIN DILLMAN, Colorado State University, JESSE WILSON, Duke University, RANDY BARTELS, NANCY LEVINGER, Colorado State University — We have developed a method of probing the low-frequency (sub-1000 cm^{-1}) vibrational modes of molecules at interfaces using third-harmonic generation (THG). The THG process is enhanced at an interface due to the differences in the third-order nonlinear susceptibilities of the materials. We have used this method to collect low-frequency second hyper-Raman spectra from BGO, BaF_2 and CdWO_4 crystals. In addition, we have observed coherent second hyper-Raman scattering arising from CCl_4 molecules at the liquid-glass interface. We are presently extending these techniques to observe resonant second hyper-Raman scattering from dye molecules adsorbed on gold nanoparticles in order to gain surface enhancement effects. We aim to use this method to characterize the environment at interfaces of reverse micelle systems. The development of this method is significant because we can sensitively probe the low-frequency vibrational modes of only those molecules at an interface.

4:30PM L34.00007 New generation ultrafast fiber-lasers with automated pulse compression for biomedical imaging, BAI NIE, Michigan State University, DMITRY PESTOV, Biophotonic Solutions Inc, ILYAS SAYTASHEV, SERGEY ARKHIPOV, Michigan State University, ANDY CHONG, HUI LIU, FRANK WISE, Cornell University, MARCOS DNATUS, Michigan State University — A double-clad Yb-doped all-normal-dispersion fiber laser is demonstrated to produce 22 nJ pulses at 42.5 MHz repetition rate. With a 3 nm intracavity spectral filter, self-similar evolution is formed in the gain segment. The formation of self-similar evolution allows the achievement of both short pulse duration and high pulse energy from a fiber laser oscillator. These pulses are characterized and compressed via multiphoton intrapulse interference phase scan to as short as 42 fs and 10 nJ/pulse. Adaptive compression underlies the achievement of 250-kW peak power, which enables efficient second and third harmonic generation with spectra spanning 30 nm and 20 nm, respectively. Using the newly developed fiber laser, multiphoton imaging on live tissues is demonstrated.

4:42PM L34.00008 Ionization and Coulomb explosion of small hydrocarbons exposed to short intense laser pulses¹, SERGIY BUBIN, KALMAN VARGA, Vanderbilt University — We have performed first principles numerical simulation of high field ionization in small hydrocarbons followed by a Coulomb explosion. The process was driven by 790 nm 27 fs laser pulses of high intensity (of the order of 10^{15} W/cm^2), for which case there exists recent experimental data [S. Roither et al., Phys. Rev. Lett. 106, 163001 (2011)]. We have analyzed the spectra of ejected protons and investigated the ionization-fragmentation mechanism that takes place when molecules are subjected to short intense laser pulses. The results of our simulations support the all-at-once (concerted) fragmentation scenario proposed by Roither et al. At the same time we also observed some quantitative differences between the theoretical and experimental spectra.

¹This work has been supported by NSF (grant CMMI-0927345)

Tuesday, February 28, 2012 2:30PM - 5:30PM —

Session L35 DCP: Focus Session: DFT IV: Ground-State DFT: New Directions 107B

2:30PM L35.00001 Progress in fractional perspectives of density functional theory, WEITAO YANG, Duke University — Density functional theory of electronic structure is widely and successfully applied in simulations throughout engineering and sciences. However, there are major failures for many predicted properties. These errors can be characterized and understood through the perspective of fractional charges and fractional spins introduced recently. The fractional perspectives offer a possible pathway forward. I will report progress in excited states, spin state splitting, open-shell singlet states, Fukui functions and band gaps.

3:06PM L35.00002 Generalized-gradient approximations with non-vanishing exchange-correlation magnetic torque, GIOVANNI SCALMANI, Gaussian, Inc., STEFANO PITTALIS, Department of Physics and Astronomy, University of Missouri-Columbia, MICHAEL J. FRISCH, Gaussian, Inc., GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri-Columbia — The description of systems of interacting electrons in the presence of magnetic fields, within spin-density functional theory (SDFT), requires the non-collinear magnetization density vector $\mathbf{m}(\mathbf{r})$ to be used as basic variable, along with the particle density $n(\mathbf{r})$. Furthermore, for a meaningful description of spin-dynamics, the magnetization density and its conjugate exchange-correlation (xc) field $\mathbf{B}_{xc}(\mathbf{r})$ must not be constrained to be locally parallel at every point in space. It is well known that the local density approximation (LDA) cannot, by construction, provide such a non-collinear configuration of the two vector fields. Here we show how popular generalized gradient approximations (GGAs), developed assuming collinear spin-density, can be used to describe non-collinear magnetization states, including the presence of non-vanishing local torque between $\mathbf{m}(\mathbf{r})$ and $\mathbf{B}_{xc}(\mathbf{r})$. Unlike previous attempts to extend the use of collinear GGAs to the domain of non-collinear magnetization densities, the approach we introduce is invariant with respect of spin-rotations, globally satisfies the *zero-torque theorem*, reduces to the proper collinear limit and is numerically stable.

3:18PM L35.00003 New gradient functional for SDFT derived from spin spirals in the uniform electron gas, F.G. EICH, E.K.U. GROSS, Max Planck Institute of Microstructure Physics, Halle, Germany — The development of functionals in SDFT depending on gradients of the spin magnetization is a long standing challenge. We present a new functional based on the spin-spiral state of the uniform electron gas. Comparing the principal idea of the new functional to the LSDA and GGAs, we highlight the intrinsic way non-collinearity is built into the proposed approximation. As key feature the functional yields exchange-correlation magnetic fields that are non-collinear w.r.t. the spin magnetization, while obeying the zero-torque theorem by construction. This means that an adiabatic application of the functional within TD-SDFT accounts for the local torque exerted by the exchange-correlation field and retains the numerical simplicity of explicit density functionals. An implementation of the functional based on the RPA-treatment of spin spirals in the electron gas is shown.

3:30PM L35.00004 Tuning the correlation energy in second-order Møller-Plesset perturbation theory with an effective electron-electron interaction potential, TIM KOWALCZYK, TROY VAN VOORHIS, Massachusetts Institute of Technology — For practical electronic structure calculations on large molecules, wave function theories (WFT) remain less popular than density functional theory (DFT) despite the systematic improvability of WFT. The greater computational cost of WFT is largely to blame and is two-fold in nature: WFT generally presents unfavorable scaling with system size relative to DFT, and WFT results converge more slowly than those of DFT with respect to basis set size. We propose that each of these issues can be partially mitigated by the introduction of an effective electron-electron interaction potential, in lieu of the true $1/r$ potential, for evaluating the correlation energy in WFT. We discuss the design and optimization of such an effective interaction, in the context of second-order Møller-Plesset perturbation theory (MP2), for two distinct purposes: to accelerate basis set convergence of MP2 correlation energies, and to re-scale the MP2 correlation to improve agreement with experiment and/or higher-level methods.

3:42PM L35.00005 Toward Improved Semilocal and Nonlocal Density Functionals for Atoms, Molecules, and Solids¹, JOHN P. PERDEW, Tulane University — Semilocal density functionals construct the exchange-correlation energy density at a point from the electron density and orbitals in the neighborhood of that point. They can be constructed nonempirically, and work best for sp-bonded systems near equilibrium. They increase in sophistication from the local spin density approximation to the generalized gradient approximation to the meta-GGA. For a molecule like CO on a transition metal surface, it appears that only a meta-GGA can give a good simultaneous description of the lattice constant and surface energy of the metal, on the one hand, and the adsorption energy of the molecule on the other [1]. I will discuss two remaining deficiencies of the revised TPSS meta-GGA [2]: its artificial order-of-limits problem, and its need for more information about non-bonded interaction. When electrons are shared over stretched bonds, full nonlocality is needed, and typically empirical parameters are also needed. This suggests that we don't yet know enough about the full nonlocality of the density functional for the exchange-correlation energy.

[1] J. Sun, M. Marsman, A. Ruzsinszky, G. Kresse, and J.P. Perdew, Phys. Rev. B 83, 121410 (2011).

[2] J.P. Perdew, A. Ruzsinszky, G.I. Csonka, L.A. Constantin, and J. Sun, Phys. Rev. Lett. 103, 026403 (2009).

¹Supported by NSF-DMR.

4:18PM L35.00006 Energy expressions for model exchange potentials: Beyond the Levy-Perdew virial relation, ALEX P. GAIDUK, VIKTOR N. STAROVEROV, University of Western Ontario — The common way to assign energies to Kohn-Sham exchange potentials is by using the Levy-Perdew virial relation. However, for model potentials that are not functional derivatives, this approach leads to energy expressions that lack translational invariance. We point out that there is a more general procedure for constructing density functionals from model potentials, of which the Levy-Perdew relation is just a special case. Using this generalization we propose a method for converting model potentials into density functionals that ensures translational invariance of the energy. To illustrate our approach we construct a competitively accurate exchange functional from the model potential of van Leeuwen and Baerends.

4:30PM L35.00007 Laplacian-based models for the exchange energy¹, ANTONIO C. CANCIO, Ball State University, CHRISTOPHER E. WAGNER, University of Florida, SHAUN WOOD, Ball State University — Recent Quantum Monte Carlo data for the exchange-correlation energy density of pseudopotential systems strongly suggest the value of using the Laplacian of the density as a variable for constructing first order corrections to the local density approximation of density functional theory. We report on an exchange functional built upon these observations and extended to the all-electron case. The model keeps the typical properties of constraint-based generalized gradient approximations (GGA) and also has a finite-valued potential at the nucleus, unlike the GGA. Problems with oscillatory behavior in the potential due to higher order derivatives are controlled by a curvature minimization constraint. The results are tested against exact potentials for the He and Ne atom. A combination of gradient and Laplacian as suggested by a gradient expansion of the exchange hole gives the best overall results.

¹Work support by National Science Foundation grant DMR-0812195.

4:42PM L35.00008 A non-empirical improvement of PBE and its hybrid PBE0¹ , ALBERTO VELA,

Departamento de Química, Cinvestav, JORGE M. DEL CAMPO, Departamento de Física y Química Teórica, UNAM, JOSÉ L. GÁZQUEZ, Departamento de Química, UAM-Iztapalapa, S.B. TRICKEY, Quantum Theory Project, Physics & Chemistry, U. Florida — We present a non-empirical re-parameterization of the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA) exchange-correlation functional and of the related PBE hybrid (PBE0) obtained by imposing the constraint that, for the hydrogen atom, the exchange energy cancels the Coulomb repulsion energy. The new parameterization is validated with well-known test sets. The results for the re-parameterized PBE GGA, called PBE_{mol}, show a substantial improvement over the original PBE in predicted heats of formation, while retaining the quality of the original PBE functional for description of all the other properties considered. The results for the hybrids indicate that, although the PBE0 functional provides a rather good description of those properties, the predictions of the re-parameterized functional are, except in the case of the ionization potentials, modestly better. Also, the results are better than B3LYP, except for the case of the ionization potentials and the harmonic frequencies.

¹AV and JLG were partially supported by the Conacyt project grant 128369, and SBT was supported in part by US DOE SC-0002139.

4:54PM L35.00009 Effect of the orbital-overlap dependence on Meta Generalized Gradient Approximation , JIANWEI SUN, JOHN PERDEW, BING XIAO, ADRIENN RUZSINSZKY, Department of Physics and Engineering Physics, Tulane University — The dimensionless inhomogeneity parameter, α , characterizing the extent of orbital overlap, is disentangled from the other dimensionless inhomogeneity parameter, s , the reduced density gradient, in terms of constructing a meta generalized gradient approximation (MGGA) for the exchange functional. We show that the formation of the intershell region inside an atom is associated with increase of α , which suggests MGGA should expect a monotonically decreasing α dependence for a wide range of density. This leads to a simple nonempirical MGGA exchange functional, which interpolates between the single-orbital regime for confinement systems, where $\alpha=0$, and the slowly varying density regime, where $\alpha \approx 1$, and then extrapolates to $\alpha \rightarrow \infty$. The new MGGA exchange functional, combined with the variant of the Perdew-Burke-Ernzerhof (PBE) GGA correlation as used in the revised Tao-Perdew-Staroverov-Scuseria (revTPSS) MGGA [1], performs equally well for atoms, molecules, surfaces, and solids, with an implication of a tight Lieb-Oxford bound.

[1] J.P. Perdew, A. Ruzsinszky, G.I. Csonka, L.A. Constantin, and J. Sun, Phys. Rev. Lett. 103, 026403 (2009).

5:06PM L35.00010 The derivative discontinuity in density functional theory from an electrostatic description of the exchange and correlation potential , XAVIER ANDRADE, ALAN ASPURU-GUZI, Department of Chemistry and Chemical Biology, Harvard University, 12 Oxford Street, Cambridge, Massachusetts 02138, USA — We present an approach that we have recently proposed [Phys. Rev. Lett. 107, 183002 (2011)] to approximate the exchange and correlation (XC) term in density functional theory. In our approach the XC potential is considered as an electrostatic potential, generated by a fictitious XC density, which is in turn a functional of the electronic density. In this picture, the exact asymptotic limit for low density regions, wrongly predicted by many XC functionals, can be imposed as a local condition. Based on this XC density representation we develop a correction scheme that fixes the asymptotic behavior of any approximated XC potential for finite systems. The procedure is simple, computationally inexpensive, and does not depend on adjusted parameters. Additionally, from the correction procedure it is possible to extract an approximation to the derivative discontinuity of XC energy. This value can be used to directly obtain the gap of the system as a ground-state property. Results are presented for the application of the method to atoms and small molecules. The correction results in a significant improvement in the value of the ionization energy and the gap, with errors that are comparable to the results given by orbital dependent functionals.

5:18PM L35.00011 Multi-Scale Approach to Simulations of Kelvin Probe Force Microscopy¹ , ALI SADEGHI, ALIREZA GHASEMI, STEFAN GOEDECKER, ALEXIS BARATOFF, THILO GLATZEL, ERNST MEYER, University of Basel — The distance dependence and atomic-scale contrast recently observed in nominal contact potential difference (CPD) signals simultaneously recorded during non-contact atomic force microscopy on surfaces of insulating and semiconducting samples have stimulated theoretical attempts to explain how the applied bias voltage affects electrostatic forces acting on the atomic scale. We attack the problem in two steps. First, the electrostatics of the macroscopic tip-cantilever-sample system is treated by a finite-difference method on an adjustable nonuniform mesh. It has the advantages of getting a systematically increasable accuracy as well as the ability of considering the cantilever which turns out to be important for insulating samples. The resulting electric field near the tip apex is then inserted into a series of wavelet-based density functional theory calculations. Results are obtained for a reactive disordered neutral silicon nano-scale tip interacting with a NaCl(001) sample. Bias-dependent forces and resulting atomic displacements are computed to an accuracy of 1 pN. Theoretical expressions for Kelvin signals and local contact potential difference (LCPD) are obtained combining both contributions to the electrostatic force and evaluated for several tip oscillation amplitudes.

¹This work has been supported by the Swiss National Science Foundation and the Swiss National Center of Competence in Research on Nanoscale Science.

Tuesday, February 28, 2012 2:30PM - 5:42PM — Session L36 DCP: Focus Session: New Energy IV 107C

2:30PM L36.00001 Molecular photovoltaics: Tricks from theory, from fission to gaps to traps , MARK RATNER, Northwestern University — No abstract available.

3:06PM L36.00002 Study of excitonic energy transport in thin-film J-aggregates , STEPHANIE VALLEAU, SEMION SAIKIN, MAN-HONG YUNG, ALAN ASPURU-GUZI, Department of Chemistry and Chemical Biology, Harvard University — The concentration and transfer of light through materials is one of the main current scientific goals in the ongoing quest for a new clean energy source. Molecular structures with optimal exciton transfer properties find widespread applications, ranging from solar cells and photonic devices to photographic and lithographic systems. J-aggregates of organic dye molecules are a good example of such structures where a strong interaction between molecular electronic transitions results in a partial exciton delocalization and a large exciton diffusion length. In this presentation I will discuss theoretical aspects of exciton dynamics in two dimensional films of J-aggregates with an emphasis on macroscopic transport properties that could be used for device modeling. As specific illustrations I will use results of our recent studies of exciton dynamics in aggregates of cyanine dyes.

3:18PM L36.00003 Control of exciton delocalization pathways using ZnTPP functionalization, ROBERT BARTYNSKI, SYLVIE RANGAN, SENIA COH, JONATHAN ROCHFORD, ELENA GALOPPINI, Rutgers University — Zn(II)-Tetraphenylporphyrin (ZnTPP) derivatives are attractive candidates for photoinduced electron-transfer mediators in dye sensitized solar cells. We have investigated the influence on solar cells efficiency, of the energy alignment and of the molecular adsorption geometry at the ZnTPP/metal-oxides interface. In this work, using x-ray, UV and inverse photoemission spectroscopies in conjunction with density functional theory (DFT) calculations, we have determined the energy alignment of molecular levels with respect to the substrate band edges for several ZnTPP derivatives adsorbed on ZnO(11-20) and TiO₂(110) surfaces. The ZnTPP derivatives were functionalized with COOH anchoring groups, to allow upright or flat adsorption on the surfaces. While the energy alignment is found similar for all of these systems, large differences in devices efficiencies are observed. We have thus explored the adsorption geometry of the same ZnTPPs at the surface of ZnO and TiO₂ using UV-visible absorption and NEXAFS spectroscopies and scanning tunnel microscopy. It is found that for ZnTPPs, upright adsorption opens deleterious exciton delocalization pathways, due to dipole/dipole interactions competing with electron transfer to the substrate. Choosing the adsorption geometry is thus critical for the electronic pathway control.

3:30PM L36.00004 Coupled polaronic and ion transport in nanocrystalline metal oxide electrodes, KEVIN ROSSO, Pacific Northwest National Laboratory — We report new computational methods and fundamental understanding in the dynamics of coupled charge and ion transport in nanoscale metal oxides. The methods attack the multi-scale problem of simulating the collective diffusivities of ions and charge compensating e⁻/h⁺ carriers in single crystal particles, across particle-particle grain boundaries, and through networks of grains for select systems. Methods include embedded quantum mechanical clusters at the DFT and MP2 levels of theory for atomic-scale polaronic and ion transport kinetics, classical DFT-based free energy calculations for grain-scale conductivity in the framework of the Poisson-Nernst-Planck formalism, and phase field simulation of charged particle diffusivity for conductivity at the grain network scale. This combination of approaches is one of a kind in terms of its multi-scale range, scaling, and computational efficiency. We are presently focused on coupled electron and Li⁺ ion transport in polymorphs of TiO₂, and also in mixed valence spinel oxides, for electrode conductivity optimization and improving energy storage materials performance for Li⁺ batteries.

4:06PM L36.00005 Electrochemical properties of Pt-Co-Zr thin films on high surface area NSTF supports, CHARLES HAYS, POYAN BAHRAMI, MICHAEL ERRICO, JAMES KULLECK, DANIEL KONOPKA, ADAM KISOR, STUART COOLEY, HAROLD GREER, California Institute of Technology, Jet Propulsion Laboratory — Nanostructured thin film supports (NSTF) are a promising fuel cell (FC) technology demonstrated by 3M [1]. We have examined the electrochemical performance of Pt-Co-Zr films deposited onto NSTF supports by dc-magnetron sputtering. In this presentation, we will present results of microstructural, composition, and electrochemical properties, for NSTF supported (Pt₃Co)_{100-x}Zr_x thin films, with 10 < x < 40 (At. %). Electrochemical measurements show that the films are electrochemically stable, and active for the oxygen-reduction-reaction (ORR), with ORR kinetic current densities at 0.9 V (vs. NHE), up to 57X greater than those of Pt(111) films measured in the same cell. The composition dependence of the ORR, and relevant physical properties will be discussed.

[1] M. K. Debe, A. J. Steinbach, G. D. Vernstrom et al, J. Electrochemical Soc. 158, B910 (2011).

Acknowledgements: The research in this presentation was carried out at the Jet Propulsion Laboratory, California Institute of Technology, under a contract with the National Aeronautics and Space Administration. We acknowledge support from the Department of Energy (DE-PS36-08G098101). We thank our collaborators Dr. M. Debe, Dr. R. Atanasoski, and G. D. Vernstrom of 3M Corp.

4:18PM L36.00006 Enhanced Surfactant Adsorption on Activated Carbon through Manipulation of Surface Oxygen Groups¹, JOHN COLLINS, DEYANG QU, MICHELLE FOSTER, University of Massachusetts, Boston — Passive energy storage is a necessary component for balancing the lifecycle budget with new forms of green energy. The work presented describes how surface oxygen groups (SOG) on granulated activated carbon have been manipulated using Nitric Acid in a controlled, stepwise fashion. The structure and surface functionality of the activated carbon samples were characterized using DRIFTS, Raman Spectroscopy and Porosimetry. Total surface area was found to increase proportionally with the removal of heteroatom material, exposing previously insulated active sites responsible for SOG attachment. Broad oxide peaks were deconvoluted and analyzed, allowing for absolute identification of evolving functionality at each oxidation stage. SOGs were maximized on the third oxidation cycle with the presence of conjugated aromatic, phenol, lactone, and carboxylic acid groups. FSN Zonyl nonionic was applied to all oxidized samples at various concentrations. Total adsorbed surfactant was quantified for each concentration / oxidation scheme using attenuated total reflection. The relative quantity and polarity of chemisorbed surfactant were qualitatively assessed for each equilibrium concentration.

¹Raman data courtesy of Thermo Fisher Scientific

4:30PM L36.00007 Coarse-grained potential models for structural prediction of carbon dioxide in confined environments, TARUN SANGHI, NARAYANA ALURU, University of Illinois at Urbana-Champaign — Geological storage of carbon dioxide is a promising option to reduce the level of carbon dioxide in the atmosphere and mitigate its effect on climate change. In geological storage, high-pressure carbon dioxide is injected into the underground porous rock formations, where it gets trapped inside the tiny nanometer size pores of the rocks. Thus, a good understanding of the microstructure of carbon dioxide inside nanoscale confinements is of great practical importance in developing an efficient technology for carbon dioxide storage. In this work, we discuss the systematic development of coarse-grained single-site (CGSS) potential models to study the structure of carbon dioxide in confined environments. These single-site potentials allow computationally efficient simulations, which are several orders of magnitude faster than all-atom MD (AAMD) simulations. The potential models are used in our earlier proposed multi-scale quasi-continuum theory, called EQT, and in coarse-grained MD (CGMD) to predict the equilibrium structure of carbon dioxide confined inside graphite slit pores. The results obtained from both EQT and CGMD are found to be in good agreement with those obtained from computationally expensive AAMD simulations.

4:42PM L36.00008 Multiscale Simulation of Electrochemical Phenomena: Fuel Cells and Batteries, RYAN JORN, Argonne National Laboratory — Results will be presented from multiscale simulations of two important systems from renewable energy technology, fuel cell proton membranes and electrochemical cells. In the first case, the solvation and transport of hydrated protons in proton exchange membranes (PEMs) such as NafionTM will be described using a novel multi-state reactive molecular dynamics (MD) approach. The multi-state MD methodology allows for the treatment of explicit (Grotthuss) proton shuttling and charge defect delocalization which, in turn, can strongly influence the properties of the hydrated protons in various aqueous and complex environments. The role of PEM hydration level and morphology on these properties will be further described. A new multiscale computational methodology for describing the mesoscopic features of the proton transport will also be described, which can be coupled to the results from the molecular-scale simulations. On the second topic, a computationally efficient method will be presented for the treatment of electrostatic interactions between polarizable metallic electrodes held at a constant potential and separated by an electrolyte. The method combines a fluctuating uniform electrode charge with explicit image charges to account for the polarization of the electrode by the electrolyte, and a constant uniform charge added to the fluctuating uniform electrode charge to account for the constant potential condition. The method is used to calculate electron transport rates using electron transfer theory; these rates are incorporated in a multiscale approach to model oxidation/reduction reactions in an electrochemical cell efficiently.

5:18PM L36.00009 Collective Behavior of Water on Platinum, DAVID LIMMER, University of California, Berkeley, ADAM WILLARD, University of Texas, Austin, DAVID CHANDLER, University of California, Berkeley — We present the results of molecular dynamics simulations of a interface between water and a platinum electrode. Using importance sampling techniques we probe a variety of collective phenomenon that emerge at the interface. We consider platinum electrodes with two different geometries and discuss how different behaviors result from a competition between geometrical frustration and favorable local interactions.

5:30PM L36.00010 Superstructured tungsten oxide photoanodes, ROBERT CORIDAN, Division of Chemistry and Chemical Engineering, California Institute of Technology, KEVIN ARPIN, PAUL BRAUN, Department of Materials Science and Engineering, University of Illinois, Urbana-Champaign, NATHAN LEWIS, Division of Chemistry and Chemical Engineering, California Institute of Technology — Tungsten oxide is a robust and stable semiconductor for photoanodic applications in aqueous solutions. Typical deposition techniques like electroplating or sputtering produce granular films which increase interfacial recombination of minority carriers. This has a deleterious effect on the photovoltaic performance of these materials. Using a variety of templating methods, we explore multiscale structuring strategies for increasing the surface area of the photoanode while maintaining significant light absorption. We describe photoelectrochemical and reflectivity measurements on structured and templated tungsten oxide photoanodes and consider how these results guide future photosynthetic electrochemical device design.

Tuesday, February 28, 2012 2:30PM - 3:54PM – Session L37 FEd: Informal Education and Public Outreach - Policy Questions 108

2:30PM L37.00001 Selectively Bringing Down the Curtain on OPERA Superluminal Neutrino Papers, ROBERT GARISTO, American Physical Society (Physical Review Letters) — Picture this: instead of watching from afar the daily flow of superluminal proposals trying to explain OPERA's preliminary data, you are the PRL Editor charged with deciding what to do with each paper. How do you address the validity of a manuscript whose starting point involves circumventing Einstein? I'll discuss the general issues of controversial claims and data-driven floods of theory papers through the unusual lens of the OPERA-motivated papers. Along our ten minute journey, I'll show some interesting correspondence.

2:42PM L37.00002 Superluminal Neutrinos: The Good Kind of Science Controversy, MICHAEL LUCIBELLA, American Physical Society — After OPERA released results indicating neutrinos were traveling faster than the speed of light, a number of scientists said that the team shouldn't have prematurely engaged in "science by press release." However, controversial claims like this, if handled properly, can actually be a boon to science. Getting the public interested in cutting edge physics is notoriously difficult, but the public is always interested in hearing about a controversy. The press conference and following debate becomes a great "teaching moment" which offers the public a unique opportunity to get an inside and in-depth look at how science works. Scientists willing to publicly engage in this kind of civil controversy are important because when other scientific controversies arise, ones with major public policy implications, the public starts out with a better understanding of how science works, and scientists have better practice managing questions from the public.

2:54PM L37.00003 Controversial Science and the Media, JAMES RIORDON, American Physical Society — The possibility that the OPERA collaboration has detected superluminal neutrinos was among the most controversial topics in physics news in decades, and one of the most widely covered stories in all of science in 2011. Word of the research initially reached journalists and the public prior to publication in peer-reviewed journals. Understandably, many physicists are concerned that the significance of controversial science may be exaggerated or distorted when news organizations report on science at such an early stage. I will offer an overview of the ways the story was promoted by the media relations personnel, and outline the rationales that motivate media relations efforts along with the associated benefits and drawbacks that can result. Finally, I will examine the accuracy and completeness of the superluminal neutrino news stories that ultimately were made available to the general public.

3:06PM L37.00004 Controversial Physics: Perfect Public Outreach Opportunity, REBECCA THOMPSON, American Physical Society — The goal of public outreach is to excite and engage the public in physics. What can be more exciting than controversy? When OPERA announced their discover of superluminal neutrinos, controversy within the physics community quickly followed. This result could overturn a century of established physics. From a public outreach perspective there was no better way to bring people usually unaware of current research into the discussion of this result. If handled well this could be used as a gateway to interest in other physics research. The public drive to learn more about this particular result can be harnessed to create interest in other cutting edge physics research and drive the public to continue their informal physics learning. If the results of OPERA and eventually proven incorrect as many physicists believe they will, that will not erase the public's new-found interest in physics but hopefully continue to fuel it.

3:18PM L37.00005 Informal Physics Education: Outreach from a National Laboratory, JOSE SANCHEZ, PATRICIA DIXON, ROXANNE HUGHES, National High Magnetic Field Laboratory — This presentation highlights strategies for K-20 teaching and learning about materials research in informal settings. The National High Magnetic Field Laboratory's Center for Integrating Research & Learning is in a unique position to conduct programs that reach K-20 students and teachers. As part of a national laboratory the Center provides the infrastructure around which informal education programs are implemented, including the nationally-recognized programming as well as facilitating scientists' educational outreach in the community. Research Experiences for Undergraduates, focuses on encouraging women and other underrepresented groups to pursue STEM careers reaching approximately 200 students many of whom have pursued careers in research as well as academia. The Research Experiences for Teachers program has provided internships for over 150 teachers; the Center also reaches over 10,000 students each year through school and community outreach. Success of informal education programs relies heavily on establishing strong mentoring relationships between scientists and K-20 students and teachers. The Center's success at maintaining diverse programming that transforms how materials education is presented beyond the traditional classroom is the focus for this presentation.

3:30PM L37.00006 ABSTRACT WITHDRAWN –

3:42PM L37.00007 Houston, we have a problem: What the Voting Public Believes about Science Funding, JODI LIEBERMAN, Senior Government Relations Specialist, APS Physics — In an election year with a tight Federal budget outlook, the views of the voting public are critical to forecasting what may be in store for the National Science Foundation, Department of Energy Office of Science and National Institute for Standards and Technology. It is these people who weigh in with their legislators to identify what is important and what should be cut. The results of some recent polling commissioned by the APS and other scientific societies reveal that the general public may not be as supportive of Federal science funding as has been previously believed. Jodi Lieberman will present the results of that polling data and how it is likely to impact the next Federal science budget.

Tuesday, February 28, 2012 2:30PM - 5:18PM – Session L39 GQI: Focus Session: Superconducting Qubits: 3D Cavities 109B

2:30PM L39.00001 How coherent are Josephson junctions?¹, HANHEE PAIK, Yale University — Superconducting quantum circuits based on Josephson junctions are a promising technology to realize a electronically controlled, solid-state based large-scale quantum information processor but their future prospects rely on the intrinsic coherence of Josephson junctions and the engineering of the isolated environment for the quantum circuits. We introduce a new architecture for superconducting quantum circuits employing a single-Josephson junction in a three dimensional waveguide cavity where we carefully engineer the environment of the qubit to effectively reduce the coupling of the qubit to the environment while maintaining sufficient coupling to the control signal. With this architecture we demonstrate that Josephson junction qubits are at least an order of magnitude more coherent with $T_2^{Ramsey} \sim 10$ to $20 \mu s$ without the use of spin echo than previously reported and highly stable, enabling us to observe the physics in a Josephson junction with a unprecedented level of precision. These results suggest that the overall quality of Josephson junctions will allow error rates of a few 10^{-4} , approaching the error correction threshold. We will also discuss how to scale this architecture and perform two-qubit gates.

¹This work was performed in collaboration with D. I. Schuster, Lev S. Bishop, G. Kirchmair, G. Catelani, A. P. Sears, B. R. Johnson, M. J. Reagor, L. Frunzio, L. I. Glazman, S. M. Girvin, M. H. Devoret and R. J. Schoelkopf

3:06PM L39.00002 Bottom-up construction of artificial molecules for superconducting quantum processors, STEFANO POLETTI, CHAD RIGETTI, JAY M. GAMBETTA, SETH MERKEL, JERRY M. CHOW, ANTONIO D. CORCOLES, JOHN A. SMOLIN, JIM R. ROZEN, GEORGE A. KEEFE, MARY B. ROTHWELL, MARK B. KETCHEN, MATTHIAS STEFFEN, IBM T.J. Watson Research Center — Recent experiments on transmon qubits capacitively coupled to superconducting 3-dimensional cavities have shown coherence times much longer than transmons coupled to more traditional planar resonators. For the implementation of a quantum processor this approach has clear advantages over traditional techniques but it poses the challenge of scalability. We are currently implementing multi-qubits experiments based on a bottom-up scaling approach. First, transmon qubits are fabricated on individual chips and are independently characterized. Second, an artificial molecule is assembled by selecting a particular set of previously characterized single-transmon chips. We present recent data on a two-qubit artificial molecule constructed in this way. The two qubits are chosen to generate a strong Z-Z interaction by matching the 0-1 transition energy of one qubit with the 1-2 transition of the other. Single qubit manipulations and state tomography cannot be done with “traditional” single tone microwave pulses but instead specifically shaped pulses have to be simultaneously applied on both qubits. Coherence times, coupling strength, and optimal pulses for decoupling the two qubits and perform state tomography are presented

3:18PM L39.00003 Quasiparticle tunneling in a single-junction transmon qubit¹, DIEGO RISTÉ, JOSEPHINE VAN LEEUWEN, LEONARDO DICARLO, Kavli Institute of Nanoscience, Delft University of Technology — The recent increase in transmon qubit quality factor into the million range [1] makes non-equilibrium quasiparticle tunneling a potentially limiting mechanism for qubit coherence. We investigate the dynamics of quasiparticle tunneling in a single-junction transmon qubit with relaxation time $T_1 = 85 \mu s$ ($Q = 2.6$ million). The qubit operates at moderate ratio of Josephson to charging energy, $E_J/E_C \sim 30$, where charge parity in the qubit islands is encoded in the qubit transition frequency. Using Ramsey-type and stimulated echo experiments, we investigate quasiparticle tunneling across the qubit junction on time scales short and long compared to T_1 . We observe that the quasiparticle tunneling time for the single-junction qubit is at least as long as T_1 , but shorter than the 1 ms repetition rate. This result is consistent with recent theory and qualitatively different from the two-junction transmon. The dephasing time $T_2^* = 10 \mu s$ is limited by slow background charge fluctuations and extended to $T_2 = 95 \mu s$ using dynamical decoupling.

[1] Paik et al. arXiv:1105.4652v4

¹Research supported by NWO, FOM, and EU Project SOLID.

3:30PM L39.00004 Varying Cavity Quality Factor in situ for a Transmon in Circuit QED, ANDREI PETRENKO, ADAM SEARS, GERHARD KIRCHMAIR, HANHEE PAIK, LUYAN SUN, GIANLUIGI CATELANI, LEONID GLAZMAN, ROBERT SCHOELKOPF, Yale University — Superconducting transmon qubits have recently been studied within 3D cavities. In addition to increasing the coherence times of the qubits this has enabled a simple scheme for varying the quality factor Q (or decay rate κ) of a cavity in situ. This decay rate plays an important role in our understanding of a number of effects in circuit quantum electrodynamics, many of which have direct bearing on qubit decoherence processes. Here we study how adjusting the cavity Q affects the coherence times of a single qubit within the 3D architecture. We demonstrate that varying the coupling enables us to not only examine the limitations of qubit T_1 due to the Purcell Effect, but also probe new decoherence mechanisms such as the dephasing due to photon shot noise. By understanding and minimizing these effects, we obtain record coherences times T_2 and T_2^{Echo} of $\sim 27 \mu s$ and $\sim 47 \mu s$ respectively.

3:42PM L39.00005 Dephasing Due to Shot Noise in the Strong Dispersive Limit of Circuit QED, ADAM SEARS, ANDREI PETRENKO, GERHARD KIRCHMAIR, HANHEE PAIK, LUYAN SUN, GIANLUIGI CATELANI, LEONID GLAZMAN, ROBERT SCHOELKOPF, Yale University — The design parameters of superconducting qubits inside resonant cavities have evolved over time to minimize decoherence, allow fast pulses and enable high fidelity readout. The two are often coupled so strongly that the dispersive shift of the qubit due to a single photon in the cavity (or AC Stark shift) is much larger than a linewidth. In this strong dispersive regime, the passage of any photons can lead to an unintended and complete measurement of the qubit state. We study photon shot noise dephasing in this limit for a transmon and derive a simple relation between the dephasing rate and the product $\bar{n}\kappa$, where $\bar{n}$ is the average cavity occupancy and κ is the cavity decay rate. We find good experimental agreement for a large range of κ , varied *in situ* using a simple mechanism, and note several ways this can influence qubit experiments.

3:54PM L39.00006 Effective model of nonlinear circuit quantum electrodynamics¹, SIMON NIGG, Physics Department, Yale University, MICHEL DEVORET, Department of Applied Physics, Yale University, STEVEN GIRVIN, Physics Department, Yale University — Superconducting electronic circuits containing nonlinear elements such as Josephson junctions are of interest for quantum information processing. The low-energy spectrum of such circuits can now be measured to a precision of better than one part per million. A precise knowledge of their Hamiltonian that goes beyond current models is thus desirable. In this talk I will show how to quantize a superconducting, weakly nonlinear circuit from the knowledge of its classical linear admittance matrix. This approach represents a change of paradigm in circuit quantum electrodynamics and may potentially become a useful alternative to the standard models based on the language of atomic physics and quantum optics.

¹I acknowledge financial support from the Swiss National Science Foundation.

4:06PM L39.00007 Designing a three mode circuit QED experiment, BRIAN VLASTAKIS, GERHARD KIRCHMAIR, HANHEE PAIK, SIMON NIGG, LUIGI FRUNZIO, STEVEN GIRVIN, MICHEL DEVORET, ROBERT SCHOELKOPF, Yale University — Circuit QED employs the coupling of nonlinear elements to resonant modes of an electronic circuit. We demonstrate that all resonant modes will attain some degree of nonlinearity from even a single nonlinear element. This can result in individually addressable transitions for each mode and allow direct control of each quantum state. Furthermore, we show that the transition frequency of any one mode will depend on the state of all other modes. These state dependent shifts can be used to directly readout the quantum state of one mode probing another. We illustrate this behavior by coupling two three-dimensional resonators to a superconducting transmon qubit and present a method to determine the Hamiltonian for this system using a nonlinear circuit QED model.

4:18PM L39.00008 Experiments on a three mode circuit QED system, GERHARD KIRCHMAIR, BRIAN VLASTAKIS, HANHEE PAIK, Applied Physics Department Yale University, SIMON NIGG, Physics Department Yale University, LUIGI FRUNZIO, Applied Physics Department Yale University, STEVEN GIRVIN, Physics Department Yale University, MICHEL DEVORET, ROBERT SCHOELKOPF, Applied Physics Department Yale University — Current research in superconducting circuit QED is working towards combining an increasing number of cavities and qubits to investigate larger scale quantum systems. Here we will discuss measurements on a system consisting of two three-dimensional microwave resonators coupled to a single transmon qubit. We demonstrate that each mode of the system has sufficient anharmonicity to coherently manipulate the state of the lowest two energy levels. This allows us to measure the coherence of a single excitation in a mode and detect the frequency shift due to excitations of the other modes. These effects are important to consider when using a resonator as a quantum memory to decouple the quantum state from the rest of the system. Furthermore we show that we can use the state dependent shifts to detect the quantum state of one mode with another. The full characterization of the system allows us to determine the Hamiltonian and compare it to the theoretical predictions obtained with a nonlinear circuit QED model.

4:30PM L39.00009 Material and Geometric Effects in 3D Transmon Qubits, MATTHEW WARE, M.P. DEFEQ, J.D. STRAND, B. XIAO, B.L.T. PLOURDE, Syracuse University, STEFANO POLETTI, CHAD RIGETTI, IBM Research, SYRACUSE UNIVERSITY COLLABORATION, IBM RESEARCH COLLABORATION — Optimization of coherent behavior is a key ingredient for any scalable architecture using qubits. Recent breakthroughs in novel qubit designs have resulted in significant improvements in coherence by coupling superconducting qubits to 3-dimensional microwave cavities. We are investigating material and geometric factors affecting the coherence of these 3D transmon qubits. Various loss mechanisms limiting the qubit coherence will be discussed. The role played by device geometry and size in determining the effective qubit-cavity coupling will also be explored.

4:42PM L39.00010 3D Microwave Cavity for Qubit Measurement, SERGEY NOVIKOV, V. ZARETSKEY, B. SURJ, Z. KIM, Dept. of Physics, Univ. of Maryland, B. S. PALMER, Lab. for Physical Sciences, F. C. WELLSTOOD, JQI, CNAM, Dept. of Physics, Univ. of Maryland — We have investigated the loss mechanisms of the TE_{101} mode (resonant frequency $f_0 = 8$ GHz) of a superconducting Al microwave cavity. The internal quality factor Q_{int} of the cavity has been measured for a range of temperatures from 23 mK to 360 mK in a low photon number regime and from 360 mK to $T_c \sim 1.1$ K in a high photon number regime, both with and without a sapphire chip in the cavity. With sapphire present, $Q_{int} \sim 10^6$ was strongly reduced by an applied magnetic field. Without sapphire, $Q_{int} \sim 4 \times 10^6$ was only weakly dependent on the applied field. The frequency stability of the cavity and the use of the cavity for qubit readout (following recent experiments by H. Paik *et al.*¹) will be discussed.

¹arXiv:1105.4652v4

4:54PM L39.00011 Characterization of superconducting accelerator cavity at millikelvin temperature for use in quantum computation, BING LI, YANG GE, University of Chicago, ALEX ROMANENKO, LANCE COOLEY, Fermi National Laboratory, DAVID SCHUSTER, University of Chicago — Quantum computation using 2D superconducting circuits has been advancing rapidly but has been limited to coherence times of a few microseconds. On the other hand, 3d superconducting cavities for accelerators routinely achieve quality factors exceeding ten billion, corresponding to coherence times exceeding one second. With the recent demonstration of coupling a superconducting qubit to a 3d resonator [1], it should be possible to take advantage of this advanced accelerator technology. However, accelerator cavities are typically used above 2 K and at 1 W input powers. The ultimate residual resistance of accelerator cavities is not yet well understood and it is unclear if they will maintain their exceptional properties at millikelvin temperatures and ultra-low powers. We present measurements of a 3.9 GHz accelerator cavity from 2K-20mK and at powers less than one attowatt. [1] Paik, *et. al.* arXiv:1105.4652

5:06PM L39.00012 Improving the Coherence Time of Microwave Cavities, MATTHEW REAGOR, HANHEE PAIK, LUYAN SUN, ERIC HOLLAND, LUIGI FRUNZIO, ROBERT SCHOELKOPF, Department of Physics and Applied Physics, Yale University — A superconducting cavity resonator is able to store quantum states of light, protect qubits from decoherence and place bounds on material losses. The resonator's utility in all three goals is inherently tied to its quality factor. We report recent progress in improving the quality factors of aluminum waveguide cavities in the quantum regime. We will also report on the use of these cavities to measure the dielectric properties of low-loss substrates and the surface impedance of bulk superconductors and thin films.

Tuesday, February 28, 2012 2:30PM - 5:18PM –

Session L40 DBIO GSNP: Focus Session: Systems Biology and Biochemical Networks II 156A

2:30PM L40.00001 Microbial interaction networks in soil and in silico, KALIN VETSIGIAN, University of Wisconsin-Madison — Soil harbors a huge number of microbial species interacting through secretion of antibiotics and other chemicals. What patterns of species interactions allow for this astonishing biodiversity to be sustained, and how do these interactions evolve? I used a combined experimental-theoretical approach to tackle these questions. Focusing on bacteria from the genus *Streptomyces*, known for their diverse secondary metabolism, I isolated 64 natural strains from several individual grains of soil and systematically measured all pairwise interactions among them. Quantitative measurements on such scale were enabled by a novel experimental platform based on robotic handling, a custom scanner array and automatic image analysis. This unique platform allowed the simultaneous capturing of ~15,000 time-lapse movies of growing colonies of each isolate on media conditioned by each of the other isolates. The data revealed a rich network of strong negative (inhibitory) and positive (stimulating) interactions. Analysis of this network and the phylogeny of the isolates, together with mathematical modeling of microbial communities, revealed that: 1) The network of interactions has three special properties: “balance”, “bi-modality” and “reciprocity”; 2) The interaction network is fast evolving; 3) Mathematical modeling explains how rapid evolution can give rise to the three special properties through an interplay between ecology and evolution. These properties are not a result of stable co-existence, but rather of continuous evolutionary turnover of strains with different production and resistance capabilities.

3:06PM L40.00002 ABSTRACT WITHDRAWN –

3:18PM L40.00003 Regulatory schemes to achieve optimal flux partitioning in bacterial metabolism¹, LEI-HAN TANG, Department of Physics, Hong Kong Baptist University and Beijing Computational Science Research Center, ZHU YANG, Department of Physics, Hong Kong Baptist University, SHENG HUI, Department of Physics, UCSD, PAN-JUN KIM, APCTP, Korea, XUE-FEI LI, Department of Physics, Hong Kong Baptist University, TERENCE HWA, Department of Physics, UCSD — The flux balance analysis (FBA) offers a way to compute the optimal performance of a given metabolic network when the maximum incoming flux of nutrient molecules and other essential ingredients for biosynthesis are specified. Here we report a theoretical and computational analysis of the network structure and regulatory interactions in an *E. coli* cell. An automated scheme is devised to simplify the network topology and to enumerate the independent flux degrees of freedom. The network organization revealed by the scheme enables a detailed interpretation of the three layers of metabolic regulation known in the literature: i) independent transcriptional regulation of biosynthesis and salvage pathways to render the network tree-like under a given nutrient condition; ii) allosteric end-product inhibition of enzyme activity at entry points of synthesis pathways for metabolic flux partitioning according to consumption; iii) homeostasis of currency and carrier compounds to maintain sufficient supply of global commodities. Using the amino-acid synthesis pathways as an example, we show that the FBA result can be reproduced with suitable implementation of the three classes of regulatory interactions with literature evidence.

¹Work supported in part by the RGC of the HKSAR under grant 201910.

3:30PM L40.00004 A Realtime Active Feedback Control System For Coupled Nonlinear Chemical Oscillators, NATHAN TOMPKINS, SETH FRADEN, Brandeis University — We study the manipulation and control of oscillatory networks. As a model system we use an emulsion of Belousov-Zhabotinsky (BZ) oscillators packed on a hexagonal lattice. Each drop is observed and perturbed by a Programmable Illumination Microscope (PIM). The PIM allows us to track individual BZ oscillators, calculate the phase and order parameters of every drop, and selectively perturb specific drops with photo illumination, all in realtime. To date we have determined the native attractor patterns for drops in 1D arrays and 2D hexagonal packing as a function of coupling strength as well as determined methods to move the system from one attractor basin to another. Current work involves implementing these attractor control methods with our experimental system and future work will likely include implementing a model neural network for use with photo controllable BZ emulsions.

3:42PM L40.00005 Stochastic gene expression with bursting and positive feedback, THIERRY PLATINI, Virginia Bioinformatics Institute, HODJAT PENDAR, RAHUL KULKARNI, Department of Physics, Virginia Tech — Stochasticity (or noise) in the process of gene expression can play a critical role in cellular circuits that control switching between probabilistic cell-fate decisions in diverse organisms. Such circuits often include positive feedback loops as critical elements. In some cases (e.g. HIV-1 viral infections), switching between different cell fates occurs even in the absence of bistability in the underlying deterministic model. To characterize the role of noise in such systems, we analyze a simple gene expression circuit that includes contributions from both transcriptional and translational bursting and positive feedback effects. Using a combination of analytical approaches and stochastic simulations, we explore how the underlying parameters control the corresponding mean and variance in protein distributions.

3:54PM L40.00006 mRNA Noise Reveals that Activators Induce a Biphasic Response in the Promoter Kinetics of Highly Regulated Genes, KATIE QUINN, Massachusetts Institute of Technology, TSZ-LEUNG TO, University of California, San Francisco, NARENDRA MAHESHRI, Massachusetts Institute of Technology — A dominant source of fluctuations in gene expression is thought to be the process of transcription. The statistics of these fluctuations arise from the kinetics of transcription. Multiple studies suggest the bulk of fluctuations can be understood by a simple process where genes are inactive for exponentially distributed times punctuated by geometric bursts of mRNA. Yet it's largely unknown how cis and trans factors affect the two lumped kinetic parameters, burst size and burst frequency, that describe this process. Importantly, how these parameters are regulated in a single gene can qualitatively affect the dynamical behavior of the network it is embedded within. Here, we ask whether transcriptional activators increase gene expression by increasing the burst size or burst frequency. We do so by deducing these parameters from steady-state mRNA distributions measured in individual yeast cells using single molecule mRNA FISH. We find that for both a synthetic and natural promoter, activators appear to first increase burst size, then burst frequency. We suggest this biphasic response may be common to all highly regulated genes and was previously unappreciated because of measurement techniques. Furthermore, its origins appear to relate to cis events at the promoter, and may arise from combinations of basal and activator-dependent bursts. Our measurements shed new light on transcriptional mechanisms and should assist in building synthetic promoters with tunable statistics.

4:06PM L40.00007 Determining the stability of genetic switches: Explicitly accounting for mRNA noise, MICHAEL ASSAF, ELIJAH ROBERTS, ZAN LUTHEY-SCHULTEN, University of Illinois at Urbana-Champaign — Cells use genetic switches to shift between alternate gene expression states, e.g. to adapt to new environments or to follow a developmental pathway. Here, we study the dynamics of switching in a generic-feedback on/off switch. Unlike protein-only models, we explicitly account for stochastic fluctuations of mRNA, which have a dramatic impact on the genetic switch dynamics. Employing a semi-classical theory to treat the underlying chemical master equations, we obtain accurate results for the quasi-stationary distributions of mRNA and protein copy numbers and for the mean switching time, starting from either state. Our analytical results agree well with extensive Monte Carlo simulations. Importantly, one can use the approach to study the effect of varying biological parameters, and of extrinsic noise, on the switch stability.

4:18PM L40.00008 Quantitative Model of microRNA-mRNA interaction, JAVAD NOORBAKHS, ALEX LANG, PANKAJ MEHTA, Boston University — MicroRNAs are short RNA sequences that regulate gene expression and protein translation by binding to mRNA. Experimental data reveals the existence of a threshold linear output of protein based on the expression level of microRNA. To understand this behavior, we propose a mathematical model of the chemical kinetics of the interaction between mRNA and microRNA. Using this model we have been able to quantify the threshold linear behavior. Furthermore, we have studied the effect of internal noise, showing the existence of an intermediary regime where the expression level of mRNA and microRNA has the same order of magnitude. In this crossover regime the mRNA translation becomes sensitive to small changes in the level of microRNA, resulting in large fluctuations in protein levels. Our work shows that chemical kinetics parameters can be quantified by studying protein fluctuations. In the future, studying protein levels and their fluctuations can provide a powerful tool to study the competing endogenous RNA hypothesis (ceRNA), in which mRNA crosstalk occurs due to competition over a limited pool of microRNAs.

4:30PM L40.00009 On the control of gene expression in small RNA post-transcriptional regulation pathway: role of conserved weak targets¹, DANIEL JOST, ANDRZEJ NOWOJEWSKI, EREL LEVINE, Department of Physics and FAS Center for Systems Biology - Harvard University — Small RNA molecules play critical regulatory roles in organisms across all kingdoms of life. Many small RNA families achieve target-specificity via base-pairing of a very short (6-8 nucleotides) "seed" region with the targeted mRNA, and consequently many genes carry a matching seed in their sequence. Evidence in bacteria and animals suggest that a single small RNA may regulate the gene expression of many different targets, although most of them very weakly. On the other hand, in all cases we are aware of where the functionality of a small RNA has been carefully studied, only a small number of target genes were identified as being phenotypically relevant. Here, we present a Langevin formalism which describes the dynamics of the different interacting entities (small RNA and targets), including the stochasticity of the underlying biochemical reactions and the effect of transport. Using analytical or numerical computations, we study the influence of (many) weak targets on the mean and noise properties of (few) principal targets. In particular, we argue that the role of these weak targets is to confer robustness to the regulation of the principal targets without significantly affecting their temporal responses to changing environments.

¹This work was supported by the National Science Foundation under Grant No. MCB1121057.

4:42PM L40.00010 Approaches to Chemical and Biochemical Information and Signal Processing, VLADIMIR PRIVMAN, Clarkson University — We outline models and approaches for error control required to prevent buildup of noise when "gates" and other "network elements" based on (bio)chemical reaction processes are utilized to realize stable, scalable networks for information and signal processing. We also survey challenges and possible future research.

[1] Control of Noise in Chemical and Biochemical Information Processing, V. Privman, Israel J. Chem. 51, 118-131 (2010).

[2] Biochemical Filter with Sigmoidal Response: Increasing the Complexity of Biomolecular Logic, V. Privman, J. Halamek, M. A. Arugula, D. Melnikov, V. Bocharova and E. Katz, J. Phys. Chem. B 114, 14103-14109 (2010).

[3] Towards Biosensing Strategies Based on Biochemical Logic Systems, E. Katz, V. Privman and J. Wang, in: Proc. Conf. ICQNM 2010 (IEEE Comp. Soc. Conf. Publ. Serv., Los Alamitos, California, 2010), pages 1-9.

4:54PM L40.00011 Organizing biochemical reactions: Lessons from cyanobacteria¹, NIAL MANGAN, Harvard University Systems Biology PhD Program, MICHAEL BRENNER, Harvard School of Engineering and Applied Sciences — Cyanobacteria are model organisms for photosynthesis and are of interest for bio-fuel production and carbon dioxide sequestration. I present a mathematical model of the carbon concentrating mechanism (CCM) in cyanobacteria. The CCM is a combination of transporters and enzymes distinctively organized in the cell, which increase the internal concentration of carbon dioxide, and improve the efficiency of converting carbon dioxide to sugar. I find that the internal carbon concentration can be completely described by solutions in two parameter regimes of the model. These solutions correspond to varying transporter and enzymatic activity, which can be directly connected to experimental measurements. I also find a dependence of the carbon concentration on the spatial organization of the reactions within the cell. Understanding the CCM in cyanobacteria gives us insight into design principles for the cellular organization of biological reactions.

¹NSF Graduate Fellowship

5:06PM L40.00012 ABSTRACT WITHDRAWN —

Tuesday, February 28, 2012 2:30PM - 5:30PM —

Session L41 DFD: Pattern Formation, Nonlinear Dynamics, Computational Fluid Dynamics
156B

2:30PM L41.00001 A Thermodynamic Model for Behavioral Intelligence, ALEXANDER WISSNER-GROSS, CAMERON FREER, Massachusetts Institute of Technology — Recent advances in cosmology and computer science have hinted at a potentially deep connection between intelligence and thermodynamics. Here we attempt to elucidate that connection by showing that a generalization of entropic forces can induce archetypically intelligent behaviors in a variety of classical mechanical systems. These results suggest a simple, but general, thermodynamic model for behavioral intelligence.

2:42PM L41.00002 Data collapse and critical dynamics in neuronal avalanche data, THOMAS BUTLER, Massachusetts Institute of Technology, NIR FRIEDMAN, KARIN DAHMEN, University of Illinois at Urbana-Champaign, JOHN BEGGS, Indiana University, LEE DEVILLE, University of Illinois at Urbana-Champaign, SHINYA ITO, Indiana University — The tasks of information processing, computation, and response to stimuli require neural computation to be remarkably flexible and diverse. To optimally satisfy the demands of neural computation, neuronal networks have been hypothesized to operate near a non-equilibrium critical point. In spite of their importance for neural dynamics, experimental evidence for critical dynamics has been primarily limited to power law statistics that can also emerge from non-critical mechanisms. By tracking the firing of large numbers of synaptically connected cortical neurons and comparing the resulting data to the predictions of critical phenomena, we show that cortical tissues in vitro can function near criticality. Among the most striking predictions of critical dynamics is that the mean temporal profiles of avalanches of widely varying durations are quantitatively described by a single universal scaling function (data collapse). We show for the first time that this prediction is confirmed in neuronal networks. We also show that the data have three additional features predicted by critical phenomena: approximate power law distributions of avalanche sizes and durations, samples in subcritical and supercritical phases, and scaling laws between anomalous exponents.

2:54PM L41.00003 Self Organized Criticality as a new paradigm of sleep regulation¹, PLAMEN CH. IVANOV, RONNY P. BARTSCH, Harvard Medical School and Division of Sleep Medicine, Brigham and Womens Hospital, Boston, MA 02115, USA — Humans and animals often exhibit brief awakenings from sleep (arousals), which are traditionally viewed as random disruptions of sleep caused by external stimuli or pathologic perturbations. However, our recent findings show that arousals exhibit complex temporal organization and scale-invariant behavior, characterized by a power-law probability distribution for their durations, while sleep stage durations exhibit exponential behavior. The co-existence of both scale-invariant and exponential processes generated by a single regulatory mechanism has not been observed in physiological systems until now. Such co-existence resembles the dynamical features of non-equilibrium systems exhibiting self-organized criticality (SOC). Our empirical analysis and modeling approaches based on modern concepts from statistical physics indicate that arousals are an integral part of sleep regulation and may be necessary to maintain and regulate healthy sleep by releasing accumulated excitations in the regulatory neuronal networks, following a SOC-type temporal organization.

¹Supported by: NIH Grant 1R01HL098437-01A1, Office of Naval Research Grant 000141010078, Brigham and Womens Hospital BRI Fund and the German Academic Exchange Service (DAAD).

3:06PM L41.00004 Frost nucleation, growth and propagation on a hydrophobic surface¹, JOSÉ GUADARRAMA-CETINA, University of Navarra, ANNE MONGRUEL, PMMH, UMR 7636 CNRS-ESPCI-University Paris 6-University Paris 7, WENCESLAO GONZÁLEZ-VIÑAS, University of Navarra, DANIEL BEYSENS, PMMH, UMR 7636 CNRS-ESPCI-University Paris 6-University Paris 7 and CEA-Grenoble — We report experimental results on the condensation of water vapor on a substrate (-9°C) at supercooled conditions. The resulting breath figure grows until the liquid to solid phase transition takes place. The frost seeds start to grow by deposition at the expense of neighboring supercooled water drops that evaporate. Sometimes the propagation (due to the growth of the ice) is faster than the evaporation of the drops, hence they transit to the solid state via a percolation mechanism. In this work [1], we analyze the growth of supercooled condensed drops (first stage), the growth of the ice crystals and the evolution of the supercooled water drops (intermediate and late stages). We also consider the liquid - solid front propagation (growth of the frost figure).

[1] J. Guadarrama-Cetina, A. Mongruel, W. González-Viñas, D. Beysens. In preparation

¹This work is partly supported by the Spanish Government (contract No. FIS2008-01126). J.G. acknowledges the financial support from the "Asociación de Amigos de la Universidad de Navarra".

3:18PM L41.00005 Pattern formation in oscillatory fluid flows, DAPHNE KLOTSAS, University of Michigan, MICHAEL SWIFT, University of Nottingham — Rigid spherical particles in oscillating fluid flows form interesting structures as a result of fluid mediated interactions. Here we show that two spheres under horizontal vibration align themselves at right angles to the oscillation and sit with a gap between them, which scales in a non-classical way with the boundary layer thickness. The details of this behavior have been investigated through experiments and simulations. We then look at a collection of spherical particles, which form chains perpendicular to the direction of oscillation. Comparing experiments and simulations we study the stages of evolution from a dispersed initial configuration to an ordered chain structure. We investigate the details of the interactions and find that the nonlinear hydrodynamic effect of steady streaming is the driving force.

3:30PM L41.00006 Dynamic effects induced by renormalization in anisotropic pattern forming systems, MATTEO NICOLI, Physique de la Matière Condensée, École Polytechnique, CNRS, Palaiseau, France, ADRIAN KELLER, STEFAN FACKSO, Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany, RODOLFO CUERNO, Departamento de Matemáticas and Grupo Interdisciplinar de Sistemas Complejos, Universidad Carlos III de Madrid, Leganés, Spain — The dynamics of patterns in large two-dimensional domains remains a challenge in nonequilibrium phenomena. Often it is addressed through mild extensions of one-dimensional equations. We show that full two-dimensional generalizations of the latter can lead to unexpected dynamic behavior. As an example we consider the anisotropic Kuramoto-Sivashinsky equation, which is a generic model of anisotropic pattern forming systems and has been derived in different instances of thin film dynamics. A rotation of a ripple pattern by 90° occurs in the system evolution when nonlinearities are strongly suppressed along one direction. This effect originates in nonlinear parameter renormalization at different rates in the two system dimensions, showing a dynamic interplay between scale invariance and wavelength selection. Potential experimental realizations of this phenomenon are identified. A. Keller, M. Nicoli, S. Fackso, and R. Cuerno, Phys. Rev. E 84, 015202(R) (2011).

3:42PM L41.00007 Self-Sustained Front Propagation in Disordered Flow, SEVERINE ATIS, HAROLD AURADOU, CNRS, DOMINIQUE SALIN, UPMC, LAURENT TALON, CNRS — We generate propagative fronts resulting from a balance between molecular diffusion and non-linear chemical reaction. These fronts behave as solitary waves with a constant velocity and a stationary concentration profile. The interaction between this self-sustained system and a disordered flow leads to complex structures formation. We have performed experiments of the front propagation over a wide range of stochastic flow rates, in porous media. We have determined the structure and the velocity distribution measured along the front. The concentration profile displays salient spatial features such as scaling laws and pattern formation.

3:54PM L41.00008 Sidebranching in the Dendritic Crystal Growth of Ammonium Chloride, ANDREW DOUGHERTY, Lafayette College — We report measurements of the dendritic crystal growth of NH_4Cl from supersaturated aqueous solution at small supersaturations. Sidebranch growth in this regime is challenging to model well, and the origin of the sidebranches is not fully understood. The early detection of sidebranches requires measurements of small deviations from the smooth steady state shape, but that shape is not well known at the intermediate distances relevant for sidebranch measurements. One model is that sidebranches result from the selective amplification of microscopic noise. We compare measurements of the sidebranch envelope with predictions of the noise-induced sidebranching model of González-Cinca, Ramírez-Piscina, Casademunt, and Hernández-Machado [Phys. Rev. E, 63, 051602 (2001)]. We find that the measured amplitude is somewhat larger than predicted, and the shape of the sidebranch envelope is also different. A second model is that sidebranches result from small oscillations of the tip. We have observed no such oscillations, but very small ones can not be ruled out. No measurement of the tip region can be completely free of contamination from early sidebranches, so it can be challenging to distinguish between an oscillating tip and a smooth tip with sidebranches starting nearby.

4:06PM L41.00009 Burning invariant manifolds in spatially disordered advection-reaction-diffusion¹, DYLAN BARGTEIL, Bucknell University/University of Maryland, TOM SOLOMON, Bucknell University, JOHN MAHONEY, KEVIN MITCHELL, University of California, Merced — We introduce burning invariant manifolds (BIMs) which act as barriers to front propagation, similar to the role played by invariant manifolds as barriers to passive transport in two-dimensional flows. We present experimental studies of BIMs in a spatially disordered, time-independent flow. We generate the flow with a magnetohydrodynamic technique that uses a DC current and a disordered pattern of permanent magnets. The velocity field is determined from this flow using particle tracking velocimetry, and reaction fronts are produced using the Ferriin-catalyzed Belousov-Zhabotinsky (BZ) chemical reaction. We use the experimental velocity field and a three-dimensional set of ODEs to predict from theory the location and orientation of BIMs. These predicted BIMs are found to match up well with the propagation barriers observed experimentally in the same flow using the BZ reaction. We explore the nature of BIMs as one-sided barriers, in contrast to invariant manifolds that act as barriers for passive transport in all directions. We also explore the role of projection singularities in the theory and how these singularities affect front behavior.

¹NSF Grants DMR-0071771, PHY-0552790

4:18PM L41.00010 Chaotic advection of immiscible fluids¹, BENJAMIN VOLLMAYR-LEE, Bucknell University, DANIEL BELLER, University of Pennsylvania, SOHEI YASUDA, Purdue University — We consider a system of two immiscible fluids advected by a chaotic flow field. A nonequilibrium steady state arises from the competition between the coarsening of the immiscible fluids and the domain bursting caused by the chaotic flow. It has been established that the average domain size in this steady state scales as an inverse power of the Lyapunov exponent. We examine the issue of local structure and look for correlations between the local domain size and the finite-time Lyapunov exponent (FTLE) field. For a variety of chaotic flows, we consistently find the domains to be smallest in regions where the FTLE field is maximal. This raises the possibility of making universal predictions of steady-state characteristics based on Lyapunov analysis of the flow field.

¹Supported by NSF grant REU-0552790

4:30PM L41.00011 Hamiltonian traffic dynamics in microfluidic-loop networks, RAPHAEL JEANNERET, DENIS BARTOLO, PMMH-ESPCI, Université Paris Diderot, BARTOLO TEAM — Recent microfluidic experiments revealed that large particles advected in a fluidic loop display long-range hydrodynamic interactions. However, the consequences of such couplings on the traffic dynamics in more complex networks remain poorly understood. In this letter, we focus on the transport of a finite number of particles in one-dimensional loop networks. By combining numerical, theoretical, and experimental efforts, we evidence that this collective process offers a unique example of Hamiltonian dynamics for hydrodynamically interacting particles. In addition, we show that the asymptotic trajectories are necessarily reciprocal despite the microscopic traffic rules explicitly break the time reversal symmetry. We exploit these two remarkable properties to account for the salient features of the effective three-particle interaction induced by the exploration of fluidic loops.

4:42PM L41.00012 Intensity statistics of branched flow, JAKOB METZGER, RAGNAR FLEISCHMANN, THEO GEISEL, Max-Planck-Institute for Dynamics and Self-Organization, Goettingen, Germany — Branched flow is a universal phenomenon of particle and wave flows which are subjected to weak, correlated disorder. It has been observed on length scales ranging from a few micrometres, affecting the transport properties of semiconductor devices [1], up to several thousand kilometres, influencing sound propagation through the ocean [2]. It is also responsible for the appearance of large and hazardous freak waves and tsunamis [3]. While the statistics of the number of such branches has recently been calculated [4], the influence on the statistics of the intensity of the waves remains an open question [5]. Here, we show how the classical ray intensity impacts on the wave intensity statistics, and illuminate the role played by the decoherence of the wavefunction.

[1] Topinka et al., Nature 410, 183 (2001), Jura et al., Nat. Phys. 3, 841 (2007)

[2] Wolfson & Tomsovic, J. Acous. Soc. Am. 109, 2693 (2001)

[3] Berry, Proc. R. Soc. A 463, 3055 (2007); Heller et al., J. Geophys. Res. 113, C09023 (2008)

[4] Metzger, Fleischmann and Geisel, Phys. Rev. Lett. 105, 020601 (2010)

[5] Höhmann et al., Phys. Rev. Lett. 104, 093901 (2010), Arecchi et al., Phys. Rev. Lett. 106, 153901 (2011), Ying et al., Nonlinearity 24, R67 (2011)

4:54PM L41.00013 Flow past a circular cylinder with momentum injection: Optimal control cylinder design, SUBHASH REDDY, PRASAD PATNAIK, Indian Institute of Technology, Madras — The primary aim of this work is to suppress vortex shedding behind a circular cylinder by placing two small rotating control cylinders very close to it and hence injecting momentum into the boundary layer. The position and circulation strengths of the control cylinders are the important aspects of our study. Solving the complete Navier-Stokes (NS) equations can be time consuming while identifying the position and circulation strength of the control cylinders. Instead, reduced order models (ROM) can be used to save the computational expenditure associated with solving the complete NS model. Physics-based approaches to reduced order modeling include many of the techniques for modeling and simplification commonly used in fluid dynamics analysis such as potential flow analysis, vortex methods etc. Each of these are approximations to the full NS equations and each can serve as effective ROMs under appropriate conditions. In the present study, we try to achieve potential flow behavior by optimum positioning of the control cylinders and hence potential flow analysis is carried out with different analytical methods like Föppl vortex model and conformal mapping techniques. For these optimum values, the analytical solution obtained is compared with the numerical viscous flow simulations.

5:06PM L41.00014 ABSTRACT WITHDRAWN —

5:18PM L41.00015 Simulating Tablet Dissolution in Complex Hydrodynamic Environment with Lattice-Boltzmann Method, ARPON RAKSIT, Harvard University, NING SUN, VADIM POZIN, DILIP GERSAPPE, Department of Materials Science and Engineering, Stony Brook University — Using the Lattice-Boltzmann method, we developed a 3D mesoscopic model to study the drug-dissolution process in a complex hydrodynamic environment involving spatially varying velocity and shear forces. The results showed turbulent flow in region above tablet, which was also obtained by visualization experiments. The dissolution profiles obtained by incorporating detailed kinetics showed good agreement with case studies from literature. The influence of the paddle speed and the size of the system were studied, and a multicomponent approach was also incorporated. Our results show how that the hydrodynamic environment would affect the dissolution process by changing the local concentration of components near the tablet and by the particle erosion under high fluid velocity. The code was also successfully parallelized so that the simulation of comparatively large system is now possible.

Tuesday, February 28, 2012 2:30PM - 4:54PM —

Session L42 DBIO: Focus Session: Physics of Cancer II – Physical Aspects 156C

2:30PM L42.00001 A Condensed Matter Physicist Looks at Cancer and the Tumor Microenvironment¹, CLARE YU, University of California, Irvine — We will discuss what physics can bring to cancer biology, and give an example by taking a closer look at the tumor microenvironment. Cancer cells do not act alone. They get their cues from the their environment which consists of the extracellular matrix and the cells (fibroblasts) that form it. These cues can be both chemical and mechanical in nature.

¹Work supported by the Princeton Physical Sciences Oncology Center

3:06PM L42.00002 Senescent cells in growing tumors, STEFANO ZAPPERI, National Research Council of Italy, IENI-CNR, Milano, Italy, CATERINA A.M. LA PORTA, Department of Biomolecular Science and Biotechnology, University of Milano, Italy, JAMES P. SETHNA, LASSP, Department of Physics, Cornell University, Ithaca NY — Tumors are defined by their intense proliferation, but sometimes cancer cells turn senescent and stop replicating. In the stochastic cancer model in which all cells are tumorigenic, senescence is seen as the result of random mutations, suggesting that it could represent a barrier to tumor growth. In the hierarchical cancer model a subset of the cells, the cancer stem cells, divide indefinitely while other cells eventually turn senescent. Here we formulate cancer growth in mathematical terms and obtain distinct predictions for the evolution of senescence in the two models. We perform experiments in human melanoma cells which confirm the predictions of the hierarchical model and show that senescence is a reversible process controlled by survivin. We conclude that enhancing senescence is unlikely to provide a useful therapeutic strategy to fight cancer, unless the cancer stem cells are specifically targeted.

3:18PM L42.00003 Clustering of brain tumor cells: a first step for understanding tumor recurrence, EVGENIY KHAİN, Department of Physics, Oakland University, M.O. NOWICKI, E.A. CHIOCCA, S.E. LAWLER, Department of Neurological Surgery, The Ohio State University Medical Center, C.M. SCHNEIDER-MIZELL, L.M. SANDER, Department of Physics, University of Michigan — Glioblastoma tumors are highly invasive; therefore the overall prognosis of patients remains poor, despite major improvements in treatment techniques. Cancer cells detach from the inner tumor core and actively migrate away [1]; eventually these invasive cells might form clusters, which can develop to recurrent tumors. In vitro experiments in collagen gel [1] followed the clustering dynamics of different glioma cell lines. Based on the experimental data, we formulated a stochastic model for cell dynamics, which identified two mechanisms of clustering. First, there is a critical value of the strength of adhesion; above the threshold, large clusters grow from a homogeneous suspension of cells; below it, the system remains homogeneous, similarly to the ordinary phase separation. Second, when cells form a cluster, there is evidence that their proliferation rate increases. We confirmed the theoretical predictions in a separate cell migration experiment on a substrate and found that both mechanisms are crucial for cluster formation and growth [2]. In addition to their medical importance, these phenomena present exciting examples of pattern formation and collective cell behavior in intrinsically non-equilibrium systems [3].

[1] A. M. Stein et al, Biophys. J., 92, 356 (2007).

[2] E. Khaın et al, EPL 88, 28006 (2009).

[3] E. Khaın et al, Phys. Rev. E. 83, 031920 (2011).

3:30PM L42.00004 Targeting tumor acidity, YANA K. RESHETNYAK, Physics, University of Rhode Island, DONALD M. ENGELMAN, Mol. Biophys & Biochem., Yale, OLEG A. ANDREEV, University of Rhode Island, URI TEAM, YALE TEAM — One of the main features of solid tumors is extracellular acidity, which correlates with tumor aggressiveness and metastatic potential. We introduced novel approach in targeting of acidic tumors, and translocation of cell-impermeable cargo molecules across cellular membrane. Our approach is based on main principle of insertion and folding of a polypeptide in lipid bilayer of membrane. We have identified family of pH Low Insertion Peptides (pHLIPs), which are capable spontaneous insertion and folding in membrane at mild acidic conditions. The affinity of peptides of pHLIP family to membrane at low pH is several times higher than at neutral pH. The process of peptides folding occurs within milliseconds. The energy released in a result of folding (about 2 kcal/mol) could be used to move polar cargo across a membrane, which is a novel concept in drug delivery. pHLIP peptides could be considered as a pH-sensitive single peptide molecular transporters and conjugated with imaging probes for fluorescence, MR, PET and SPECT imaging, they represent a novel in vivo marker of acidity. The work is supported by NIH grants CA133890 and GM073857 to OAA, DME, YRK.

3:42PM L42.00005 Stress Modulus of Cancer Cells¹, KEITH BONIN, MARTIN GUTHOLD, XINYI GUO, JUSTIN SIGLEY, Wake Forest University — Our main goal is to study the different physical and mechanical properties of cells as they advance through different stages of neoplastic transformation from normal to the metastatic state. Since recent reports indicate there is significant ambiguity about how these properties change for different cancer cells, we plan to measure these properties for a single line of cells, and to determine whether the changes vary for different cellular components: i.e. whether the change in physical properties is due to a change in the cytoskeleton, the cell membrane, the cytoplasm, or a combination of these elements. Here we expect to present data on the stress modulus of cancer cells at different stages: normal, mortal cancerous, immortal cancerous, and tumorigenic. The cells are Weinberg cell line Human Mammary Epithelial (HME) cells. Atomic force microscope (AFM) probes with different diameters are used to push on the cell membrane to measure the local, regional and global cell stress modulus. Preliminary results on normal HME cells suggests a stress modulus of 1.5 ± 0.8 kPa when pushing with $7 \mu\text{m}$ spherical probes. We anticipate reporting an improved value for the modulus as well as results for some of the Weinberg cancer cells.

¹This work is supported by NSF Materials and Surface Engineering grant CMMI-1152781.

3:54PM L42.00006 Cancer-stroma evolutionary dynamics in stress-gradient microenvironment, AMY WU, Princeton University, GUILLAUME LAMBERT, New York University, ROBERT AUSTIN, JAMES STURM, Princeton University, ZAYAR KHIN, ARIOSTO SILVA, Moffitt Cancer Center, PRINCETON PHYSICAL SCIENCES-ONCOLOGY CENTER TEAM, PRINCETON INSTITUTE FOR THE SCIENCE AND TECHNOLOGY OF MATERIALS TEAM — In order to study the evolution of drug resistance in cancer, it is important to mimic the tumor microenvironment, in which cells are exposed to not uniform concentrations but rather gradients of drugs, nutrients, and other factors Compared to traditional in-vitro methods, microfluidic structure enables better control of the temporal and spatial profile of gradients. Here we demonstrate a microfluidic Doxorubicin gradient environment with heterogeneous landscape, and culture multiple myeloma (8226-S, expressing RFP) and bone marrow stroma (HS-5, expressing GFP) cell lines together. The myeloma cells are not directly motile, but they are able to migrate via the adhesion to motile stroma cells. The indirect motility mechanism of the myeloma cells is crucial for the adaptation to stress environment. Finally, we will report the co-culture dynamics under the stress of doxorubicin gradients, observing for cellular migrations and growth

4:06PM L42.00007 Dynamic density functional theory of solid tumor growth: Preliminary models, JOHN LOWENGRUB¹, UC Irvine — Cancer is a complex system whose dynamics and growth result from nonlinear processes coupled across wide ranges of spatio-temporal scales. The current mathematical modeling literature addresses issues at various scales but the development of theoretical methodologies capable of bridging gaps across scales needs further study. We present a new theoretical framework based on Dynamic Density Functional Theory (DDFT) extended, for the first time, to the dynamics of living tissues by accounting for cell density correlations, different cell types, phenotypes and cell birth/death processes, in order to provide a biophysically consistent description of processes across the scales. We present an application of this approach to tumor growth.

¹This is joint work with Arnaud Chauviere, Haralampos Hatzikirou, and Vittorio Cristini.

4:18PM L42.00008 The physics of Eukaryotic cell crawling through elastic media, ELNAZ ALIPOUR, BAUM-SNOW, CHARLES WOLGEMUTH, University of CT Health Center — Understanding the motion of cells through deformable media, such as the extra-cellular matrix (ECM), is important for understanding many biological processes, such as cancer metastasis, wound healing, and organismal development. Crawling eukaryotic cells exert dipole-distributed traction stresses on the external environment. These stress distributions pull backwards at the front of the cell and forward at the rear of the cell. Recent experiments have shown the magnitude of the deformations induced in a collagen matrix by migrating cancer cells. We propose a model to understand cell movements through the ECM, by considering a dipole-crawler moving through an isotropic, linear elastic medium. This model captures the major features of the deformations that are induced by motile cancer cells in collagen. In addition, the model suggests that the deformations that are induced in the matrix can provide a mechanism by which distal cells can interact with one another through matrix-mediated interactions. We, therefore, study the forces, torques, and trajectories of two cells migrating through the ECM. Our analysis suggests a mechanism that may be relevant for the collective migration of cells during cancer metastasis and other processes where numerous cells move through the ECM.

4:30PM L42.00009 Monte Carlo Simulations for Radiobiology, NICOLE ACKERMAN, Stanford University, Dept of Physics, MAGDALENA BAZALOVA, Stanford University, Dept of Radiation Oncology, KEVIN CHANG, Stanford University, Dept of Bioengineering, EDWARD GRAVES, Stanford University, Dept of Radiation Oncology — The relationship between tumor response and radiation is currently modeled as dose, quantified on the mm or cm scale through measurement or simulation. This does not take into account modern knowledge of cancer, including tissue heterogeneities and repair mechanisms. We perform Monte Carlo simulations utilizing Geant4 to model radiation treatment on a cellular scale. Biological measurements are correlated to simulated results, primarily the energy deposit in nuclear volumes. One application is modeling dose enhancement through the use of high-Z materials, such gold nanoparticles. The model matches in vitro data and predicts dose enhancement ratios for a variety of in vivo scenarios. This model shows promise for both treatment design and furthering our understanding of radiobiology.

4:42PM L42.00010 A two-phase mixture model of avascular tumor growth, DENIZ OZTURK, M. BURCIN UNLU, SIRIN YONUCU, UGUR CETINER, Bogazici University, Bebek, 34342 Istanbul / Turkey, MEDICAL & BIOLOGICAL PHYSICS RESEARCH GROUP TEAM — Interactions with biological environment surrounding a growing tumor have major influence on tumor invasion. By recognizing that mechanical behavior of tumor cells could be described by biophysical laws, the research on physical oncology aims to investigate the inner workings of cancer invasion. In this study, we introduce a mathematical model of avascular tumor growth using the continuum theory of mixtures. Mechanical behavior of the tumor and physical interactions between the tumor and host tissue are represented by biophysically founded relationships. In this model, a solid tumor is embedded in inviscid interstitial fluid. The tumor has viscous mechanical properties. Interstitial fluid exhibits properties of flow through porous medium. Associated with the mixture saturation constraint, we introduce a Lagrange multiplier which represents hydrostatic pressure of the interstitial fluid. We solved the equations using Finite Element Method in two-dimensions. As a result, we have introduced a two-phase mixture model of avascular tumor growth that provided a flexible mathematical framework to include cells' response to mechanical aspects of the tumor microenvironment. The model could be extended to capture tumor-ECM interactions which would have profound influence on tumor invasion.

Tuesday, February 28, 2012 2:30PM - 5:30PM —

Session L43 DBIO DPOLY: Invited Session: Precursors to the Folding and Aggregation of Biological Molecules 157AB

2:30PM L43.00001 Postranslational modifications significantly alter the binding-folding pathways of proteins associating with DNA, GAREGIN PAPOIAN, The University of Maryland — Many important regulators of gene activity are natively disordered, but fully or partially order when they bind to their targets on DNA. Interestingly, the ensembles of disordered states for such free proteins are not structurally featureless, but can qualitatively differ from protein to protein. In particular, in random coil like states the chains are swollen, making relatively few contacts, while in molten globule like states a significant collapse occurs, with ensuing high density of intra-protein interactions. Furthermore, since many DNA binding proteins are positively charged polyelectrolytes, the electrostatic self-repulsion also influences the degree of collapse of the chain and its conformational preferences in the free state and upon binding to DNA. In our work, we have found that the nature of the natively disordered ensemble significantly affects the way the protein folds upon binding to DNA. In particular, we showed that posttranslational modifications of amino acid residues, such as lysine acetylation, can alter the degree of collapse and conformational preferences for a free protein, and also profoundly impact the binding affinity and pathways for the protein DNA association. These trends will be discussed in the context of DNA interacting with various histone tails and the p53 protein.

3:06PM L43.00002 Mesoscopic Aggregation in Protein Solutions¹, VASSILIY LUBCHENKO, University of Houston — Long-lived mesoscopic clusters of a dense protein liquid are observed in concentrated solutions of numerous proteins. These clusters are a necessary kinetic intermediate for the formation of solid aggregates of native and misfolded protein molecules. We propose a novel physicochemical mechanism, by which the clusters consist of an off-equilibrium mixture of single protein molecules and long-lived protein-containing complexes. The puzzling mesoscopic size of the clusters is determined by the lifetime of the complexes and their diffusivity. We have predicted and observed a number of interesting kinetic and thermodynamic behaviors that are associated with the mesoscopic clusters. These behaviors include: (a) Ostwald-like ripening of the clusters (b) a crossover to long-range density fluctuations at high concentrations; (c) a universal, diffusion-like scaling of the autocorrelation function of light scattered off the protein solution; (d) non-trivial dependencies of the cluster size and volume fraction on the protein concentration in the solution. Our analysis of the anisotropic Coulomb interactions suggests for mesoscopic clusters to form in lysozyme solutions, protein molecules must undergo conformational changes.

¹Supported by NSF, Beckman Foundation, Welch Foundation, Sloan Foundation

3:42PM L43.00003 Protein misfolding and aggregation, DAVE THIRUMALAI, University of Maryland — No abstract available.

4:18PM L43.00004 The impact of conformational transformations on the pathways and kinetics of protein self-assembly into extended matrices¹, JIM DE YOREO, Lawrence Berkeley Nat'l Lab — The concept of a folding funnel with kinetic traps is used to describe folding of individual proteins. Using in situ AFM to investigate both collagen fibril and S-layer membrane assembly on mica, we show this concept is equally valid during self-assembly of proteins into extended matrices. Moreover, considering the conformational changes required to achieve the ordered structure is critical to understanding the pathway to the final state and the kinetics of assembly. In the collagen system, both the pathway and the final conformational state can be finely tuned by varying the ionic strength. This alters the relative strengths of the collagen-collagen and collagen-mica binding free energy, which we quantify using dynamic force spectroscopy. Moreover, when conditions result in the ordered D-band structure of collagen, the emergence of order catalyzes the further transformation leading to non-linear attachment kinetics. In the S-layer system, there is a kinetic trap associated with conformational differences between a long-lived transient state and the final stable state. Both ordered tetrameric states emerge from clusters of an amorphous precursor phase, however, they then track along two different pathways. One leads directly to the final low-energy state and the other to the kinetic trap. Over time, the trapped state transforms into the stable state. By analyzing the time and temperature dependencies of formation and transformation we find the energy barriers to formation of either state to be nearly identical, but once the high-energy state forms, the barrier to transformation to the low-energy state is large. Thus the transient state exhibits the characteristics of a kinetic trap in a folding funnel.

¹This work was performed at the Molecular Foundry, Lawrence Berkeley National Laboratory, with support from the Office of Science, Office of Basic Energy Sciences, of the U.S. DoE under Contracts No. DE-AC52-07NA27344 and DE-AC02-05CH11231.

4:54PM L43.00005 The role of proteins and peptides in shaping the structure and microstructure of biogenic and biomimetic crystals, BOAZ POKROY, Department of Materials Engineering and the Russell Berrie Nanotechnology Institute, Technion Israel Institute of Technology, Haifa, Israel — In the course of biomineralization organisms form crystals which demonstrate superior characteristics as compared to their non-biogenic counterparts. One of the main reasons for this is that these crystals are actually hybrid nano-composites. In fact, each biogenic single crystal is not only encapsulated by an intercrystalline organic phase but in addition there are intracrystalline proteins within each individual single crystal. These proteins are the key players in the formation of biominerals and are vital in the precursor phase of their formation. I will show that both in biogenic and biomimetic crystals, these proteins have a major effect on their atomic structure and microstructure. This effect is in the form of lattice distortions which relax upon mild annealing. The distortions can be detected by means of high-resolution synchrotron diffraction. The activation energy of the relaxation of the lattice distortions is rather low and is comparable to the energy needed for protein unfolding. Furthermore, it will be shown that these intracrystalline proteins can stabilize metastable phases of calcium carbonate and even stabilize a previously unidentified twin law in calcite.

Tuesday, February 28, 2012 2:30PM - 5:30PM —

Session L44 DPOLY: Focus Session: Nano to Mesoscale Structure in Ordered Soft Matter: Liquid Crystal Phases 157C

2:30PM L44.00001 DILLON MEDAL BREAK —

3:06PM L44.00002 Nano to Meso-scale Structure in Liquid Crystals: the Cybotactic Nematic Phase of Bent-core Mesogens

, ORIANO FRANCESCANGELI, Polytechnic University of Marche, SIMAU Department, Via Brecce Bianche, 60131 Ancona, Italy — The extent of molecular order and the resulting broken symmetry determine the properties and mesophase type of liquid crystals (LCs). Thermotropic bent-core mesogens (BCMs) represent a new class of LCs exhibiting substantially different physical properties than traditional linear (calamitic) materials. In recent years BCMs have become the focus of intense experimental and theoretical investigation, with several exciting new developments. These include chiral mesophases composed of achiral BCMs, giant flexoelectricity, biaxial nematic (N) order, a ferroelectric response in the N phase, and a large flow birefringence. A key issue that is currently widely debated concerns the actual nature of the N phase of BCMs which gives rise to some of the above mentioned effects and is unambiguously identified by a peculiar low-angle X-ray diffraction pattern (the “four-spot pattern”). The consensus emerging is that this N phase of BCMs constitutes a new type of mesophase, namely, a cybotactic nematic (N_{cyb}) phase unrelated to pretransition cybotaxis, in agreement with experimental [1-3] and theoretical findings [4]. This N_{cyb} phase is composed of nanometer-size clusters of BCMs exhibiting a relatively high degree of internal order—orientational as well as translational order (strata) imposed by close packing the BCM nonlinear shape. This peculiar supramolecular structure of the N_{cyb} mesophase of BCMs—evanescent, biaxial clusters of tilted and stratified nonlinear mesogens percolating the nematic fluid—accounts for their unusual properties, e.g., biaxial order [4], ferroelectric response [1], and extraordinary field-induced effects [5]. In this talk I will give an overview of the most recent developments and the current state of research on this subject.

[1] O. Francescangeli *et al.*, Adv. Funct. Mater. **19**, 2592 (2009).

[2] O. Francescangeli and E.T. Samulski, Soft Matter **6**, 2413 (2010)

[3] O. Francescangeli *et al.*, Soft Matter **7**, 895 (2011).

[4] A.G. Vanakaras and D.J. Photinos, J. Chem. Phys. **128**, 154512 (2008).

[5] O. Francescangeli *et al.*, Phys. Rev. Lett. **107**, 207801 (2011).

3:42PM L44.00003 Nanoscale Positional Order Correlations: Swarms, Cybotactic Groups, Clusters, and Pretransitional Fluctuations in Liquid Crystals¹

, SATYENDRA KUMAR, DENA AGRA-KOOIJMAN, Kent State University, BHARAT ACHARYA, Platypus Technologies, LLC — Short-range molecular associations in organic liquids were first described as “cybotactic” groups [1] followed by the development of the swarm theory [2] to explain the structure, strong light scattering, and flow behavior of the nematic (N) liquid crystal phase. However, these ideas became inconsequential with the advent of the Oseen-Frank’s continuum theory [3]. In 1970, de Vries reinvented cybotactic groups for the N phase of bis-(4'-n-octyloxybenzal)-2-chloro-1,4-phenylenediamine. These were eventually understood to be SmC pretransitional fluctuations, i.e., small correlated regions of the lower symmetry phase near the transition. Thermotropic biaxial mesophases have resurrected the faith in cybotacticity in the guise of a new word - “clusters”. Previous x-ray studies of normal organic fluids, and calamitic, lyotropic, and bent-core mesogens show that these clusters fall into three groups depending on the relative contributions of normal liquid structure and pretransitional fluctuations. A comparison with other organic and inorganic fluids will also be made.

[1] G.W. Stewart, Phys. Rev. **35**, 726 (1930).

[2] L.S. Ornstein and W. Kast, Trans. Farad. Soc. **29**, 931 (1933).

[3] FC Frank, Discuss. Faraday Soc. **25**, 19 (1958); W. Oseen, Ark. Mat., Astron. Fys. **19**, 1 (1925).

¹Supported by the BES, US DOE, Grant DE-SC0001412.

3:54PM L44.00004 Randomized Grain Boundary Liquid Crystal Phase

, D. CHEN, University of Colorado at Boulder, H. WANG, M. LI, Jilin University, M. GLASER, J. MACLENNAN, N. CLARK, University of Colorado at Boulder, UNIVERSITY OF COLORADO AT BOULDER TEAM, JILIN UNIVERSITY TEAM — The formation of macroscopic, chiral domains, in the B4 and dark conglomerate phases, for example, is a feature of bent-core liquid crystals resulting from the interplay of chirality, molecular bend and molecular tilt. We report a new, chiral phase observed in a hockey stick-like liquid crystal molecule. This phase appears below a smectic A phase and cools to a crystal phase. TEM images of the free surface of the chiral phase show hundreds of randomly oriented smectic blocks several hundred nanometers in size, similar to those seen in the twist grain boundary (TGB) phase. However, in contrast to the TGB phase, these blocks are randomly oriented. The characteristic defects in this phase are revealed by freeze-fracture TEM images. We will show how these defects mediate the randomized orientation and discuss the intrinsic mechanism driving the formation of this phase. This work is supported by NSF MRSEC Grant DMR0820579 and NSF Grant DMR0606528.

4:06PM L44.00005 Resonant X-ray Scattering Studies of Smectic and Columnar Bent-Core Liquid Crystal Phases¹

, RONALD PINDAK, Brookhaven National Laboratory, PHILIPPE BAROIS, VIRGINIE PONSINET, Universite Bordeaux, CESAR FOLCIA, JOSU ORTEGA, Universidad del País Vasco, LIDONG PAN², SHUN WANG, University of Minnesota, SUNTAO WANG³, Brookhaven National Laboratory, CHENG-CHER HUANG, University of Minnesota — Resonant X-ray scattering provides a direct probe of orientational structures in liquid crystals with periodicities that range from molecular dimensions (0.1 nm) to dimensions that can be observed with visible light (1.0 micron). We have recently applied this technique to study the orientational ordering of bent-core molecules in the smectic B₂ phase and the columnar B₁ phase. Using resonant scattering “forbidden” reflections due to glide or screw symmetry elements can be measured and an analysis of their polarization state enabled us to identify a chiral anticlinic antiferroelectric B₂ phase (Smectic C_{AP}A) coexisting with an achiral synclinic antiferroelectric B₂ phase (Smectic C_{SP}A) [1]. We were also able to determine the structure of a columnar B₁ phase and study the transition mechanism between the B₁ and B₂ phases [2].

[1] V. Ponsinet, *et al.*, Phys. Rev. E **84**, 011706 (2011).

[2] C. Folcia, *et al.*, Phys. Rev. E **84**, 010701R (2011).

¹Supported by DOE contract DE-AC02-98CH10886, NSF grant DMR-0605760, MICINN-FEDER project. MAT2009-14636-C03.

²current affiliation: Johns Hopkins University

³current affiliation: Cornell University

4:18PM L44.00006 Polyhedral Liquid Crystalline Vesicles¹

, MARK BOWICK, Syracuse University — Vesicles with internal liquid-crystalline order can assume a variety of shapes depending on the ratio of the Frank moduli to the bending rigidity. Using both analytic and numerical tools one can show that the possible low free energy morphologies include nano-fibers, faceted tetrahedral vesicles, ellipsoidal vesicles and cylindrical vesicles. The tetrahedral vesicle is a particularly fascinating example of a faceted liquid-crystalline membrane. Faceted liquid vesicles may lead to the design of supra-molecular structures with tetrahedral symmetry and new classes of nano-carriers.

¹NSF DMR-0808812

4:30PM L44.00007 Packing Cheerios: Simulation studies of torus-shaped hard particles¹, AN-DREW KONYA, ROBIN SELINGER, Kent State University — We perform simulation studies of hard torus-shaped particles under compression or in granular flow. A major challenge in performing simulations of non-spherical hard particles is determination of possible overlap between particle pairs. To simplify this calculation, we model a torus particle as an assembly of overlapping hard spheres arranged in a ring, and implement GPU acceleration to create an efficient Monte Carlo algorithm. For particles shaped approximately like Cheerios, with major radius $R=1$ and minor radius $r=0.6$, the hexagonal columnar crystal structure has packing fraction of about 2/3, but—as easy to observe in your cereal box—the system is easily trapped in a glassy disordered state. Preliminary simulation studies of the disordered state formed via rapid compression show short-range orientational correlations in which neighboring particles are either parallel or at right angles. We also examine structures that form when particles rain down onto a flat surface. Results are compared with the known liquid crystal phases of oblate ellipsoids and experiments on discotic colloidal phases.

¹Supported by NSF DMR-1106014.

4:42PM L44.00008 Effect of CNTs and Induced Chirality on Smectic- Smectic Liquid Crystal Phase Transitions, P. KALAKONDA, G.S. IANNACCHIONE, WPI, R. BASU, C. ROSENBLATT, CWRU, R.P. LEMIEUX, Queens U., CA — High-resolution calorimetry results are presented of carbon nanotubes (CNTs) and the liquid crystal (LC) 9004 nano-colloidal dispersions as a function of temperature, scan rate, and CNT concentration (0, 0.025, 0.05, 0.20 wt%). The CNT used have an enantiomeric excess that has been shown to induce chirality into this LC. The pure LC exhibits the phase sequence $I-N-SmA-SmC-SmB-Cr$ on cooling with the expected heat capacity C_p signatures, except for the $SmA-SmC$ transition, manifesting a double- C_p peak ~ 2 K apart at low effective scan rates (< 0.5 K min⁻¹). The introduction of CNTs results in the $I-N$, $N-SmA$, and $SmA-SmC$ double C_p features shifting to higher temperatures by ~ 1 K and remain sharp. However, the $SmC-SmB$ and $SmB-Cr$ transitions shift to lower temperatures by $\sim 3-4$ K and broaden dramatically with increasing CNT content. We interpret these observations as a consequence of the $\pi-\pi$ interactions between the phenyl rings of 9004 and the graphene surfaces that induces bulk chirality, and the pinning of the director parallel to the CNT long-axis far from the surface. The balance of these two mechanisms may stabilize phases that lack any in-smectic-plane ordering.

4:54PM L44.00009 ABSTRACT WITHDRAWN —

5:06PM L44.00010 Mesophase behavior and effect of polydispersity in assemblies of polyhedral particles¹, FERNANDO ESCOBEDO, UMANG AGARWAL, Cornell University — Mesophase behavior of polyhedral particles is uniquely linked to the inherent interactions embedded in their geometrical shape. A two-parameter model based on particle shape anisotropy and order of symmetry has been proposed for predicting phase behavior of polyhedral particles. The focus of the current work is to explore the phase behavior of a distinct class of polyhedral shapes, which emerge at different growth stages of PbSe nanocrystal formation. The body of knowledge that is emerging from these studies may prove useful in designing optimal self-assembly strategies for many desired nanostructures; e.g., as in our ongoing efforts in understanding the nanocrystal superlattice formation for solar cell applications. Moreover the effect of particle size polydispersity is explored by simulating the assembly of two representative shapes exhibiting totally different mesophase behavior. It is found that while mesophases are quite resilient to particle size anisotropy, the ordered structures are a complex function of the polydispersity and geometric attributes.

¹Support from Department of Energy grant no. ER46517

5:18PM L44.00011 Submolecular organization of de Vries smectics with tuned frustration between SmA- and SmC- promoting elements¹, DENA MAE AGRA-KOOIJMAN, S DEY, Kent State University, Q. SONG, Queens University, Canada, D. NONNENMACHER, F. GIESSELMANN, Universität Stuttgart, Germany, R. LEMIEUX, Queens University, Canada, SATYENDRA KUMAR, Kent State University — Structure-property relationships and the $SmA-SmC$ (AC) transition were investigated with x-ray diffraction in de Vries smectics compounds with tuned frustration between SmA and SmC promoting elements in the molecules. These are isometric analogues of a compound with a 2-phenylpyrimidine core that combines a trisiloxane-terminated alkoxy side-chain with a chloro-terminated alkoxy side-chain. The results reveal the local molecular structure in which, both siloxane and hydrocarbon segments are segregated and oriented parallel to the director in the SmA phase. But the siloxane segments oriented at an angle ($\sim 14^\circ$) different from the remaining hydrocarbon part of the molecule. This provides the first direct evidence of a kinked molecular conformation and nano-segregation of the molecule in the SmC phase. The two parts of the molecule possess different orientational order, siloxane part being more disordered, in both phases. The rate of change of the tilt angle with temperature appears to be different in the three compounds investigated.

¹Work supported by the Office of Basic Energy Sciences, DOE, Grant No. DE-SC0001412.

Tuesday, February 28, 2012 2:30PM - 5:30PM —
Session L45 DPOLY: Friction and Brushes 159

2:30PM L45.00001 DILLON MEDAL BREAK —

3:06PM L45.00002 Velcro[®] as a Mesoscopic Model System for Stick-Slip Motion¹, LISA MARIANI, CARA ESPOSITO, PIOTR HABDAS, PAUL ANGIOLILLO, Saint Joseph's University — The Amontons-Coulomb (AC) laws of friction, established during the 18th Century, serve to explain many of the phenomenological observations of friction in the macroscopic world. The AC laws for friction do not adequately explain certain systems, which undergo stick-slip motion, however. The hook-and-loop system (Velcro), in particular, exhibits easily observed stick-slip motion. Velcro evinces clear evidence of stick-slip dynamics that is independent of sliding velocity in accordance with Coulomb but, the maximum static friction force $F_s^{\max}$ and kinetic friction F_k are keenly dependent on "area of contact" (hook number) in contrast to accepted law, but consistent with recent studies of frictional dynamics in nanoscopic systems. Both the $F_s^{\max}$ and F_k as a function of area follow power law dependences with an exponent of approximately 2/3. Moreover, the fluctuations of the kinetic friction F_k also follow a power law dependence with an exponent of approximately 1/2 in accordance with random walk theory. On the other hand, the $F_s^{\max}$ and F_k both follow a linear dependence with applied load in accordance with the classical theory of AC.

¹Howard Hughes Medical Institute, Sigma Xi, McNulty Foundation

3:18PM L45.00003 The Use of Microscale Geometry to Tailor Stimulus-Responsive Surface Friction, LIN HAN, JIE YIN, LIFENG WANG, KHEK-KHIANG CHIA, ROBERT COHEN, MICHAEL RUBNER, MARY BOYCE, CHRISTINE ORTIZ, Massachusetts Institute of Technology — The capability to tailor stimulus-responsive surface friction, including sensitivity profile, range, temporal response and deformation mechanisms, holds great potential for an array of engineering and biomedical applications. In this study, the pH-dependent friction of layer-by-layer assemblies of poly(allylamine hydrochloride) and poly(acrylic acid) (PAH/PAA) were quantified for structures of a continuous planar film and anisotropic microtube forests via lateral force microscopy. By comparing experiments to microstructure-specific finite element modeling, a mechanistic change from surface adhesion-dominated friction ($\mu=0.11$) to viscoelasticity-governed shear ($\mu=0.017$) was predicted upon ionic crosslink density reduction of PAH/PAA from pH 5.5 to 2.0 for the film ($6.5\times$ decrease). The responsiveness of μ was further tuned by the tube forest geometry to be $3.5\times$. At pH 5.5, μ ($=0.094$) was lower than the film due to discrete tube bending/buckling and smaller tip-sample interface stress. At pH 2.0, μ ($=0.027$) was higher because of inter-tube contact and weaker substrate effect. This study provides an excellent platform to quantitatively access and design dynamic substrates with tailorable stimulus-responsive surface friction.

3:30PM L45.00004 Viscous friction of hydrogen-bonded matter, AYKUT ERBAS, North Carolina State University, DOMINIK HORINEK, University of Regensburg, ROLAND R. NETZ, Free University of Berlin — Amontons' law successfully describes friction between macroscopic solid bodies for a wide range of velocities and normal forces. For the diffusion and forced sliding of adhering or entangled macromolecules, proteins and biological complexes, temperature effects are invariably important and a similarly successful friction law at biological length and velocity scales is missing. Hydrogen bonds are key to the specific binding of bio-matter. Here we show that friction between hydrogen-bonded matter obeys in the biologically relevant low-velocity viscous regime a simple equation: the friction force is proportional to the number of hydrogen bonds, the sliding velocity, and a friction coefficient γ_{HB} . This law is deduced from atomistic molecular dynamics simulations for short peptide chains that are laterally pulled over hydroxylated substrates in the presence of water and holds for widely different peptides, surface polarities and applied normal forces. The value of γ_{HB} is extrapolated from simulations at sliding velocities in the range from $v = 10^{-2}$ m/s to 100 m/s by mapping on a simple stochastic model and turns out to be of the order of $\gamma_{HB} \simeq 10^{-8}$ kg/s. 3 hydrogen bonds act collectively.

3:42PM L45.00005 Molecular mechanisms of friction at soft polymer interfaces¹, FREDERIC RESTAGNO, CELINE COHEN, CHRISTOPHE POULARD, LILIANE LEGER, Laboratoire de physique des solides - CNRS/Univers. Paris-Sud — Polymer molecules strongly anchored to a solid substrate and interdigitated into bulk crosslinked elastomer have been shown recently to efficiently promote adhesion and friction between substrate and elastomer. Concerning friction, the regime of low surface coverage in surface anchored chains has been fully and quantitatively accounted for by the pull off mechanisms, where individual chains are dynamically extracted from the elastomer. Then, the stretching energy of these chains dominates the friction losses. We focus here on the dense surface coverage regime. We present systematic experiments performed on the polydimethylsiloxane (PDMS) - silica system, and determine molecular weight and sliding velocity dependences of the friction stress. We show that the friction is dominated by the shear thinning of the grafted layer confined between the elastomer and the substrate, and responding to the shear sollicitation like a melt, but with very long relaxation times. We also show that the friction stress appears highly sensitive to the molecular organization inside the surface anchored polymer layer, comparing end grafted and strongly adsorbed layers having otherwise the same molecular characteristics (molecular weight of the chains, and thickness of the surface anchored layer).

¹We thank the RTRA "Triangle de la physique" for financial support.

3:54PM L45.00006 Frictional properties of the end-grafted polymer layer in presence of salt solution, MARYAM RAFTARI, ZHENYU ZHANG, Department of Physics and Astronomy, University of Sheffield, Sheffield S3 7RH, UK, GRAHAM J. LEGGETT, Department of Chemistry, University of Sheffield, Sheffield S3 7HF, UK, MARK GEOGHEGAN, Department of Physics and Astronomy, University of Sheffield, Sheffield S3 7RH, UK — We have studied the frictional behaviour of grafted poly[2-(dimethylamino)ethyl methacrylate] (PDMAEMA) films using friction force microscopy (FFM). The films were prepared on native oxide-terminated silicon substrates using the technique of atom transfer radical polymerization (ATRP). These brushes had constant grafting density (1.18 nm^2), and of a thickness of $\sim 66 \text{ nm}$, as measured by ellipsometry. We show that single asperity contact mechanics (Johnson-Kendall-Roberts (JKR) and Derjaguin-Müller-Toporov (DMT) models) as well as a linear (Amontons) relation between applied load and frictional load all apply to these systems depending on the concentration of salt and the nature of the FFM probe. Measurements were made using gold-coating and polymer functionalized silicon nitride triangular probes. Polymer functionalized probe included growth the PDMAEMA with same method on tips. The frictional behaviour are investigated between PDMAEMA and gold coated and PDMAEMA tips immersed in different concentrations of KCl, KBr and KI.

4:06PM L45.00007 Nanofluidity of Polymer Melt: Two velocity hydrodynamics, SERGEI OBUKHOV, University of Florida, ALBERT JOHNER, CNRS Institut Charles Sadron, Strasbourg, France — According to the traditional macroscopic theory, the flow of the entangled polymer melt is associated with the relaxation processes in the network of entanglements. Each entanglement is formed by polymer chains, and these chains are moving randomly along their reptation tubes. Because of this random motion of polymers each entanglement has a finite lifetime. The lifetime is equal to the time needed for a polymer to leave its original tube. We should point out, that the motion of individual polymer chain in a tube is assumed to be completely random (diffusive). It means, that according to traditional theory, in average there is no systematic displacement of polymers with respect to the network of entanglements. The local polymer flow velocity in this theory is just the instant local velocity of individual entanglements forming this network. But the drift of individual polymers provides additional mechanism of a flow of a polymer melt, which becomes dominant at small scale. We suggest two velocity hydrodynamic equations which describe combined contribution of these two mechanisms. For illustration of this method we solve the problem of mobility of a small particle in a polymer melt.

4:18PM L45.00008 Poly(ethylene oxide) Chains Are Not "Hydrophilic" When They Exist As Polymer Brush Chains, HOYOUNG LEE, DAE HWAN KIM, KEVIN N. WITTE, KIMBERLY OHN, JE CHOI, School of Chemical Engineering, Purdue University, KYUNGIL KIM, MATI MERON, BINHUA LIN, CARS, The University of Chicago, BULENT AKGUN, SUSHIL SATIJA, NIST Center for Neutron Research, NIST, YOU-YEON WON, School of Chemical Engineering, Purdue University — By using a combined experimental and theoretical approach, a model poly(ethylene oxide) (PEO) brush system, prepared by spreading a poly(ethylene oxide)-poly(*n*-butyl acrylate) (PEO-PnBA) amphiphilic diblock copolymer onto an air-water interface, was investigated. The polymer segment density profiles of the PEO brush in the direction normal to the air-water interface under various grafting density conditions were determined from combined X-ray and neutron reflectivity data. In order to achieve a theoretically sound analysis of the reflectivity data, we developed a new data analysis method that uses the self-consistent field theoretical modeling as a tool for predicting expected reflectivity results for comparison with the experimental data. Using this new data analysis method, we discovered that the effective Flory-Huggins interaction parameter of the PEO brush chains is significantly greater than that corresponding to the theta condition, suggesting that contrary to what is more commonly observed for PEO in normal situations, the PEO chains are actually not "hydrophilic" when they exist as polymer brush chains, because of the many body interactions forced to be effective in the brush situation.

4:30PM L45.00009 ABSTRACT WITHDRAWN —

4:42PM L45.00010 Tunable Surface Properties from Bioinspired Polymers, WENDY VAN ZOELLEN, ADRIANNE M. ROSALES, University of California, Berkeley, RONALD N. ZUCKERMANN, The Molecular Foundry, Lawrence Berkeley National Laboratory, RACHEL A. SEGALMAN, University of California, Berkeley — Tunability of surface properties is of importance for a variety of coating applications, including antifouling coatings. We have investigated the surface properties of polypeptoids, a class of non-natural biomimetic polymers based on an N-substituted glycine backbone, that combine many of the advantageous properties of bulk polymers with those of synthetically produced proteins, including controllable chain shape, sequence, and self-assembled structure. We demonstrate the influence of the amount and sequence of hydrophobic monomers in a predominantly hydrophilic peptoid chain on surface properties. Especially the surface reconstruction behavior of block copolymers of these amphiphilic polypeptoids with polystyrene upon contact with water will be addressed. It has been found that surface reconstruction of peptoid chains that contain a sequence of only three fluorinated monomers and up to forty-two hydrophilic monomers occurs within seconds, whereas reorganization of surfaces containing five fluorinated monomers was an order of magnitude slower. Surfaces with higher fluorine content also showed lower settlement of spores of the green algae *Ulva*.

4:54PM L45.00011 Concentration Fluctuations of a Semidilute Polymer Solution in Good Solvent Near a Repulsive Surface, CATHERINE YEH, PHILIP PINCUS, Department of Physics, University of California, Santa Barbara, ALEXANDRA ZIDOVSKA, Dept. of Systems Biology, Harvard Medical School and School of Engineering and Applied Sciences/Dept. of Physics, Harvard University — The concentration profile of a semidilute polymer solution in good solvent near a repulsive surface has been previously calculated.¹ In this work we consider fluctuation corrections to the mean field concentration profile in the presence of a repulsive surface using the Cahn-Hilliard square-gradient approach extended to polymer interfaces. Our results predict that at strongly repulsive surfaces, a polymer in good solvent exhibits concentration fluctuations associated with the surface in addition to fluctuations of the bulk polymer solution. We compare our predictions with current experiments which have measured fluctuations in the concentration of interphase chromatin (DNA with its associated proteins) inside the nucleus of mammalian cells *in vivo* using ultrafast high space resolution spinning disc confocal microscopy.

¹J. F. Joanny, L. Leibler, P.-G. de Gennes, J. Polym. Sci. 17, 1073 (1979)

5:06PM L45.00012 Kinetics of Polymer Interfacial Reaction, SHUO ZHANG, JEFFREY KOBERSTEIN, Columbia University — Germanium crystals modified with high quality azide functional monolayers are used to directly monitor in situ the kinetics of interfacial “click” reactions with complementary alkyne end-functional poly(n-butyl acrylate) (PnBA) and polystyrene (PS) by attenuated total reflectance infrared spectroscopy (ATR-IR). In the presence of copper (I), the azide-modified Ge substrates react quantitatively with PnBA and PS via a 1,3-dipolar cycloaddition reaction. Time-resolved ATR-IR measurements show two regimes of kinetic behavior, as predicted by theory. In the first regime the rate is rapid and is controlled by diffusion of the polymer through the solvent, scaling with the square root of time. The rate slows considerably in the second regime, limited by penetration of the reacting polymer through the covalently bound polymer brush layer, scaling with the natural logarithm of time. The influence of polymer size and solvent quality are reported.

5:18PM L45.00013 Influence of Substrate Surface Energy on the Morphological Evolution of PS/PMMA Blend Thin Films, YIFU DING, DAE-UP AHN, ZHEN WANG, IAN CAMPBELL, MARK STOYKOVICH, University of Colorado at Boulder — In this study, the morphological evolutions of PS/PMMA blend thin films are systematically characterized during thermal annealing on both preferential and non-preferential surfaces. The evolution of phases on preferential surfaces was dictated by the preferential wetting of the components, and the coarsening process of the PMMA domains. PS droplets with high spatial correlation were formed in a moderately asymmetric PS/PMMA blend because of PS dewetting via a controlled nucleation mechanism. In contrast, a more asymmetric blend evolved into PS droplets via a random nucleation process, such that the PS droplets did not exhibit spatial correlation and had a broad size distribution. The morphological evolution of the blends on relatively non-preferential surfaces was also dictated by domain coarsening, but proceeds without the formation of PMMA wetting layer. As a result, a diverse set of non-equilibrium, micro- and nanoscale morphologies were observed.

Tuesday, February 28, 2012 2:30PM - 5:30PM –
Session L46 DPOLY: Dillon Medal Symposium 160ABC

2:30PM L46.00001 John H. Dillon Medal Lecture: Self-assembly of rod-coil block polymers, RACHEL SEGALMAN, University of California, Berkeley — While the self-assembly of coil-like block copolymers into morphologies with well-defined nanometer-sized periodicities is now classic, the translation of this strategy to functional polymers with non-Gaussian chain shapes is significantly more complicated. Control and predictive understanding of nanoscale structure in rod-coil block copolymer systems are of particular importance in both conjugated polymers (for optoelectronic devices) and biomimetic polymers. Our work is targeted at gaining a fundamental understanding of the thermodynamics and kinetics of self-assembling functional rod-coil block copolymer systems, and then applying this to conjugated polymers to understand structure-property relationships in plastic electronics. We demonstrate that phase space for weakly segregated model systems is described by the Flory-Huggins block interaction parameter (χN), the Maier-Saupé parameter (μN) (which parameterizes rod-rod interactions and also scales with temperature), the coil volume fraction (φ_{coil}), and a geometrical asymmetry term (ν) to account for aspect ratio differences in the rod and coil. Further, we also find that careful molecular design to moderate molecular interactions is essential in creating controllable systems. In particular, both sidechain substitution and sequence control can be used to control melting temperatures and liquid crystalline interactions in order to create a processing window in which self-assembly can occur.

3:06PM L46.00002 Wrinkles and Folds as Photonic Structures in Polymer Photovoltaics, YUEH-LIN LOO, JONG BOK KIM, Chemical and Biological Engineering, PILNAM KIM, HOWARD STONE, Mechanical and Aerospace Engineering, NICOLAS PEGARD, JASON FLEISCHER, Electrical Engineering, Princeton University, SOONG JU OH, CHERIE KAGAN, Materials Science and Engineering, University of Pennsylvania — We exploit the elastic instabilities of polymer surfaces under compressive mechanical stress to generate wrinkles and deep folds with prescribed dimensions and at pre-specified coverage over large areas. These wrinkles and deep folds act as photonic structures; they increase light coupling into and trapping within polymer photovoltaics. Devices on these surfaces show a 79% increase in the external quantum efficiency (EQE) in the visible compared to analogous devices on flat surfaces. More significantly, we observe an exponential increase in near-infrared light absorption in these devices. In both experiments and numerical simulations, we find that these structures extend the useful range of energy conversion by >200 nm, corresponding to a 600% increase in the EQE in the near-infrared where light is otherwise minimally absorbed. While we demonstrate this concept with polymer photovoltaics, the controlled introduction of compressive stress provides a straightforward and economical route to large-scale patterning of photonic structures for flexible opto-electronics.

3:18PM L46.00003 Molecular Exchange Dynamics in Block Copolymer Micelles¹ , FRANK BATES, JIE LU, SOOHYUNG CHOI, TIMOTHY LODGE, University of Minnesota — Poly(styrene-*b*-ethylene propylene) (PS-PEP) diblock copolymers were mixed with squalane (C₃₀H₆₂) at 1% by weight resulting in the formation of spherical micelles. The structure and dynamics of molecular exchange were characterized by synchrotron small-angle x-ray scattering (SAXS) and time resolved small-angle neutron scattering (TR-SANS), respectively, between 100 °C and 160 °C. TR-SANS measurements were performed with solutions initially containing deuterium labeled micelle cores and normal cores dispersed in a contrast matched squalane. Monitoring the reduction in scattering intensity as a function of time at various temperatures revealed molecular exchange dynamics highly sensitive to the core molecular weight and molecular weight distribution. Time-temperature superposition of data acquired at different temperatures produced a single master curve for all the mixtures. Experiments conducted with isotopically labeled micelle cores, each formed from two different but relatively monodisperse PS blocks, confirmed a simple dynamical model based on first order kinetics and core Rouse single chain relaxation. These findings demonstrate a dramatic transition to nonergodicity with increasing micelle core molecular weight and confirm the origins of the logarithmic exchange kinetics in such systems.

¹Support for this work was provided by Infinium

3:30PM L46.00004 Direct Imaging of Nanoscale Ionic Clusters in a Polymer Electrolyte Membrane , NITASH BALSARA, University of California, Berkeley, KENNETH DOWNING, SERGEY YAKOVLEV, Lawrence Berkeley National Laboratory — One of the factors hindering development of technologies such as fuel cells that rely on polyelectrolyte membranes (PEMs) is the lack of quantitative morphological characterization. While it has been recognized that clustering of ionic groups, can impede proton transport rates, model-free methods to quantify clustering in PEMs have not been developed. We present the first electron micrographs of sulfonic acid clusters in a polymer electrolyte membranes (PEM). The clusters are spherical with an average diameter of 1.4 nm and a standard deviation of 0.25 nm. Obtaining images of densely packed clusters of this size in a soft material is non-trivial due to their overlap in projection. Imaging of the sulfur-rich clusters by dark field microscopy was facilitated by the spontaneous formation of thin, cluster-containing layers on the top and bottom surfaces of free-standing films.

3:42PM L46.00005 Mechanisms underlying conductivity of lamellar block copolymer electrolytes , VENKAT GANESAN, VICTOR PRYAMITSYN, The University of Texas at Austin — Recent experiments have reported intriguing trends for the molecular weight (MW) dependence of the conductivity of block copolymer lamellae which are opposite that exhibited by homopolymer matrices. Using coarse-grained simulations of the transport of penetrant ions, we probe the possible mechanisms underlying such behavior. Our results indicate that the MW dependence of the conductivity of homopolymeric and block copolymeric matrices owe their origins to different mechanisms. On the one hand, the solubility of penetrants in block copolymer matrices themselves exhibit a MW dependence which arises from the MW dependence of the thickness of the conducting phase relative to the interfacial zones. Moreover, distinct mechanisms are shown to be responsible for the mobilities of ions in homopolymer and block copolymers. In the former, the mobility effects associated with the free ends of the polymers play an important role. In contrast, in block copolymer lamellae, the interfacial zone between the blocks presents a zone of hindered mobility for ions and manifests as a molecular weight dependence of the ionic mobility. Together, the preceding mechanisms are shown to provide a plausible explanation for the experimentally observed trends for the conductivity of block copolymer matrices.

3:54PM L46.00006 Physical Aspects of Photodynamic Corneal Collagen Crosslinking , JULIA KORNFIELD, California Institute of Technology — Healthy vision depends on the stability of the shape of the cornea, which provides most of the lens power of the optical system of the eye. Diseases in which the cornea progressively undergoes irregular deformation over time (e.g., keratoconus) can be treated clinically by inducing additional protein-protein crosslinks using a photosensitizing drug and a tailored dose of light. Unfortunately, the treatment moving through clinical trials is toxic to cells in and on the cornea. A path to a safer treatment is offered by the nanostructure of the corneal stroma—reminiscent of a HEX phase in block copolymers with 30nm diameter collagen cylinders spaced 60nm center-to-center in a hydrogel matrix of proteoglycans and water. We show that using a photosensitizing drug that sequesters itself in the collagen fibrils can minimize the toxicity of therapeutic protein-protein cross-linking. Photorheology and transport measurements are used to quantify the parameters of a simple physical model that is useful for optimizing clinical protocols.

4:06PM L46.00007 Directed Assembly of Block Copolymer Cylinders: Fundamental Physical Limits to Cylinder Spacing¹ , VINDHYA MISHRA, GLENN H. FREDRICKSON, Department of Chemical Engineering, UCSB, EDWARD J. KRAMER, Departments of Materials and Chemical Engineering, UCSB — Understanding the fundamental 2D physics of disordering and defect generation in block copolymer films is important in setting the limits for directed assembly based block copolymer lithography. Our experiments on monolayer films of cylindrical morphology block copolymer show that the monolayer structure disorders at a lower temperature compared to the bulk order-disorder transition temperature by thermal generation of a critical density of dislocations (point defects in the monolayer). We demonstrate experimentally and theoretically how this process sets lower limits on the monolayer cylinder spacing and thus pattern spacing that can be achieved by directed assembly of a given block copolymer using graphoepitaxy. Self-consistent field theoretic simulations are used to predict the compressional elastic constant B of the cylinder monolayer and cylinder spacing a as a function of χN and f , the minor block volume fraction. In turn these are used to estimate the formation energies E_d ($\sim Ba^3$) of dislocations in cylinder monolayers of various block copolymers.

¹We acknowledge funding from NSF DMR-07-04539 and DMR-09-04499

4:18PM L46.00008 Measurement of Diffusion in Entangled Rod-Coil Triblock Copolymers , B.D. OLSEN, M. WANG, Massachusetts Institute of Technology — Although rod-coil block copolymers have attracted increasing attention for functional nanomaterials, their dynamics relevant to self-assembly and processing have not been widely investigated. Because the rod and coil blocks have different reptation behavior and persistence lengths, the mechanism by which block copolymers will diffuse is unclear. In order to understand the effect of the rigid block on reptation, tracer diffusion of a coil-rod-coil block copolymer through an entangled coil polymer matrix was experimentally measured. A monodisperse, high molecular weight coil-rod-coil triblock was synthesized using artificial protein engineering to prepare the helical rod and bioconjugation of poly(ethylene glycol) coils to produce the final triblock. Diffusion measurements were performed using Forced Rayleigh scattering (FRS), at varying ratios of the rod length to entanglement length, where genetic engineering is used to control the protein rod length and the polymer matrix concentration controls the entanglement length. As compared to PEO homopolymer tracers, the coil-rod-coil triblocks show markedly slower diffusion, suggesting that the mismatch between rod and coil reptation mechanisms results in hindered diffusion of these molecules in the entangled state.

4:30PM L46.00009 Taking a Hard Look at Soft X-ray Scattering , ALEXANDER HEXEMER, CHENG WANG, LBNL — For many years neutron and X-ray scattering has been a trusted tool for polymer scientist. In the hard X-ray regime contrast for scattering has been limited to the difference in electron density between different components. At the Advanced Light Source we have been developing a techniques that combines the advantages of traditional scattering with chemical sensitive spectroscopy. Using soft X-rays at selected photon energies we can tune the contrast between different polymers based on there chemical makeup. We have applied this to a variety of polymer systems.

4:42PM L46.00010 Neither crystalline nor amorphous: measuring disorder in polymers and assessing its effect on charge transport, ALBERTO SALLEO, JONATHAN RIVNAY, RODRIGO NORIEGA, Stanford University, MICHAEL TONEY, Stanford Synchrotron Radiation Lightsource — Conjugated polymers displaying high mobility are semicrystalline. Thin films of these materials are comprised of ordered regions (crystallites) and disordered regions. Because of the inherent anisotropy of polymers, the crystallites exhibit varying degrees of disorder in different directions. I will show a quantitative measurement of disorder as applied to these materials, which allows us to quantify a paracrystalline parameter g . This parameter can be used to rank polymers. I will show how g is related to the electronic structure of the polymer and with the presence of electronic traps in particular. By studying the dependence of g on molecular weight we can get to a definition of polymer behavior in an electronic transport sense.

4:54PM L46.00011 Shear Alignment of Perpendicular Lamellae in Block Copolymer Thin Films¹, RICHARD REGISTER, SASWATI PUJARI, Princeton University, PAUL CHAIKIN, New York University — Thin supported block copolymer films, containing a single layer of cylindrical microdomains lying parallel to the substrate, can be effectively aligned by applying a shear stress to the molten, ordered film. Such films have been used effectively as contact masks for pattern transfer via reactive ion etching, permitting the fabrication of in-plane nanowire arrays, where the nanowires are aligned over macroscopic (cm) distances. Such a nanowire array could also be formed from a film which contains lamellae whose interdomain interfaces lie perpendicular to the substrate; such a template film would in principle allow for the formation of nanostructures of high aspect ratio, provided that the lamellae can be aligned along a single in-plane direction while retaining their perpendicular orientation. We have generated such films of perpendicular lamellae in a polystyrene-poly(methylmethacrylate) diblock, PS-PMMA, by neutralizing the substrate with a random terpolymer brush. Shearing the film, using a moving polydimethylsiloxane (PDMS) pad in contact with the film surface, can indeed produce alignment over cm-scale distances; however, the orientational order is poorer and the defect density higher than in typical cylinder-forming systems, and a significantly higher stress is required. After peeling off the PDMS pad, both PS and PMMA blocks are exposed at the surface in thinner films, but for films thicker than one domain spacing, the lower-energy PS block tends to cap the film surface, overlaying aligned perpendicular lamellae.

¹support from PCCM (NSF-MRSEC, DMR-0819860)

5:06PM L46.00012 Role of nanoscale morphology on the nano and macro-scale performance of polythiophene based polymer solar cells, PETER GREEN, JOJO AMONOO, EMMANOUIL GLYNOS, CHELSEA CHEN, Materials Science and Engineering, University of Michigan, Ann Arbor — Maximization of the short circuit current, J_{SC} , the open circuit voltage, V_{OC} , and the fill factor (FF) to achieve highest power conversion efficiencies (PCEs) in donor/acceptor, polymer/polymer, solar cells is dependent on optimization of variables associated with the active material's chemical and morphological structure. Control of the nanoscale structure of polythiophene (P3HT)/phenyl-C61-butyric acid methyl ether (PC₆₁BM) active materials was achieved through use of a novel low temperature processing strategy. With the use of energy filtered transmission electron microscopy (EF-TEM), electron and X-ray diffraction, together phase contrast, deflection and photocurrent measurements at the nanoscale, we were able to tailor nanoscale morphologies to achieve increases in the J_{SC} by a factor of 1.2 and the PCE by 30%, beyond that using conventional heat treatments for processing.

5:18PM L46.00013 Semiconducting block copolymers as nano-structuring agents for high-efficiency and annealing-free bulk hetero-junction organic solar cells, GEORGES HADZIOANNOU, SÉBASTIEN-JUN MOUGNIER, CEDRIC RENAUD, CYRIL BROCHON, GUILLAUME FLEURY, DARGIE DERIBEW, ERIC CLOUTET, University of Bordeaux, LAURENCE VIGNAU, ENSCBP, LCPO UMR 5629 CNRS TEAM, IMS UMR 5218 CNRS TEAM — Three main requirements for the industrial development of the polymer solar cells have to be addressed in order to obtain a competitive technology: a fabrication process compatible with common polymer printing technologies, an enhanced life time stability and an improved power conversion efficiency (PCE). The active layer nano-structure in bulk heterojunction organic solar cells plays a key role on the properties of charge transfer, transport and consequently on the PCE. Ideally a bi-continuous network of donor-acceptor domains with a length scale comparable to the exciton diffusion length is required. To obtain an optimized nano-structured active layer, an annealing process (thermal and/or solvent) is commonly performed leading to an increase of the photovoltaic performance. Currently, the implementation of common printing technologies for the fabrication of polymer solar cells on a mechanically flexible polymer substrate is impeded by this annealing step. In order to overcome the limitations above a novel approach based on an annealing-free fabrication process will be presented making use of a block copolymer as a nano-structuring agent for the polymer/fullerene derivative blend.

Tuesday, February 28, 2012 2:30PM - 5:30PM —
Session L48 DPOLY DBIO: Polymers and DNA Coated Colloid Particles 161

2:30PM L48.00001 DILLON MEDAL BREAK —

3:06PM L48.00002 Structure and Assembly of Polymeric Dots Formed by Conjugated Polymers, NARESH OSTI, DILRU RATNAWEERA, THUSITHA ETEMPAWALA, UMESH SHRESTHA, DVORA PERAHIA, Clemson University — Rigid conjugated polymers assume extended conformation in dilute solution and often behave as colloidal suspensions. When forced into a collapsed configuration, they form highly fluorescing particles, or poly-dots, which have demonstrated potential as intracellular imaging markers, as well as building blocks for light harvesting devices. The current work investigates the structure and stability of poly-dots of *di-alkyl para polyphenyleneethynylene* (PPE) conjugated polymers in solution and follows their assembly at interfaces. Small angle neutron scattering measurements of the poly-dots in water have shown that at low concentrations, stable unimolecular spherical poly-dots are formed with a polydispersity that corresponds to that of the polymer itself. With increasing concentration, yet, below the critical micelle concentration of these rod-like polymers in good solvents, the size and density of the NPs increases, however the spherical symmetry is retained. The nature and length of the substituents affect the internal density and the degree of swelling of the poly dots. Atomic Force Microscopy results show that these PPE poly-dots assemble into arrays with different symmetries, depending on molecular parameters and assembly conditions.

3:18PM L48.00003 Molecular dynamics study of polymer-silica nanoparticle hybrids: Building blocks for directed assembly, SABINA MASKEY, Clemson University, FLINT PIERCE, GARY GREEST, Sandia National Laboratories, DVORA PERAHIA, Clemson University — Molecular dynamic simulations have been used to study the conformation and interactions of a polymer nanoparticle hybrid that consists of *para* dialkyl phenyleneethynylenes (PPEs) grafted to a silica nanoparticle, with the goal of deriving the factors that control their assembly. PPEs are electro-optically active polymers whose conformation determines their degree of conjugation and their assembly mode which in turn affects the electro-optical properties of the nanoparticle-polymer complexes. When confined to a nanoparticle surface, the PPE chains are fully extended in good solvents but cluster as the quality of the solvents is decreased. Tuning the degree of clustering by tuning the solvent-polymer interaction is expected to direct the assembly of the particles. Results for the conformation of grafted PPE molecules on a single nanoparticle and the forces between two nanoparticles as a function of solvent quality will be presented.

3:30PM L48.00004 Structural and Dynamical Characteristics of Polyelectrolyte Dendrimer Solutions Revealed by Neutron Scattering and Atomistic Simulation, BIN WU, Oak Ridge National Laboratory, YUN LIU, National Institute of Standards and Technology, LIONEL PORCAR, PETER FALUS, Institut Laue-Langevin, CHANGWOO DO, Oak Ridge National Laboratory, MICHAELA ZAMPONI, Forschungszentrum Julich, KUNLUN HONG, GREGORY SMITH, WEI-REN CHEN, Oak Ridge National Laboratory — Solutions of polyelectrolyte dendrimers were investigated using small angle neutron scattering (SANS) and dynamical measurements including quasi-elastic neutron scattering, neutron spin-echo and high resolution NMR. The goal of the experiments was to understand the structural and dynamical responsiveness polymer toward the variation of molecular charge. Experimental spatial correlation functions and temporal correlation functions such as intermediate scattering functions and the dynamic structure factor were evaluated quantitatively. Complementary atomistic simulations were developed for providing the microscopic interpretation of the scattering measurements and for investigating the material characteristics that are not accessible experimentally. Based on this synergistic approach, we attempt to provide a detailed understanding of the microscopic mechanisms underlying the observed electrostatic responsive properties in these very important classes of materials.

3:42PM L48.00005 A theoretical study of the phase behavior of spherical colloids decorated with adhesive domains, HOMIN SHIN, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — We propose a nonlinear self-consistent phonon theory for the self-assembly of spherical particles with patterned adhesive surfaces, such as Janus colloids. The approach is first tested against the known crystallization behavior of hard spheres, and also homogeneous particles that interact via short range attractions. Janus colloid pair interactions are described by an anisotropic extension of the Baxter adhesive sphere potential where particles attract only if their hydrophobic domains are in contact. Given various crystalline symmetries, the effective harmonic potential experienced by a colloid confined to its Wigner-Seitz cell is self-consistently computed. The characteristic vibrational displacements or localization lengths are determined by the lattice symmetry as well as the strength and surface pattern of adhesive interactions. The crystal free energy is then computed, and thermodynamic stability evaluated, including pressure-driven solid-solid transitions, and the fluid-solid coexistence boundary based on the Baxter solution of the Percus-Yevick integral equation for adhesive hard sphere liquids. A primary goal is to evaluate the influence of patch size, attraction strength, and geometric patterning on the formation of heterogeneous crystalline phases.

3:54PM L48.00006 In situ electrochemical small-angle neutron scattering (eSANS) for quantitative structure and redox properties of polymer-coated nanoparticles¹, VIVEK PRABHU, Polymers Division, NIST, VYTAS REIPA, Biochemical Sciences Division, NIST, PETER BÖNNESEN, ADAM RONDINONE, ERIC FORMO, Center for Nanophase Materials Sciences, ORNL — Rapid growth in nanomaterial applications (energy, cosmetics and healthcare products) highlights limitations of available physicochemical characterization methods. An in situ electrochemical small-angle neutron scattering (eSANS) methodology was devised that enables direct measurements of nano and colloid material dispersion structure while undergoing reduction-oxidation (redox) reactions. By combining the electrochemical signal with contrast variant SANS, the structure of the polymer-nanoparticle complexes can be examined under electrochemical conditions. Specially-synthesized poly(ethyleneglycol)-stabilized zinc oxide nanoparticles were examined by eSANS showing an irreversible change in nanoparticle-complex structure during the potential cycle. We will report on the kinetics of the nanoparticle transformation as measured at BL-6 EQSANS, Spallation Neutron Source, Oak Ridge National Laboratory.

¹ORNL Center for Nanophase Materials Sciences and Spallation Neutron Source under user proposal 2011-125, sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, DOE

4:06PM L48.00007 Topological Interaction by Entanglement of DNA, LANG FENG, Center for Soft Matter Research, New York University, RUOJIE SHA, NADRIAN SEEMAN, Chemistry department, New York University, PAUL CHAIKIN, Center for Soft Matter Research, New York University — We find and study a new type of interaction between colloids, Topological Interaction by Entanglement of DNA (TIED), due to concatenation of loops formed by palindromic DNA. Consider a particle coated with palindromic DNA of sequence “P1.” Below the DNA hybridization temperature (T_m), loops of the self-complementary DNA form on the particle surface. Direct hybridization with similar particle covered with a different sequence P2 do not occur. However when particles are held together at $T > T_m$, then cooled to $T < T_m$, some of the loops entangle and link, similar to a Olympic Gel. We quantitatively observe and measure this topological interaction between colloids in a $\sim 5^\circ\text{C}$ temperature window, $\sim 6^\circ\text{C}$ lower than direct binding of complementary DNA with similar strength and introduce the concept of entanglement binding free energy. To prove our interaction to be topological, we unknot the purely entangled binding sites between colloids by adding Topoisomerase I which unconcatenates our loops. This research suggests novel history dependent ways of binding particles and serves as a new design tool in colloidal self-assembly.

4:18PM L48.00008 Measuring in situ primary and competitive hybridization events on microspheres, VALERIA MILAM, JAMES HARDIN, Georgia Institute of Technology — Understanding hybridization events at surfaces is crucial for optimizing nucleic acid detection platforms as well as DNA-mediated colloidal assembly. We used flow cytometry to measure time-dependent primary and competitive hybridization events of perfectly matched and mismatched targets on microsphere surfaces. In addition to more conventional sample preparation involving multiple wash and resuspension steps prior to measurement, we sampled the reaction volume directly for in situ measurements to minimize potential dissociation events between weaker partner strands during wash steps. Similar to prior reports for oligonucleotide solutions, the nearly identical rates for primary hybridization events on microsphere surfaces were independent of target sequence and reached an equilibrium value within 30 min. The extent of in situ primary hybridization events for immobilized probes, however, deviated from solution model predictions. In situ competitive hybridization events were at least 100-fold slower than primary hybridization events and did not appear to reach equilibrium. The kinetics of competitive hybridization events on microspheres are consistent with predicted effects stemming from toehold effects or base length differences between primary and secondary targets.

4:30PM L48.00009 You can always get what you want, ZORANA ZERAVCIC, School of Engineering and Applied Sciences, Harvard University, SAHAND HORMOZ, Kavli Institute for Theoretical Physics, University of California, JESSE COLLINS, VINOTHAN MANOHARAN, MICHAEL BRENNER, School of Engineering and Applied Sciences, Harvard University — Colloidal particles coated with DNA strands can self assemble into complex structures. Which structures are formed and with what yield depends on the specifics of the design rules. We numerically study the directed self assembly of DNA coated colloidal particles. By testing different design rules for self-assembly with short-range interactions and studying the stability of equilibrium structures, we uncover the principles for always getting a desired assembled structure.

4:42PM L48.00010 Rigid and Soft Minima of DNA-colloid Clusters, JESSE COLLINS, ZORANA ZERAVCIC, Harvard SEAS, VINOTHAN MANOHARAN, Harvard SEAS and Physics, MICHAEL BRENNER, Harvard SEAS — What are the limits of self-assembly via short-ranged, isotropic potentials? We investigate how carefully tuning the interaction matrix—breaking the permutation symmetry—of a small number of particles leads to unique ground states and novel energy landscape features, including soft local and global minima. We coat microspheres with highly specific and thermodynamically optimized DNA-sequences, and observe a few of these at a time organize in wells and droplets. DIC and other imaging techniques reveal 3D cluster structure, and fluorescence reveals the identity of each bead in the cluster. Although our experiments equilibrate timely over only a small temperature window, they elucidate how discrete sphere packing geometry governs both the statistical equilibrium and theoretical “zero T” cluster probabilities. Finally, I'll describe how relaxing some constraints can shift equilibria and flatten maxima on the energy landscapes of these specific spheres.

4:54PM L48.00011 Uniform colloidal clusters from random aggregation of bidisperse spheres¹, NICHOLAS B. SCHADE, MIRANDA C. HOLMES-CERFON, Harvard University, ELIZABETH R. CHEN, None, DINA ARONZON, JESSE W. COLLINS, JONATHAN A. FAN, VINOTHAN N. MANOHARAN, Harvard University — Using a combination of experiment and simulation, we investigate the structures that form when colloidal spheres cluster around smaller spheres. We use either oppositely charged particles or particles coated with complementary DNA sequences to form the clusters, and we observe them under optical microscopy. We find that random sphere parking serves as a useful model for cluster self-assembly in these systems and that the sphere diameter ratio controls the distribution of cluster sizes. In particular, near a critical diameter ratio, random parking produces tetrahedral clusters in theoretically unlimited yield. Experimentally we observed 90% tetramer yield near this geometrical singularity. We investigate how this method can be used to assemble tetrahedral plasmonic resonators from metallo-dielectric nanospheres in order to create a bulk, isotropic, optical metamaterial.

¹We acknowledge support from NSF grant no. ECCS-0709323 as well as the DOE Office of Science Graduate Fellowship Program.

5:06PM L48.00012 The Internal Structure of Nanoparticle Dimers Linked by DNA, FERNANDO VARGAS LARA, Physics Department, Wesleyan University, Middletown, CT, CHING-JUNG CHENG, OLEG GANG, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY, FRANCIS W. STARR, Physics Department, Wesleyan University, Middletown, CT — The self-assembly of inorganic units controlled by the interactions of biological molecules, like DNA, has received attention for the possibility to specify higher-order structure, with potential biological, optical and electronic applications. In biology, self-assembly of complex materials (eg. bone, spider silk) frequently occurs in a stepwise, hierarchical fashion. Here, we consider a first step towards a hierarchical approach for synthetic nanostructures of nanoparticles (NPs) linked by DNA. The most basic unit in this multiscale approach is a dimer of NPs linked by DNA. We use a coarse-grained molecular model to explain experimental measurements of the separation of two DNA-coated NPs connected by linking single-stranded DNA (ssDNA). We show that the dimer separation is primarily controlled by the number of DNA links between NPs. If these links are not constrained to lie along the axis between NPs, the separation is limited by off-axis connections that force the NPs to be closer. We also determine how the number of connections alters the effective persistence length of the ssDNA that connects the dimer. We discuss how these dimers might be used for subsequent assembly at larger scales.

5:18PM L48.00013 Specific interactions in complex mixtures: effects on the thermodynamic stability of multicomponent protein solutions, WILLIAM JACOBS, DAAN FRENKEL, University of Cambridge — Multicomponent protein solutions, such as the cytosol, comprise complex networks of specific interactions in a crowded environment of molecules with nonspecific interactions, with dissociation constants spanning many orders of magnitude. We investigate the phase behavior of a multicomponent lattice model with both specific and non-specific interactions. We use bit strings to encode the binding strength between interacting patches on particles at neighboring lattice sites. The boundary of the well-mixed dilute phase is calculated for a statistical ensemble of mixtures using semi-grand Monte Carlo simulations and multicanonical histogram reweighting techniques. We examine the sensitivity of this phase boundary to the distribution of component interactions and demonstrate that the phase behavior is extremely sensitive to the high-end tail of the distribution of interaction strengths.

Tuesday, February 28, 2012 2:30PM - 5:18PM –
Session L49 DPOLY: Focus Session: Fluctuation-Induced Forces in Soft Matter and Polymeric Systems - Charge, Shape and Nucleation 162A

2:30PM L49.00001 DILLON MEDAL BREAK —

3:06PM L49.00002 Ion-induced interactions between charged macroions and dielectric inhomogeneities, JOS ZWANIKKEN, MONICA OLVERA DE LA CRUZ, Northwestern University — We present a theoretical study of the interactions between macroions in ionic solutions, that are induced by the surrounding electrolyte. In a first scenario, we consider responsive nanoparticles with positively and negatively charged surface groups, and predict that thermal fluctuations of the net surface charge are responsible for an effective attraction, as a chemical analogue of the atomic London-forces. In a second scenario, we consider nanoparticles in solvents with a low dielectric permittivity, where the Coulomb interactions between ions easily exceed the thermal energy. We predict an ionic condensation in the confinement between two nearby nanoparticles, where the suppression of fluctuations leads to a locally dense state of ions, and a consequent strong effective attraction between the nanoparticles. The induced potential between the nanoparticles is also related to the ion-nanoparticle interactions, by e.g. Van der Waals, surface charge, or image charge attractions. Recently developed theoretical methods are discussed, based on earlier work [1,2].

[1] J. W. Zwanikken, and M. Olvera de la Cruz, Phys. Rev. E 82, 050401(R) (2010).

[2] J. W. Zwanikken, P. K. Jha, and M. Olvera de la Cruz, J. Chem. Phys. 135, 064106 (2011);

3:18PM L49.00003 Dielectric many-body effects in arrays of charged cylindrical macromolecules, DANIEL W SINKOVITS, University of Illinois at Urbana-Champaign, KIPTON BARROS, Los Alamos National Laboratory, JURE DOBNIKAR, University of Cambridge and Jožef Stefan Institute (IJS), MATEJ KANDUČ, Technische Universität München and IJS, ALI NAJI, Institute for Research in Fundamental Sciences (IPM), RUDOLF PODGORNIK, IJS and University of Ljubljana, ERIK LUIJTEN, Northwestern University — Nonuniform dielectric constants are a ubiquitous aspect of condensed-matter systems, but nevertheless widely ignored in simulations. Analytical work suggests that the polarization effects resulting from these inhomogeneities can produce many-body interactions that qualitatively alter the behavior of systems driven by electrostatic interactions, but such work relies on approximations. Recently, we have developed an algorithm that computes the fluctuating polarization charge at the interface between dielectric materials during a molecular dynamics simulation, without approximation. Here, we apply this approach to investigate arrays of charged cylindrical macromolecules in the presence of explicit counterions. We study the dielectric many-body effects as a function of separation, dielectric constant variation, and counterion valency. Our findings have implications for the aggregation of polyelectrolytes such as F-actin or DNA.

3:30PM L49.00004 ABSTRACT WITHDRAWN —

3:42PM L49.00005 Influence of probe shape on polymer configurations and entropic forces, YACOV KANTOR, Tel Aviv University — The free energy of long polymers is frequently dominated by entropy with the interaction energy playing a minor role. In the absence of an energy scale, the corresponding forces are then governed by the thermal energy scale $k_B T$ and by the length scales associated with the experimental set-up. Recent advances in single molecule manipulation techniques have brought the accuracy of position and force determination into the range where the measurement of relatively small deformations becomes possible. In these situations the detailed shape of probes to which the molecule is attached must be taken into account. The behavior of a polymer of size R_0 attached to the rounded tip of a probe (sphere, paraboloid, spherocylinder) with radius of curvature R , differs qualitatively for large and small values of the ratio $s = R_0/R$. The scaled compliance (inverse force constant) S/R_0^2 , is anisotropic and quite large in the direction parallel to the surface when $s \sim 1$ [1]. When a cone with a polymer attached to its sharp tip approaches a plate, then for cone-plate separation $h \ll R_0$ the polymer-mediated force between them [2] is given by $F = Ak_B T/h$. The coefficient A can be related to geometry-dependent correlation exponents of long polymers. We computed A for phantom polymers, and for self-avoiding polymers by ϵ -expansion, as well as by numerical simulations in 3 dimensions.

[1] R. Bubis, Y. Kantor and M. Kardar, Europhys. Lett. **88**, 48001, 2009.

[2] M. F. Maghrebi, Y. Kantor and M. Kardar, Europhys. Lett., *in press*, 2011 (arXiv:1109.5658).

4:18PM L49.00006 Topological obstacles and the forces on them in systems of strongly interacting directed polymers, DAVID ZEB ROCKLIN, University of Illinois at Urbana-Champaign, PAUL M. GOLDBART, SHINA TAN, Georgia Institute of Technology — Owing to their extended structure and impenetrability, polymers are strongly influenced by topological obstacles. To shed light on this issue we consider a model system of noncrossing directed polymers in two dimensions. As first exploited by de Gennes [1], the configurations of this system can be mapped onto the worldlines of noninteracting fermions—an analogy that enables the application to the polymer system of techniques initially developed for one-dimensional quantum systems. Via this approach, we discuss how an obstacle that forces a fixed number of polymers to pass to one side of a single topological constraint is associated with a large fluctuation of the quantum system. In addition, via the use of techniques from quantum hydrodynamics, we find that such a constraint on a system of noncrossing polymers generates an effective, long-ranged repulsion between the polymers. This repulsion causes a void to appear in the polymer fluid and generates a super-Hookean force opposing the constraint. [1] P.-G. de Gennes, J. Chem Phys. **48**, 2257-2259 (1968).

4:30PM L49.00007 Critical exponents in the presence of a tip, MOHAMMAD F. MAGHREBI, MIT, YACOV KANTOR, Tel Aviv University, MEHRAN KARDAR, MIT — The behavior of Landau-Ginzburg model of a critical system, appropriate to describe SAW polymers, in the presence of a conical boundary is studied within mean field and by epsilon expansion in $d=4-\epsilon$ dimensions. New exponents emerge for correlation functions near the boundaries, in this case the tip of the cone. In the limit of a sharp cone we find a new exponent which we interpret for a SAW polymer by using its fractal dimension.

4:42PM L49.00008 Trapping fluctuations in confined carbon dioxide near the supercritical ridge, MANFRED HEUBERGER, ERICH SCHURTENBERGER, EMPA, Materials Science and Technology, CH-9014 St. Gallen — We investigate the properties of a confined supercritical carbon dioxide film. Density fluctuations are theoretically predicted near the critical point and along the supercritical extension of the liquid-gas coexistence line (ridge). We have confined carbon dioxide between two atomically smooth surfaces in a new generation of surface forces apparatus. The nanometers to micrometer films are found to be laterally divided into nano domains of two distinct refractive indices. The two-refractive index structure is apparent, yet different on behavior, above or below the supercritical ridge. This non-equilibrium phase separated film exhibits long-range attractive forces (up to 500 nm), which results from an interfacial energy between the different domains. High refractive nano domains can be trapped and stretched to lengths of several micrometers, until we observe coalescence of the domains. Our observations suggest that density fluctuations can be trapped and pinned between surfaces in the form of nano strings of significantly different molecular order.

4:54PM L49.00009 Homogeneous crystal nucleation from the melts of flexible n -alkanes by molecular simulation, PENG YI, GREGORY C. RUTLEDGE, Massachusetts Institute of Technology — Homogeneous crystal nucleation from a dense melt is particularly interesting for chain molecules due to their anisotropy and conformational flexibility. We report our molecular simulation study of the homogeneous crystal nucleation from n -alkane melts. For short n -alkane (C20) (J.Chem.Phys. **135**, 024903), the nucleation trajectory was sampled using brute force molecular dynamics (MD) simulations at about 20% supercooling and the nucleation free energy was sampled using the Monte Carlo (MC) umbrella sampling method for temperatures ranging from 10% to 20% supercooling. In the MD simulation, we identified the induction period unambiguously and calculated the nucleation rate through a mean-first-passage time analysis. A typical critical nucleus consists of a bundle of stretched segments organized into a cylindrical shape. The remaining CH₂ groups form a disordered interfacial layer. By fitting the free energy curve sampled by MC to the cylindrical nucleus model, the crystal-melt interfacial free energies are calculated. We have found good agreement between the melting temperature and the interfacial free energies obtained in our simulation and those from experiment. For a long n -alkane above the entanglement length (C150), MD simulation of nucleation was performed at super-cooling as small as 15%. Chain folding was observed during the nucleation stage, and thickening of crystallites was observed during the subsequent crystal growth. The resulting crystal-amorphous interface is characterized in terms of loops, bridges and tails.

5:06PM L49.00010 ABSTRACT WITHDRAWN —

Tuesday, February 28, 2012 2:30PM - 5:30PM —

Session L50 DMP DPOLY: Focus Session: Organic Electronics and Photonics - Morphology

162B

2:30PM L50.00001 DILLON MEDAL BREAK —

3:06PM L50.00002 Real-time observation of optoelectronic properties during poly(3-alkylthiophene) crystallization, VICTOR HO, BRYAN BOUDOURIS, University of California, Berkeley, LESLIE JIMISON, Stanford University, MICHAEL TONEY, Stanford Synchrotron Radiation Lightsource, ALBERTO SALLEO, Stanford University, RACHEL A. SEGALMAN, University of California, Berkeley — Poly(3-alkylthiophenes) (P3ATs) are commonly used semiconducting polymers in organic electronic applications where the nanoscale morphology of the active layer largely dictates device performance. However, during solution processing, a large driving force for crystallization results in thin film morphologies that are kinetically trapped and cannot be easily controlled. We show that rational side chain design, particularly the use of branched alkyl chains, can reduce the melting transition increasing thermal control relative to P3HT. Importantly, the lower crystallization transition temperature provides the opportunity to monitor crystallization in real-time using grazing-incidence x-ray diffraction and UV-vis absorption spectroscopy, and the relative degree of crystallinity is observed to increase gradually over the course of crystallization. In contrast to the gradual increase in crystallinity and optical properties, the field-effect mobility monitored during crystallization exhibits a sharp increase of approximately two orders of magnitude. We propose that the difference in time scales may be due to the formation of a percolated network between electrodes, and that increases in the degree of crystallinity beyond this point are not probed by the transistor geometry.

3:18PM L50.00003 In Situ Annealing Study of Organic Photovoltaic Morphology via Non-invasive Polarized Neutron Reflectivity, BRETT GURALNICK, MICHAEL MACKAY, University of Delaware, BRIAN KIRBY, CHARLES MAJKRZAK, NIST Center for Neutron Science — Polarized neutron reflectivity, a non-invasive technique, allows the unambiguous density distribution within a thin film to be determined. By utilizing this technique with organic photovoltaics it is possible to study the same device pre- and post-annealing. We studied a bulk heterojunction cell consisting of an organic semiconductor (P3HT) and a nanoparticle electron acceptor (PCBM). We found a shift in the location of PCBM within the organic film which migrates toward the anode and cathode following annealing. However, while some PCBM can reach the substrate interface it never fully blooms to the air interface and pure P3HT resides at the surface for the thick (200 nm) films used in this study. These results differ from previous research in that the same device was characterized allowing a true study on the effect of annealing to be performed.

3:30PM L50.00004 Solvent Studies for Solution Processing of Polymer-Fullerene Bulk Heterojunctions, MARGARET J. SOBKOWICZ, University of Massachusetts Lowell Plastics Engineering Department, RONALD L. JONES, R. JOSEPH KLINE, DEAN M. DELONGCHAMP, National Institute of Standards and Technology Polymers Division — A major advantage of polymer solar cells over higher-efficiency photovoltaic alternatives is the low cost of printing technologies. Solution-based film preparation relies on the self-assembly of the polymer and fullerene phases as the layer dries from the casting ink into a bulk heterojunction morphology. The nanoscale morphology must facilitate optimal charge separation and transport; thus solution processing parameters heavily influence the device performance. Current technology uses chlorinated aromatic solvents and small processing windows with stringent requirements on ink properties. In this study, the stability of various ink formulations is investigated to develop more reliable, sustainable alternatives. Model solutions of poly(3-hexylthiophene) (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM) are prepared using a range of solvents and solvent mixtures. P3HT solution crystallization behavior is investigated using differential scanning calorimetry, UV-visible absorbance measurements and neutron and light scattering. The behavior of the solutions under shear is investigated in order to predict the success of disparate printing and coating techniques.

3:42PM L50.00005 Morphology in Hybrid Oxide/Polymer Core-Shell Nanowire Photovoltaics, JIE JIANG, SOHRAB ISMAIL-BEIGI, Yale University — We use first principles theory (DFT) to gain insight into the Poly(3-hexylthiophene) (P3HT)-ZnO nanowire binding morphology where the P3HT is bound to ZnO via SiO_3 linkers [1]: understanding the experimentally realized morphology is the first step in trying to predict and enhance electronic energy alignments conducive to photovoltaic operation. For large diameter ZnO nanowires, the morphology is that of P3HT bound to the $(10\bar{1}0)$ surface of ZnO. The existence of a lattice mismatch of the ZnO surface and the polymer backbone creates a competition between linker binding and strain energy. We solve this realization of the classic Frenkel-Kontorova model based on ab initio parameters to obtain the lowest energy binding morphology on the surface. For small ZnO nanowire diameters, curvature effects become important: the P3HT polymer must bend around the nanowire, and the reduction of linker spacing due to curvature enlarges the lattice mismatch for helical wrappings. We use DFT to estimate these curvature energies, and we predict a morphology change from helical wrapping to linear alignment with the nanowire axis at a diameter close to 25 nm. [1] S. Zhang, Adv. Mater. (in press, 2011).

3:54PM L50.00006 An Improved Forcefield for Molecular Modeling of Crystalline Poly(3-Hexyl Thiophene)¹, RAM BHATTA, Department of Chemistry, University of Akron, YENENEH YIMER, Department of Polymer Science, University of Akron, DAVID PERRY, Department of Chemistry, University of Akron, MESFIN TSIGE, Department of Polymer Science, University of Akron — A fundamental understanding of molecular structure and dynamics of poly(3-hexyl thiophene) (P3HT), one of the most promising organic solar cell materials, is crucial for improving the efficiency of organic solar cells containing P3HT as the donor. Molecular dynamics (MD) simulations can produce the correct structures and dynamics of P3HT provided that robust forcefields are employed for this system. The forcefields that are currently used for MD simulations of P3HT are mostly taken from the analogous thiophene molecule, bi-thiophene. However, such forcefields may lack to produce the correct morphology and stacking properties of P3HT. We present the results of MD simulations using an improved forcefield for P3HT. In the improved forcefield the torsional and partial atomic charge parameters for both the alkyl side chains and backbone were derived from ab initio calculations. Our results from MD simulations are compared with available experimental and theoretical data and the range of accessible structures is explored.

¹This work is supported by the NSF (DMR0847580).

4:06PM L50.00007 Device simulation of morphologies that are consistent with small angle scattering and reflectometry, DANIEL OLDS, PHILLIP DUXBURY, Michigan State University — Through the use of a dynamic Monte Carlo simulation, we are able to evaluate the efficiency of bulk heterojunction morphologies of P3HT/PCBM based photovoltaic devices that are consistent with neutron reflectometry and SANS data. We have developed a method to efficiently generate simulated small angle scattering data from hypothetical nanoscale systems such as polymer-fullerene bulk heterojunctions found in organic photovoltaic devices. We will show how this method can be used to accurately calculate the scattering information of well known systems such as a polydisperse collection of hard and soft spheres. We will then demonstrate this method on the calculated device morphologies, and show how the simulated scattering can grant insight into the validity of assumptions based on traditional fitting methods.

4:18PM L50.00008 Three dimensional device simulations to model conducting probe AFM measurements of organic semiconductors with fibrous morphologies, KANOKKORN PIMCHAROEN, DANIAL OLDS, JIEBING SUN, PENG PENG ZHANG, PHILLIP DUXBURY, Michigan State University — Organic semiconductors offer a promising material for many optoelectronic devices, with device performance depending significantly on the nanoscale morphology. Atomic force microscopy (AFM) is one of the major instruments for investigating the dependence of current-voltage response on nanoscale structures. We are developing computational methods for fundamental study of charge transport probed by these measurements, using continuum device models and Kinetic Monte Carlo simulations. The simulations are performed on complex three dimensional model morphologies that are consistent with the topology observed in AFM measurements. The calculated IV response of these models is compared with CP-AFM measurements.

4:30PM L50.00009 Self-Limiting Crystal Microstructure in Poly(3-hexylthiophene), CHAD SNYDER, RYAN NIEUWENDAAL, DEAN DELONGCHAMP, JESSICA HENRY, Polymers Division, National Institute of Standards and Technology — Polymeric semiconductors, such as poly(3-hexylthiophene-2,5-diyl) (P3HT), hold great potential for a variety of technologies. These solution processable materials are promising as active layers for low cost or large area flexible electronic or optoelectronic devices that can be prepared through high-throughput deposition processes, such as inkjet or roll-to-roll printing. Of the myriad of materials currently under examination, P3HT is one of the most widely studied materials because of its electronic properties and commercial availability. However, most, if not all, commercially available P3HT is produced with some non-negligible level of regiodefects that has a predefined impact on its crystalline fraction. We examine the effect of regiodefects in P3HT on the semicrystalline microstructure, i.e., lamellar thickness and distribution, and overall crystallinity, and discuss the impact of these effects on potential device performance and bulk heterojunction morphology.

4:42PM L50.00010 X-ray and neutron reflectivity and electronic properties of PCBM-poly(bromo)styrene blends and bilayers with poly(3-hexylthiophene)¹, STUART KIRSCHNER, NATHANIEL SMITH, KEVIN WEPASNICK, HOWARD KATZ, Johns Hopkins University, BRIAN KIRBY, JULIE BORCHERS, NIST Center for Neutron Research, DANIEL REICH, Johns Hopkins University — We used neutron reflectivity to complement x-ray reflectivity characterization of PCBM-based layers formed on poly(3-hexylthiophene) (P3HT). Single-layer analyses were used to provide reliable scattering length density values for bilayer fitting. Atomic force microscopy analyses showed trends similar to the reflectivity experiments when observing upper surfaces. Styrene polymers added to PCBM in small concentrations (ca. 10 percent) led to processing advantages while retaining substantial electron mobility, about 0.001 cm²/V s. The further introduction of a relatively heavy bromo atom substituent on the styrene rings greatly increased the film smoothness, as revealed by increases of the oscillation amplitudes in the reflectivity. In addition, the bromine heavy atom increased x-ray reflectivity scattering length density of the upper layer. Finally, we confirm that P3HT is capable of extracting PCBM from a subsequently deposited overlying layer, consistent with predictions based on published phase diagrams of the P3HT-PCBM system.

¹This research was supported in part by NSF grant ECCS-0823947.

4:54PM L50.00011 Controlled phase separation in conjugated polymer blends using quadruple hydrogen bonding interactions¹, YEN-HAO LIN, RAFAEL VERDUZCO, Rice University — All-polymer photovoltaic blends have significant promise for low-cost, solution processed photovoltaics, but large-scale phase separation can lead to non-optimal active layer structures for charge-separation and transport. We propose a novel strategy for controlling phase separation in conjugated polymer blends using quadrupole hydrogen bonding interactions. We investigate a series of end-modified conjugated and coil-like polymers in blends, including poly(3-hexyl thiophene) (P3HT), poly(styrene), poly(ethylene glycol), poly(9,9-dioctyl fluorene). Polymers are end-terminated with the multiple hydrogen bonding group 2-ureido-4(1H)-pyrimidinone (UPy) using isocyanate chemistry. Atomic force microscopy and grazing incidence x-ray scattering show phase separation is suppressed and, in some cases, P3HT crystallite orientation is improved in films for blends of UPy functionalized polymers. These results show the quadruple hydrogen bonding groups can prevent large-scale phase separation and direct the orientation of polymer chains.

¹This work was supported by the Welch Foundation for Chemical Research (Grant No. C-1750)

5:06PM L50.00012 Synthesis and Characterization of All-Conjugated Block Copolymers Prepared via Click Chemistry¹, RAFAEL VERDUZCO, KENDALL SMITH, Rice University — All-conjugated block copolymers with both hole-conducting and electron-conducting polymer blocks can be used to address fundamental questions regarding the structure, optoelectronic properties, and photovoltaic performance of organic photovoltaic blends, but synthetic challenges have precluded comprehensive studies on such systems. Here, we present a novel synthetic approach for preparing all-conjugated block copolymers and detailed studies of their nanoscale structure and optical properties. Our synthetic approach is based on copper-catalyzed azide-alkyne “click” chemistry and enables us to prepare block copolymers with a poly(3-alkylthiophene) block covalently linked to a conjugated polymer prepared by Suzuki polycondensation polymerization, including poly(9,9-dioctyl fluorene), poly(9,9-dioctyl fluorene-alt-benzothiadiazole) and poly((9,9-dioctylfluorene)-2,7-diyl-alt-[4,7-bis(thiophen-5-yl)-2,1,3-benzothiadiazole]-2',2"-diyl) (PFOTBT). A combination of x-ray diffraction, grazing-incidence x-ray scattering, atomic force microscopy, and fluorescence quenching measurements give insight into their microstructure and potential for use in high-performance all-polymer photovoltaics.

¹This work was supported by the Welch Foundation for Chemical Research (Grant No. C-1750)

5:18PM L50.00013 Undulation instability in drop-cast poly(3-hexylthiophene) film originated from self-assembly, MIN SANG PARK, School of Materials Science and Engineering, Georgia Institute of Technology, AVISHEK AIYAR, School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, JUNG OK PARK, School of Materials Science and Engineering, Georgia Institute of Technology, ELSA REICHMANIS, School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, MOHAN SRINIVASARAO, School of Materials Science and Engineering, Georgia Institute of Technology — In this study, we characterize the undulated structures which appear at the edge of drop-cast regio-regular poly(3-hexylthiophene) (rr-P3HT, head-to-tail > 95%) film using optical microscopy and atomic force microscopy. We propose that these periodic structures originate from the undulations of the layered structure of liquid crystal-air interface. Evidence of rr-P3HT solution forming liquid crystalline phases at higher concentrations was obtained by the observation of distinct birefringence and characteristic textures under crossed polarizers using an optical microscope. Synchrotron x-ray diffraction pattern provides additional structural information at the undulated area compared with those at the area without undulated pattern. Based on these experimental results, we propose rr-P3HT solution can form a lyotropic liquid crystal at specific concentrations. This work was partially supported by NSF funding (DMR-0706235).

Tuesday, February 28, 2012 2:30PM - 5:42PM —

Session L51 DCMP DFD: Self Assembly: Mostly Colloids, Lipids and Surfactants Boston Convention Center 154

2:30PM L51.00001 Basic parameters affecting nanoparticle self-assembly: An experimental approach, CHAKRA JOSHI, The University of Toledo, Department of Chemistry, YEVGEN KRYUKOV, JACQUES AMAR, University of Toledo, Department of Physics and the Wright Center for Photovoltaics Innovation and Commercialization, TERRY BIGIONI, The University of Toledo, Department of Chemistry and the Wright Center for Photovoltaics Innovation and Commercialization — Understanding the basic parameters that govern the nanoparticle self-assembly process is important for high-quality monolayer formation and technological advances. A complete theory that explains nanoparticle self assembly, in the bulk and at the liquid-air interface, is lacking. In this paper, dodecanethiolated gold nanoparticles were used as a model system for studying the forces that govern self assembly. These nanoparticles are known to make compact and highly-ordered monolayers at the liquid-air interface via a mechanism that is analogous to epitaxial growth of atomic layers. Epitaxial theory was used as a starting point to study the nanoparticle self-assembly at the liquid-air interface. Experimental measurements were successfully interpreted using an epitaxy-based analysis, including flux of nanoparticles onto the liquid air-interface, decay rate of the island density, and the dependence of critical nucleus size on nanoparticle diameter. Furthermore, anomalous diffusion was observed as was a remarkable ordering of islands at the liquid-air interface. This ordering was determined to be due to a long-range repulsive force between islands.

2:42PM L51.00002 Self-assembly of gold nanoparticles at water/vapor interface, GARY S. GRETT, J. MATTHEW D. LANE, Sandia National Laboratories — The self-assembly of coated gold nanoparticles at the water/vapor interfaces are studied using explicit-atom molecular dynamic simulations. While it is often assumed that uniformly coating spherical nanoparticles with short organic ligands lead to symmetric nanoparticles, we find that the high curvature of small nanoparticle and the relatively short dimensions of the coatings can produce highly asymmetric coatings. At an interface this asymmetry of the ligands tends to orient the nanoparticles with the surface to minimize free energy. First results for individual gold nanoparticles of diameter 2-8 nm coated with alkanethiol ligands of various lengths and different end group will be presented. Results for the self-assembly of the multiple nanoparticles at the water/vapor interfaces will then be presented for the diameter 2 and 4 nm nanoparticles which show how these asymmetric and oriented coatings affect the interactions between nanoparticles and the structure of the resulting aggregate. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

2:54PM L51.00003 Electric Field Driven Self-Assembly of Colloidal Rods, JAIME JUAREZ, KUNDAN CHAUDHARY, QIAN CHEN, STEVE GRANICK, JENNIFER LEWIS, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — The ability to assemble anisotropic colloidal building blocks into ordered configurations is of both scientific and technological importance. We are studying how electric field-induced interactions guide the self-assembly of these blocks into well aligned microstructures. Specifically, we present observations of the assembly of colloidal silica rods ($L/D \sim 4$) within planar electrode cells as a function of different electric field parameters. Results from video microscopy and image analysis demonstrate that aligned microstructures form due to the competition between equilibrium interactions of induced dipoles and non-equilibrium processes (i.e., electro-osmosis). Under the appropriate electric field conditions ($\sim$ kHz AC fields), aligned colloidal rod fluids form over large areas on the electrode surface. The superposition of a DC electric field to this aligned colloidal rod fluid initiates their condensation into a vertically oriented crystalline phase. Ongoing work is now focused on exploring how temporal changes to electric fields influence colloidal rod dynamics and, hence, the assembly kinetics of aligned colloidal monolayers.

3:06PM L51.00004 Electron-induced Three Dimensional Self-assembly and Disassembly of Molecules on a Gold Surface, QING LI, Oak Ridge National Laboratory, CHENGBO HAN, North Carolina State University, MIGUEL FUENTES-CABRERA, HUMBERTO TERRONES, BOBBY SUMPTER, Oak Ridge National Laboratory, JERRY BERNHOLC, North Carolina State University, JIEYU YI, ZHENG GAI, ART BADDORF, PETRO MAKSYMOWYCH, MINGHU PAN, Oak Ridge National Laboratory — The immensely successful methodology of molecular self-assembly on surfaces has produced thousands of new applications and paved ways to new research areas, such as molecular electronics and the dip-pen nanolithography. Here we demonstrate a seminal example of non-thermal control over molecular self-assembly, where hot-electrons transform a largely disordered layer of hydrocarbon molecules, into a highly ordered, densely packed and three-dimensional monolayer on a gold surface. Subsequently, hot-electron/hot-hole injection can heal the defects within the self-assembled layer, and even entirely and reversibly disassemble it. From a theoretical analysis we have identified that electron-induced processes allow the formation of a very strongly-bonded molecule, and yet it is inaccessible by thermally-activated reactions due to a large number of competing processes. This work thus demonstrates the feasibility of accessing and controlling non-thermal reaction pathways that may lead to unique and controllable order-disorder transitions in supported molecular layers.

3:18PM L51.00005 Self assembly of anisotropic colloidal particles, DANIEL FLOREA, HANS WYSS, Eindhoven Technical University — Colloidal particles have been successfully used as "model atoms", as their behavior can be more directly studied than that of atoms or molecules by direct imaging in a confocal microscope. Most studies have focussed on spherical particles with isotropic interactions. However, a range of interesting materials such as many supramolecular polymers or biopolymers exhibit highly directional interactions. To capture their behavior in colloidal model systems, particles with anisotropic interactions are clearly required. Here we use a colloidal system of nonspherical colloids, where highly directional interactions can be induced via depletion. By biaxially stretching spherical PMMA particles we create oblate spheroidal particles. We induce attractive interactions between these particles by adding a non-adsorbing polymer to the background liquid. The resulting depletion interaction is stronger along the minor axis of the oblate spheroids. We study the phase behavior of these materials as a function of the ellipsoid aspect ratio, the strength of the depletion interactions, and the particle concentration. The resulting morphologies are qualitatively different from those observed with spherical particles. This can be exploited for creating new materials with tailored structures.

3:30PM L51.00006 Adsorption of Core-Shell Nanoparticles at Liquid-Liquid Interfaces, EMANUELA DEL GADO, LUCIO ISA, ETH Zurich, ESTHER AMSTAD, Harvard, KONRAD SCHWENKE, PATRICK ILG, MARTIN KROEGER, ETH Zurich, ERIK REIMHULT, BOKU Wien, SURFACE TECHNOLOGY, ETH ZURICH TEAM, MICROSTRUCTURE AND RHEOLOGY, ETH ZURICH TEAM, POLYMER PHYSICS, ETH ZURICH TEAM, NANOBIO TECHNOLOGY, BOKU TEAM — The use of nanoparticles as building blocks for the self-assembly of functional materials has been rapidly increasing in recent years. In particular, two-dimensional materials can be effectively self-assembled at liquid interfaces thanks to particle localization and mobility at the interface in combination with tailoring of specific interactions. Many recent advances have been made in the understanding of the adsorption and assembly at liquid interfaces of small hydrophobic nanoparticles, stabilized by short-chain rigid dispersants, but the corresponding studies on core-shell nanoparticles sterically stabilized by extended hydrophilic polymer brushes are presently missing. Such particles offer significant advantages in terms of fabrication of functional, responsive and bio-compatible materials. We present here a combination of experimental and numerical data together with an intuitive and simple model aimed at elucidating the mechanisms governing the adsorption of iron oxide nanoparticles (5-10nm) stabilized by low molecular weight poly(ethylene glycol) (1.5-10 kDa). We show that the adsorption dynamics and the structure of the final assembly depend on the free energy of the particles at the interface and discuss the thermodynamics of the adsorption.

3:42PM L51.00007 ABSTRACT WITHDRAWN —

3:54PM L51.00008 Encapsulation by Janus Oblate Spheroids¹, WEI LI, YA LIU, Lehigh University, GENEVIEVE BRETT, Skidmore College, JAMES GUNTON, Lehigh University — The micro/nano encapsulation technology has acquired considerable attention in the fields of drug delivery, biomaterial engineering, and material science. Based on recent advances in chemical particle synthesis, we propose a preliminary model of encapsulation system induced by self-assembly of Janus oblate ellipsoids, the particles with oblate ellipsoidal cores and two semi-surfaces coded with dissimilar chemical properties. Using Monte Carlo simulation, we investigate the encapsulation system with spherical particles as encapsulated guests in different densities. We study the anisotropic effect brought by encapsulating agent's geometric shape and chemical composition on encapsulation morphology and efficiency. In the relative high encapsulation efficiency we observe from the simulation, we believe this method of encapsulation is of potential value in practical use.

¹This work was supported by grants from the Mathers Foundation and the National Science Foundation (Grant DMR-0702890). One of us (GB) was supported by the NSF REU Site Grant in Physics at Lehigh University.

4:06PM L51.00009 Particle Deposition in Drying Drops of Colloidal Suspensions Containing Different Surfactants¹, TIM STILL, PETER J. YUNKER, A.G. YODH, University of Pennsylvania — When a drop of water containing small solid particles dries, most of the solid material is deposited in a ring-shape stain after evaporation (the so-called coffee ring), driven by initial contact line pinning and a subsequent outward-flow. The fluid dynamics and, hence, the deposition mechanism in such suspensions can be dramatically changed when surfactants are introduced into the system. In a colloidal model-system, the ionic sodium dodecyl sulfate (SDS) produces a concentration-driven Marangoni flow counteracting the outward-flow of the coffee ring effect. SDS locally concentrates at the air/water interface next to the contact line, leading to a reduced local surface tension. Thus, a circulating flow ('Marangoni eddy') is introduced that prevents particles from deposition. This flow is visualized by the movements of the dragged particles using video microscopy. Other surfactants can influence this highly non-equilibrium systems in completely other ways. E.g., the non-ionic Poloxamer block-copolymer surfactants lead to a uniform particle deposition, which we explain by hydrophilization of the colloidal particles. Controlling the solid deposition in drying drops is of major importance for many technical applications.

¹We acknowledge financial support from MRSEC DMR11-20901 and DAAD.

4:18PM L51.00010 Formation of Lipid-Based Nanodiscs and Their Dependence of Temperature and Chemical Composition¹, YING LIU, YONGKUN YANG, MU-PING NIEH, UNIVERSITY OF CONNECTICUT — Phospholipid mixtures composed of 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC), 1,2-dihexanoyl-sn-glycero-3-phosphocholine (DHPC) and 1,2-dipalmitoyl-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt)(DPPG) and 1,2-distearoyl-sn-glycero-3-phosphoethanolamine-N-[methoxy(polyethylene glycol)-2000] (ammonium salt) (PEGylated DSPE) and cholesterol were found to form nanodiscs (bicelles) in both non-ionic and phosphate buffer solutions. The structure of the aggregates is resolved using dynamic light scattering, transmission electron microscopy and small angle neutron scattering. The effects of temperature and chemical composition (e.g., PEGylated DSPE and cholesterol) on the structural variation and polydispersity will be discussed in this presentation. These nanodiscs have the potential of serving as a model delivery carrier for hydrophobic molecules for their biological compatibility and capability of incorporating with targeting molecules.

¹Thanks NSF - CMMI 1131589

4:30PM L51.00011 How to control GUV shape transformations, KEJIA CHEN, ADAM SZMELTER, SUNG CHUL BAE, STEVE GRANICK, University of Illinois at Urbana-Champaign — Using a microfluidic platform, we expose giant unilamellar vesicles (GUVs) to programmed time-varying profiles of osmotic pressure. In response to these conditions that intentionally do not approach equilibrium, water flows in and out, and the excess area changes in response. Shape transformations are observed that were not previously reported, nor predicted theoretically.

4:42PM L51.00012 Aqueous Gemini Surfactant Self-Assembly into Complex Lyotropic Phases, MAHESH MAHANTHAPPA, GREGORY SORENSON, Department of Chemistry, University of Wisconsin-Madison, 1101 University Ave., Madison, WI 53703 — In spite of the potentially wide-ranging applications of aqueous bicontinuous lyotropic liquid crystals (LLCs), the discovery of amphiphiles that reliably form these non-constant mean curvature morphologies over large phase windows remains largely serendipitous. Recent work has established that cationic gemini surfactants exhibit a pronounced tendency to form bicontinuous cubic (e.g. gyroid) phases as compared to their parent single-tail amphiphiles. The universality of this phenomenon in other surfactant systems remains untested. In this paper, we will report the aqueous LLC phase behavior of a new class of anionic gemini surfactants derived from long chain carboxylic acids. Our studies show that these new surfactants favor the formation of non-constant mean curvature gyroid and primitive ("Plumber's Nightmare") structures over amphiphile concentration windows up to 20 wt% wide. Based on these observations, we will discuss insights gained into the delicate force balance governing the self-assembly of these surfactants into aqueous bicontinuous LLCs.

4:54PM L51.00013 Shear-Driven Circulation Patterns in Lipid Membrane Vesicles, FRANCIS WOODHOUSE, AURELIA HONERKAMP-SMITH, RAYMOND GOLDSTEIN, DAMTP, University of Cambridge — Recent experiments [C. Vézy, G. Massiera, and A. Viallat, *Soft Matter* 3, 844 (2007)] have shown that when a near-hemispherical lipid vesicle attached to a solid surface is subjected to a simple shear flow it exhibits a pattern of membrane circulation much like a dipole vortex. This is in marked contrast to the toroidal circulation that would occur in the related problem of a drop of immiscible fluid attached to a surface and subjected to shear. This profound difference in flow patterns arises from the lateral incompressibility of the membrane, which restricts the observable flows to those in which the velocity field in the membrane is two-dimensionally divergence free. We theoretically study these circulation patterns within the simplest model of membrane fluid dynamics. A systematic expansion of the flow field is developed for differing bulk fluid viscosities incorporating a non-zero membrane shear viscosity and curvature effects. It is shown how such studies can allow measurements of the membrane viscosity from flow field data. New experimental results utilising this method are discussed.

5:06PM L51.00014 Self standing nanoparticulate networks by self assembly surfactant H₁ mesophase, GURUSWAMY KUMARASWAMY, NCL, Pune, India, KAMENDRA SHARMA, SAYAM SEN GUPTA, NCL — We show that nanoparticles (size > 10 nm) that are dispersed in nonionic surfactant/water system, assemble into networks on cooling into the H₁ phase, independent of particle surface chemistry. Coating the particles with a crosslinkable polymer, and covalent coupling of the coated particle assemblies in the H₁ phase allows us to form free standing particulate networks that are stable after surfactant removal. Thus, dynamic templating of surfactant H₁ domains is a facile technique that involves near ambient temperatures, and a benign water wash for template removal. The network mesh size can be varied from the sub-micron to tens of microns by controlling the cooling rate. Particle networks can be flow-oriented prior to crosslinking, and interpenetrating networks can also be formed. We will show examples of macroporous nanoparticulate networks formed using nanoparticles of inorganic oxides, polymer latices, as well as bionanoparticles such as proteins.

5:18PM L51.00015 SAXS on ice crystals reveals fractal structure on nanometer length scales, JESSE HOPKINS, RYAN BADEAU, MATTHEW WARKENTIN, ROBERT THORNE, Cornell University — We have used small angle x-ray scattering (SAXS) to probe ice formation in supercooled aqueous solutions and water. The SAXS shows that the ice formed in supercooled aqueous solutions and water has power law behavior that is invariant across a wide range of solute type, concentration, and temperature. We interpret this power law as scatter from fractal structures in the ice. The consistency of this power law across four different solutes and in pure water, and at temperatures between 150 K and 220 K suggests an underlying similarity between macroscopically/visually different forms of ice on length scales of 10-100 nm. Time dependent SAXS curves reveal two scattering regimes, one occurring at early times and one dominating at later times, which we interpret within the context of fractal scatterers. Finally, we use scaling collapses on the data to extract information about the time and temperature dependence of the ice growth. We interpret this within the established framework of the ice nucleation and growth community.

5:30PM L51.00016 Molecular Dynamics simulations of flow-structure interactions in fluids containing cylindrical micelles and micelle-nanoparticle complexes¹, RADHAKRISHNA SURESHKUMAR, Syracuse University, Syracuse, NY, ASHISH SANGWAI, Intel Corporation, Hillboro, OR, ABHINANDEN SAMBASIVAM, Syracuse University, Syracuse, NY, SYRACUSE UNIVERSITY TEAM — Coarse-grained (CG) force fields, benchmarked against fully atomistic ones, are used in Molecular Dynamics simulations to predict shape transitions and binary interactions in cationic surfactant micelles as well as to understand the molecular mechanisms of self-assembly of micelles with noble metal nanoparticles germane to plasmonics. Non-equilibrium MD simulations are conducted to probe the effect of flow shear on cylindrical micelle dynamics and estimate properties such as tumbling frequency, relaxation time and scission energy. Simulations are also performed to understand flow-mediated alignment and merger of two cylindrical micelles which is hypothesized to be the mechanism underlying the formation of shear-induced structures in micellar fluids.

¹NSF CBET 1049454

Tuesday, February 28, 2012 2:30PM - 5:30PM –
Session L52 GSNP DFD: Focus Session: Extreme Mechanics - Origami, Creasing, and Folding
153C

2:30PM L52.00001 Extreme Folding, ERIK DEMAINE, Massachusetts Institute of Technology — Our understanding of the mathematics and algorithms behind paper folding, and geometric folding in general, has increased dramatically over the past several years. These developments have found a surprisingly broad range of applications. In the art of origami, it has helped spur the technical origami revolution. In engineering and science, it has helped solve problems in areas such as manufacturing, robotics, graphics, and protein folding. On the recreational side, it has led to new kinds of folding puzzles and magic. I will give an overview of the mathematics and algorithms of folding, with a focus on new mathematics and sculpture.

3:06PM L52.00002 Geometry in the mechanics of origami, MARCELO A. DIAS, CHRISTIAN D. SANTANGELO, University of Massachusetts Amherst — We present a mechanical model for curved fold origami in which the bending energies of developable regions are balanced with a phenomenological energy for the crease. The latter energy comes into play as a source of geometric frustration, allowing us to study shape formation by prescribing crease patterns. For a single fold annular configuration, we show how geometry forces a symmetry breaking of the ground state by increasing the width of the ribbon. We extend our model to study multiple fold structures, where we derive geometrical constraints that can be written as recursive relations to build the surface from valley to mountain, and so on. We also suggest a mechanical model for single vertex folds, mapping this problem to an elastica on the sphere.

3:18PM L52.00003 Photo-Origami – Using Light to Bend, Fold, and Buckle¹, JENNIE RYU, University of Colorado, MATTEO D'AMATO, University of Trento, KEVIN LONG, Sandia National Laboratories, XIAODONG CUI, H. JERRY QI, MARTIN DUNN, University of Colorado — We describe photo-origami, a method to program spatially- and temporally-variable mechanical, chemical, and optical fields into a polymer that enable controllable, sequenced, macroscopic bending and folding to create three-dimensional structures. We combine mechanical and optical stimuli to locally rearrange the polymer's network topology which allows us to program a residual stress state into the film; upon release of mechanical constraints, we realize a wide variety of desired shapes. We demonstrate, through a combination of theory, simulation-based design, synthesis, and experiment, the operative phenomena and capabilities of photo-origami. We demonstrate architectures that rely on bending, folding, instabilities, and post-buckling behavior to achieve their three-dimensional form, starting from a flat sheet. We also describe a theory that couples the hereditary nature of photophysics, chemistry, and large-deformation mechanics and enables simulations of the fabricated structures that are in good agreement with the experiments.

¹AFOSR, National Science Foundation, Sandia National Laboratories

3:30PM L52.00004 Pleated and Creased Structures¹, LEVI DUDTE, ZHIYAN WEI, L. MAHADEVAN, Harvard University — The strategic placement of curved folds on a paper annulus produces saddle-shaped origami. These exotic geometries resulting from simple design processes motivate our development of a computational tool to simulate the stretching, bending and folding of thin sheets of material. We seek to understand the shape of the curved origami figure by applying the computational tool to simulate a thin annulus with single or multiple folds. We aim to quantify the static geometry of this simplified model in order to delineate methods for actuation and control of similar developable structures with curved folds. Miura-ori pattern is a periodic pleated structure defined in terms of 2 angles and 2 lengths. The unit cell embodies the basic element in all non-trivial pleated structures - the mountain or valley folds, wherein four folds come together at a single vertex. The ability of this structure to pack and unpack with a few degrees of freedom leads to their use in deployable structures such as solar sails and maps, just as this feature is useful in insect wings, plant leaves and flowers. We probe the qualitative and quantitative aspects of the mechanical behavior of these structures with a view to optimizing material performance.

¹Grant Acknowledgement: Harvard NSF MRSEC, DARPA, Kavli Institute, Wyss Institute

3:42PM L52.00005 Hierarchical Stress Focusing in Elastic Ridge, LEE WALSH, BENNY DAVIDOVITCH, University of Massachusetts — A crumpled or confined elastic sheet contains many stress-focusing structures and singularities, primarily ridges and vertices, which may contain much of the strain. We seek to determine the degree and quality of stress focusing within the geometry of a single ridge. Previous work on the ridge assumes the asymptotic limit of infinitely sharp vertices. However, in a physically realistic sheet any vertex or intersection of ridges will naturally have a finite radius of curvature greater than the sheet's thickness. We simulate these more physically realistic boundary conditions in a ridge using Surface Evolver.

3:54PM L52.00006 Stress focusing and collapse of a thin film under constant pressure¹, EUGENIO HAMM, NICOLAS CABEZAS, Universidad de Santiago de Chile — Thin elastic sheets and shells are prone to focus stress when forced, due to their near inextensibility. Singular structures such as ridges, vertices, and folds arising from wrinkles, are characteristic of the deformation of such systems. Usually the forcing is exerted at the boundaries or at specific points of the surface, in displacement controlled experiments. On the other hand, much of the phenomenology of stress focusing can be found at micro and nanoscales, in physics and biology, making it universal. We will consider the post-buckling regime of a thin elastic sheet that is subjected to a constant normal distributed force. Specifically, we will present experiments made on thin elastoplastic sheets that collapse under atmospheric pressure. For instance, in vacuum-sealing technology, when a flat plastic bag is forced to wrap a solid volume, a series of self-contacts and folds develop. The unfolded bag shows a pattern of scars whose structure is determined by the geometry of the volume and by the exact way it stuck to its surface, by friction. Inspired by this everyday example we study the geometry of folds that result from collapsing a hermetic bag on regular rigid bodies.

¹Fondecyt 1110584 and Anillo ACT95

4:06PM L52.00007 Creasy modeling of a compressed elastic surface, TUOMAS TALLINEN, L. MAHADEVAN, Harvard University — Compression of an elastic layer attached to a rigid substrate leads to nucleation and growth of creases. We explore crease formation by a numerical model allowing control of compressive strain, anisotropy and bulk modulus. We address questions on arrangement and geometry of creases and model also the stabilizing effect of surface tension at small scales.

4:18PM L52.00008 Creasing instability of elastomers under uniaxial compression, DAYONG CHEN, RYAN HAYWARD, Polymer Science and Engineering Department at UMass-Amherst — Soft polymers placed under compressive stress can undergo an elastic creasing instability in which sharp folds spontaneously form on the free surfaces. This process may play an important role in contexts as diverse as brain morphogenesis, failure of tires, and electrical breakdown of soft polymer actuators, but our understanding of this instability is still quite limited. We describe a simple experimental system to study creasing of thin elastomer films under uniaxial compression. The equilibrium depths, spacings and shapes of creases are characterized and found to show excellent agreements with numerical results. Further, we use this system to explore the important roles played by surface energy and adhesion in the onset and hysteretic behavior of creases.

4:30PM L52.00009 Sulcus formation in a compressed elastic half space, JOHN BIGGINS, L. MAHADEVAN, Harvard University — When a block of rubber, biological tissue or other soft material is subject to substantial compression, its surfaces undergo a folding instability. Rather than having a smooth profile, these folds contain cusps and hence have been called creases or sulci rather than wrinkles. The stability of a compressed surface was first investigated by Biot (1965), assuming the strains associated with the instability were small. However, the compression threshold predicted with this approach is substantially too high. I will introduce a family of analytic area preserving maps that contain cusps (and hence points of infinite strain) that save energy before the linear stability threshold even at vanishing amplitude. This establishes that there is a region before the linear stability threshold is reached where the system is unstable to infinitesimal perturbations, but that this instability is quintessentially non-linear and cannot be found with linear strain elasticity.

4:42PM L52.00010 Compression induced folding of a sheet: An integrable system, HAIM DIAMANT, Tel Aviv University, THOMAS A. WITTEN, University of Chicago — The apparently intractable shape of a fold in a compressed elastic film lying on a fluid substrate is found to have an exact solution. Such systems buckle at a nonzero wave vector set by the bending stiffness of the film and the weight of the substrate fluid. Our solution describes the entire progression from a weakly displaced sinusoidal buckling to a single large fold that contacts itself. The pressure decrease is exactly quadratic in the lateral displacement. We demonstrate a subtle connection to the sine-Gordon problem, which reveals a new symmetry in the folding phenomenon.

4:54PM L52.00011 Wrinkles or creases in a bi-layer structure, LIHUA JIN, School of Engineering and Applied Sciences, Kavli Institute, Harvard University, ANESIA BURNS, RYAN HAYWARD, Department of Polymer Science & Engineering, University of Massachusetts, ZHIGANG SUO, School of Engineering and Applied Sciences, Kavli Institute, Harvard University — Wrinkles and creases are different modes of instability. In this work, we try to answer for a bi-layer structure with different modulus ratios and thickness ratios of the film and substrate whether wrinkles or creases form first when the bi-layer is under uniform compression. The onset of wrinkles corresponds to a bifurcation point, and we use the linear perturbation method to analyze the critical strain for the onset of wrinkles. Since the initiation of creases is autonomous, we directly apply the critical condition for crease initiation in a half space calculated by the finite element method in the literature to the situation of a bi-layer structure with finite thickness. By comparing the critical strains for the formation of wrinkles and creases under different modulus and thickness ratios, a phase diagram of the formation of wrinkles or creases is obtain. Although the critical strains for both wrinkle and crease initiation depend on the state of strain, remarkably the phase diagram is independent of the state of strain. As a result, creases tend to set in for more compliant and thicker films, while wrinkles tend to set in for stiffer and thinner films. Especially, when the modulus ratio of the film and substrate is smaller than 1.67, creases always form earlier than wrinkles, no matter what the thickness ratio is. We further verify the result experimentally by compressing a bi-layer of polymers with different modulus and thickness ratios.

5:06PM L52.00012 Wrinkles and Folds in Ultra-Thin Polymer Films¹, YURI EBATA, University of Massachusetts, Amherst, ANDREW B. CROLL, North Dakota State University, ALFRED J. CROSBY, University of Massachusetts, Amherst — Wrinkles and folds are observed in many biological systems during morphogenesis processes. However, the mechanics of how these wrinkles and folds form are not completely understood. Studying the mechanics of wrinkles and folds will not only provide us with fundamental insights of nonlinear deformation processes but also allow for the fabrication of unique patterned surfaces that can be controlled reversibly. In this study, we examine wrinkles and folds of polystyrene films of thickness ranging from 5 nm to 180 nm attached to uniaxially-strained polydimethylsiloxane substrates. The strain is released incrementally to apply increasing compressive strain to the attached film. The wavelength and the amplitude of local out-of-plane deformation are measured as global compression is increased to distinguish between different buckling modes. The transition from wrinkling to folding is observed by tracking the statistics of amplitude distribution sampled across a large lateral area, and a critical strain map is constructed to observe how film thickness affect the resulting buckling modes.

¹NSF-DMR 0907219

5:18PM L52.00013 Relaxation mechanisms in the unfolding of thin sheets, BENJAMN THIRIA, PMMH-ESPCI, MOKHTAR ADDA-BEDIA, LPS-ENS — When a thin sheet is crumpled, creases form in which plastic deformations are localized. Here we study experimentally the relaxation process of a single fold in a thin sheet subjected to an external strain. The unfolding process is described by a quick opening at first, and then a logarithmic slow relaxation of the crease. In the latter regime, the necessary force needed to open the folded sheet at a given displacement is found to decrease logarithmically in time, allowing its description through an Arrhenius activation process. We accurately determine the parameters of this law and show its general character by performing experiments on both Mylar and paper sheets.

Tuesday, February 28, 2012 2:30PM - 5:30PM – Session L53 GSNP DCMP: Frontiers of Statistical Physics 153B

2:30PM L53.00001 Lars Onsager Prize Lecture: A Random Walk Through Theoretical Physics, IAN AFFLECK, University of British Columbia — A historical account will be given of my efforts to apply conformal field theory techniques to experimentally relevant models of condensed matter. This began with a so far unsuccessful attempt to find the exact critical exponents for the localization transition in the integer quantum Hall effect, using techniques developed by field/string theorists. It was followed by a program to classify critical behavior of Heisenberg antiferromagnetic spin chains of arbitrary spin magnitude. It eventually led to a general theory of the low energy behavior of quantum impurity models including exact solutions for non-Fermi liquid critical points.

3:06PM L53.00002 Dannie Heineman Prize for Mathematical Physics Lecture: Understanding Nonequilibrium via Rare Fluctuations, GIOVANNI JONA-LASINIO, Dipartimento di Fisica, Università di Roma “La Sapienza” and INFN, Roma, Italy — Irreversible processes are a hot subject in statistical mechanics. During the last decade through the effort of several people, including the recipient of the prize and his collaborators, a progress in understanding stationary nonequilibrium states has been achieved. The key has been the study of rare fluctuations. The talk will review some basic ideas, results and perspectives.

3:42PM L53.00003 Experimental confirmation of Landauer's principle¹ , JOHN BECHHOEFER, YONGGUN JUN², Simon Fraser University — Landauer's principle, formulated in 1961, postulates that irreversible logical or computational operation such as memory erasure must dissipate heat, no matter how slowly they are performed. For example, to "reset to one" a memory that can be in state 0 or 1 requires at least $kT \ln 2$ of work, which is dissipated as heat. In 1982, Bennett pointed out a link to Maxwell's Demon: Were Landauer's principle to fail, it would be possible to repeatedly extract work from a heat bath. We report the first confirmation of Landauer's principle in an experimental system, where a virtual double-well potential is created via a feedback loop. We observe the position of a charged, fluorescent, colloidal particle in water and calculate and then apply a force $= -\text{grad } U(x,t)$ via an electric field. In a first experiment, the probability of "erasure" (resetting to one) is unity, and at long cycle times, we observe that the work is compatible with $kT \ln 2$. In a second, the probability of erasure is zero; the system may end up in two states; and, at long cycle times, the measured work tends to zero.

¹Supported by NSERC, Canada

²Present address: Department of Developmental and Cell Biology, School of Biological Sciences, Univ. of Calif., Irvine

3:54PM L53.00004 The Basis of the Second Law of Thermodynamics in Quantum Field Theory¹ , DAVID SNOKE, GANGQIANG LIU, Department of Physics and Astronomy, University of Pittsburgh, STEVEN GIRVIN, Department of Physics, Yale University — We derive the quantum Boltzmann equation for a closed system with a two-particle collision process on the basis of quantum field theory. In the thermodynamic limit, the system evolves deterministically and irreversibly towards equilibrium, on the time scale of the scattering time of the particles. This irreversibility is related to the loss of information which comes from the vanishing off-diagonal phase coherence in the system. By calculating the time evolution of the off-diagonal elements of the generalized density matrix, we show that these terms decay rapidly due to the interaction. In the case of Bose-Einstein condensates, all phase coherence is not lost. We deduce the onset of phase coherence in a Bose-Einstein condensate, which gives rise to macroscopic wavelike behaviors of Bose systems. We also derive the H-theorem by combining our results with standard definitions of entropy.

¹We thank A. Duncan, D. Boyanovsky, and K. Sengupta for helpful discussions. This work has been partly supported by the National Science Foundation through grant DMR-0706331.

4:06PM L53.00005 The Stochastic Geometry of non-Gaussian Fields , THOMAS BEUMAN, Institute Lorentz, Leiden University, ARI TURNER, University of Amsterdam, VINCENZO VITELLI, Institute Lorentz, Leiden University — Gaussian random fields pervade various areas of physics and have distinctive and well understood stochastic properties. Here we study the stochastic geometry of a random surface, whose height is given by a nonlinear function of a Gaussian field. We find that, as a result of the non-Gaussianity, the density of maxima and minima no longer match and calculate the relative imbalance between the two. We perform similar calculations for the density of umbilical points, which are topological defects of the lines of curvature. Our results apply to the analysis of speckle patterns generated by nonlinear random waves and more generally to detect and quantify non-Gaussianities present in any scalar field that can be represented as a smooth two-dimensional surface.

4:18PM L53.00006 Differential geometry of the space of Ising models , BENJAMIN MACHTA, RICKY CHACHRA, Department of Physics, Cornell University, MARK TRANSTRUM, Department of Bioinformatics and Computational Biology at the MD Anderson Cancer Center, JAMES SETHNA, Department of Physics, Cornell University — We use information geometry to understand the emergence of simple effective theories, using an Ising model perturbed with terms coupling non-nearest-neighbor spins as an example. The Fisher information is a natural metric of distinguishability for a parameterized space of probability distributions, applicable to models in statistical physics. Near critical points both the metric components (four-point susceptibilities) and the scalar curvature diverge with corresponding critical exponents. However, connections to Renormalization Group (RG) ideas have remained elusive. Here, rather than looking at RG flows of parameters, we consider the reparameterization-invariant flow of the manifold itself. To do this we numerically calculate the metric in the original parameters, taking care to use only information available after coarse-graining. We show that under coarse-graining the metric contracts very anisotropically, leading to a "sloppy" spectrum with the metric's Eigenvalues spanning many orders of magnitude. Our results give a qualitative explanation for the success of simple models: most directions in parameter space become fundamentally indistinguishable after coarse-graining.

4:30PM L53.00007 Growth Inside a Corner: Limiting Interface Shape , JASON OLEJARZ, PAUL KRAPIVSKY, SIDNEY REDNER, Boston University, KIRONE MALLICK, CEA Saclay, France — We investigate a simple model for crystal growth in which elemental cubes are stochastically deposited onto the inside of a three-dimensional corner. The interface of this crystal evolves into a deterministic limiting shape in the long-time limit. We incorporate known results from the corresponding two-dimensional system and use geometrical symmetries of the three-dimensional problem to conjecture an equation of motion for the interface profile which we solve analytically. The agreement between the result of the calculation and simulations of the growth process is excellent. We also present a generalization of our equation of interface motion to arbitrary spatial dimension.

4:42PM L53.00008 The magnetisation distribution of the Ising model for $d \geq 5$, PER LUNDOW, ANDERS ROSENGREN, KTH - Royal Institute of Technology — The magnetisation distribution of the Ising model for $d > 4$ is excellently fitted by a generalised binomial distribution. We have computed exactly an ansatz expression which can be fitted to the distribution near T_c . Though the ansatz is long and complicated it only has three parameters, besides the number of vertices, which then provides us with details about the distribution. This method also provided us with an estimate of T_c for $d = 6$. For extremely dense regular graphs, such as a complete bipartite graph, we can show what the parameter values are and that these values give asymptotically correct behaviour of eg the susceptibility and the free energy. Also a possible approach for $d \leq 4$ will be briefly discussed as well as boundary effects for $d = 5$.

4:54PM L53.00009 A Topological Phase Transition in Models of River Networks , JACOB OPPENHEIM, MARCELO MAGNASCO, Rockefeller University — The classical Scheidegger model of river network formation and evolution is investigated on non-Euclidean geometries, which model the effects of regions of convergent and divergent flows - as seen around lakes and drainage off mountains, respectively. These new models may be differentiated by the number of basins formed. Using the divergence as an order parameter, we see a phase transition in the number of distinct basins at the point of a flat landscape. This is a surprising property of the statistics of river networks and suggests significantly different properties for riverine networks in uneven topography and vascular networks of arteries versus those of veins among others.

5:06PM L53.00010 Finite size scaling of the dynamical free-energy in the interfacial regime of a kinetically constrained model, VIVIEN LECOMTE, Laboratoire Probabilités et Modèles Aléatoires (LPMA), CNRS UMR 7599, Universités Paris 6 et Paris 7, France, THIERRY BODINEAU, DMA, Ecole Normale Supérieure (UMR 8553), 45 rue d'Ulm, Paris, France, CRISTINA TONINELLI, Laboratoire Probabilités et Modèles Aléatoires (LPMA), CNRS UMR 7599, Universités Paris 6 et Paris 7, France — Glassy phenomena have proven difficult to understand: they present a variety of features – slow dynamics, ageing, dynamical heterogeneity, frustration – which make their study arduous from a theoretical point of view. Kinetically Constrained Models (KCMs) are a simple class of lattice gas whose dynamics present features similar to those of glassy phenomena, with the advantage that no disorder is present in the model – making them easier to study. A dynamical approach has been recently proposed: it consists in determining the large deviation function associated to the probability distribution function of time-integrated observables quantifying the “activity” of histories followed by the system. We determine the finite size corrections to the large deviation function of the activity in a KCM (the Fredrickson-Anderson model in one dimension), in the regime of dynamical phase coexistence. Numerical results agree with an effective model where the boundary between active and inactive regions is described by a Brownian interface. We show that the scalings of this physical picture are reflected in the finite size scaling of the dynamical free energy of the model. We expect the same picture to hold in other kinetically constrained models where the particle number is not conserved.

5:18PM L53.00011 Effective Temperature Dynamics of Radiation Induced Amorphization, IDO REGEV, Center for non linear studies and Theoretical division, Los Alamos National Laboratory, XIANGDONG DING, TURAB LOOKMAN, Theoretical division, Los Alamos National Laboratory 61097340 — Materials exposed to radiation suffer structural changes over time. Typically, after exposure to radiation, a crystal will gradually lose its periodic structure and become amorphous. A theory of radiation amorphization should provide a description of the structural evolution. We study radiation amorphization in a simple molecular dynamics model and show that one can describe the amorphous steady-state using a structural effective temperature (different from the thermal bath temperature). We derive a theory that predicts the value of the steady-state effective-temperature as a function of the thermal bath temperature for a constant intensity of radiation. The theory agrees well with simulations results.

Tuesday, February 28, 2012 2:30PM - 5:30PM – Session L54 DCMP: Superconductivity: Mostly Devices and Applications 152

2:30PM L54.00001 Proximity Induced Superconductivity in Ferromagnetic Nanowires: Magnetoresistance Oscillations and Steps in I-V Characteristics¹, MEENAKSHI SINGH, Pennsylvania State University, MINGLIANG TIAN, University of Science and Technology of China, Hefei, JIAN WANG, Pennsylvania State University, HE LIN, Beijing Normal University, Beijing, MOSES CHAN, Pennsylvania State University — Ferromagnetic order requires electronic spins to be aligned parallel whereas singlet superconducting order requires spins to be aligned antiparallel. This spin incompatibility limits the superconducting proximity effect to ~ 1 nm in bulk ferromagnets. In ferromagnetic nanowires contacted with superconducting W electrodes however, the proximity effect is seen to extend to ~ 400 nm [Wang et al., Nat. Phys. 6, 389 (2010)]. The mechanism behind the long range proximity in these systems is not certain. We have studied single crystalline Co nanowires contacted with normal electrodes with a single superconducting W strip patterned on the nanowire. The long range proximity effect is found to persist in this geometry. Robust magnetoresistance oscillations were found when an external field parallel to the axis of the wire was applied. In addition, regularly spaced peaks were seen in the dI/dV vs. V characteristics of the sample. The origin of the oscillations and the peaks is not understood.

¹This work was supported by NSF under grant no. DMR-0820404.

2:42PM L54.00002 Imaging point-like defects in two dimensional superconductors: theory and experiment, HILARY NOAD, JULIE BERT, KATJA NOWACK, BEENA KALISKY, ILYA SOCHNIKOV, THOMAS LIPPMAN, Stanford Institute for Materials and Energy Science, Stanford University, Stanford CA 94305, JOHN KIRTLEY, Department of Applied Physics, Stanford University, Stanford CA 94305, KATHRYN MOLER, Stanford Institute for Materials and Energy Science, Stanford University, Stanford CA 94305 — Point defects in two-dimensional superconductors produce significant local variations in the superconducting properties. A model [1] of point defects in a weak, two-dimensional superconductor, based on London's equations, shows that defects appear as haloes of decreased diamagnetic susceptibility as seen by the imaging kernel of a scanning SQUID susceptometer. We report theoretical limits on the defect strength and superconducting Pearl length Λ required for defects to be visible. We compare these models to our experimental data showing similar haloes in the superconducting state of several types of superconducting films as a function of magnetic field, gate voltage, temperature, and height. Our ability to image these defects offers new possibilities for studying the interplay between materials properties and superconducting phenomena in thin film systems.

[1] V.G. Kogan and J.R. Kirtley, Phys. Rev. B **83**, 214521 (2011).

2:54PM L54.00003 Half-quantum vortices in superconducting networks¹, ILYA SOCHNIKOV, KATHRYN MOLER, Department of Physics and Department of Applied Physics, Stanford University, Stanford, California 94305, USA, VICTOR VAKARYUK, Argonne National Laboratory, Argonne, Illinois 60439, USA — We study numerically the magnetic field and temperature dependence of vortex occupation in superconducting wire networks assuming that the underlying material allows for the presence of half-quantum vortices. We focus on thermodynamic stability of half-quantum vortices, which are believed to be present in large size networks even when a stability of a single isolated half-quantum vortex is not expected. The spatial arrangements of half- and full vortices in networks are studied as well.

¹V. V. acknowledges the support from CES-EFRC DoE, Award DE-AC0298CH1088.

3:06PM L54.00004 DNA templating for *in situ* growth and measurement of 1D superconducting wires, LIUQI YU, JINGJIAO GUAN, PENG XIONG, Florida State University — Controllable and reproducible fabrication of sub-10 nm metal wires is of broad scientific and technological interest. One notable example is nanowires of disordered superconductors; such a small width is generally required to place them in the 1D regime where questions remain on the nature of superconductivity and superconducting fluctuations. Molecular templating based on macromolecules, such as carbon nanotubes and DNA strands, offers a relatively straightforward and reliable method of producing nm-wide wires. Here, we report the fabrication of nanowire templates using a unique procedure of DNA stretching.¹ DNA wires are assembled onto Si/SiO₂/Si₃N₄ substrates across trenches with an overhang, fabricated via e-beam lithography and combination of dry and wet etching. The location and orientation of the DNA wires can be well controlled. The template will be used as the substrate for *in situ* growth and electrical measurement of 1D superconductor nanowires in a custom dilution refrigerator. The experiments are expected to enable a close examination of the emergence and evolution of superconductivity in true 1D limit as the wire cross-section is varied in situ on one and the same sample.

¹J.J. Guan *et al*, Adv. Mater. 19, 1212 (2007).

3:18PM L54.00005 The role of dissipation in quantum phase slip production in superconducting nanowires, DIMA MOZYRSKY, Los Alamos National Laboratory — We study dynamics of quantum phase slips (QPS) in ultrathin superconducting wires. At sufficiently low temperatures momentum conservation is known to pose a constraint on QPS creation, which can be lifted due to inhomogeneous external potential or due to production of quasiparticles. We argue that while the former mechanism is weak in nanowires with diameters significantly exceeding the Fermi wavelength (which is the case for most up-to-date QPS experiments), the dissipation caused by quasiparticles is likely to be the major source for the QPS generation. We argue that dissipation can be enhanced in superconductors with broken time reversal symmetry, and therefore such systems are likely to exhibit phase slips at ultralow temperatures. Our studies may clarify recent experiments (Nature Physics 5, 503 (2009)) showing the evidence of QPS at sufficiently high values of bias-current.

3:30PM L54.00006 Quantum oscillations in superconducting mesoscopic rings of Sr_2RuO_4 ¹, XINXIN CAI, YIQUN YING, NEAL STALEY, Pennsylvania State University, YAN XIN, NHMFL, Florida State University, DAVID FOBES, TIJIANG LIU, ZHIQIANG MAO, Tulane University, YING LIU, Pennsylvania State University — Sr_2RuO_4 has attracted considerable amount of attention recently because of its potential application in topological quantum computing as a $p_x \pm ip_y$ superconductor. Cantilever magnetometry measurements carried out on doubly connected Sr_2RuO_4 samples of a micron size were found to exhibit jumps in magnetization suggesting the presence of both integer and half-integer flux quanta. To search for quantum oscillations with periods corresponding to integer and half-integer flux, we prepared micron size rings of Sr_2RuO_4 from thin flakes of Sr_2RuO_4 obtained by mechanical exfoliation and carried out transport measurements at low temperatures. Photolithography technique was applied to make contact probes on the flake and focused ion beam (FIB) was used in the fabrication. Disorder introduced by the FIB process employing high-energy beams of Ga ions was characterized by transmission electron microscopy. We succeeded in the preparation of superconducting rings of roughly 1 μm in diameter with 200~400nm line width. Strong oscillations of ring resistance with a conventional period of full flux quantum have been observed. In some samples a different period of oscillations was also found at high field range. The nature of these oscillations will be discussed.

¹This work is supported by DOE under grant DE-FG02-04ER46159

3:42PM L54.00007 Superconductivity of a Sn film controlled by an array of Co nanowires, ZHIYUAN WEI, ZUXIN YE, DAYA RATHNAYAKA, IGOR LYUKSYUTOV, WENHAO WU, DONALD NAUGLE, Texas A&M University, DEPARTMENT OF PHYSICS TEAM — Superconducting properties of a hybrid structure composed of ferromagnetic Co nanowire arrays and a superconducting Sn film have been investigated. Ordered Co nanowires arrays with 60 nm, 150 nm and 200 nm diameter were electroplated into the pores of self organized anodic aluminum oxide (AAO) membranes. Hysteretic dependence of the Sn film superconducting properties on applied magnetic field and critical current enhancement at moderate fields has been observed. This behavior strongly depends on the ratio of the Sn film thickness to the Co nanowire diameter.

3:54PM L54.00008 Measurements on Superconducting Nanorings Smaller than the Coherence Length¹, STEPHEN SNYDER, MICHAEL J. ERICKSON, JOSEPH KINNEY, YEONBAE LEE, J.J. NELSON, ALLEN GOLDMAN, University of Minnesota — The Little-Parks experiment on superconducting cylinders is an important demonstration of fluxoid quantization in superconductors. The transition temperature oscillations in magnetic field have a period of $h/2e$ for the micro cylinders in their studies, which was further evidence for Cooper pairing at the time [W. A. Little, R. D. Parks, *PRL* **9**, 9 (1964)]. However recent theoretical works have suggested that in superconducting loops smaller than the coherence length this period changes from $h/2e$ to h/e , for details see [F. Loder, et al. *PRB* **78**, 174526 (2008)] and references therein. The destructive regime has also been observed experimentally in cylinders whose diameter is small compared to the coherence length [Y. Liu, et al. *Science* **294**, 2332 (2001)]. We present experimental work in an effort to achieve this limit in Al nanorings prepared by electron beam lithography. These measurements achieve a regime hitherto unexplored in nanorings with interesting consequences.

¹This work was supported by the U.S. Department of Energy under Grant No. DE-FG02-02ER46004.

4:06PM L54.00009 Flux noise in SQUIDS: calculations of geometrical dependence¹, SEAN O'KELLEY, KEENAN PEPPER, STEVEN ANTON, JEFFREY BIRENBAUM, JOHN CLARKE, UC Berkeley — Low frequency ($1/f$) magnetic flux noise in SQUIDS is understood to arise from the random reversal of electron spins localized at the surface of the superconducting film. Analytical results¹ that assume independent electron spins predict that the spectral density at 1 Hz scales with the washer geometry approximately as R/W in the limit $R/W \gg 1$. Here, R is the outer radius and W is the linewidth. We present numerical calculations that reproduce the analytical result in the appropriate limit and extend these results to arbitrary values of R/W . In addition, a logarithmic dependence on W , evident when R/W is fixed and W is varied, is reproduced and discussed. The contribution of spins at the edge of the film is also computed. We compare the predicted geometrical scaling to our recent measurements of several SQUIDS with varying geometries. Our calculation that is valid for all values of R/W enables us to investigate a possible breakdown of the independent spin model in our experimental data. ¹R. C. Bialczak et al., Phys. Rev. Lett. **99**, 187006 (2007).

¹Work supported by ARO and IARPA.

4:18PM L54.00010 Geometry and temperature dependence of low frequency flux noise in dc SQUIDS¹, JEFFREY BIRENBAUM, S.M. ANTON, S.R. O'KELLEY, UC Berkeley, V. BOLKHOVSKY, D.A. BRAJE, G. FITCH, M. NEELEY, W.D. OLIVER, MIT Lincoln Laboratory, F.C. WELLSTOOD, Univ of Maryland, JOHN CLARKE, UC Berkeley — Measurements of low frequency magnetic flux noise in dc SQUIDS demonstrate a spectral density $S_\Phi(f) = A^2/f^\alpha$ in which the magnitude A scales only weakly with the washer geometry and typically $0.5 < \alpha < 1$. An analytical model assuming non-interacting spins localized to the surface of the SQUID loop predicts that $A^2 \propto R/W$ for $R/W \gg 1$. Here, R and W are the outer radius and linewidth, respectively. Our numerical calculations extend the analytical results to arbitrary washer geometries. We compare both models to flux noise measurements on several dc SQUIDS fabricated simultaneously on a single chip using a Nb trilayer process. Multiple SQUIDS were measured within a single cool-down. The SQUID geometries were divided into two categories: fixed $W=500$ nm with $3 < R/W < 24$ and fixed $R/W = 3$ with $1.5 \mu\text{m} < R < 24 \mu\text{m}$. Our measurements are in approximate agreement with the theoretical predictions for temperatures between 100 mK and 4 K, despite the fact that the slope α —for which we have no theoretical model—varies with temperature. We present measured values of α as functions of both geometry and temperature. Finally, we interpret our results within the framework of the non-interacting spin model.

¹This work was supported by ARO and IARPA.

4:30PM L54.00011 Investigation of $1/f$ flux noise in superconducting circuits, STEVEN SENDELBAACH, ANTONIO PUGLIELLI, Department of Physics, University of Wisconsin-Madison, CHANG-BEOM EOM, JACOB PODKAMINER, KWANG HWAN CHO, Department of Materials Science and Engineering, University of Wisconsin-Madison, ROBERT MCDERMOTT, Department of Physics, University of Wisconsin-Madison — Low-frequency $1/f$ flux noise is a dominant source of dephasing in the Josephson phase and flux qubits. Recent work has revealed the presence of a high density of unpaired spins at the surfaces of superconducting thin films; it is now believed that these spins are the source of the noise, although the microscopic noise mechanism is not understood. Here we describe experiments on SQUIDS and Josephson phase qubits designed to shed light on the underlying noise mechanism, and we describe efforts to develop novel materials with reduced levels of noise.

4:42PM L54.00012 Critical Exponents and Cluster Analysis on STM Studies of a Cuprate Superconductor, BENJAMIN PHILLABAUM, ERICA CARLSON, Purdue University, KARIN DAHMEN, University of Illinois at Urbana-Champaign — In this presentation we will show results from a new kind of analysis for surface probes allowing us to gather some information about the bulk behavior of the sample that is studied. This presentation will introduce the analysis in as general a way as practical and use a particular example to concretely demonstrate how it can be applied. The particular example is the case of a local nematic order observed in a Scanning Tunneling Microscopy (STM) experiment on a BSCCO sample from which we determine which model best describes the behavior of nematic orientation using critical exponents derived from the properties of clusters and correlations of these orientations. These results would highlight key physical contributions to the nematic's orientation and guide further studies into the underlying physics. We fully expect similar impact on the study of other systems for which this analysis can be performed.

4:54PM L54.00013 Extracting the Bosonic Spectra of Pb Using Superconducting-Tip STS and Comparing it with the Cuprates, F.C. NIESTEMSKI, Stanford University, S. JOHNSTON, IFW Dresden, A.W. CONTRYMAN, C.D. CAMP, T.P. DEVEREAUX, H.C. MANOHARAN, Stanford University — In high-temperature superconductors the meaning of the common feature labeled "peak-dip-hump" is still a point of great debate. In terms of scanning tunneling spectroscopy (STS) this refers to the shape of satellite features that occur outside the coherence peaks in the dI/dV spectra. There are many conflicting interpretations and labeling schemes for this feature in both the hole- and electron-doped cuprates. The path to resolving this confusion is to study a well-understood BCS superconductor to better observe the way that the STM measures bosonic information. Utilizing the ultra-low electronic noise of our home-built low-temperature STM, and utilizing a superconducting tip for increased spectral resolution, we recreate the original McMillan and Rowell S-I-S junction¹ with the STM equivalent (S-Vacuum-S). This method provides very high energy resolution for both the filled and empty electronic states in both the superconducting and normal state. We compare this data to first-principle Eliashberg calculations and relate this data to "peak-dip-hump" in the high T_c case.

¹W. L. McMillan and J. M. Rowell Phys. Rev. Lett., **14**, 108-112 (1965)

5:06PM L54.00014 Comparison between Simmons's Equations and Quantum Tunneling Experimental Results in A Thin Film, LIANXI MA, Blinn College, TEXAS A&M UNIVERSITY COLLABORATION — The theoretical predictions of J.G. Simmons's equations are compared with quantum tunneling experimental results and a discrepancy is found at bias voltage $V_b = U/e$, where U is the barrier's potential height and e is the electron charge. Specifically, he divided the bias voltage into 2 regions: $V_b < U/e$ and $V_b > U/e$, and the $I - V$ characteristics are different in these two regions. The derived equations show a kink on differential conductance dI/dV vs. V_b at $V_b = U/e$, because starts at this bias the thickness of the insulation film decreases with V_b in addition to the lowering of the barrier's average height. Therefore, the differential conductance decreases more rapidly in the region $V_b > U/e$ than in the region $V_b < U/e$. However, in tunneling experiment in which Pt is used as conductor and solid neon as insulator, we have not observed such kink even the bias was increased to 4 volts. Our speculation is either 1) there should not be a kink on conductance at $V_b = U/e$ so Simmons's equations need to be modified; 2) the kink should exist but bias voltage is not high enough to observe it in the experiments.

5:18PM L54.00015 Size effect on supercurrent screening in large array superconducting anti-dot thin films¹, HSIANG-HSI KUNG, TING-HUI CHEN, CHIA-TSO HSIEH, CHI-CHIH HO, Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan R.O.C., KEN-HUI LIN, Institute of Physics and Research Center of Applied Science, Academia Sinica, Nankang, Taipei, Taiwan R.O.C., WEN-TAU JUAN, WEI-LI LEE, Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan R.O.C. — We fabricated well-ordered and large array niobium (Nb) anti-dot thin films using a monolayer of polymer/nanosphere hybrid as a template. The hole diameter and center-to-center distance can be tuned independently. By applying a perpendicular magnetic field, we observed pronounced oscillations with field in both magnetization and resistivity due to the criteria of the flux quantization, which is reminiscent of the well-known Little-Parks experiment in a thin-walled superconducting cylinder. By varying the hole diameter, the detailed size effect on supercurrent screening can be explored and will be discussed.

¹National Science Council in Taiwan and research program on nanoscience and nanotechnology at Academia Sinica, Taipei

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Session M1 GIMS: GIMS Business Meeting 203

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Session M8 GMAG: GMAG Business Meeting 208

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Session M25 GSCCM: GSCCM Business Meeting 257A

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Session M28 FIAP: FIAP Business Meeting 258C

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Session M29 GQI: GQI Business Meeting 259A

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Session M33 GERA: GERA Business Meeting 106

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Session M34 DCP: DCP Business Meeting 107B

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Session M42 DBIO: DBIO Business Meeting 156C

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Session M46 DPOLY: DPOLY Business Meeting 160ABC

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Session M52 GSNP: GSNP Business Meeting 153C

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Tuesday, February 28, 2012 7:00PM - 8:00PM —

Session M60 DCMP: DCMP Business Meeting Westin Boston Waterfront Paine

7:00PM M60.00001 DCMP BUSINESS MEETING —

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Session M61 DMP: DMP Business Meeting Westin Boston Waterfront Revere

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Tuesday, February 28, 2012 8:00PM - 9:30PM —

Session N1 The IBM Computer Watson: Its Future Challenges After Winning at Jeopardy 253
ABC

8:00PM N1.00001 How Watson was Developed? Whats Inside and Watsons Future in Medical
Diagnosis , DAVID MCQUEENEY, IBM Research — .

8:36PM N1.00002 Making Computers Like Watson Faster, Smaller and Smarter Bits and
Atoms , NEIL GERSHENFELD, The Center for Bits and Atoms —

9:12PM N1.00003 Question and Answer —

Wednesday, February 29, 2012 8:00AM - 11:00AM – Session P2 GSNP: Invited Session: Large Fluctuations Far From Equilibrium 204AB

8:00AM P2.00001 Characterizing Order in Glassy Systems, DOV LEVINE, Technion - IIT — Crystals and quasicrystals can be characterized by an order that is a purely geometric property of an instantaneous configuration, independent of particle dynamics or interactions. Glasses, on the other hand, are ostensibly amorphous arrangements of particles. A natural and long-standing question has been whether they too have, albeit in a hidden way, some form of geometric order. I will examine a recent proposal for a coherence length that applies to systems which are typically characterized as amorphous, as well as to those that are conventionally ordered. The question of whether exotic order can arise in physical systems will be addressed.

8:36AM P2.00002 Drift, diffusion and barrier crossing of small objects on a surface assisted by an external noise: roles of non-linear friction, MANOJ CHAUDHURY, Lehigh University — We study experimentally the behaviors of several driven diffusive systems that involve the sliding and rolling of small solid objects or liquid drops on a surface with an external noise and an external field. The displacement statistics here are non-Gaussian at short observation time, but they tend towards a Gaussian behavior at long time scale. Furthermore, in each of these cases, the drift velocity increases sub-linearly, but the diffusivity increases super-linearly with the strength of the noise. These observations reflect the underlying non-linear friction control of their stochastic dynamics. Specific experiments have also been designed to study the hopping of a small object over a physical barrier assisted by an external noise. These results mimic the classical Arrhenius behavior from which an effective temperature may be deduced. However, the regimes controlled by a Coulombic like friction and a linear kinematic friction need to be treated somewhat differently. All the drifted diffusive systems studied here exhibit substantial negative fluctuations of displacement at a short observation time that diminishes at longer time scale. Using the integrated fluctuation theorem, we characterize the persistence time of negative fluctuations in terms of the diffusivity and the drift velocity that can be measured experimentally.

9:12AM P2.00003 Noise induced stabilization in population dynamics¹, ALEX KAMENEV, University of Minnesota — We investigate a model where strong noise in a sub-population creates a metastable state in an otherwise unstable two-population system. The induced metastable state is vortex-like, and its persistence time grows exponentially with the noise strength. A variety of distinct scaling relations are observed depending on the relative strength of the sub-population noises.

¹supported by NSF grant DMR-0804266

9:48AM P2.00004 Speeding up spontaneous disease extinction, MICHAEL KHASIN¹, University of Michigan — The dynamics of epidemic in a susceptible population is affected both by the random character of interactions between the individuals and by environmental variations. As a consequence, the sizes of the population groups (infected, susceptible, etc.) fluctuate in the course of evolution of the epidemic. In a small community a rare large fluctuation in the number of infected can result in extinction of the disease. We suggest a novel paradigm of controlling the epidemic, where the control field, such as vaccination, is designed to maximize the rate of spontaneous disease extinction. We show that, for a limited-scope vaccination, the optimal vaccination protocol and its impact on the epidemics have universal features: (i) the vaccine must be applied in pulses, (ii) the spontaneous disease extinction is synchronized with the vaccination. We trace this universality to general properties of the response of large fluctuations to external perturbations.

¹in collaboration with Mark Dykman, Michigan State University, and Baruch Meerson, Hebrew University of Jerusalem

10:24AM P2.00005 Cooperativity-Driven Singularities in Cooperative Asymmetric Exclusion¹, SIDNEY REDNER, Boston University — We investigate the effect of cooperative interactions on the asymmetric exclusion process. In the simplest case a particle can hop to its vacant right neighbor only if its left neighbor is occupied. We show that an initial density downstep develops into a rarefaction wave that can have a jump discontinuity at the leading edge, while an upstep results in a shock wave. We also investigate a more general model in which the particle velocity can be an increasing function of the density. Within a hydrodynamic theory, initial density upsteps and downsteps can evolve into: (a) shock waves, (b) continuous compression or rarefaction waves, or (c) a mixture of shocks and continuous waves. These unusual phenomena arise because the current versus density relation has an inflection point, so that the group velocity can either be an increasing or a decreasing function of the density on either side of the inflection point.

¹Supported by NSF grant DMR-0906504

Wednesday, February 29, 2012 8:00AM - 11:00AM – Session P3 DCMP: Invited Session: Alkaline Iron Selenides vs Iron Pnictides: Properties and Their Implications 205AB

8:00AM P3.00001 Neutron Scattering Study on the New 245 Iron Selenide Superconductors¹, WEI BAO, Renmin University of China, Beijing 100872, China — We determine using neutron and x-ray diffraction method the sample composition, crystalline structure and magnetic order of the recently discovered $A_2Fe_4Se_5$ superconductors ($A=K, Rb, Cs, Tl/K$ or Tl/Rb). Contrary to initial belief that these materials are heavily electron-doped variety of the $BaFe_2As_2$ family of Fe-based superconductors, they are almost charge balanced with the Fe valence close to $2+$ as in the 11 iron selenide superconductors, and crystalize in an Fe vacancy-ordered lattice structure [1,2]. Coexisting with superconductivity is a novel block antiferromagnetic order which conforms to the tetragonal crystalline symmetry and possesses a very large ordered magnetic moment $3.3\mu_B$ per Fe and a very high ordering temperature above 500 K [1]. Such Fe vacancy ordered crystal structure and coexisting antiferromagnetism and superconductivity occur in all 5 types of new iron selenide superconductors discovered so far. With Fe vacancy number departs from the chemical formulas $A_2Fe_4Se_5$, an imperfect version of the Fe vacancy order results at base temperature while phase separation into two vacancy-ordered phases exists at the intermediate temperature range [4]. The Fe site disorder renders the materials insulating and destroys the superconductivity as spin-glass disorder does in previous 11 iron selenide superconductors [5].

[1] W. Bao et al., Chin. Phys. Lett. **28**, 086104 (2011).

[2] P. Zavalij et al., Phys. Rev. B **83**, 132509 (2011).

[3] F. Ye et al., Phys. Rev. Lett. **107** 137003 (2011).

[4] W. Bao et al., arXiv: 1102.3674 (2011).

[5] T.J. Liu et al., Nat. Materials **9**, 716 (2010).

¹Supported by National Natural Science Foundation of China grant No 11034012 and National Basic Research Program of China grant No 2011CBA00112.

8:36AM P3.00002 Distinct Fermi Surface Topology and nearly Isotropic Superconducting Gap in $A_x\text{Fe}_{2-y}\text{Se}_2$ ($A=\text{K, Tl, Rb}$) Superconductors¹, XINGJIANG ZHOU, Institute of Physics, Chinese Academy of Sciences, Beijing 100190 — High resolution angle-resolved photoemission measurements have been carried out to study the electronic structure and superconducting gap of the newly discovered $A_x\text{Fe}_{2-y}\text{Se}_2$ [$A=\text{K, (Tl,K)}$ and (Tl,Rb)] superconductors[1,2,3] 1. Distinct Fermi surface topology, consisting of two electron-like Fermi surface sheets around the $\Gamma(0,0)$ point and an electron-like Fermi surface sheet near the $M(\pi,\pi)$ point, was revealed in all these samples. This is in strong contrast to the Fermi surface topology of other Fe-based superconductors where hole-like Fermi surface sheets are present near the $\Gamma(0,0)$ point. 2. Both the electron-like Fermi surface sheet near M point and the large electron-like Fermi surface sheet near Γ point show nearly isotropic superconducting gap without nodes 3. The doping evolution of the electronic structure from insulating samples to the superconducting samples is consistent with a phase separation picture. The information on the Fermi surface topology and superconducting gap of this new $A_x\text{Fe}_{2-y}\text{Se}_2$ superconductor will provide key insights and constraints to understand the superconductivity mechanism in iron-based superconductors.

[1]. D. X. Mou, X. J. Zhou et. al, Phys. Rev. Lett. **106**, 107001 (2011).

[2]. L. Zhao, X. J. Zhou et. al, Phys. Rev. B **83**, 140508(R) (2011).

[3]. L. Yu, X. J. Zhou et al., unpublished.

¹Work done in collaboration with Daixiang Mou, Lin Zhao, Li Yu, Minghu Fang, G. F. Chen, X. L. Chen, Zuyan Xu and Chuangtian Chen

9:12AM P3.00003 Pairing strength and symmetries of 122 iron selenides in comparison with iron pnictides¹, PALLAB GOSWAMI, National High Magnetic Field Laboratory and Florida State University — High temperature superconductivity with comparable transition temperatures has been observed in the vicinity of an antiferromagnetic phase, in both 122-alkaline iron selenides and 122-iron pnictides. In contrast to iron pnictides, where the parent state is an antiferromagnetic semimetal, the parent state of 122-iron selenides is a large moment, antiferromagnetic insulator. This provides a clear indication of strong electronic correlations. The 122-selenides possess only electron pockets, while the pnictides have both hole and electron pockets. In addition, the observed block spin magnetic order in 122-selenides can not be explained by Fermi surface nesting. At the same time, the comparable T_c suggests a commonality in the underlying mechanism for superconductivity in the two classes of materials. Motivated by these observations and considerations, we present a comparative strong coupling analysis of the pairing strength and symmetries in these two classes of materials [1,2]. The analysis of appropriate five orbital $t - J_1 - J_2$ models, reveals a similar pairing phase diagram for both materials, with $A_{1g} s(x^2y^2)$ and $B_{1g} d(x^2 - y^2)$ as two dominant pairing channels. The pairing amplitudes in both materials are of comparable strength, making it natural for a comparable maximum T_c . In contrast to the pnictides case, an $A_{1g} s(x^2 + y^2)$ state is not competitive, making the dominant pairing channels fully gapped. We also discuss the magnetism of the vacancy-ordered insulating 122 iron selenides [3], showing that the observed block-spin state occurs over a wide parameter range. The predicted magnetic excitation spectrum has been verified by inelastic neutron scattering experiments. Our study also reveals some commonality with the magnetism of the parent iron pnictides [4].

Work was done in collaboration with Rong Yu, Predrag Nikolic, Jian-Xin Zhu, Qimiao Si and Elihu Abrahams.

[1] Rong Yu, Pallab Goswami, Qimiao Si, Predrag Nikolic, and Jian-Xin Zhu, "Pairing strength and symmetries of 122 iron selenides in comparison with iron pnictides," to be published; arXiv:1103.3259.

[2] Pallab Goswami et al, "Superconductivity in Multi-orbital $t - J_1 - J_2$ Model and its Implications for Iron Pnictides," Europhys. Lett. **91**, 37006 (2010).

[3] Rong Yu, Pallab Goswami, and Qimiao Si, "The magnetic phase diagram of an extended $J_1 - J_2$ model on a modulated square lattice and its implications for the antiferromagnetic phase of $\text{K}_y\text{Fe}_x\text{Se}_2$," Phys. Rev. B **84**, 094451 (2011).

[4] Pallab Goswami et al, "Spin Dynamics of a $J_1 - J_2$ Antiferromagnet and its Implications for Iron Pnictides," Phys. Rev. B **84**, 155108 (2011).

¹NSF

9:48AM P3.00004 Pairing state in AFe_2Se_2 from spin fluctuation theory, PETER HIRSCHFELD, University of Florida — No abstract available.

10:24AM P3.00005 NMR investigation of iron-selenide and iron-arsenide high T_c superconductors, TAKASHI IMAI, McMaster University and Canadian Institute for Advanced Research — We have investigated the electronic, magnetic, and superconducting properties of the iron-selenide high T_c superconductor $\text{K}_x\text{Fe}_{2-y}\text{Se}_z$ ($T_c = 33$ K) with ^{77}Se NMR [1]. We will compare the results with those observed for FeSe in ambient and applied pressures ($T_c > 9$ K) [2], and with iron-arsenides [3]. Similarities and dissimilarities will be pointed out, with primary focus on the anomalous normal state properties. Our latest work on $\text{K}_x\text{Fe}_{2-y}\text{Se}_z$ was carried out in collaboration with D. Torchetti, M. Fu, D. Christensen, K. Nelson (McMaster), H. Lei, and C. Petrovic (Brookhaven National Lab).

[1] D. Torchetti et al., PR **B83**, 104508 (2011).

[2] T. Imai et al. PRL **102**, 177005 (2009).

[3] F.L. Ning et al., PRL **104**, 037001 (2010); JPSJ **78**, 103711 (2009).

Wednesday, February 29, 2012 8:00AM - 11:00AM – Session P4 DAMOP: Multi-Component BECs and Mixtures 205C

8:00AM P4.00001 Analytical solutions to the spin-1 Bose-Einstein condensates, SHI-JIE YANG, ZHI-HAI ZHANG, Department of Physics, Beijing Normal University — We present classes of exact stationary solutions for the one-dimensional coupled nonlinear Gross-Pitaevskii equations which describe the $F = 1$ spinor Bose-Einstein condensates, both with and without the Zeeman splitting. The spin magnetization configurations and the spin currents are investigated. The soliton or the soliton train complexes are naturally produced.

8:12AM P4.00002 Geometry of Spinor Condensates with Large Spins, OMNARAYANI NAYAK, University of California, Berkeley, ARI TURNER, University of Amsterdam — Laser cooled atoms with spin can become magnetically ordered in a variety of ways, like electrons in a frustrated lattice, but the phases are more geometrical in this setting. For spin one, two and three atoms, states have been predicted with a nematic symmetry (the symmetry of a toothpick), a hexagon, and an octahedron, as well as other possibilities. As the spin becomes larger, the phase diagrams become more and more complicated. I will present a geometrical way of predicting regularities in the phases as the spin increases. For a certain form of interaction, we find a phase diagram for arbitrarily large spin. (In particular, a nematic phase does not occur beyond spin 2.) We have used a mapping to a classical problem of interacting particles arranging themselves on a sphere.

8:24AM P4.00003 Pomeranchuk cooling of $SU(N)$ ultracold fermions in optical lattice¹, ZI CAI, HSIANG-HSUAN HUNG, Department of physics, UCSD, DONG ZHENG, Department of physics, Tsinghua University, CONGJUN WU, Department of physics, UCSD — We investigate thermodynamic properties of a half-filled $SU(2N)$ Fermi-Hubbard model in two-dimensional square lattice using the determinantal Quantum Monte Carlo simulation. We address the question how the large number of hyperfine-spin components makes thermodynamic properties of $SU(N)$ ultracold fermions different from the conventional Hubbard model with $N=2$. Various thermodynamic quantities such as entropy, charge fluctuations, and spin correlations have been calculated. We devote special attention to the interaction-induced adiabatic cooling: an analogue of the Pomeranchuk effect in Helium-3.

¹This work was supported by the NSF DMR-1105945 and the AFOSR-YIP program

8:36AM P4.00004 Determinant Quantum Monte Carlo simulations on quantum magnetism of the $SU(2N)$ ultra-cold fermions¹, DONG ZHENG, Department of Physics, Tsinghua University, HSIANG-HSUAN HUNG, Department of electrical and computer engineering, University of Illinois at Urbana-Champaign, ZI CAI, CONGJUN WU, Department of Physics, University of California, San Diego — We investigate the quantum magnetism of the repulsive $SU(2N)$ -Hubbard model on a two-dimensional square lattice at half-filling. At $2N = 4$, our numerical results suggest that there exists a long-range Neel ordering at large U . In this regime, both of the antiferromagnetic structure factor per site and the farthest two-point spin-spin correlation functions are saturated to finite values in the thermodynamic limit. The single-particle excitations are finite and the spin gaps vanish. All of above evidences support the presence of the Neel ordering in the $SU(4)$ -Hubbard model. For $2N > 4$, such features are not explicitly observed.

¹NSF DMR-1105945

8:48AM P4.00005 Multi-component integrable models in cold atoms, YUZHU JIANG, Beijing Computational Science Research Center, Beijing 100084, China, JUNPENG CAO, YUPENG WANG, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, PR China, HAIQING LIN, Beijing Computational Science Research Center, Beijing 100084, China — The quantum gases are intensively studied for the inspiring advances in ultra-cold atomic physics. Various kinds of lattice and gas systems are created in different dimensions. The multi-component cold atomic systems have rich phase diagrams. Our works focus on the one-dimensional integrable quantum systems. We find a series of integrable models of $Sp(2s+1)$ fermions and $SO(2s+1)$ bosons and solve them via Bethe ansatz techniques, where s the hyperfine spin of the atoms. We find the paired bosons exist in both repulsive and attractive $SO(3)$ integrable bosonic gases with hyperfine spin-1. For the $Sp(2s+1)$ repulsive fermions, there are no bound states in the ground state, while 2-string bound solutions appear in the spin sector. We also calculate the spin-wave velocities and low temperature specific heat of the repulsive fermions. These systems have spin-charge separation property of Luttinger liquid. Different from the $SU(2s+1)$ repulsive models, the spin-wave velocities of the $Sp(2s+1)$ models are no longer the same. The holes of 1-strings (real rapidities) of different branches in the spin sector have a same spin-wave velocity v_1 and the ones of 2-strings share a same spin-wave velocity v_2 . The two velocities are different.

9:00AM P4.00006 Haldane Phase of Ultra Cold Atom Gas Loaded on Pseudo-One-Dimensional Optical Lattice, KEITA KOBAYASHI, MASAHIKO OKUMURA, Center for Computational Science & e-System Japan Atomic Energy Agency, YUKIHIRO OTA, REKIN, SUSUMU YAMADA, MASAHIKO MACHIDA, Center for Computational Science & e-System Japan Atomic Energy Agency — Ultracold Fermi gas loaded on optical lattice (FGOL) has attracted considerable attention since its temperature, interaction, and filling factor are flexibly controllable and various quantum phases are accessible. In this study, we examine properties of pseudo-one-dimensional (P1D) FGOL obtained by including effects of the transverse excitations. At first, we prove that the P1D system at half-filling can be theoretically mapped on spin-1 Heisenberg chain. Secondly, we reveal by using DMRG scheme that Haldane phase emerges in the P1D FGOL. Finally, we clarify effects of trap potential and spin imbalance on not only the central Haldane phase but also various different magnetic structures around the Haldane phase.

9:12AM P4.00007 Half-quantum vortex state and its excitations in a spin-orbit coupled spinor Bose-Einstein condensate¹, B. RAMACHANDHRAN, Department of Physics and Astronomy, and Rice Quantum Institute, Rice University, Houston, TX 77005, USA, BOGDAN OPANCHUK, XIA-JI LIU, ACQAO and Centre for Atom Optics and Ultrafast Spectroscopy, Swinburne University of Technology, Melbourne 3122, Australia, HAN PU, Department of Physics and Astronomy, and Rice Quantum Institute, Rice University, Houston, TX 77005, USA, HUI HU, ACQAO and Centre for Atom Optics and Ultrafast Spectroscopy, Swinburne University of Technology, Melbourne 3122, Australia — We investigate theoretically the condensate state and collective excitations of a spin-orbit coupled spinor Bose gas in two-dimensional harmonic traps. In the weakly interacting regime, when the inter-species interaction is larger than the intra-species interaction ($g_{\uparrow\downarrow} > g$), we find that the condensate state has a half-quantum-angular-momentum vortex configuration (half-vortex state) with spatial rotational symmetry and skyrmion-type spin texture. We investigate the stability of half-vortex state in the regime when g is greater than a threshold g_c , and in the regime when $g_{\uparrow\downarrow} < g$, by solving the Bogoliubov equations for collective density oscillations. In addition, we also investigate the dynamical properties of the half-vortex state. We present the phase diagram as a function of interatomic interaction and spin-orbit coupling.

¹HP is supported by the NSF, the Welch Foundation (Grant No. C-1669) and the DARPA OLE program.

9:24AM P4.00008 Searching for Non-abelian Phases in Bose-Einstein Condensate of Dy, BIAO LIAN, HUI ZHAI, Institute for Advanced Study, Tsinghua University — Recently Bose-Einstein condensate of a spin 8 element, Dysprosium, has been realized. We compute the mean-field ground state and Bogoliubov excitation of Dy condensate for different scattering lengths and in presence of a magnetic field, and find various non-abelian phases in the parameter space. We suggest an experimental scheme for detecting the remaining discrete point group symmetry of these phases simply by looking at population of each spin components and the degeneracy of Goldstone modes. A BEC whose remaining symmetry is a non-abelian group can support exotic non-abelian vortices.

9:36AM P4.00009 Quasiparticles in a Bose-Fermi mixture in optical lattice, KAZUTO NODA, ROBERT PETERS, NORIO KAWAKAMI, Kyoto University, THOMAS PRUSCHKE, University of Goettingen — We investigate a mixture of interacting bosons and fermions using a generalized dynamical mean-field theory combined with the numerical renormalization group. We focus on many-body effects in the presence of the superfluidity. It is elucidated that fermionic particles are strongly renormalized by low-energy bosonic excitations via the boson-fermion interaction, giving rise to an anomalous peak structure in the density of states for fermions. We also address how the renormalization effects appear in the phases with long-range order such as a supersolid phase.

9:48AM P4.00010 Ultracold bosons in the presence of a second species in the Tonks-Girardeau regime: dynamics and quantum features¹, MIGUEL ANGEL GARCIA-MARCH, THOMAS FOGARTY, THOMAS BUSCH, Department of Physics, University College Cork — We develop a framework to study the interaction between two ultracold bosonic species in different regimes. One species is in the low correlation limit forming a Bose-Einstein condensate (BEC), while the other is in the strongly correlated Tonks-Girardeau regime. We use a Bose-Hubbard-like model where, due to the momentum distribution of the Tonks gas, many single particle states are considered and study the dynamics of the system by numerical simulation of the equations obtained. The atoms in the Tonks gas act as impurities submerged in the BEC, and the excitations created by their interactions with the BEC gas can be understood in terms of polarons. We focus on the fundamental quantum properties of the system and investigate the effects the condensed environment has on the Tonks-Girardeau gas as a function of the interspecies scattering strength.

¹This work is supported by SFI under grant number 10/IN.1/I2979

10:00AM P4.00011 The Many-Body Correlation of Bose-Fermi Mixture in the Ring Trap, RYOSUKE SHIBATO, Department of Physics, Tokyo Metropolitan University, TAKUSHI NISHIMURA, Division of Advanced Sciences, Ochanai Academic Production, Ochanomizu University — Since the realization of Bose-Einstein Condensation in alkali atoms in 1995, studies on cold atomic gases have greatly advanced. The cold atoms are precisely controlled by electromagnetism and optics, and flexible to design quantum systems. In 2001, A. Görlitz's group has realized the Bose-Einstein condensates in the quasi-one-dimensional system [1]. One have now obtained the ideal system to study the one-dimensional many-body physics experimentally. The purpose of our study is to clarify the effect of quantum many-body correlation beyond the mean-field approximation. To accomplish this purpose, we first prepare the bosons and fermions in the ring trap [2]. We prepare the initial state in the trap with the small distortion and obtained that both kinds of particles tend to be localized. After taking off this distortion, we solved the time-dependent Schrödinger equation. We derived the energy spectrum, density profile, and studied pair-correlation effect. Our results predict that the many-body correlation emerges, which has never been observed experimentally up to now.

[1] A. Görlitz et al., Phys. Rev. Lett. 87, 130402 (2001)

[2] O. Morizot et al., Phys. Rev. A. 74, 023617 (2006)

10:12AM P4.00012 Cooling by corralling: a route to antiferromagnetism in optical lattices¹, YEN LEE LOH, University of North Dakota — Cold atoms in optical lattices have emerged as a promising tool for emulating condensed matter Hamiltonians. Current experiments have observed “Mott insulating” behavior in the Fermi-Hubbard model at an average entropy $S/N \approx 1k_B/\text{atom}$. Our quantum Monte Carlo simulations [1], in agreement with other methods, show that $S/N \approx 0.65k_B/\text{atom}$ is low enough to produce antiferromagnetism (AF) at the center of a harmonic trap. However, further progress in the field requires even lower entropies that are beyond the reach of traditional cooling techniques. I have proposed a way to attain very low temperatures and entropies ($S/N < 0.03k_B/\text{atom}$) by trapping fermions in a corral formed from another species of atoms [2]. This Fermi system can then be evolved into an antiferromagnet by morphing the lattice into a set of double wells, quasi-adiabatically. Quantum dynamics simulations have, so far, given promising results.

[1] Thereza Paiva, Yen Lee Loh, Mohit Randeria, Richard T. Scalettar, and Nandini Trivedi, “Fermions in 3D optical lattices: Cooling protocol to obtain antiferromagnetism,” PRL 107, 086401 (2011).

[2] Yen Lee Loh, “Proposal for achieving very low entropies in optical lattice systems,” arxiv:1108.0628.

¹DARPA #60025344 under OLE program

10:24AM P4.00013 Magnetic order in the doped Hubbard model and the crossover from two- to three-dimensions: a Hartree-Fock study¹, JIE XU, ERIC J. WALTER, SHIWEI ZHANG, College of William and Mary — We report unrestricted Hartree-Fock (UHF) results for the ground state of the single-band Hubbard model in three-dimensions (3D), with repulsive onsite interactions and nearest-neighbor hopping. Magnetic and charge properties are determined by full numerical solutions of the self-consistent UHF equation in large supercells, and quantified as a function of hole doping h . We focus on weak to intermediate interaction strengths, where UHF has been shown to capture the main characteristics of the magnetic correlations in two-dimensions (2D). ² We find linear spin-density wave (SDW) states with AFM order and a long wavelength modulation whose wavelength is inversely proportional to h . We also study the dimensional crossover from 2D to 3D as the inter-plane distance is increased.

¹Supported by NSF and ARO.

²J. Phys.: Condens. Matter, in press (arXiv:1107.0976v2).

10:36AM P4.00014 Continuous measurement quantum state tomography of atomic spins, CARLOS RIOFRIO, IVAN DEUTSCH, Department of Physics and Astronomy, Center for Quantum Information and Control, University of New Mexico, AARON SMITH, BRIAN ANDERSON, HECTOR SOSA, POUL JESSEN, College of Optical Sciences, Center for Quantum Information and Control, University of Arizona — Quantum state tomography is a fundamental tool in quantum information science and technology. It requires estimates of the expectation values of an “informationally complete” set of observables. This is, in general, a very time-consuming process that requires a large number of measurements to gather sufficient statistics. There are, however, systems in which the data acquisition can be done more efficiently. An ensemble of quantum systems can be prepared and driven by external fields while being continuously and collectively probed, producing enough information in the time evolving measurement record to estimate the initial state. Such protocol has the advantage of being fast and robust. In this talk, we present a study of a continuous-measurement quantum-state tomography protocol and its application to controlling large spin ensembles. We perform reconstruction of quantum states prepared in the 16 dimensional ground-electronic hyperfine manifolds of an ensemble of 133Cs atoms, controlled by microwaves and radio-frequency magnetic fields and probed via polarization spectroscopy. We present theoretical and experimental results of its implementation and discuss two estimation methods: constrained maximum likelihood and compressed sensing.

10:48AM P4.00015 Measuring spin correlations in optical lattices, K.G.L. PEDERSEN, B.M. ANDERSEN, Niels Bohr Institute, University of Copenhagen, Denmark, G.M. BRUUN, Department of Physics and Astronomy, Aarhus University, Denmark, O.F. SYLJUÅSEN, Department of Physics, University of Oslo, Norway, A.S. SØRENSEN, Niels Bohr Institute, University of Copenhagen, Denmark — The study of ultracold atoms in optical lattices has produced several groundbreaking results. A major, but presently unrealized goal, is to study quantum magnetism using atoms in optical lattices. We suggest three different experimental methods for probing both short- and long-range spin correlations of atoms in optical lattices. The first method involves an adiabatic doubling of the periodicity of the underlying lattice to probe neighboring singlet (triplet) correlations for fermions (bosons) by the occupation of the resulting vibrational ground state. The second method utilizes a time-dependent superlattice potential to generate spin-dependent transport by any number of prescribed lattice sites, and probes correlations by the resulting number of doubly occupied sites. The third method relies on the difference in tunneling times for the vibrational ground state and the first excited state. Correct timing then allows for the spin correlations to be fingerprinted. For experimentally relevant parameters, we demonstrate how all three methods yield large signatures of antiferromagnetic correlations of strongly repulsive fermionic atoms in a single shot of the experiment.

Wednesday, February 29, 2012 8:00AM - 11:00AM –

Session P5 DCMP: Surfaces, Interfaces, and Thin Films: Kinetics, Dynamics, and Reactions

206A

8:00AM P5.00001 Direct versus hydrogen assisted CO dissociation on metal surfaces, DOMINIC ALFONSO, National Energy Technology Laboratory - Department of Energy — We present investigations of the formation of precursor hydrocarbon species relevant to production of liquid hydrocarbons on low index surfaces of various important noble and transition metals. The formation could occur via the so-called carbide mechanism where direct CO dissociation takes place, followed by stepwise hydrogenation of C yielding CH_x species. Formation of precursor CH_x species could also potentially take place through hydrogenated CO intermediates. First-principles calculations of energetics and barriers of CO conversion to hydrocarbons species were performed using plane-wave periodic density functional theory. Our calculations indicate that the two pathways are generally competitive on transition metals. A microkinetic model, with input thermodynamics and kinetic parameters estimated from electronic structure calculations, has been developed. The two pathways will be further examined using microkinetic approach to determine whether the aforementioned finding holds at realistic conditions.

8:12AM P5.00002 Multi-lattice approach to first-principles kinetic Monte Carlo simulations: Application to catalytic CO oxidation at Pd(100), MAX HOFFMANN, TU München, MATTHIAS SCHEFFLER, Fritz-Haber-Institut, Berlin, Germany, KARSTEN REUTER, TU München — First-principles kinetic Monte Carlo (1p-kMC) simulations enable a quantitative microkinetic modeling of heterogeneous chemical reactions while accounting for the full spatial distributions at the surface. Application to reaction-induced surface morphological transitions is hitherto prevented by the inability to describe the system within prevalent fixed-lattice 1p-kMC and the excessive cost of off-lattice 1p-kMC variants. To this end we develop a novel multi-lattice 1p-kMC approach and apply it as a case in point to the CO oxidation at Pd(100). In the catalytically active state this system is suspected to undergo transitions from the pristine metal surface to a PdO surface-oxide film. As a first step towards a comprehensive simulation we focus on the initial oxide destruction step induced by clustering of oxygen vacancies. First simulations confirm the stability of the oxide film at stoichiometric feed as predicted by preceding fixed-lattice 1p-kMC simulations [1].

[1] J. Rogal, K. Reuter, and M. Scheffler, Phys. Rev. Lett. 98, 046101 (2007).

8:24AM P5.00003 The role of non-conventional supports for single-atom Platinum-based catalysts in fuel cell technology: A theoretical surface science approach, ALOYSIUS SOON, RENQIN ZHANG, Yonsei University, Seoul, Korea — Platinum-based heterogeneous catalysts are known to play a key role in the fuel cell technology, such as their use in the low-temperature proton exchange membrane (PEM) fuel cells. However, the high cost and low lifecycle of these PEM fuel cells are the major hindrances to its large-scale commercial production. To elevate the high-cost and to optimize its catalytic activity, it was recently proposed that catalysts with single-Pt atom dispersions and a more durable, corrosion-resistant TiN support could play an important role in the next generation of Pt-based PEM fuel cells [1]. As a first step towards a microscopic understanding of single-Pt atom-dispersed catalysts on these new supports, we present density-functional theory (DFT) calculations to investigate the adsorption properties of Pt atoms on pristine TiN(001). Optimized atomic geometries, energetics, and analysis of the electronic structure of the Pt/TiN system are reported for various surface coverages of Pt. We find that atomic Pt does not bind preferably to the clean TiN surface, but under operational conditions, TiN surface vacancies play a crucial role in anchoring the Pt atom for its catalytic function. [1] B. Qiao, *et al.* Nat. Chem. 3 (2011) 634; B. Avsarala and P. Haldar, Int. J. Hydrog. Energy 36 (2011) 3965

8:36AM P5.00004 Water-Pd Interface in Catalytic Biomass Conversion: Atomic-Scale Structure and Properties, YAKE WANG, SHUXIA YIN, XIN LIU, DARWIN SHIELDS, SANWU WANG, Department of Physics and Engineering Physics, The University of Tulsa — Biomass pyrolysis and other relevant catalytic reactions often occur at the liquid-solid interface. It is therefore of great importance to investigate the interfacial structure and other properties in order to achieve a deep understanding about the catalytic reactions for biomass conversion. We used *ab initio* molecular dynamics simulations to study the interfaces formed by liquid water and the palladium surfaces. Such interfaces are involved in many catalytic reactions for biomass conversion. We report results about the structural properties of the water/Pd(100) and water/Pd(111) interfaces, the interaction between liquid water and the metal surfaces, and how the interaction affects the structure. We found that while the interaction between water and the metal surface is weak, it could still cause considerable effects. In particular, the interaction promotes the formation of close-packed local clusters of liquid water.

8:48AM P5.00005 Multilayer epitaxial graphene oxide: structural and chemical properties from a combined theoretical and experimental XPS study, SI ZHOU, SUENNE KIM, ELISA RIEDO, ANGELO BONGIORNO, Georgia Inst of Tech — Multilayer graphene oxide (GO) is a material holding great promise in future energy storage and nano-electronic technologies. This material remains qualitatively known to date. In this work, we present a combined density functional theory (DFT) and experimental X-ray photo-emission spectroscopy (XPS) study of the structural, chemical, and thermal stability of multilayer GO grown epitaxially on silicon carbide. This investigation shows that at room temperature multilayer GO is a metastable material. GO films undergo spontaneous modifications and chemical reduction with a relaxation time of about one month. These processes lead multilayer GO toward a longer-living quasi-equilibrium state, consisting a structure deprived of epoxide groups, rich of hydroxyl groups, and with a O/C ratio of 0.38. Our study suggests that the presence of excess H chemisorbed on the graphitic sheets is the origin of the metastable character of multilayer GO. These H species favor the reduction of epoxide groups and the consequent transformation of hydroxyls into water molecules intercalated between the graphitic layers. Our DFT calculations show that these molecular transformations are controlled by diffusion processes.

9:00AM P5.00006 Switching of molecules at metal surfaces¹, PETRA TEGEDER, Freie Universitaet Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — Understanding the switching ability of molecules on surfaces upon excitation with external stimuli is a prerequisite for the development of functional molecular devices with possible applications to information processing, storage, or switching. While the switching mechanisms in many classes of molecular switches are thoroughly studied and understood in solution, their counterparts on surfaces still remain largely unresolved. In particular, many switching processes are suppressed or irreversible when the molecules are anchored to a metallic substrate. The adsorption configuration and steric hindrance are only one factor influencing the switching capability. More important is the electronic coupling strength between adsorbate and substrate and accordingly the lifetime of molecular excited states which is significantly reduced at metal surfaces. I will discuss several examples of optically and thermally induced conformational changes in molecular switches at noble metal surfaces.

¹Funding by the DFG through the SFB658 is acknowledged

9:12AM P5.00007 Competing Atomic and Molecular Mechanisms of Thermal Oxidation of Si versus SiC, XIAO SHEN, Vanderbilt University, BLAIR R. TUTTLE, Penn State Behrend College, SOKRATES T. PANTELIDES, Vanderbilt University — Thermal oxidation is a universal process in solids and is of practical importance in semiconductor technology. The oxidation of Si and SiC provide a unique opportunity for studying the oxidation mechanism because the products are the same oxide SiO₂. The oxidation of Si follows a linear-parabolic law with molecular oxygen identified as the oxidant. The oxidation of SiC obeys the same linear-parabolic law as Si but with different rates and temperature dependences. Using results from first-principle calculations, we first show that an atomic oxygen mechanism can account for the oxidation of Si-face SiC. We then discuss implications of the results and identify the determining factors in the competition between atomic and molecular mechanism. This work is supported by NSF GOALI grant DMR-0907385.

9:24AM P5.00008 Scanning tunneling microscopy uncovers the mechanism of silicon oxidation in aqueous solutions, MELISSA HINES, MARC FAGGIN, KUN BAO, ANKUSH GUPTA, BRANDON ALDINGER, Cornell University — Because of their immense technological importance, silicon oxidation reactions have been studied intensely for decades under a variety of conditions. However, the disordered nature of the reaction product, silicon oxide, makes these reactions notoriously difficult to understand. In this work, silicon oxidation is coupled with a subsequent etching reaction, allowing the oxidation reactions to literally write an atomic-scale record of their reactivity into the etched surface – a record that can be decoded into site-specific reaction rates, and thus chemical understanding, with the aid of simulations and infrared spectroscopy. This record overturns the long-standing and much-applied mechanism for the (low-temperature) oxidation of the technologically important face of silicon, Si(100), and shows that the unusually high reactivity of a previously unrecognized surface species leads to a self-propagating etching reaction that produces near-atomically-flat surfaces terminated by a single monolayer of hydrogen atoms. This finding shows that, contrary to expectation, the low-temperature oxidation of Si(100) is a highly site-specific reaction and suggests strategies for the uniform functionalization of the technologically relevant face of silicon by low-temperature reactions.

9:36AM P5.00009 Metal pulled-off effect: A unique explanation of different oxidation process on Cu and Al surfaces, JUNYI ZHU, JOONGOO KANG, SU-HUAI WEI, National renewable Energy Lab — One interesting oxidation phenomenon is the difference of the oxidation of Cu and Al. Cu forms disordered domains, large surface reconstructions and oxide islands on the surface with some O atoms diffuse into inner layers to further oxidize inner Cu atoms. Al forms a dense oxide layer which protects the inner Al atoms from oxidation. In this talk, we demonstrate a possible electronic origin of this oxidation difference by using the first-principles method to calculate the initial oxidation of different metal surfaces and nanoclusters. On Cu 55 Icosahedron surface, we found that 2 O atoms at neighboring sites form a structure with a Cu atom in the middle pulled off from the surface. We also found the similar pull-offs on Cu, Pd, Zn surfaces, but not on Al surface, which is not a transition metal. This pulled off effect is explained by the strong metal d and O p coupling. We also checked different O concentration on Cu (111) surface and on Cu cluster surface and found that O atoms form chain or ring like structures. Our first principle molecular dynamic calculation confirms that these structures are stable. With this pull-off effect, additional O atoms can further oxidize inner Cu atoms and make Cu relative easy to oxidize. This finding enhances the scientific understanding of the initial oxidation of metallic nano-particles and surfaces, which may have important applications in catalysis, thermal storage and other surface science fields.

9:48AM P5.00010 Electrical and Structural Properties of Thin Films Fabricated by E-Beam Lithography from Gold Nanoparticle Resists¹, STEFAN DICKERT, MYOUNG-HWAN PARK, COLIN JERMAIN, VINCENT ROTELLO, MARK TUOMINEN, University of Massachusetts Amherst — Drop- and spin-coated solutions of ligand-coated nanoparticles act as novel “direct write” e-beam resist, which can be prepared with metallic, magnetic and semiconducting nanoparticles. We prepared thin films from gold nanoparticles, in which we varied the film thickness. Small angle X-Ray scattering experiments as well as SEM imaging of the samples were performed to determine structural properties of the nanoparticles films at various stages of the fabrication process, after drop coating, ebeam exposure and annealing. We further performed DC charge transport measurements in the 2-350K temperature range and report different conductivity mechanisms based on the film thickness, ranging from insulating to Mott hopping conduction to metallic.

¹This research is supported by NSF grant CMMI-1025020.

10:00AM P5.00011 Self-Diffusion of small Ag and Ni islands on Ag(111) and Ni(111) using the self-learning kinetic Monte Carlo method¹, SYED ISLAMUDDIN SHAH, GIRIDHAR NANDIPATI, ABDELKADER KARA, TALAT S. RAHMAN, University of Central Florida — We have applied a modified Self-Learning Kinetic Monte Carlo (SLKMC) method [1] to examine the self-diffusion of small Ag and Ni islands, containing up to 10 atom, on the (111) surface of the respective metal. The pattern recognition scheme in this new SLKMC method allows occupancy of the fcc, hcp and top sites on the fcc(111) surface and employs them to identify the local neighborhood around a central atom. Molecular static calculations with semi empirical interatomic potential and reliable techniques for saddle point search revealed several new diffusion mechanisms that contribute to the diffusion of small islands. For comparison we have also evaluated the diffusion characteristics of Cu clusters on Cu(111) and compared results with previous findings [2]. Our results show a linear increase in effective energy barriers scaling almost as 0.043, 0.051 and 0.064 eV/atom for the Cu/Cu(111), Ag/Ag(111), and Ni/Ni(111) systems, respectively. For all three systems, diffusion of small islands proceeds mainly through concerted motion, although several multiple and single atom processes also contribute. [1] Oleg Trushin et al. Phys. Rev. B 72, 115401 (2005) [2] Altaf Karim et al. Phys. Rev. B 73, 165411 (2006)

¹This work was supported by DOE-BES under grant DE-FG02-07ER46354

10:12AM P5.00012 Collective Excitations in Ultrathin Magnesium Films on Silicon¹, XIAO GUANG LI, Fudan University, Shanghai, China, U of Tennessee, U of Sci. & Tech. of China, DI XIAO, Oak Ridge National Laboratory, JIAN SHEN, Fudan University, Shanghai, China, HANNO WEITERING, U of Tennessee, Oak Ridge National Laboratory, ZHENYU ZHANG, U of Sci. & Tech. of China, Harvard U — We present a systematic study of plasmon excitation in ultrathin Mg overlayer on Si(111) substrate. Our numerical results qualitatively reproduce the experimentally observed plasmon spectra of the Mg/Si systems [1]. The underlying physics of the formation of various absorption peaks can be understood using the simple hybridization concept. Based on this concept, the coexistence of surface and bulk plasmons in the experimental observation turns out to be a clear evidence for the existence of multiple surface plasmons due to the quantum confinement in Mg thin films [2]. In addition, we clearly see the plasmon enhanced substrate absorption, which comes from the screening of the substrate to the oscillatory charges.

[1] Ao Teng et al.(to be published).

[2] Xiaoguang Li et al.(to be published).

¹Supported by NNSF of China, USNSF, DMSE/BES of USDOE.

10:24AM P5.00013 Scaling Properties of Exciton Binding Energies in Two-Dimensional Insulating Films¹, HAIPING LAN, PING CUI, Univ. of Sci. and Tech. of China, ZHENYU ZHANG, Univ. of Sci. and Tech. of China, Harvard University — Using the GW and Bethe-Salpter Equation (BSE) methods with inclusion of many-electron effects, we carry out a systematic study of the quasiparticle energy and optical absorption spectra of various two-dimensional (2D) thin-film insulators, including boron nitride, graphane, fluorographene, fluorosilicene, etc. All the calculated band gaps of these systems are increased by the GW corrections, and their optical responses are dominated by the strongly bound excitons, which can be attributed to the enhanced Coulomb attraction in 2D. Most strikingly, we find a well-defined linear scaling dependence between the exciton binding energy and band gap, and this scaling relationship is in stark contrast with the established ones in 3D and 1D insulating systems. The likely underlying physical mechanism for the linear scaling relationship will also be discussed.

¹Supported by NNSF of China, USNSF, and DMSE/BES of USDOE.

10:36AM P5.00014 Spatially and Temperature Resolved Photoluminescence (PL) Of Excitons in Highly Oriented Phthalocyanine Films, NAVEEN RAWAT, ZHENWEN PAN, LANE MANNING, Physics Dept and the Material Science Program, UVM, Burlington, VT, ANTHONY WETHERBY, RORY WATERMAN, Chemistry Dept, UVM, Burlington, VT, RANDY HEADRICK, MADALINA FURIS, Physics Dept and the Material Science Program, UVM, Burlington, VT — Phthalocyanines and their derivatives are interesting alternative to polymer materials for the development of electronic devices such as organic thin field effect transistors, organic Light Emitting Diodes and photovoltaic cells. The present study focuses on spatially resolved, temperature-dependent PL of highly-oriented metal free and Zn -Octa-butoxy phthalocyanine (OBPc) polycrystalline thin films. Samples were fabricated using an in-house solution processing method¹ that results in mm-sized grains which can be individually probed using a focused laser beam. The experiments indicate the lowest optically active excitonic state which dominates the PL spectrum at 5K is optically-forbidden at room temperature. Linear Dichroism microscopy experiments indicate a reorientation of molecular planes below T~200K which may favor a mixing of Frenkel and intermolecular excitons, changing the nature of excitonic ground state.

¹R. L. Headrick et al, APL, 92, 063302 (2008)

10:48AM P5.00015 Grain Boundary Exploration of Excitonic States in Organic Crystalline Thin Films, LANE MANNING, NAVEEN RAWAT, ZHENWEN PAN, CODY LAMARCHE, ISHVIENE COUR, RANDY HEADRICK, MADALINA FURIS, University of Vermont — The electronic states of Metal-Phthalocyanine (MPc) crystalline thin films are investigated. These samples are fabricated by solution processed pen-writing deposition technique.¹ Specifically, a linear dichroism mapping is performed, and excitonic emission is studied both close to and far from the large grain boundaries found in these phthalocyanine thin films. Multiple M-Pc samples are examined, including nickel, zinc and cobalt. In phthalocyanine crystalline films, it is believed that a monomer-like emission feature exclusively associated with a grain boundary is observed. The presence of this feature and its intensity are correlated with the relative orientation of neighboring grains at the boundary. The experiments are performed using a combined Linear Dichroism/Photoluminescence Microscopy experiment developed at the University of Vermont.

¹R. Headrick et al, APL, 92, 063302 (2008)

Wednesday, February 29, 2012 8:00AM - 11:12AM – Session P6 DMP: Graphene Optical Phenomena 206B

8:00AM P6.00001 Graphene-based photonic crystals¹, ROMAN YA. KEZERASHVILI, OLEG L. BERMAN, VLADIMIR S. BOYKO, Physics Department, New York City College of Technology, City University of New York — A novel type of photonic crystals formed by embedding a periodic array graphene and dielectric material into a background dielectric medium is discussed. One-dimensional (1D) photonic crystal formed by an array of periodically located stacks of alternating graphene and dielectric stripes, while the two-dimensional (2D) one is formed by constituent stacks of alternating graphene and dielectric discs. The electromagnetic wave propagation in 1D crystal analyzed in the framework of the Kronig-Penney model. The frequency band structure of 1D graphene-based photonic crystal is obtained analytically as a function of the filling factor and the thickness of the dielectric between graphene stripes. The photonic frequency corresponding to the electromagnetic wave localized by a defect that breaks the symmetry of the system is obtained. For 2D crystal the photonic band structure and transmittance are calculated. The graphene-based photonic crystals can be used effectively as the frequency filters and waveguides for the far infrared region of electromagnetic spectrum. Due to substantial suppression of absorption of low-frequency radiation in doped graphene the damping and skin effect in the photonic crystal are also suppressed. The advantages of the graphene-based photonic crystal are discussed.

¹The work was supported by PSC CUNY grant: Award # 64197-00 42.

8:12AM P6.00002 Graphene Plasmonic Terahertz Filters and Polarizers, FENGNIAN XIA, HUGEN YAN, XUESONG LI, BHUPESH CHANDRA, GEORGE TULEVSKI, YANQING WU, MARCUS FREITAG, WENJUAN ZHU, PHAEDON AVOURIS, IBM T. J. Watson Research Center — Graphene has remarkably strong interaction with light, especially in the terahertz frequency range. Free carriers in graphene exhibit Drude behavior and the Drude weight can be tuned by electrostatic or chemical doping. Graphene can support surface plasmons. In this paper, we'll show that with multiple stacked CVD graphene layers, terahertz filters and polarizers can be realized by patterning them into micro-disks and ribbons. The influence of dipole-dipole interaction on the extinction spectra will be discussed.

8:24AM P6.00003 ABSTRACT WITHDRAWN –

8:36AM P6.00004 Surface-plasmon polaritons on graphene-metal surface, COSKUN KOCABAS, OMER SALIHOGLU, SINAN BALCI, Bilkent University, Department of Physics, ADVANCED RESEARCH LABORATORY TEAM — In this presentation we present a new application of graphene in the field of plasmonics. We studied excitation of surface-plasmon polaritons on graphene-metal surface. The metal surface is functionalized by transfer printing of a graphene layer grown by chemical vapor deposition on copper foils. Surface plasmon resonance (SPR) characteristics of monolayer and multilayer graphene on the metal surface are presented. The results reveal the essential features predicted by the calculations based on transfer matrix method. As an application, we fabricated a surface plasmon resonance sensor integrated with a microfluidic device to study nonspecific physical interaction between graphene layer and proteins. We obtained association and dissociation coefficient of BSA adsorbed on graphene layer. We believe that graphene functionalized SPR sensors could provide a new platform to study interactions between graphene and molecules.

8:48AM P6.00005 New Aspects of Photocurrent Generation at Graphene pn Junctions Revealed by Ultrafast Optical Measurements¹, GRANT AIVAZIAN, DONG SUN, AARON JONES, JASON ROSS, University of Washington, WANG YAO, University of Hong Kong, DAVID COBDEN, XIAODONG XU, University of Washington — The remarkable electrical and optical properties of graphene make it a promising material for new optoelectronic applications. However, one important, but so far unexplored, property is the role of hot carriers in charge and energy transport at graphene interfaces. Here we investigate the photocurrent (PC) dynamics at a tunable graphene pn junction using ultrafast scanning PC microscopy. Pump-probe measurements show a temperature dependent relaxation time of photogenerated carriers that increases from 1.5ps at 290K to 4ps at 20K; while the amplitude of the PC is independent of the lattice temperature. These observations imply that it is hot carriers, not phonons, which dominate ultrafast energy transport. Gate dependent measurements show many interesting features such as pump induced saturation, enhancement, and sign reversal of probe generated PC. These observations reveal that the underlying PC mechanism is a combination of the thermoelectric and built-in electric field effects. Our results enhance the understanding of non-equilibrium electron dynamics, electron-electron interactions, and electron-phonon interactions in graphene. They also determine fundamental limits on ultrafast device operation speeds (~500 GHz) for graphene-based photodetectors.

¹We acknowledge DARPA YFA.

9:00AM P6.00006 Relaxation dynamics of photoexcited carriers in graphene probed by optical pump-THz probe spectroscopy, LIANG ZHAO, Case Western Reserve University, KIN FAI MAK, NICK PETRONE, JIM HONE, TONY HEINZ, Columbia University, JIE SHAN, Case Western Reserve University — The relaxation of hot carriers in graphene is a subject of much current interest. The role of electronic and phonon relaxation channels is a topic of particular focus, with phenomena such as carrier multiplication, in which multiple charge carriers are generated from absorption of a single photon, having been predicted.¹ In this work, we apply the optical pump-THz probe spectroscopy to investigate the relaxation dynamics of photoexcited carriers in large-area single-layer graphene samples grown by chemical vapor deposition (CVD). The complex optical conductivity induced by optical excitation is determined over a broad range of THz frequencies as a function of the pump-probe delay time. To probe carrier relaxation dynamics, we compare the transient optical conductivity to a single-particle model for the intraband response. The effect of pump fluence and the static doping density on the carrier dynamics will be discussed.

¹T. Winzer, A. Knorr, and E. Malic, Nano Letts. 10, 4839 (2010).

9:12AM P6.00007 Excitonic Effects and Optical Absorption Spectrum of Doped Graphene, FELIPE JORNADA, University of California at Berkeley, JACK DESLIPPE, STEVEN LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory — First-principles calculations based on the GW-Bethe-Salpeter Equation (GW-BSE) approach and subsequent experiments have shown large excitonic effects in the optical absorbance of graphene. Here we employ the GW-BSE formalism to probe the effects of charge carrier doping and of having an external electric field on the absorption spectrum of graphene. We show that the absorbance peak due to the resonant exciton exhibits systematic changes in both its position and profile when graphene is gate doped by carriers, in excellent agreement to very recent measurements¹. We analyze the various contributions to these changes in the absorption spectrum, such as the effects of screening by carriers to the quasiparticle energies and electron-hole interactions. This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, and the U.S. DOD - Office of Naval Research under RTC Grant No. N00014-09-1-1066. Computer time was provided by NERSC.

¹Tony F. Heinz, private communications.

9:24AM P6.00008 Magneto-phonon resonance in graphene, YOUNGHEE KIM, J.-M. POUMIROL, National High Magnetic Field Laboratory, Tallahassee, FL 32310, USA, A. LOMBARDO, Engineering Department, Cambridge University, Cambridge, CB3 0FA, UK, N.G. KALUGIN, Department of Materials and Metallurgical Engineering, New Mexico Tech, Socorro, NM 87801, USA, J. KONO, Department of Electrical & Computer Engineering, Rice University, Houston, TX 77005, USA, T. GEORGIOU, A.K. GEIM, K.S. NOVOSELOV, School of Physics & Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, UK, A.C. FERRARI, Engineering Department, Cambridge University, Cambridge, CB3 0FA, UK, D. SMIRNOV, National High Magnetic Field Laboratory, Tallahassee, FL 32310, USA — Recently, much attention has been paid to electron-phonon coupling in graphene. In particular, significant re-normalization and broadening of long-wavelength optical phonons are predicted to occur through resonant interaction with Landau-quantized Dirac fermions. We report a high-field magneto-Raman spectroscopy study of single-layer graphene in magnetic fields up to 45 T. The Raman G peak exhibits clear splitting at approximately 30 T, which we attribute to the fundamental magneto-phonon resonance associated with (0,1) inter Landau level transitions. The coupled electron-phonon modes exhibit characteristic anti-crossing behavior allowing for an accurate determination of the electron-phonon coupling strength in graphene.

9:36AM P6.00009 Coherent photocurrent control in a graphene bilayer in a magnetic field, KIRAN RAO, JOHN SIPE, University of Toronto — We consider theoretically the coherent control of a Bernal-stacked graphene bilayer in a perpendicular magnetic field. When the system is exposed to a two-color optical pulse, photocurrents of electrons and holes are induced through interference between one- and two-photon excitation processes. The generated photocurrents are time-dependent as a result of the two processes placing electrons or holes in different Landau levels. The direction and phase of the terahertz current oscillation can be tuned through the polarization and relative phase parameter of the optical pulses. We compare the results to those obtained in the absence of a magnetic field [1] and also to the results for monolayer graphene.

[1] J. Rioux, G. Burkard and J. E. Sipe, Phys. Rev. B 83, 195406 (2011).

9:48AM P6.00010 Giant optical nonlinearity of graphene in a strong magnetic field¹, XIANGHAN YAO, ALEXEY BELYANIN, Texas A&M University — We demonstrate theoretically that graphene placed in a strong magnetic field possesses by far the highest third-order optical nonlinearity among all known materials. The giant nonlinearity originates from unique electronic properties and selection rules near the Dirac points, which gives rise to resonantly enhanced nonlinear response. We present rigorous and intuitive quantum-mechanical density-matrix formalism for calculating linear and nonlinear optical properties of graphene, valid for arbitrarily strong magnetic and optical field [1]. The calculated magnitude of the third-order nonlinearity is of the order of 0.01 esu for the field of several Tesla in the mid/far-infrared spectral range. Due to this giant nonlinearity, even one monolayer of graphene gives rise to appreciable nonlinear frequency conversion efficiency for incident mid/far-infrared radiation.

[1] X. Yao and A. Belyanin, Giant optical nonlinearity of graphene in a strong magnetic field, Phys. Rev. Lett. submitted; arXiv: 1110.4869.

¹This work was supported in part by NSF Grants ECS-0547019, OISE-0968405, and EEC-0540832.

10:00AM P6.00011 Mid-Infrared Magneto-Optical Kerr and Faraday Studies in Gated Monolayer and Rotated Bilayer CVD Graphene, C.T. ELLIS, N. TESAROVA, ALOK MUKHERJEE, A. STABILE, SUNY Buffalo, Dept. of Physics, YUFENG HAO, R.S. RUOFF, The University of Texas at Austin, Dept. of Mechanical Engineering and the Materials Science and Engineering Program, G. SAMBANDAMURTHY, J. CERNE, SUNY Buffalo, Dept. of Physics — Previous studies of multi-layer graphene grown on C-face SiC have proven that mid-IR (111-135 meV) Polar Magneto-Optical Kerr Effect (PMOKE) measurements provide a unique and sensitive way to probe the Landau Level (LL) structure of graphene. Graphene PMOKE measurements, which are proportional to the Hall conductivity (σ_{xy}), have revealed large changes in the Kerr angle due to the chiral nature of LL transitions in mono- and multi-layer graphene, as well as the dependence of these Kerr features on the position of the Fermi level. In this work we present new results that extend these measurements to more ideal samples consisting of large area (5x5mm), epitaxial single layer CVD grown graphene that has been deposited onto a Si/SiO₂ substrate. Unlike epitaxial SiC graphene these new samples can be back-gated and also allow magneto-optical measurements to be made in transmission (Faraday geometry). The ability to tune parameters such as the Fermi energy, probing photon energy, magnetic field strength, and temperature allows us to better understand graphene through its mid-IR Hall conductivity and to test for theoretical predictions of an infrared quantum Hall effect in graphene (Morimoto, PRL, 2009). This work is supported by NSF-DMR1006078 and by the Office of Naval Research.

10:12AM P6.00012 Substrate effects and photon energy dependence of ultrafast carrier relaxation in graphene¹, ADAM ROBERTS, DANIEL CORMODE, University of Arizona, JOHN FOREMAN, US Army Aviation and Missile RD&E Center, HENRY EVERITT, Duke University, US Army Aviation and Missile RD&E Center, BRIAN LEROY, ARVINDER SANDHU, University of Arizona — Ultrafast photo-excitation in graphene creates non-equilibrium carrier distributions and provides an avenue for the measurement of couplings between electronic and lattice degrees of freedom. Previous studies have explored the carrier relaxation dynamics in graphene on various substrates albeit primarily in the linear dispersion regime. We investigate the ultrafast carrier dynamics of graphene both in the linear band regime and near the saddle point. We perform femtosecond-resolved degenerate pump-probe differential transmission experiments to extract the timescales for electronic relaxation from different starting points on the band structure. The use of degenerate pump-probe allows us to obtain exact relaxation timescales corresponding to the local band structure without contributions from other carriers. We use multiple transparent substrates, such as fused silica, quartz, sapphire etc. to probe the substrate-graphene interactions at various points along the local electronic band structure. We find that in the UV regime, the relaxation dynamics in graphene shows remarkable dependence on the substrate, with relaxation timescales ranging from a few to hundreds of picoseconds. We will also compare our measurements with those obtained in freestanding graphene samples.

¹ Graduate support from DoD SMART Scholarship.

10:24AM P6.00013 Excitonic Effects on Optical Absorption Spectra of Doped Graphene, LI YANG, Washington University in St. Louis — We have performed first-principles calculations to study optical absorption spectra of doped graphene with many-electron effects included. Both self-energy corrections and electron-hole interactions are reduced due to the enhanced screening in doped graphene. However, self-energy corrections and excitonic effects nearly cancel each other, making the prominent optical absorption peak fixed around 4.5 eV under different doping conditions. On the other hand, an unexpected increase of the optical absorbance is observed within the infrared and visible-light frequency regime (1 ~ 3 eV). Our analysis shows that a combining effect from the band filling and electron-hole interactions results in such an enhanced excitonic effect on the optical absorption. These unique variations of the optical absorption of doped graphene are of importance to understand relevant experiments and design optoelectronic applications.

10:36AM P6.00014 Dirac Plasmas in Graphene, HUGEN YAN, FENGNIAN XIA, XUESONG LI, BHUPESH CHANDRA, GEORGE TULEVSKI, YANQING WU, MARCUS FREITAG, WENJUAN ZHU, PHAEDON AVOURIS, IBM T. J. Watson Research Center — Collective excitation of Dirac Fermions in graphene has many similarities to that of conventional semiconductor two dimensional electron gas (2DEG). For instance, the resonance frequency is proportional to $q^{1/2}$, where q is the wave-vector. However, there are some fundamental differences. In this paper, we'll present our far-infrared spectroscopy studies of Dirac plasma in graphene. Localized plasmons in graphene disks and micro-ribbons are excited by far-infrared photons. The resonance frequency scales as $n^{1/4}$, where n is the sheet carrier density. This is distinctively different from conventional semiconductor. In addition, plasmons in graphene superlattice are compared to their counterparts in semiconductor superlattice.

10:48AM P6.00015 Experimental and theoretical investigations on SERS enhancement mechanism of graphene, QINGZHEN HAO, Physics Department, SETH MORTON, Chemistry Department, BEI WANG, Physics Department, YANHUI ZHAO, Engineering Science and Mechanics Department, LASSE JENSEN, Chemistry Department, TONY JUN HUANG, Engineering Science and Mechanics Department, The Pennsylvania State University — Graphene has recently been shown to improve the Surface-enhanced Raman Scattering (SERS) performance of traditional nanostructured metallic substrates. Here we present an experimental and theoretical study on its SERS enhancement mechanism. We observed that SERS enhancement of graphene can be tuned by changing its Fermi level via doping. Both molecular doping and gate doping experiments show that hole-doped graphene yields a larger SERS enhancement in methylene blue (MB) than electron-doped one. The MB-graphene system is then modeled using both a fully quantum mechanical (QM) description as well as a QM-polarizable force field model wherein the graphene is modeled using a Drude-Lorentz function. In the first model, charge transfer (CT) excitations between MB and a graphene cluster can be accounted for, while in the second model we can account for the "infinite" size of the graphene sheet. Both of the models confirm the role of graphene Fermi level on its SERS enhancement. Our preliminary results suggest that graphene SERS enhancement would likely be coming from a ground-state chemical enhancement.

11:00AM P6.00016 Exciting and probing plasmons in graphene by local defects, ANATOLY EFIMOV, KIRILL VELIZHANIN, Los Alamos National Laboratory — The short wavelength of collective excitations, i.e., plasmons, in doped graphene (~10-20 nm) is very attractive for multiple applications. However, the same short wavelength makes photoexcitation of plasmons in graphene a very challenging task. In this work, we discuss various types of local defects including semiconductor quantum dots, metallic nanoclusters, edges and holes in graphene as means to "squeeze" the large wavelength of optical excitation down to the nanometer scale, thus, providing an effective coupling between free photons and plasmons in graphene. In the case of semiconductor quantum dots, we show how plasmons in graphene can be excited and probed by Förster resonance energy transfer from the optically excited quantum dot to the graphene sheet. Specifically, we demonstrate how the calculated dispersion relation of plasmons in graphene as well as of other electronic excitations can be accurately extracted by controlling the backgate voltage and the distance between the quantum dot and graphene [1].

[1] K. A. Velizhanin, A. Efimov "Probing plasmons in graphene by resonance energy transfer," Phys. Rev. B, 085401, 84 (2011).

Wednesday, February 29, 2012 8:00AM - 10:48AM —
 Session P7 DMP DCOMP: Focus Session: Computational Design of Materials: Graphene - Electronic Structure and Transport 207

8:00AM P7.00001 Electronic transport properties of a graphene monolayer covered by another layer with infinite or finite width, DANIEL VALENCIA, JI LUO, JUN-QIANG LU, University of Puerto Rico Mayaguez — Intrinsic graphene, a zero-gap semiconductor, is one of the most promising materials for nanodevices. In this work, the electronic transport properties of a graphene monolayer covered by another infinite or finite layer were studied. The results of the transmission spectrum and the local density of states (LDOS) showed a weak interaction between the two layers when the top layer is infinite or semi-infinite. Thus the transport properties of the monolayer do not change much. However, when the monolayer is covered by a finite-width nanoribbon, the change in its transmission spectrum is dependent on the width of the ribbon. In order to understand the origin of this phenomenon we calculated the transmission spectrum of one individual channel, and observed that the changes are due to antiresonance in the electronic transmission, which is caused by interlayer interference between the wavefunctions.

8:12AM P7.00002 Electronic transport proprieties of graphene few-layers¹, JUNQIANG LU, CARLOS SIERRA, DANIEL VALENCIA, University of Puerto Rico at Mayaguez — We study electronic transmission spectrums of graphane few-layers (up to 6 layers) with AA or AB stacking by using of first-principle transport calculations. The results demonstrate flat transmission spectrum for even layers while linear transmission for odd layers, which can be understood by different band structures of graphene few-layers due to the interlayer interaction.

¹JQL acknowledges the support from the Institute for Functional Nanomaterials, University of Puerto Rico.

8:24AM P7.00003 Quantum Transport Properties of Modified Graphene Nanoribbons with Boron Nitride Domains at the Mesoscopic Scale, ALEJANDRO LOPEZ-BEZANILLA, ORNL — Graphene nanoribbons are seen as promising building blocks for engineering graphene based field effect transistor (GNR-FET). The quest for fabricating efficient GNR-FETs requires a trade-off between a sufficiently wide energy gap and a reasonably large charge mobility. The solution might be the chemical codoping of one-atom thick layers of C with B and N atoms. These hybrid systems are attracting much attention as they can provide an efficient way to create new materials with complementary properties to those of graphene and h-BN. I will present a study of charge transport in graphene nanoribbons with BN domains randomly distributed along the ribbon surface. My results describe how the conductance of the hybrid systems is altered as a function of the incident electron energy and the BN domain density which leads to transport band gap opening. We explore the transport regimes comparing different degrees of BN codoping and BN domain size for ribbons of various widths and lengths on the order of the micrometer. A comparison with other types of defects such as oxygen atoms in epoxy configuration and functional groups covalently attached to the ribbon surface will be discussed as well.

8:36AM P7.00004 First-principles study of charge transfer doping and electronic transport in single-walled carbon nanotubes¹, XIANGGUO LI, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida, Gainesville, Florida 32611, USA — It is well known that charge transfer doping can greatly enhance the conductivity in single-walled carbon nanotube thin films. Recent experiments showed that the tube-tube contact resistance dominates the impedance in the films. To understand effects of doping on the tube-tube contact, we studied the tube-tube distance changes and electron transport properties upon doping (K and Br) using first-principles calculations. Our results suggest that the effect of doping on the tube-tube distance depends not only on the type of dopants but also on the electronic properties of the carbon nanotubes.

¹Acknowledgement: DOE/BES-DE-FG02-02ER45995; NERSC and UF/HPC

8:48AM P7.00005 Computational Study of the Thermal and Electronic Transport Properties of Rigidly-Interconnected Carbon Nano Foam, SORA PARK, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, DAVID TOMÁNEK, Physics and Astronomy Department, Michigan State University — We study the thermal and electronic transport properties of rigidly-interconnected structures having sp^2 carbon minimal surface called schwarzites. The system consists of core parts composed of schwarzite and interconnection parts with (4,4) carbon nanotube segments [1]. Using direct molecular dynamics simulations with the Tersoff potential, we compute the thermal conductivity of various configurations to explore the dependence on the number of core parts and on the length of interconnection parts. Our calculations show that each core part plays as a scattering center, which reduces the phonon mean free path and thus the thermal conductivity. We also investigate the electronic transport properties of the system by applying the non-equilibrium Green function approach in combination with density functional theory. We explore the effects of different core connectivity and structural defects introduced near the core parts on the electrical conductance. These thermal and electronic properties may be connected to the thermoelectric properties of the schwarzite system.[1] S. Park, K. Kittimanapun, J. S. Ahn, Y.-K. Kwon and D. Tománek, J. Phys.: Condens. Matter **22**, 334220 (2010).

9:00AM P7.00006 Klein, anti-Klein tunneling and pseudo-spintronics in graphene heterojunctions¹, REDWAN SAJJAD, AVIK GHOSH, University of Virginia — Electrons in monolayer graphene act like massless spin-1/2 Dirac fermions. Backscattering is suppressed due to the pseudospin orthogonality of the forward and reverse scattering modes. The resulting Klein tunneling provides unit transmission for normally incident electrons at a pn junction, regardless of barrier height. By combining voltage gating with a tunnel barrier, we can realize a gate tunable metal insulator transition that promotes subthermal switching [1] and also makes the conduction unipolar. In contrast, bilayer graphene electrons act like parabolic spin-1 systems with perfect reflection for normal incidence (anti-Klein tunneling). For n^+n or p^+p junction, the transmission maximizes for normal incidence like single layer, but unlike monolayer graphene, it's barrier-dependent. We also perform atomistic numerical calculation of graphene sheets with experimentally relevant size (hundreds of nanometer) using non-equilibrium Green's function formalism and we show that the conductance can be varied substantially with gate voltage for multiple sequenced pn junctions with smoothly varying potential.

[1] Sajjad and Ghosh, APL 99, 123101 (2011).

¹The authors acknowledge funding from NSF-NRI.

9:12AM P7.00007 Curvature-induced spin-orbit coupling and spin relaxation in a chemically-clean single-layer graphene¹, JAE-SEUNG JEONG, School of Physics, Korea Institute for Advanced Study, Seoul 130-722, Korea, JEONGKYU SHIN, HYUN-WOO LEE, Department of Physics and PCTP, Pohang University of Science and Technology, Pohang 790-784, Korea — Based on the second-order perturbation theory, we show that curvature induced by corrugations or periodic ripples in single-layer graphenes generates two types of effective spin-orbit coupling. In addition to the spin-orbit coupling reported previously that couples with sublattice pseudospin and corresponds to the Rashba-type spin-orbit coupling, there is an additional spin-orbit coupling that does not couple with the pseudospin. The additional spin-orbit coupling depends on the direction of principal curvature, which is similar with the curvature-induced spin-orbit coupling of carbon nanotubes that depends on the chiral angle. However, the spin-orbit coupling of single-layer graphenes can not be obtained from the trivial extension of the spin-orbit coupling of carbon nanotubes owing to their distinct topological structure. Via the numerical calculation, we show that both types of the curvature-induced spin-orbit coupling make the same order of contribution to spin relaxation in chemically-clean single-layer graphene with nanoscale corrugation. The spin relaxation dependence on the corrugation roughness is also investigated.

¹This work was financially supported by the NRF (2010-0014109) and BK21.

9:24AM P7.00008 Fractional topological phases, triplet superconductivity and spontaneous time reversal symmetry breaking in strained graphene, POUYAN GHAEMI, Department of Physics, University of Illinois, Urbana, IL 61801, USA, JEROME CAYSSOL, LOMA (UMR-5798), CNRS and University Bordeaux, F-33045 Talence, France, DONNA SHENG, Department of Physics and Astronomy, California State University, Northridge, California 91330, USA, ASHVIN VISHWANATH, Department of Physics, University of California, Berkeley, CA 94720, USA — Despite wide interests to realize fractional time-reversal symmetric phases, an experimentally realizable system with these exotic topological orders is still lacking. Recent experiment has confirmed that strain can be used to control the electronic states of graphene and create flat pseudo-Landau levels in the absence of external magnetic field. In this talk, I show that graphene under strain is a natural playground for the observation of exotic phases such as fractional valley Hall insulator as well as flat band superconductivity. For neutral graphene, we find a competition between the Ising valley ferromagnet and the spin ferromagnet ruled by the value of short range Hubbard and long range Coulomb interactions. At fractional filling with different intervalley and intravalley interactions, a spin triplet superconductor, a valley-polarized Laughlin state or a time-reversal symmetric fractional valley-Hall state could be realized.

9:36AM P7.00009 Satellite Structures in Spectral Functions of Silicon and Graphene from *ab initio* GW and Cumulant Expansion Calculations¹, DEREK VIGIL CURREY, JOHANNES LISCHNER, STEVEN LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — The GW approximation is a well-established method for obtaining accurate quasiparticle properties in a wide range of materials. Its suitability for satellite structures (e.g., those measured in photoemission spectroscopies), however, has rarely been addressed in detail for real materials and the fact that GW overestimates the position of the plasmon satellite peaks in the spectral function of silicon indicates the need for an improved method for satellites. One such method is the cumulant expansion. The cumulant expansion is a method that includes, approximately, higher-order processes beyond GW that are important for satellite properties. We present here full-frequency results for the satellite and quasiparticle properties of silicon and doped graphene using the GW and the cumulant expansion methods, and discuss the improvements in satellite properties given by the cumulant expansion. We also compare our results to earlier model calculations on doped graphene.

¹This work was supported by NSF Grant No. DMR10-1006184 and U.S. DOE Contract No. DE-AC02-05CH11231. Computational resources have been provided by the NERSC and NICS. Derek Vigil Currey acknowledges funding from the DOD's NDSEG fellowship.

9:48AM P7.00010 Static and dynamical response of graphene, TOBIAS STAUBER, GUILLERMO GOMEZ SANTOS, Universidad Autonoma de Madrid — We discuss the static and dynamical response of graphene. First, we show that including the full hexagonal lattice leads to anisotropic Friedel oscillations and paramagnetic orbital susceptibility around the neutrality point [1]. We then apply the dynamical current-current correlation function to discuss graphene's fluorescence quenching including also transverse decay channels and full retardation [2]. We finally discuss the optical properties of double layer graphene.

[1] G. Gómez-Santos and T. Stauber, Phys. Rev. Lett. 106, 045504 (2011).

[2] G. Gómez-Santos and T. Stauber, Phys. Rev. B 84, 165438 (2011).

10:00AM P7.00011 First-principles study of graphene - carbon nanotube contacts, BRANDON COOK, KALMAN VARGA, Vanderbilt University — The electron transport properties of carbon nanotube – graphene junctions are investigated with first-principles total energy and electron transport calculations. By combining the advantageous material properties of graphene and nanotubes one can create all carbon hybrid architectures with properties that are particularly well suited to applications. The p-type Schottky barrier height is calculated in model junctions with (8,0) and (10,0) nanotubes in a top-contact configuration. Results indicate a lower barrier in carbon nanotube – graphene junctions than in other carbon nanotube – metal systems.

10:12AM P7.00012 Electronic Band Structures of Graphene Nanomeshes, WILLIAM OSWALD, ZHIGANG WU, Department of Physics, Colorado School of Mines — Owing to its many remarkable properties, graphene is very promising for electronic and opto-electronic applications for size miniaturization and improving performance; however, bulk graphene is a semi-metal with zero band gap, and many methods have been proposed to open up a sizable band gap. In this work, we carry out first-principles calculations based on the density functional theory (DFT) to investigate electronic band structures of graphene nanomeshes (GNMs), the defected graphene containing a high-density array of nanoholes, studying the bandgap opening mechanism and evaluating band gap as functions of structural parameters, including hole size, hole shape, hole-hole distance, and hole arrangement. Our results suggest that while the band gap opening is a result of quantum confinement at nanomesh necks, the size of band gap depends strongly on the detailed GNM structures. For the simplest hexagonal holes, two thirds of GNMs remain semi-metallic and the rest one third are semiconductors.

10:24AM P7.00013 Quantum Mechanics on a Möbius Strip: Energy Levels, Symmetries, and Level Splitting in a Magnetic Field, ZHAO LI, RAMDAS RAM-MOHAN, Physics Department, Worcester Polytechnic Institute — We investigate the energy levels of an electron on a Möbius strip. Schrödinger's equation on this curved surface is shown to have terms that do not have invariance under parity transformation in parameter space for the strip. The double degeneracy of energy levels that exists for flat cylindrical rings is shown to be removed for the pairs of energies in the Möbius strip due to parity symmetry breaking. The orbital angular momentum is found to have approximately not only integer but also half-integer values of $\hbar$. The splitting of the energy levels in an external magnetic field is displayed. The effects of multiple twists are investigated to further clarify that the parity symmetry breaking is the effect of the curved geometry, while the appearance of half-integer angular momentum states is a topological effect. The implications for twisted rings composed of graphene will be discussed, and carrier transport through the Möbius strip will be considered. This work was supported by AFRL/DARPA under grant FA8650-10-1-7046.

10:36AM P7.00014 QED Kapitza conductance of nano-carbon thermal interconnects¹, SLAVA V. ROTKIN, Physics Department, Lehigh University, ALEXEY G. PETROV, Ioffe Institute — The theory for the near-field Kapitza conductance across the interface of a nano-carbon material and the quartz is thoroughly investigated. The near-field photon tunneling is shown to contribute to the total heat flux between the hot and cold sides of the interface on the order of or even larger than the normal thermal conductance. Quartz is chosen as the most common example of non-conductive and strongly polar substrate material with the well known polarization properties, though the theory is not restricted to quartz only. Our approach allowed us to derive a unified expression for QED Kapitza conductance of the nanocarbon thermal interconnect material, such as graphene, a nanotube, or a nanotube forest and predict thermal phenomena, such as the heat rectification, as a function of the materials properties of the interface.

¹This work is supported by DoD (AFOSR # FA9550-11-1-0185).

Wednesday, February 29, 2012 8:00AM - 11:00AM – Session P8 DMP GMAG: Focus Session: Spin Liquids I 208

8:00AM P8.00001 Quantum Ice : Experimental Signatures, NIC SHANNON, Clarendon Laboratory, University of Oxford, Oxford OX1 3PU, UK; Okinawa Institute of Science and Technology, Okinawa, Japan 904-0495, OWEN BENTON, H H Wills Physics, University of Bristol, Bristol BS8 1TL, UK, OLGA SIKORA, H H Wills Physics, University of Bristol, Bristol BS8 1TL, UK; Okinawa Institute of Science and Technology, Okinawa, Japan 904-0495, KARLO PENC, Research Institute for Solid State Physics and Optics, H-1525, Budapest, Hungary, PAUL MCCLARTY, FRANK POLLMANN, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, PETER FULDE, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany; Asia Pacific Center for Theoretical Physics, Pohang, Korea — “Quantum Spin Ice” materials have attracted considerable attention as three-dimensional examples of quantum spin liquids. Recently, we have used zero-temperature Quantum Monte Carlo simulation to explore one possible scenario for these materials, confirming the possibility of a “quantum ice” state driven by quantum tunnelling between an extensive number of different spin-ice configurations [1]. Here we address the simple question : what would such a quantum ice look like in experiment ? We focus in particular on the fate of “pinch point” singularities seen in neutron scattering experiments on spin ice materials, showing how these are suppressed and ultimately eliminated as the system is cooled to its ground state [1,2].

[1] N. Shannon *et al.*, arXiv:1105.4196

[2] O. Benton *et al.*, in preparation.

8:12AM P8.00002 Quantum Ice : A Quantum Monte Carlo Study, OLGA SIKORA, HH Wills Physics, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK, Okinawa Institute of Science and Technology, Japan, OWEN BENTON, HH Wills Physics, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK, NIC SHANNON, HH Wills Physics, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, University of Oxford, UK; Okinawa Institute of Science and Technology, Japan, KARLO PENC, Research Institute for Solid State Physics and Optics, H-1525 Budapest, P.O.B. 49, Hungary, PAUL MCCLARTY, FRANK POLLMANN, RODERICH MOESSNER, MPI PKS, Dresden, Germany, PETER FULDE, MPI PKS, Dresden, Germany, Asia Pacific Center for Theoretical Physics, Pohang, Korea — The magnetic “ice” state found in spin ice materials has recently generated great excitement for its magnetic monopole excitations. However the deconfined nature of these monopoles depends crucially on the macroscopic degeneracy of the classical ice ground state. And at very low temperatures we might expect this degeneracy to be lifted by quantum tunneling between different ice configurations. Here we present the results of large-scale Green's function Monte Carlo simulation of ice-type models which include quantum tunneling. We find compelling evidence of an extended quantum U(1)-liquid ground state with deconfined monopole excitations in both the quantum dimer model [1,2] and the quantum ice model on the diamond lattice [3]. This quantum U(1) liquid proves to be remarkably robust against the inclusion of long range dipolar interactions.

[1] O. Sikora *et al.*, Phys. Rev. Lett. **103**, 247001 (2009) [2] O. Sikora *et al.*, Phys. Rev. B **84**, 115129 (2011) [3] N. Shannon *et al.*, arXiv:1105.4196

8:24AM P8.00003 Three-dimensional generalized Kitaev models¹, ZHOUSHEN HUANG, DANIEL AROVAS, University of California, San Diego — We generalize Kitaev's honeycomb lattice spin model to a gamma matrix model on three-dimensional cubic octahedron and pyrochlore lattices. We find the ground state Z_2 flux configuration, reducing the problem to free Majorana fermion hopping. For the cubic octahedron lattice, which has reflection planes, the ground states must obey Lieb's theorem, i.e. the Z_2 fluxes are reflection symmetric. By adding flux-flux interaction terms, a variety of interesting phases can be stabilized, including metallic, semimetallic, and both trivial and topological insulating phases.

¹Supported by NSF grant DMR-1007028.

8:36AM P8.00004 High pressure sequence of Ba₃NiSb₂O₉ structural phases: new $S=1$ quantum spin-liquids based on Ni²⁺, LUIS BALICAS, National High Magnetic Field Laboratory — A quantum spin-liquid (QSL) is a ground-state where strong quantum-mechanical fluctuations prevent a phase-transition towards conventional magnetic order and makes the spin ensemble to remain in a liquid-like state. Most QSL candidates studied to date are two-dimensional frustrated magnets with either a triangular or a kagome lattice composed of $S=1/2$ spins. Here, we report the use of a high pressure, high temperature technique to transform the antiferromagnetically ordered ($T_N=13.5$ K) 6H-A phase of Ba₃NiSb₂O₉ into two new QSL candidates with larger $S=1$ (Ni²⁺) moments: the 6H-B phase of Ba₃NiSb₂O₉ which crystallizes in a triangular lattice and the 3C-phase of Ba₃NiSb₂O₉ which forms a three-dimensional edge-shared tetrahedral lattice. Both compounds show no evidence for magnetic order down to $T=0.35$ K despite Curie-Weiss temperatures θ_{CW} of -75.5 K (6H-B) and -182.5 K (3C), respectively. Below ~ 25 K the magnetic susceptibility of the 6H-B phase is found to saturate at a constant value $\chi=0.013$ emu/mol which is followed below 7 K, by a linear in temperature dependence for the magnetic contribution to the specific heat (C_M) which displays a giant coefficient $\gamma=168$ mJ/mol-K² comparable to values observed in heavy-fermion metallic systems. Taken together, both observations indicate the development of a Fermi-liquid like ground-state characterized by a Wilson ratio of 5.6 in this otherwise insulating material. It also points to the formation at finite temperatures of a well defined Fermi surface of $S=1$ spin-excitations which behave as charged quasiparticles. For the 3C phase one observes $C_M \propto T^2$ indicating a unique $S=1$ three-dimensional QSL ground-state as previously reported for Na₃Ir₄O₈ although this later compound is composed of Ir⁴⁺ ions having $S=1/2$.

Work done in collaboration with J. G. Cheng, G. Li, J. S. Zhou, J. B. Goodenough, C. Xu and H. D. Zhou.

¹LB acknowledges support from DoE-BES award DE-SC0002613

9:12AM P8.00005 Generalizations of the Kitaev-Heisenberg model and connections to experiment, ITAMAR KIMCHI, University of California, Berkeley, YI-ZHUANG YOU, Institute for Advanced Study, Tsinghua University, Beijing, China, ASHVIN VISHWANATH, University of California, Berkeley — Generalizations of Kitaev-Heisenberg spin models are both interesting on their own right and potentially relevant for the Mott insulating layered Iridates $A_2\text{IrO}_3$ ($A=\text{Na},\text{Li}$) and other complex oxides of 5d transition metal compounds. To describe Na_2IrO_3 and Li_2IrO_3 we propose the Kitaev-Heisenberg- J_2 - J_3 model, a combination of the Kitaev honeycomb model and the Heisenberg model with all three nearest neighbor couplings J_1 , J_2 and J_3 . A rich phase diagram is obtained at the classical level, including the experimentally suggested *zigzag* ordered phase; as well as the *stripy* phase, which extends from the Kitaev-Heisenberg limit to the J_1 - J_2 - J_3 one. Combining the experimentally observed spin order with the optimal fitting to the uniform magnetic susceptibility data gives an estimate of possible parameter values, which in turn reaffirms the necessity of including both the Kitaev and farther neighbor couplings in describing the materials. Generalizations for other spin-orbit coupled Mott insulating 5d transition metal oxides with Kitaev-Heisenberg type models exhibit related magnetically ordered phases as well as different spin liquid phases.

9:24AM P8.00006 Topological phases of the 2D AKLT like model via study of degenerate singular value spectra, CHING-YU HUANG, FENG-LI LIN, Department of Physics, National Taiwan Normal University, Taipei, 116, Taiwan — We study the two-dimensional quantum spin-3/2 systems on the honeycomb lattice, which include the 2D AKLT model. We use the infinite time-evolving block decimation (iTEBD) method to numerically solve the ground state wave function by adopting the tensor product states (TPS) ansatz. We then evaluate the singular value spectra, entanglement entropy, and the Neel order by the method of tensor renormalization group (TRG). With all these results we determine the phase diagram of the spin-3/2 model. Our result shows the singular value spectra become doubly degenerate in a belt region including the AKLT point, and indicates the existence of possible topological phases. The double degeneracy of singular value spectra is related to the recent observation in [C.-Y. Huang and F.-L. Lin, Phys. Rev. B 84, 125110 (2011)] of using it to characterize the topological phase. We also cross check this statement by calculating the topological Renyi entropy. The 2D AKLT state has been shown to be a universal resource for measurement-based quantum computation. Our results indicate this state is topological in nature and should be robust against local perturbations.

9:36AM P8.00007 Finite temperature phase diagram of the classical Heisenberg-Kitaev model., NATALIA PERKINS, CRAIG PRICE, Physics Department, UW Madison — We study finite-temperature properties of classical version of the Heisenberg-Kitaev model on the honeycomb lattice. This model is a prominent example of anisotropic spin-orbital models, which can possibly describe the low-energy physics of Na_2IrO_3 and Li_2IrO_3 . In these compounds, Ir^{4+} ions are in a low spin $5d^5$ configuration and form weakly coupled hexagonal layers. Our main result is a finite-temperature phase diagram obtained by classical Monte Carlo simulations. Because of highly anisotropic Kitaev interaction, the spin symmetry of the model is reduced to the discrete symmetry, which may be regarded as $Z_3 \times Z_2$. As the discrete symmetry can be broken at finite temperature even at 2D, the model undergoes phase transitions as a function of temperature. At low temperature phase, thermal fluctuations induce order-by-disorder, just as the quantum fluctuations do at zero temperature. As a result, magnetically ordered ground states of the Heisenberg-Kitaev model persist up to a certain critical temperature. Finally, we discuss the relevance of obtained results for experimental findings in real compounds.

9:48AM P8.00008 Dynamical Jahn-Teller effect in spin-orbital coupled system, JOJI NASU, SUMIO ISHIHARA, Department of Physics, Tohoku University — Orbital degree of freedom is one of the most attractive themes in strongly correlated electron system. A coupling between the orbital and the lattice vibration is known as a Jahn-Teller effect (JTE). The dynamical aspect of the Jahn-Teller interaction is often neglected in solid, because it is strongly suppressed by the cooperative JTE. Recently, $\text{Ba}_3\text{CuSb}_2\text{O}_9$ has been reported as a candidate of the spin liquid. A Cu^{2+} has the e_g orbital degree of freedom and is surrounded by the O^{2-} octahedron. The octahedra on the neighboring sites do not have the common O ions. This fact implies that the cooperative JTE is weak, and the dynamical JTE is expected to play some key roles on orbital and magnetic properties. The purpose of this research is to study the dynamical JTE in a spin-orbital coupled system. In particular, we focus on the competitive or cooperative phenomena between the superexchange interaction and the dynamical JTE. The superexchange interactions are derived from the $d-p$ model on a honeycomb lattice. We have confirmed this interaction stabilizes the antiferro-spin and ferro-orbital configurations for the realistic parameters. The dynamical JTE described as the orbital-lattice coupling is obtained by extracting the low energy states of the vibronic Hamiltonian. We analyze the model including the two kinds of interactions by using the Bethe approximation. We find that the magnetic order is unstable in wide parameter region and the spin-dimer state with the orbital order is realized. Furthermore the orbital order is strongly suppressed by the dynamical JTE.

10:00AM P8.00009 Quantum spin liquid in frustrated one dimensional LiCuSbO_4 ¹, MARTIN MOURIGAL, Johns Hopkins University, SIAN E. DUTTON, MANORANJAN KUMAR, ZOLTAN G. ZOOS, Princeton University, JIAJIA WEN, COLLIN L. BROHOLM, Johns Hopkins University, NIELS H. ANDERSEN, Risø-DTU, QING HUANG, NIST Center for Neutron Research, MOHAMED ZBIRI, Institut Laue Langevin, RASMUS TOFT-PETERSEN, Risø-DTU, ROBERT J. CAVA, Princeton University — A quantum magnet, LiCuSbO_4 , with chains of edge-sharing $S=1/2$ CuO_6 octahedra is reported. Short-range ordering is observed while no phase transition or spin freezing occurs down to 100 mK in zero magnetic field. Specific heat indicates a distinct low-temperature high-field phase near the 12 T saturation field. Neutron scattering shows incommensurate spin correlations with $q=0.47 \pm 0.01 \pi/a$ and places an upper limit of 70 μeV on a potential spin gap. Exact diagonalization of easy plane $S=1/2$ chains with competing nearest neighbor ferro- and next-nearest neighbor antiferromagnetic interactions ($J_1=-75$ K, $J_2=34$ K) accounts for the $T>2$ K bulk and neutron data. Close to a quantum critical point, free from long-range order and with an achievable saturation field, LiCuSbO_4 is a promising candidate material to test long-standing predictions for chiral and nematic states in quantum spin chains

¹This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-08ER46544

10:12AM P8.00010 Exotic $S=1$ spin liquid state with fermionic excitations on triangular lattice, MAKSYM SERBYN, SENTHIL TODADRI, PATRICK A. LEE, Massachusetts Institute of Technology — Motivated by recent experiments on the material $\text{Ba}_3\text{NiSb}_2\text{O}_9$ we consider a spin-one quantum antiferromagnet on a triangular lattice with the Heisenberg bilinear and biquadratic exchange interactions and a single-ion anisotropy. Using a fermionic “triplon” representation for spins, we study the phase diagram within mean-field theory. In addition to a fully gapped spin-liquid ground state, we find a state where one gapless triplon mode with Fermi surface coexists with $d+id$ topological pairing of the other triplons. Despite the existence of a Fermi surface, this ground state has fully gapped bulk spin excitations. Such a state has linear in-temperature specific heat and constant in-plane spin susceptibility, with an unusually high Wilson ratio.

10:24AM P8.00011 Spin Liquid Phases for Spin-1 systems on the Triangular lattice, CENKE XU, University of California Santa Barbara, FA WANG, Massachusetts Institute of Technology, YANG QI, Tsinghua University, LEON BALENTS, Kavli Institute for Theoretical Physics, University of California Santa Barbara, MATTHEW FISHER, University of California Santa Barbara — Motivated by recent experiments on material $\text{Ba}_3\text{NiSb}_2\text{O}_9$, we propose two novel spin liquid phases (A and B) for spin-1 systems on a triangular lattice. At the mean field level, both spin liquid phases have gapless fermionic spinon excitations with quadratic band touching, thus in both phases the spin susceptibility and C_v/T saturate to a constant at zero temperature, which are consistent with the experimental results on $\text{Ba}_3\text{NiSb}_2\text{O}_9$. On the lattice scale, these spin liquid phases have $\text{Sp}(4) \sim \text{SO}(5)$ gauge fluctuation; while in the long wavelength limit this $\text{Sp}(4)$ gauge symmetry is broken down to $\text{U}(1) \times \text{Z}_2$ in type A spin liquid phase, and broken down to Z_4 in type B phase. We also demonstrate that the A phase is the parent state of the ferro-quadrupole state, nematic state, and the noncollinear spin density wave state.

10:36AM P8.00012 Stability of the U(1) Dirac spin liquid state on the kagome lattice ,

MICHAEL LAWLER, Binghamton University, BRYAN CLARK, Princeton University, JESSE KINDER, Case Western Reserve University, Cornell University, ERIC NEUSCAMMAN, UC Berkeley, Cornell University, GARNET CHAN, Cornell University — The ground state of the spin 1/2 nearest neighbor Heisenberg antiferromagnet on the kagome lattice is still unknown. Recent DMRG calculations[1] have challenged the proposal[2] that this ground state is an algebraic spin liquid with Dirac fermions and photons as elementary excitations. We numerically study all time reversal invariant Gutzwiller projected variational wave functions for this system and find a state with mild symmetry breaking as the lowest energy state. To avoid getting stuck in a local minimum, we begin our Monte-Carlo calculation from all Z2 spin liquid states cataloged in Ref. [3]. Analyzing the resulting wave function, we find it lies very close to the U(1) Dirac state proposed in Ref. [2] in terms of its gauge fluxes, but with lower energy. We believe these results strongly emphasize the dominance and stability of the U(1) Dirac spin liquid state among Gutzwiller projected wave functions. However, our state has higher energy than the DMRG matrix product state, so correlations beyond those captured by it must play a fundamental role in the characterization of the ground state. [1]S. Yan, D.A. Huse, and S.R. White, Science 332, 1173 (2011) [2]Y. Ran, M. Hermele, P.A. Lee, and X.-G. Wen, PRL, 98, 117205 (2007) [3]Y.-m. Lu, Y. Ran, and P. Lee, PRB, 83, 12 (2011)

10:48AM P8.00013 Theory of spin liquids in integer spin pyrochlores , SUNGBIN LEE, University of California,

Santa Barbara, SHIGEKI ONODA, Condensed Matter Theory Laboratory, RIKEN, LEON BALENTS, Kavli Institute for Theoretical Physics, University of California, Santa Barbara — Rare earth pyrochlores, with a chemical formula $A_2B_2O_7$, exhibit many interesting features in A site spin system. Depending on A site rare earth elements, spin ice and magnetically ordered phases are shown in several experiments. Moreover, they have been also focused as possible candidates of U(1) spin liquid. In order to explore such versatile phases, we study the pseudospin-1/2 model, which is quite generic to describe rare earth pyrochlores with integer spins, in the presence of spin-orbit coupling and crystalline electric field. Using a new "gauge mean field theory," we show the possible ground states, corresponding to several phases listed above. We also briefly discuss the experimental suggestions based on our theory.

Wednesday, February 29, 2012 8:00AM - 11:00AM –

Session P9 GMAG DMP: Focus Session: Magnetic Oxide Thin Films And Heterostructures: Manganite Thin Films 209

8:00AM P9.00001 Magnetic non-uniformity in $(La_{0.4}Pr_{0.6})_{0.67}Ca_{0.33}MnO_3$ films and measurement of the strain-magnetization coupling coefficient¹ , S. SINGH, M.R. FITZSIMMONS, T. LOOKMAN, Los Alamos National Laboratory, H. JEEN, Oak Ridge National Laboratory, M.A. ROLDAN, Complutense University, Madrid 28040, Spain, M. VARELA, Oak Ridge National Laboratory, A. BISWAS, University of Florida — We have characterized the non-uniformity of chemical and magnetic properties of $(La_{0.4}Pr_{0.6})_{0.67}Ca_{0.33}MnO_3$ (LPCMO) films grown on $NdGaO_3$ using polarized neutron reflectometry (PNR). Our data indicate that the films exhibit coexistence of different magnetic phases as a function of depth. The variation of magnetism with depth is correlated with a variation of chemical composition with depth. Using PNR we also measured the magnetization depth profile of the LPCMO film as a function of applied bending stress. From these measurements we were able to obtain values for the coupling coefficients relating strain to the variation of the magnetization depth profile. Our results suggest that application of compressive (tensile) bending stress increases (suppresses) magnetization. We will discuss the implications of our results on the prevailing theories of the role of strain on phase separation in manganites.

¹Work was supported by the Office of Basic Energy Science, U.S. Department of Energy, BES-DMS funded by the Department of Energy's Office of Basic Energy Science and the National Science Foundation (DMR-0804452) (HJ and AB).

8:12AM P9.00002 The dead layer in $La_{0.67}Sr_{0.33}MnO_3$ thin films , HANS BOSCHKER, JAAP KAUTZ, MARK HUIJBEN, Mesa+ Institute for Nanotechnology, JO VERBEECK, RICARDO EGOAVIL, SARA BALS, STAF VAN TENDELOO, EMAT Antwerp, GERTJAN KOSTER, DAVE BLANK, GUUS RIJNDERS, Mesa+ Institute for Nanotechnology, MESA+ TEAM, EMAT TEAM — $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) films have an interfacial dead layer that is attributed to either changes in the Mn valence state at the interface, a change in the Mn orbital ordering at the interface or a change in the magnetic exchange interaction due to a structural reconstruction at the interface. We studied the dead layer in LSMO films grown on $SrTiO_3$ (STO) substrates. To directly compare the effect of the polar discontinuity on the dead layer, we removed the polar discontinuity by compositional interface engineering. We also studied films in the (110) direction. We found the presence of the dead layer in all types of films and interface configurations. The LSMO (001) samples with compositional interface engineering have the thinnest dead layer (2 nm). Using electron energy loss spectroscopy, we found no deviations in the Mn valence state at the interface. Using linear dichroism in x-ray absorption spectroscopy, we also found no deviations in the orbital ordering. Therefore, we suggest that the dead layer is caused by the structural reconstruction at the interface. An outlook towards preventing the structural reconstruction and further improving the interfacial properties of the LSMO thin films will be given.

8:24AM P9.00003 Angular dependence of the anomalous Hall effect in $La_{0.8}Sr_{0.2}MnO_3$ films , NETANEL NAFTALIS, NOAM HAHAM, Department of Physics, Nano-magnetism Research Center, Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, JASON HOFFMAN, MATTHEW MARSHALL, CHARLES AHN, Department of Applied Physics, Yale University, LIOR KLEIN, Department of Physics, Nano-magnetism Research Center, Institute of Nanotechnology and Advanced Materials, Bar-Ilan University — The anomalous Hall effect (AHE) is an intriguing magnetotransport phenomenon linked to various intrinsic and extrinsic mechanisms. While for some conductors quantitative understanding of this phenomenon has been achieved, the understanding of the AHE in the manganites is far from comprehensive. We measured the transverse resistivity (ρ_{xy}) of thin films of $La_{0.8}Sr_{0.2}MnO_3$ at temperatures between 5 to 200 K and magnetic fields up to 9 T as a function of the angle θ between the film normal and the magnetic field. We find that for fields above 4 T, for which the magnetization (M) is practically parallel to the magnetic field, $\rho_{xy} = A \cos \theta + B \cos(3\theta)$. The first term is attributed to the ordinary and anomalous Hall effect, and the unexpected $\cos(3\theta)$ term is attributed only to the anomalous Hall effect. We show that the angular dependence of the longitudinal resistivity, ρ_{xx} , and of the magnitude of M cannot explain the existence of a $\cos(3\theta)$ term. We discuss the implication of this term on the possible mechanisms of the anomalous Hall effect in this compound.

8:36AM P9.00004 Effect of electronic reconstruction on the superconducting properties in high T_C superconducting spin valve structures¹, YAOHUA LIU, L.Y. ZHU, A. HOFFMANN, S.G.E. TE VELTHUIS, Argonne National Laboratory, USA, N.M. NEMES, C. VISANI, J. TORNOS, C. LEON, J. SANTAMARIA, Universidad Complutense de Madrid, Spain, M.R. FITZSIMMONS, M. ZHERNENKOV, Los Alamos National Laboratory, USA — We have studied the angular dependence of the magnetoresistance (MR) and magnetization alignment in $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ (LCMO)/ $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO)/LCMO trilayers in the superconducting transition region. The top and bottom LCMOs have different easy-axis coercivities (H_C 's) so that the mutual alignment between the two LCMO's magnetizations is tunable with in-plane rotation of the magnetic field. When the amplitude of the applied field is between the two H_C 's, the MR shows a quasi-four-fold symmetry, an angular hysteresis between clockwise and anticlockwise rotations, and a unidirectional offset along the initial saturation direction. We find that the MR is not correlated with the LCMO's magnetization alignment. More interestingly, the angular dependence of the MR is understandable by the alignment between the applied magnetic field and the (exponential tail of the) induced exchange fields in YBCO, the latter of which originate from the electronic reconstruction at the LCMO/YBCO interfaces. Our results support the scenario recently proposed by Salafranca and Okamoto [Phys. Rev. Lett. **105**, 256804 (2010)], which explains the inverse superconducting spin switch effect in this system.

¹Supported by US-DOE, Office of Science, BES, contract No. DE-AC02-06CH11357 and DE-AC52-06NA25396, and by the Spanish MICINN.

8:48AM P9.00005 STEM-EELS and theoretical analysis of the electronic structure in cuprate-manganite heterostructures¹, J. SALAFRANCA, J. TORNOS, C. LEÓN, J. SANTAMARIA, Universidad Complutense de Madrid, Spain, M. VARELA, S.J. PENNYCOOK, Oak Ridge National Laboratory, TN, E. DAGOTTO, University of Tennessee, TN; Oak Ridge National Laboratory, TN — Scanning transmission electron microscopy in combination with electron energy loss spectroscopy allows sub-nanometer scale resolution mapping of the formal oxidation state of the transition metal ions in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}/\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ superlattices. The experiments show an unexpected excess of valence electrons near the interface. We compare these results with tight binding model calculations where Coulomb interactions are included within Hartree approximation. Neither the polar catastrophe mechanism nor the mismatch of chemical potentials between the two materials are sufficient to account for the observed profile. We study the effect of oxygen vacancies near the interface and find that they can explain the measured electronic structure.

¹Acknowledgements: Research sponsored by the European Research Council Starting Investigator Award program (JS) and the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division (MV,ED,SJP).

9:00AM P9.00006 Phase Diagram of Thin Film Oxides Growth by Pulsed Laser Deposition¹, HANGWEN GUO, University of Tennessee, Knoxville; Oak Ridge National Laboratory, DALI SUN, Oak Ridge National Laboratory, JIAN SHAO, Fudan University, China, ZAC WARD, ZHENG GAI, IVAN KRAVCHENKO, Oak Ridge National Laboratory, WENBIN WANG, University of Tennessee, Knoxville; Oak Ridge National Laboratory, JIAN SHEN, University of Tennessee, Knoxville; Fudan University, China, XIAOSHAN XU, Oak Ridge National Laboratory — We present a qualitative analysis of the microscopic thermo-dynamical origin of thin film oxides growth using the pulsed laser deposition technique. A phase diagram containing different growth mechanisms has been established. By tuning growth parameters experimentally in $[\text{LaSr}]\text{MnO}_3/\text{SrTiO}_3$ system, we observe an excellent fit of thin film morphologies to our growth phase diagram. Our results offer guidance on controlling morphology, stoichiometry and crystallinity of oxides thin films.

¹Research sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy

9:12AM P9.00007 Domain Structures in Perovskite Oxide Superlattices¹, YAYOI TAKAMURA, Dept. Chemical Engineering and Materials Science, University of California, Davis — Perovskite oxides possess a wide range of technologically relevant functional properties including ferromagnetism, ferroelectricity, and superconductivity. Furthermore, the interfaces of perovskite oxides have been shown to exhibit unexpected functional properties not found in the constituent materials. These functional properties arise due to various structural and chemical changes as well as electronic and/or magnetic interactions occurring over nanometer length scales at the interfaces. In order to understand how these interfacial effects impact the ferromagnetic (FM) properties of the half metal $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (LSMO), we have examined superlattices composed of LSMO sublayers alternating with either the antiferromagnetic (AFM) insulator $\text{La}_{0.7}\text{Sr}_{0.3}\text{FeO}_3$ (LSFO) or the non-magnetic metal $\text{La}_{0.5}\text{Sr}_{0.5}\text{TiO}_3$ (LSTO). A comprehensive approach consisting of bulk magnetization, magneto-transport measurements, and scanning transmission electron microscopy as well as soft x-ray magnetic spectroscopy and microscopy has been used to fully characterize the properties of the interfaces. We find that the nature of the charge transfer across the interfaces affects the FM properties of LSMO, such that at a given sublayer thickness, the LSMO/LSTO system displays a similar Curie temperature but a higher saturation magnetization than the LSMO/LSFO system. For a specific range of sublayer thicknesses, the LSMO/LSFO system displays a unique spin-flop coupling where the FM moments and the AFM spin axis maintain a perpendicular orientation relative to one another. Through this coupling mechanism, the direction of the AFM spin axis can be reoriented with an applied magnetic field. In this talk, I will discuss how these interfacial phenomena contribute to the types of FM and AFM domain patterns observed in the individual layers in the superlattices.

¹Funding for this work was provided by the National Science Foundation (DMR 0747896). Portions of this work was carried out at the Center for Nanophase Materials Science and the Advanced Light Source.

9:48AM P9.00008 Temperature dependent optical properties of thin films of the doped manganite $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$ ¹, NAWREEN ANAND, NAVEEN MARGANKUNTE, DAVID TANNER, Department of Physics, University of Florida, HYOONGJEEN JEEN, Oak Ridge National Laboratory, Tennessee, AMLAN BISWAS, Department of Physics, University of Florida — Reflectivity as a function of temperature has been measured for thin film samples of the manganite $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$ across the metal-insulator transition. The optical properties in the infrared and visible range were determined by fits to a Drude-Lorentz model, using exact formulas for the thin film optics and the measured properties of the substrate. The phonon modes were identified and verified with lattice dynamical calculations for distorted orthorhombic crystal structure of the material. The reflectance has a strong temperature dependence in the far infrared and in the region of the phonons, rising as the temperature is lowered and the film becomes metallic. In the near-infrared and visible range, there are conductivity peaks due to electronic band transition shifts to the lower frequencies with decreasing temperature. We also observe the spectral weight shift with temperature.

¹Supported by the US DOE through contract DE-FG02-02ER45984 and NSF DMR 0804452.

10:00AM P9.00009 Induced ferromagnetism in $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{LaFeO}_3$ interfaces and its role on magnetic tunnel junctions¹, FLAVIO Y. BRUNO, C. VISANI, CNRS, France, A. RIVERA-CALZADA, J. TORNOS, N.M. NEMES, Universidad Complutense de Madrid, Spain, S. VALENCIA, R. ABRUDAN, Helmholtz-Zentrum-Berlin für Materialien und Energie, Germany, Y. LIU, J.W. FREELAND, S.G.E. TE VELTHUIS, Argonne National Laboratory, USA, M. GARCIA-HERNANDEZ, ICMN, Spain, M. VARELA, S.J. PENNYCOOK, Oak Ridge National Laboratory, USA, J. SANTAMARIA, Universidad Complutense de Madrid, Spain, J.E. VILLEGAS, M. BIBES, A. BARTHELEMY, CNRS, France — Magnetic tunnel junctions with antiferromagnetic barriers have so far been poorly studied. We have investigated $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (LSMO)/ LaFeO_3 (LFO)/LSMO magnetic tunnel junctions (MTJ) where LFO is an antiferromagnetic tunnel barrier. We examined the tunneling magnetoresistance (TMR) behavior of junctions as a function of temperature finding a 30% maximum at 100K. If the top ferromagnetic electrode is replaced by a non-ferromagnetic metal (Au) we still observe a TMR effect, which we attribute to spin filtering. We will show that this effect is connected to the presence of an induced (ferro)magnetic moment in the nominally antiferromagnetic LFO barrier at the interface with LSMO, which was detected by XMCD measurements. Finally, we will conclude discussing the new opportunities offered by such type of interfaces to obtain large spin filtering effects.

¹Research at ORNL sponsored Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division (MV, SJP)

10:12AM P9.00010 Magnetic studies on thin films of $\text{La}_{0.65}\text{Pb}_{0.35}\text{MnO}_3$ ¹, STEVEN TIDROW, THOMAS MION, MAGDALENA DORINA CHIPARA, The University of Texas Pan American, ANDREI SOKOLOV, LIU SY-HWANG, RALPH SKOMSKI, PETER DOWBEN, SHIREEN ADENWALLA, University of Nebraska-Lincoln, MIRCEA CHIPARA, The University of Texas Pan American, DAVID J SELLMYER, University of Nebraska-Lincoln, THE UNIVERSITY OF TEXAS PAN AMERICAN TEAM, UNIVERSITY OF NEBRASKA-LINCOLN TEAM — Magnetic and structural investigations on thin films of $\text{La}_{0.65}\text{Pb}_{0.35}\text{MnO}_3$ deposited on a LaAlO_3 substrate are reported. Transmission electron microscopy showed an almost epitaxial growth of the perovskite film, indicating fourfold symmetry for both substrate and thin film. Low Energy Electron Diffraction and Wide Angle X-Ray Scattering support transmission electron microscopy and scanning tunneling microscopy results. Magneto-optical Kerr effect data are consistent with the fourfold symmetry. Ferromagnetic Resonance experiments performed in the X band revealed a more complex structure. The angular dependence of the resonance line width, resonance line intensity, and double integral of the resonance line support a slightly distorted four-fold symmetry whereas the angular dependence of the resonance line position has a two-fold symmetry. This discrepancy was ascribed to the mismatch between the film and the substrate and it is considered as a proof of the sensitivity of ferromagnetic resonance.

¹The research was funded by: NSF-MRSEC grant to the University of Nebraska-Lincoln and U.S. Army Research Office grant #W911NF-08-1-0353 awarded to the University of Texas Pan-American.

10:24AM P9.00011 Using ultrafast optical pump-probe spectroscopy to reveal coexisting magnetic orders in epitaxial RMnO_3 films, JINGBO QI, LI YAN, STUART TRUGMAN, JIAN-XIN ZHU, QUANXI JIA, ANTOINETTE TAYLOR, ROHIT PRASANKUMAR, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, CENTER FOR INTEGRATED NANOTECHNOLOGIES, LOS ALAMOS NATIONAL LABORATORY TEAM — Recent discoveries of spin-driven ferroelectricity in perovskite manganites, RMnO_3 (R =rare-earth ions), have attracted enormous interest in the research of multiferroics. Although extensive experimental and theoretical studies have already been done on single crystal RMnO_3 , there are only a few reports describing the properties of RMnO_3 thin films. Here, we choose two typical materials in RMnO_3 manganites as examples: SmMnO_3 and TbMnO_3 . Previously, ultrafast optical pump-probe spectroscopy has proven to be an ideal technique for unraveling the interplay between different orders in the time domain. In this work, we used this technique to study ultrafast dynamics in epitaxial SmMnO_3 and TbMnO_3 films grown on SrTiO_3 substrates. At low temperatures, we observed an extraordinarily slow rising process, with a timescale of tens of picoseconds, followed by another decay process with a relaxation time of hundreds of picoseconds. Analysis of the time constants associated with these two processes as a function of temperature reveals that antiferromagnetic, ferromagnetic, and ferroelectric orders can coexist in these materials.

10:36AM P9.00012 Influence of growth mode & substrate doping on the reversed remanent magnetic configuration in $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ films, D.A. ARENA, C.S. NELSON, National Synchrotron Light Source, Brookhaven Nat. Lab, J.-S. LEE, C.-C. KAO, SSRL, SLAC Nat. Accelerator Lab, E. NEGUSSE, Physics Dept, Montana State Univ., T.S. SANTOS, Center for Nanoscale Materials, Argonne Nat. Lab — Charge transfer effects which can occur at oxide interfaces can modify the properties of oxide thin films. In such a system, an unusual reversed orientation of the remanent magnetic state was observed recently for $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ on Nb-doped SrTiO_3 (001) deposited via pulsed laser deposition¹. We observe a similar effect for $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ grown via molecular beam epitaxy, a deposition method with different growth kinetics, onto both Nb-doped and undoped SrTiO_3 (STO) substrates. The reversed magnetic state occurs in both samples, and a region of slightly increased charge density was revealed with x-ray reflectivity. Intriguingly, the onset of the reversed remanent state occurred at different temperatures: $\sim 125\text{K}$ for the Nb:STO substrate and $\sim 240\text{K}$ for the undoped STO substrate. High resolution x-ray diffraction reveals a subtle relationship with the cubic-to-tetragonal structural transition of the STO substrate at $\sim 105\text{K}$. Our results point to an additional mechanism for controlling the magnetism in mixed-valence oxide films².

¹J.-S. Lee *et al.*, *Phys. Rev. Lett.* **105**, 257204 (2010)

²J.-S. Lee *et al.*, *J. Phys. D: Appl. Phys.* **44**, 245002 (2011)

10:48AM P9.00013 Magnetic Exchange Between Superconducting and Ferromagnetic Oxide Layers, SEAN GIBLIN, JON TAYLOR, ISIS Facility, UK, JON DUFFY, University of Warwick, UK, STEPHEN DUGDALE, University of Bristol, UK, T. NAKAMURA, SPring-8 Japan, Japan, JACOBO SANTAMARIA, Universidad de Complutense de Madrid, Spain — The origins of high temperature superconductivity and the rich phase diagrams in complex oxides are still a matter of contention that have stimulated many novel experimental studies and observations. Recently the improvement of layer by layer growth techniques of thin films has enabled investigations of both bulk and surface properties. For most common superconductors the order parameter is thought to be antagonistic to that of the exchange mechanism in ferromagnets. Accurately grown thin films have enabled these competing interactions to be probed experimentally. In particular, the growth of epitaxial oxide layers, with well-characterized atomically flat interfaces, consisting of superconducting layers of $\text{YBa}_2\text{Cu}_3\text{O}_7$ (YBCO) and lattice-matched ferromagnetic $\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3$ (LCMO) has flourished. Using XMCD we demonstrate that the known superexchange between Mn and Cu across the YBCO/LCMO is modified when an apparent critical thickness of the superconducting layer is reduced. All samples show an apparent exchange below the superconducting transition but above it is dependent on the YBCO thickness. Possible origins of this behaviour will be discussed.

Wednesday, February 29, 2012 8:00AM - 11:00AM —
Session P10 DAMOP GQI: Invited Session: Quantum Simulations 210A

8:00AM P10.00001 Quantum simulations and artificial gauge fields with ultracold atoms , IAN SPIELMAN, NIST — Here I present our experimental work synthesizing gauge fields for Bose-Einstein condensates (BECs). I will first summarize our earlier work creating a scalar (abelian) gauge field (akin to the electromagnetic vector potential) and then focus in detail our current work creating a matrix valued (although still abelian) gauge field. I will discuss this gauge field in the language of spin-orbit coupling where it consists of an equal sum of Rashba and Dresselhaus couplings. Specifically, we couple two internal states of rubidium 87 with a pair of “Raman” lasers and load our BEC into the resulting adiabatic eigenstates. In agreement with theory, we observe that below a critical coupling strength our BEC has well defined spin degrees of freedom and acts like a spin-orbit-coupled spin-1/2 Bose gas. As a function of the Raman laser strength, a new exchange-driven interaction between the two dressed spins develops, which drives a (quantum) phase transition from a state where the two dressed spin states spatially mix, to one where they phase separate. Our 3D mean field theory accurately locates the critical laser strength for this transition.

8:36AM P10.00002 Quantum simulations with trapped Ca^+ ions , RAINER BLATT, Innsbruck University — No abstract available.

9:12AM P10.00003 Circuit QED Simulation of Interacting Bosons with Microwave Polaritons¹ , STEVEN GIRVIN, Yale University — A polariton is a coherent superposition of a photon and an electronic excitation such as an exciton. Polaritons can have very low mass (associated with the photon component) and repulsive interactions (associated with the exciton component). Recent experimental progress has observed Bose-Einstein condensation and superfluidity in polaritons in semiconductor quantum wells. In this talk I will discuss the possibility that many-body physics and quantum phase transitions of interacting polaritons [1-3] can be observed in arrays of microwave resonators containing superconducting qubits [4-6]. If the qubits are not far-detuned from the cavities, the natural excitations are coherent superpositions of cavity and qubit excitations and they have interactions acquired from the anharmonicity of the qubits. These interactions can lead to quantum phase transitions in the limit of weak dissipation. It may even be possible to simulate the fractional quantum Hall effect for bosons by coupling the polaritons between sites using superconducting structures which act as ‘circulators’ that break time-reversal and charge-conjugation symmetry. In light of recent progress in achieving very long-coherence times for superconducting qubits and strong qubit coupling to microwave photons, experimental prospects for observing quantum phase transitions in microwave resonator lattices will be described.

[1] A. D. Greentree, et al., *Nat. Phys.* **2**, 856 (2006).

[2] M. J. Hartmann et al., *Nat. Phys.* **2**, 849 (2006).

[3] D. G. Angelakis, M. F. Santos, and S. Bose, *Phys. Rev. A* **76**, 031805 (2007).

[4] J. Koch and K. Le Hur, *Phys. Rev. A* **80**, 023811 (2009).

[5] ‘Time-reversal symmetry breaking in circuit-QED based photon lattices,’ Jens Koch, Andrew A. Houck, Karyn Le Hur, and S. M. Girvin, *Phys. Rev. A* **82**, 043811 (2010).

[6] ‘Synthetic gauge fields and homodyne transmission in Jaynes-Cummings lattices,’ A. Nunnenkamp, Jens Koch, and S. M. Girvin, *New J. Phys.* **13** 095008 (2011).

¹Work supported by the NSF, ARO, LPS and NSA. This work is a collaboration with Jens Koch, Karyn Le Hur, Andreas Nunnenkamp, Andrew Houck and Claudia DeGrandi.

9:48AM P10.00004 Quantum Hall physics with photons and its application¹ , MOHAMMAD HAFEZI, Joint Quantum Institute — Phenomena associated with the topological properties of physical systems can be naturally robust against perturbations. This robustness is exemplified by quantized conductance and edge state transport in the quantum Hall and quantum spin Hall effects. Here we demonstrate how quantum spin Hall Hamiltonians can be simulated with linear optical elements using a network of coupled resonator optical waveguides (CROW) in two dimensions. Key features of quantum Hall systems, including the characteristic Hofstadter butterfly and robust edge state transport, can be obtained in such systems. As a specific application, we show that topological protection can be used to improve the performance of optical delay lines and to overcome some limitations related to disorder in photonic technologies. Furthermore, the addition of an optical non-linearity to our proposed system leads to the possibility of implementing a fractional quantum Hall state of photons, where phenomenon such as fractional statistics may be observable.

¹This work was partially supported by the US Army Research Office MURI award W911NF0910406

10:24AM P10.00005 Mixed Bose-Fermi Mott Phases and Phase Transitions¹ , EHUD ALTMAN, Weizmann Institute of Science — A recent experiment with an ultra-cold mixture of ^{174}Yb and ^{173}Yb atoms in an optical lattice [S. Sugawa et al. *Nature Physics* **7**, 642 (2011)] found a remarkable quantum phase that can be described as a mixed Mott insulator. Such a an incompressible state established at integer combined filling of the two species, must have residual low energy Fermionic degrees of freedom associated with relative motion of the two species. I will discuss the novel quantum states formed by the composite Fermions in the mixed Mott insulator as well as the unconventional phase transitions separating these states from the compressible Bose-Fermi mixture established at weak interactions. Finally I will propose to utilize the mixed Mott insulator as a quantum simulator for models of the doped Mott insulator relevant to high T_c superconductivity. The new approach, where the bosonic atoms play the role of doped holes offers significant advantages over direct simulation of the Hubbard model. In particular the mixed Mott plateau naturally provides a flat trap potential to the doped holes, while the hole doping is easily tuned by varying the relative fraction of the bosons.

¹Support from the Israel Science Foundation and from DIP is gratefully acknowledged

Wednesday, February 29, 2012 8:00AM - 11:00AM —
Session P11 DMP: Focus Session: Graphene Structure, Stacking, Interactions: Strain and Stacking 210B

8:00AM P11.00001 Non-Abelian gauge potentials in graphene bilayers , JOSE GONZALEZ, PABLO SAN-JOSE, Instituto de Estructura de la Materia, CSIC, Madrid, FRANCISCO GUINEA, Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid — We discuss the effect of spatial modulations in the interlayer hopping of graphene bilayers, such as those that arise upon shearing or twisting. We show that their single-particle physics, characterized by charge localization and recurrent formation of zero-energy bands as the pattern period L increases, is governed by a non-Abelian gauge potential arising in the low-energy electronic theory due to the coupling between layers. We find that such gauge-type couplings give rise to a confining potential that, for certain discrete values of L , localizes states at zero energy in particular regions of the Moire patterns. We also draw the connection between the recurrence of the flat zero-energy bands and the non-Abelian character of the potential.

8:12AM P11.00002 Electronic Topological Transition in Sliding Bilayer Graphene, YOUNG-WOO SON, SEON-MYUNG CHOI, YOON PYO HONG, SUNGJONG WOO, Korea Institute for Advanced Study, Seoul, Korea, SEUNG-HOON JHI, POSTECH, Pohang, Korea — We demonstrate theoretically that the topology of energy bands and Fermi surface in bilayer graphene undergoes a very sensitive transition when an extremely tiny lateral interlayer shift occurs in arbitrary directions. The phenomenon originates from a generation of an effective non-Abelian vector potential in the Dirac Hamiltonian by the sliding motions. The characteristics of the transition such as pair annihilations of massless Dirac fermions are dictated by the sliding direction owing to a unique interplay between the effective non-Abelian gauge fields and Berry's phases associated with massless electrons. The transition manifests itself in various measurable quantities such as anomalous density of states, minimal conductivity, and distinct Landau level spectrum.

8:24AM P11.00003 Fictitious gauge fields in bilayer graphene, EROS MARIANI¹, ALEX PEARCE, University of Exeter (UK), FELIX VON OPPEN, Freie Universitaet Berlin (Germany) — We discuss the effect of elastic deformations on the electronic properties of bilayer graphene membranes. Distortions of the lattice translate into fictitious gauge fields in the electronic Dirac Hamiltonian which are explicitly derived for arbitrary elastic deformations. We include gauge fields associated to intra- as well as inter-layer hopping terms and discuss their effects on the strain-induced Lifshitz transition and on the electron-phonon resistivity. Of special interest is the appearance of a linear coupling for flexural modes which is shown to dominate the temperature-dependent resistivity in suspended samples with low tension.

¹College of Engineering, Mathematics and Physical Sciences, Stocker Road EX4 4QL, Exeter (UK)

8:36AM P11.00004 Effective theory of rotationally faulted multilayer graphene, MARKUS KINDERMANN, Georgia Institute of Technology — The crystal structure of graphene multilayers with an interlayer twist is characterized by Moiré patterns with various commensurabilities. Also the electronic structure of the material, which grows for instance epitaxially on SiC, is remarkably rich. In this talk an effective low-energy description of such multilayers will be discussed. In certain limits the theory reduces to a (single-layer) Dirac model with space-dependent potentials and mass term. The consequences of this theory will be explored and comparison with experiment will be made. The discussion of experimental consequences will focus on the Landau quantization in a magnetic field, where much experimental data is available. For instance, a spatially modulated splitting of the zeroth Landau level in the material has been observed through scanning tunneling spectroscopy [1]. That splitting finds a natural explanation in the space-dependent mass term of the presented theory [2]. Also a large low-field splitting of higher Landau levels recently observed in graphene multilayers [3] will be shown to follow from that theory. Finally, a theoretically expected [4] amplitude modulation of the Landau level wavefunctions on the top layer of the material will be discussed.

[1] D. L. Miller, K. D. Kubista, G. M. Rutter, M. Ruan, W. A. de Heer, M. Kindermann, P. N. First, and J. A. Stroscio, *Nature Physics* **6**, 811 (2010).

[2] M. Kindermann and P. N. First, *Phys. Rev. B* **83**, 045425 (2010).

[3] Y. J. Song, A. F. Otte, Y. Kuk, Y. Hu, D. B. Torrance, P. N. First, W. A. de Heer, H. Min, S. Adam, M. D. Stiles, A. H. MacDonald, and J. A. Stroscio, *Nature* **467**, 185 (2010).

[4] M. Kindermann and E. G. Mele, *Phys. Rev. B* **84**, 161406(R) (2011).

9:12AM P11.00005 High-temperature topological insulator states in strained graphene, DMITRY ABANIN, Harvard University, DMITRO PESIN, University of Texas, Austin — Recently, it was realized that the electronic properties of graphene can be manipulated via mechanical deformations, which opens prospects for both studying the Dirac fermions in new regimes and for device applications. More specifically, non-uniform strains give rise to pseudomagnetic fields that are opposite in the two valleys of Dirac fermions. Certain natural configurations of strain generate large nearly uniform pseudo-magnetic field, leading to flat spin- and valley-degenerate Landau levels (LL). Here we consider the effect of the Coulomb interactions in strained graphene with nearly uniform pseudo-magnetic field. We show that the spin/valley degeneracies of the LL get lifted, giving rise to topological insulator-like states. We find that both anomalous quantized Hall states and quantum spin Hall states can be realized. These many-body states are characterized by quantized conductance and persist to high temperature scale set by the Coulomb interactions. This work provides a new route to designing robust topological insulator states in mesoscopic graphene and other 2D Dirac materials.

[1] D. A. Abanin, D. A. Pesin, submitted.

9:24AM P11.00006 Theory of topological phases in multilayer Graphene, XIAO LI, ZHENHUA QIAO, QIAN NIU, Department of Physics, The University of Texas at Austin — We present microscopic theories of possible topological phases (i.e. quantum anomalous Hall effect, quantum valley Hall effect, and two-dimensional topological insulators) in bilayer graphene systems. We show the phase diagrams as well as the resulting nontrivial edge states in these systems. We further generalize our findings to trilayer graphene systems, where similar topological states may exist. Finally, we give low energy effective models to reveal the underlying physics of these topological states.

9:36AM P11.00007 The correct solution for strain-induced pseudo vector potentials in graphene, ALEXANDER L. KITT, Boston University, Boston, MA, VITOR M. PEREIRA, National University of Singapore, Singapore, ANNA K. SWAN, BENNETT B GOLDBERG, Boston University, Boston, MA — Prior calculations of the strain-induced pseudo vector potential considered only the change in the nearest neighbor hopping energy in their derivations [1,2]. Here we show that including lattice deformations introduces new terms of the same order in strain. These terms are different at each K point, causing each population of electrons to feel different strain induced pseudo magnetic fields. We use isotropic strain, a situation where lattice deformations solely determine the pseudo vector potential, to illustrate the conceptual importance of these new terms. Finally, we exhibit how the additional terms force us to rethink the strain geometries that were previously thought to generate particular pseudo magnetic fields.

[1] A.H. Castro Neto, et al. *Rev. Mod. Phys.* **81**, 109 (2009). [2] M.A.H. Vozmediano, M.I. Katsnelson, and F. Guinea, *Phys. Rep.* **496**, 109 (2010).

9:48AM P11.00008 Two-Dimensional Topological Insulator State and Topological Phase Transition in Bilayer Graphene, ZHENHUA QIAO, WANG-KONG TSE, Department of Physics, The University of Texas at Austin, Austin, Texas 78712 USA, HUA JIANG, International Center for Quantum Materials, Peking University, Beijing 100871, China, YUGUI YAO, School of Physics, Beijing Institute of Technology, Beijing 100081, China, QIAN NIU, Department of Physics, The University of Texas at Austin, Austin, Texas 78712 USA — In this talk, we show that gated AB-stacking bilayer graphene can host a quantum phase transition from a quantum valley Hall (QVH) insulator to a two-dimensional strong topological insulator (TI) as a function of Rashba spin-orbit (SO) coupling. Different from a conventional TI phase, the edge modes of our strong TI phase exhibit both spin and valley filtering, and thus share the properties of both TI and QVH insulators. The strong TI phase remains robust in the presence of weak intrinsic SO coupling.

10:00AM P11.00009 Disorder-induced inhomogeneity in bilayer graphene¹, DAVID ABERGEL, University of Maryland — We describe the effect of charge density inhomogeneity (electron and hole puddles) and a spatially fluctuating band gap caused by charged impurity disorder in bilayer graphene. We derive a phenomenological averaging technique to calculate $\frac{d\mu}{dn}$ in the presence of this disorder and apply it recent experimental measurements in suspended bilayer graphene. This work was done in collaboration with S. Das Sarma, E. Hwang, and H. Min.

¹Support from US-ONR, NRI-SWAN, and UMD-CNAM

10:12AM P11.00010 Raman spectra of strained bilayer graphene, DUHEE YOON, SUNYOUNG JEGAL, YUJIN CHO, Department of Physics, Sogang University, Seoul 121-742, Korea, YOUNG-WOO SON, Korea Institute for Advanced Study, Seoul 130-722, Korea, HYEONSIK CHEONG, Department of Physics, Sogang University, Seoul 121-742, Korea — In the Raman spectra of strained single layer graphene, modified electron and phonon dispersions result in the splitting of the double resonance 2D Raman band. It originates from significant changes in the resonant conditions owing to both the distorted Dirac cones and anisotropic modifications of the phonon dispersion under uniaxial strains [D. Yoon et al., Phys. Rev. Lett. **106**, 155502 (2011)]. In unstrained bilayer graphene, the Raman 2D band consists of 4 Lorentzian peaks corresponding to the double resonance Raman scattering processes between the two conduction bands and the two valence bands. Under uniaxial strain, each of the four peaks in the Raman 2D band. We examined the polarization behaviors of the split 2D band and analyzed using a model similar to the one used for single layer graphene.

10:24AM P11.00011 Field Effects on the Optical Vibrations in Bilayer Graphene, JIA-AN YAN, Department of Physics, Astronomy and Geosciences, Towson University, Towson, MD 21252 USA — A first-principles study of the optical phonon modes in bilayer graphene (BLG) under a perpendicular electric field is presented. It is found that the electric field breaks the inversion symmetry of BLG and mixes the eigenvectors of the in-phase and out-of-phase optical modes. Detailed analysis shows that the mixing effect is more evident on the out-of-plane optical modes than on the in-plane modes. The field effects on the electron-phonon coupling in BLG will also be discussed.

10:36AM P11.00012 Six-band nearest-neighbor tight-binding model for the π -bands of bulk graphene and graphene nanoribbons¹, TIMOTHY BOYKIN, The University of Alabama in Huntsville, MATHIEU LUISIER, Integrated Systems Laboratory, GERHARD KLIMECK, Purdue University, XUEPING JIANG, NEERAV KHARCHE, YU ZHOU, SAROJ NAYAK, Rensselaer Polytechnic Institute (RPI), RPI COLLABORATION — The commonly used single- p_z orbital first nearest-neighbor tight-binding model faces two main problems: (i) it fails to reproduce asymmetries in the bulk graphene bands; (ii) it cannot provide a realistic model for hydrogen passivation of the edge atoms. As a result, some armchair graphene nanoribbons (AGNRs) are incorrectly predicted as metallic. A new nearest-neighbor, three orbital per atom p/d tight-binding model [1] is built to address these issues. The parameters of the model are fit to bandstructures obtained from first-principles density-functional theory and many-body perturbation theory within the GW approximation, giving excellent agreement with the ab initio AGNR bands. This model is employed to calculate the current-voltage characteristics of an AGNR MOSFET and the conductance of rough-edge AGNRs, finding significant differences versus the single- p_z model. Taken together these results demonstrate the importance of an accurate and computational efficient band structure model for predicting the performance of graphene-based nanodevices. [1] T. B. Boykin, M. Luisier, G. Klimeck, X. Jiang, N. Kharche, Y. Zhou and S. Nayak, J. Appl. Phys. 109, 104304 (2011)

¹NSF, NSF PetaApps, NRI MIND, NICS, IFC, CCNI

10:48AM P11.00013 Electronic structures of geometrically restricted nanocarbons, ARTEM BASKIN, PETR KRAL, University of Illinois at Chicago — We use large scale ab-initio calculations to explore the electronic structures of graphene, graphene nanoribbons, and carbon nanotubes periodically perforated with nanopores. We disclose common features in electronic structures of these porous nanocarbons (PNCs) with nanopores of different size, shapes, and localization. We develop a unified picture that permits to analytically predict and systematically characterize metal-semiconductor transitions in PNCs, allowing mapping of their electronic structures on those in pristine nanocarbons [1]. In contrast to other studies, we show that porous graphene can be metallic for certain arrangements of the pores. When we replace pores by defects (such as SW 55-77), we observe similar features in the electronic structures of the formed nanocarbons. We also study magnetic ordering in these nanocarbons and show that the position of pores/defects can influence the ordering of localized electronic spin states. These periodically modified nanocarbons with highly tunable band structures have great potential applications in electronics and optics. [1] A.I. Baskin and P. Kral, Sci. Rep.1, 36 (2011).

Wednesday, February 29, 2012 8:00AM - 9:30AM –

Session P12 Tutorial for Authors and Referees 210C

8:00AM P12.00001 Tutorial for Authors and Referees — Editors from Physical Review Letters and Physical Review will provide information and tips for our less experienced referees and authors. This session is aimed at anyone looking to submit to or review for any of the APS journals, as well as anyone who would like to learn more about the authoring and refereeing processes. Topics for discussion will include advice on how to write good manuscripts, similarities and differences in writing referee reports for PRL and PR, and other ways in which authors, referees, and editors can work together productively. Following a short presentation from the editors, there will be a moderated discussion. Refreshments will be served.

Wednesday, February 29, 2012 8:00AM - 11:00AM –

Session P13 DMP GMAG: Focus Session: Low-Dimensional and Molecular Magnetism - Single-Molecule Magnets - Dynamics, structure and interactions 211

8:00AM P13.00001 Quantum Tunneling of Magnetization in Trigonal Single-Molecule Magnets, JUNJIE LIU, Department of Physics, University of Florida, ENRIQUE DEL BARCO, Department of Physics, University of Central Florida, STEPHEN HILL, NHMFL and Department of Physics, Florida State University — We perform a numerical analysis of the quantum tunneling of magnetization (QTM) that occurs in a spin $S = 6$ single-molecule magnet (SMM) with idealized C_3 symmetry. The deconstructive points in the QTM are located by following the Berry-phase interference (BPI) oscillations. We find that the $\hat{O}_4^3 (= \frac{1}{2}[\hat{S}_z, \hat{S}_+^3 + \hat{S}_-^3])$ operator unfreezes odd- k QTM resonances and generates three-fold patterns of BPI minima in all resonances, including $k = 0$! This behavior cannot be reproduced with operators that possess even rotational symmetry about the quantization axis. We find also that the $k = 0$ BPI minima shift away from zero longitudinal field. The wider implications of these results will be discussed in terms of the QTM behavior observed in other SMMs.

8:12AM P13.00002 Exploration of the Berry phase interference in a single-molecule magnets of trigonal symmetry, H.M. QUDDUSI, Department of Physics, University of Central Florida, J. LIU, Department of Physics, University of Florida, P.L. FENG, Department of Chemistry and Biochemistry, University of California at San Diego, E. DEL BARCO, Department of Physics, University of Central Florida, S. HILL, National High Magnetic Field Laboratory and Department of Physics, Florida State University, D.N. HENDRICKSON, Department of Chemistry and Biochemistry, University of California at San Diego — The quantum behavior of single-molecule magnets (SMM) is mainly governed by their molecular composition and crystallographic symmetries, thus playing an essential role in the tunneling dynamics. We present low temperature magnetometry measurements on a trigonal symmetric, low nuclearity Mn₃ SMM. The experiments are designed to explore the behavior of the tunnel splittings within the transverse field magnitude/direction phase space, by applying a transverse field (0-1 T) along different directions within the hard anisotropy plane of the molecules. The expected quantum interference pattern can be understood as an outcome of a competition between different intramolecular magnetic interactions. A multi-spin description using non-collinear zero-field splitting tensors and intra molecular dipolar interactions between the manganese ions is employed to explain the symmetry patterns.

8:24AM P13.00003 Investigation of the Barriers of Blocking of Magnetization In Strongly Anisotropic SMM By Ab Initio Methods, LIVIU CHIBOTARU, LIVIU UNGUR, University of Leuven — A large amount of data concerning the blocking barriers of reversal of magnetization in various complexes with strongly anisotropic metal ions (Ln^{III} , Co^{II}) became recently available. Understanding the mechanisms of formation of these barriers is of primary importance for an efficient design of Ln-based single-molecule magnet (SMM) and represents a challenging task for the theory. Here an ab initio based approach for the investigation of blocking barriers will be presented. The methodology will be applied for the construction of the blocking barriers and the understanding of the variation of SMM properties in the series of mixed 3d-4f trinuclear complexes Co-Ln-Co, Ln=Gd, Tb, Dy. In particular, the reasons for a more pronounced SMM behavior manifested by the gadolinium complex will be elucidated. Another example is a recently synthesized Dy_3 complex, for which the origin of magnetization steps in the hysteresis loops will be explained.

[1] T. Yamaguchi, J.-P. Costes, Y. Kishima, M. Kojima, Y. Sunatsuki, N. Bréfuel, J.-P. Tuchagues, L. Vendier, W. Wernsdorfer *Inorg. Chem.* **2010**, 49, 9125–9135.

8:36AM P13.00004 Decoherence: Intrinsic, Extrinsic, and Environmental¹, PHILIP STAMP, University of British Columbia — Environmental decoherence times have been difficult to predict in solid-state systems. In spin systems, environmental decoherence is predicted to arise from nuclear spins, spin-phonon interactions, and long-range dipolar interactions [1]. Recent experiments have confirmed these predictions quantitatively in crystals of Fe_8 molecules [2]. Coherent spin dynamics was observed over macroscopic volumes, with a decoherence Q -factor $Q_\phi = 1.5 \times 10^6$ (the upper predicted limit in this system being $Q_\phi = 6 \times 10^7$). Decoherence from dipolar interactions is particularly complex, and depends on the shape and the quantum state of the system. No extrinsic “noise” decoherence was observed. The generalization to quantum dot and superconducting qubit systems is also discussed. We then discuss searches for “intrinsic” decoherence [3,4], coming from non-linear corrections to quantum mechanics. Particular attention is paid to condensed matter tests of such intrinsic decoherence, in hybrid spin/optomechanical systems, and to ways of distinguishing intrinsic decoherence from environmental and extrinsic decoherence sources.

[1] Morello, A. Stamp, P. C. E. & Tupitsyn, Phys. Rev. Lett. **97**, 207206 (2006).

[2] S. Takahashi et al., Nature **476**, 76 (2011).

[3] Stamp, P. C. E., Stud. Hist. Phil. Mod. Phys. **37**, 467 (2006).

[4] Stamp, P.C.E., Phil. Trans. Roy. Soc. A (to be published)

¹PITP, NSERC, CIFAR

9:12AM P13.00005 The Effect of Uniaxial Pressure on the Spin Hamiltonian of Mn12-Ac Single-Molecule Magnet¹, JAMES ATKINSON², JONATHAN FRIEDMAN, Department of Physics, Amherst College, Amherst, Massachusetts 01002, C. BEEDLE, D. HENDRICKSON, Department of Chemistry & Biochemistry, UCSD, La Jolla, California 92093, Y. MYASOEDOV, E. ZELDOV, Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel, K. PARK, Department of Physics, Virginia Tech, Blacksburg, Virginia 24061 — We study the effect of uniaxial pressure on the magnetic hysteresis loops of the single-molecule magnet Mn12-Ac. We find that the application of pressure along the easy axis increases the fields at which quantum tunneling of magnetization occurs. Density functional theory (DFT) calculations yield the pressure dependence of the energy barrier for spin reversal that is consistent with the experimental results. The observations, when constrained by the DFT calculations, indicate that the pressure induces changes in both the second-order anisotropy constant D and the fourth-order anisotropy constant A .

¹Work supported by NSF grants DMR-0449516 and DMR-1006519.

²Current address: Department of Physics, University of Central Florida, Orlando, Florida 32816

9:24AM P13.00006 Mitigation of decoherence in crystals of a $\text{Ho}_x\text{Y}_{1-x}\text{W}_{10}$ ($x = 0.001$ to 0.25) single-molecule magnet, SANHITA GHOSH, SAITI DATTA, STEPHEN HILL, National High Magnetic Field Laboratory and Deptt. of Physics, Florida State University, Tallahassee, FL 32310, ENRIQUE DEL BARCO, Deptt. of Physics, University of Central Florida, Orlando, FL 32816, SALVADOR CARDONA-SERRA, EUGENIO CORONADO, Instituto de Ciencia Molecular, Universidad de Valencia, Polígono la Coma s/n, 46980 Paterna, Spain — Mononuclear lanthanide-based single-molecule magnets (SMMs) have attracted considerable recent attention due to their potential application in quantum information processing devices [Nat. Nanotechnol. **2**, 312 (2007)]. In these systems, the magnetization is associated with a single rare-earth ion, which facilitates mitigation of spin decoherence due to nuclear hyperfine and electron dipolar interactions via isotope purification and dilution. Their large magnetic moments enable coherent manipulation at low driving fields. We report multi-frequency electron paramagnetic resonance (EPR) studies on a Ho polyoxometalate (POM). Simulations indicate appreciable transverse spin-orbit anisotropy, resulting in a gap in the spectrum of several GHz between pairs of levels having the same nuclear projection (effectively a tunneling gap between excited electron-nuclear spin states). Measurements at 9 GHz reveal electron-spin-echoes at low temperatures. Remarkably, a T_2 time of several hundred nanoseconds is found for concentrated samples, with much longer values found in diluted samples containing deuterated solvent. We show that these long coherence times are related to the tunneling gap, which results in an insensitivity of the spin dynamics to dipolar field fluctuations.

9:36AM P13.00007 Single-molecule magnets “without” intermolecular interactions, W. WERNSDORFER, Institut Neel, CNRS, Grenoble, France, L. VERGNANI, M.J. RODRIGUEZ-DOUTON, A. CORNIA, INSTM, Uni-Modena e Reggio Emilia, Italy, P. NEUGEBAUER, A.L. BARRA, LNCMI, CNRS, Grenoble, France, L. SORACE, R. SESSOLI, INSTM, Uni-Firenze, Italy — Intermolecular magnetic interactions (dipole-dipole and exchange) affect strongly the magnetic relaxation of crystals of single-molecule magnets (SMMs), especially at low temperature, where quantum tunneling of the magnetization (QTM) dominates. This leads to complex many-body problems [1]. Measurements on magnetically diluted samples are desirable to clearly sort out the behaviour of magnetically-isolated SMMs and to reveal, by comparison, the effect of intermolecular interactions. Here, we diluted a Fe_4 SMM into a diamagnetic crystal lattice, affording arrays of independent and iso-oriented magnetic units. We found that the resonant tunnel transitions are much sharper, the tunneling efficiency changes significantly, and two-body QTM transitions disappear. These changes have been rationalized on the basis of a dipolar shuffling mechanism and of transverse dipolar fields, whose effect has been analyzed using a multispin model. Our findings directly prove the impact of intermolecular magnetic couplings on the SMM behaviour and disclose the magnetic response of truly-isolated giant spins in a diamagnetic crystalline environment.

[1] W. Wernsdorfer, et al, PRL **82**, 3903 (1999); PRL **89**, 197201 (2002); Nature **416**, 406 (2002); IS Tupitsyn, PCE Stamp, NV Prokof'ev, PRB **69**, 132406 (2004).

9:48AM P13.00008 How Weak Dipole Interactions Can Enhance of the Collective Coupling of an Ensemble of Single-molecule Magnets to a Microwave Cavity¹, JONATHAN FRIEDMAN, Amherst College Department of Physics, Amherst, MA 01002 — When N identical spins are on resonance with a resonant mode of an electromagnetic cavity, the coupling strength (Vacuum Rabi splitting) is enhanced by $\sqrt{N}$ [1]. Add some inhomogeneity so that the spins' resonant frequencies are distributed around the cavity frequency with width σ_ω , and this enhancement will remain as long as $\sigma_\omega < \sqrt{N}g_1$, where g_1 is the coupling strength of a single, isolated spin to the cavity [2]. Recent experiments have shown that $\sim 10^{16}$ spins in a crystal of the single-molecule magnet Fe_8 nevertheless exhibit the enhanced collective coupling to a cavity, despite substantial inhomogeneous broadening. I present numerical calculations that show that weak dipole interactions between the spins can enhance the coupling of the spins to the cavity, allowing collective coupling even when the inhomogeneous broadening is large (i.e. when $\sigma_\omega > \sqrt{N}g_1$).

[1] M. Tavis and F. W. Cummings, Phys. Rev. **170**, 379 (1968).
 [2] R. Houdre, R. P. Stanley and M. Illegems, Phys. Rev. A **53**, 2711 (1996).

¹Work supported by NSF grant no. DMR-1006519

10:00AM P13.00009 Quantum deflagration in Mn_{12} -acetate in the presence of a transverse field, PRADEEP SUBEDI, New York University, SAUL VELEZ, University of Barcelona, SHIQI LI, MYRIAM SARACHIK, CCNY, CUNY, JAVIER TEJADA, University of Barcelona, ANDREW KENT, New York University, SHREYA MUKHERJEE, GEORGE CHRISTOU, UF-Gainesville — Mn_{12} -acetate single crystal have been shown to exhibit abrupt reversal of the magnetic moment through propagation of a narrow front at subsonic velocities, termed magnetic deflagration [1]. Experiments where avalanches in Mn_{12} -acetate are triggered at a fixed applied field have shown that the velocity of the front has maxima at resonant fields (kH_o , $\text{H}_o = 0.45 \text{ T}$, $k > 1$), due to thermally assisted tunneling of magnetization [2]. Application of a transverse field increases the tunnel splitting, which increases the magnetic relaxation and allows us to explore the deflagration for the first time at small longitudinal fields ($k=0$ and 1). Using time resolved measurements of local magnetization by an array of micron sized Hall sensors at temperature of 350 mK , we present the measurements on both spontaneously ignited and triggered deflagration for a large transverse field ($> 3 \text{ T}$) allowing us to explore directly the effect of a significant tunneling splitting on both the ignition and the velocity of the front. [1] Y. Suzuki, et. al PRL **95**, 147201 (2005)
 [2] A. Hernandez-Minguez, et. al, PRL **95**, 217205 (2005)

10:12AM P13.00010 Demagnetizing effect in local magnetic measurements¹, BO WEN, CUNY-CCNY/GC, PRADEEP SUBEDI, NYU, YOSI YESHURUN, Bar-Ilan Univ., MYRIAM SARACHIK, CUNY-CCNY, ANDREW KENT, NYU, ANDREW MILLIS, Columbia Univ., ENRIC PARDO, Slovak Academy of Sciences, SHREYA MUKHERJEE, GEORGE CHRISTOU, Univ. of Florida — It is well-known that magnetic measurements need to be corrected for the presence of demagnetizing fields that depend on both χ and the sample shape. Calculated demagnetization factors are generally available in tabular form for standard shapes, such as ellipsoids, spheres, and parallelepipeds, thereby providing corrections for measurements of the magnetization of the entire sample. However, appropriate corrections are not available for measurements obtained by local probes, such as micron-size Hall sensors. In this talk we present calculations of the local demagnetizing field profile and show how these results can be applied to interpret local magnetization measurements in Mn_{12} -ac.

¹NSF-DMR-0451605, ARO-W911NF-08-1-0364, NSF-DMR-1006282, CHE-0910472 and Deutsche Forschungsgemeinschaft through a Deutsch-Israelische Projektkooperation

10:24AM P13.00011 Simulation of AC Susceptibility and Electronic Structure of Mn-containing Molecular Magnets¹, MARK PALENIK, JORGE H. RODRIGUEZ, Department of Physics, Purdue University — The family of Mn_{12} -Acetate molecular magnets has been recently enhanced by the synthesis of new members with $S = 20/2$ and $S = 19/2$ ground states. These closely related systems display similar but not identical AC susceptibility patterns which we have modelled in terms of their real (χ') and imaginary (χ'') components. The fits of AC data, as a function of frequency, show subtle differences between the parameters that control the spin dynamics in the $S = 20/2$ and $S = 19/2$ systems. To further understand the dynamic parameters we have performed electronic structure calculations based on spin density functional theory (SDFT) on both systems. Results from SDFT calculations, which describe the ground state and magnetic structures, have been correlated to the AC data to gain insight about the subtle differences in their magnetization dynamics.

¹Funded, in part, by NSF CAREER award CHE-0349189

10:36AM P13.00012 Exact and quasi exact numerical methods for giant magnetic molecules, JÜRGEN SCHNACK, University of Bielefeld, Germany — The determination of the energy spectra of large magnetic molecules is a demanding numerical problem. In this contribution we demonstrate that theory has advanced very much in recent years. We first show that it is possible to diagonalize the Heisenberg Hamiltonian by employing the spin-rotational symmetry $\text{SU}(2)$ in combination with arbitrary point-group symmetries [1]. This goes far beyond earlier approaches and enables us to evaluate thermodynamic observables such as the magnetization and spectroscopic data for molecules as large as the famous ferric wheel Fe_{10} with a Hilbert space dimension of more than 60 Millions. Then we explain how the finite-temperature Lanczos method can be applied to magnetic molecules in order to determine thermodynamic functions for Hilbert spaces as large as up to 1 Billion [2]. The new method enables us to discuss the magnetic properties of the highly frustrated Keplerate molecule $\{\text{W}_{72}\text{V}_{30}\}$ which behaves like a finite size Kagome lattice antiferromagnet.

[1] R. Schnalle and J. Schnack, Int. Rev. Phys. Chem. **29** (2010) 403; R. Schnalle, J. Schnack, Phys. Rev. B **79** (2009) 104419.
 [2] J. Schnack, O. Wendland, Eur. Phys. J. B **78** (2010) 535-541.

10:48AM P13.00013 Low temperature magnetic properties of antiferromagnetic rings V6 and V7 studied by NMR¹, YUJI FURUKAWA, Iowa State University, HIROKI OSHIO, TAKUTO MATSUMOTO, University of Tsukuba, Japan — The recent progress in synthesizing odd-member antiferromagnetic (AF) ring molecules gives us the opportunity to investigate spin frustration effects on magnetic properties in systems with small number of magnetic ions. $\text{Na}_7[(\text{VO})_7\text{Na}_7(\text{H}_2\text{O})_7(\beta\text{-CD})_{14}]_2]59\text{D}_2\text{O}$ (in short, V7) is known to be one of the odd-member AF rings, in which seven V^{4+} ($S=1/2$) ions make an almost coplanar ring shape. Magnetic susceptibility measured at $T=1.8\text{--}300\text{K}$ follows a Curie-Weiss law with a Weiss temperature of -0.5K . This indicates an AF interaction between V^{4+} spins is of order of 0.5K . In order to investigate ground state magnetic properties of the spin frustrated V7 ring, we have carried out proton NMR measurements at low temperatures down to 0.05K using a dilution refrigerator. We also carried out proton NMR in another non-frustrated ring system (V6) which is comprised by six V^{4+} ions for a comparison. NMR spectrum line width in V7 increases with decreasing temperature down to 0.05K . On the other hand, for V6, line width shows a peak around 0.2K and decreases below the temperature. These results clearly indicate that these systems have a different magnetic ground state and the ground state of V6 is a spin singlet state but V7 has a magnetic ground state.

¹Work at the Ames Laboratory was supported by the Department of Energy-Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

Wednesday, February 29, 2012 8:00AM - 11:00AM – Session P14 GMAG DMP FIAP: Focus Session: Spins in Semiconductors - Quantum Dots and Qubits 212

8:00AM P14.00001 Magnetic Polarons and Bipolarons in Quantum Dots¹, RAFAL OSZWALDOWSKI, University at Buffalo — Magnetically doped (typically by Mn) semiconductor quantum dots (QDs) allow a control of magnetic ordering in ways not available in the bulk. For example, onset of magnetism can be realized by adding a single carrier or changing symmetry of the quantum confinement, even at a fixed carrier number [1]. Recent experiments revisit the concept of magnetic polaron [2], formed when a single carrier added to a QD aligns the Mn spins through exchange interaction. The experiments [3,4] show that the induced magnetization persists at relatively high temperatures. First, we discuss a QD system, in which the experimental magnetic polaron energy, in addition to its relatively high value, shows a surprisingly weak temperature dependence [4]. We explain this effect by magnetic anisotropy of the QD. Next, we turn to the case where a magnetic QD contains two carriers. We find theoretically that Mn spins align, forming a magnetic 'bipolaron', even when the ground state has zero carrier-spin [5]. The corresponding state breaks spatial symmetry, unlike in the case of a single magnetic polaron. We propose experimental tests of our prediction. We also explore the stability of the broken-symmetry state with zero net magnetization versus other patterns of magnetization [6]. Finally, we show some interesting consequences of diffusive coupling of a magnetic QD to a reservoir of carriers [7]. This work was done in collaboration with P. Stano, J. Pientka, A. Petukhov, and I. Zutic.

[1] R. M. Abolfath, et al. Phys. Rev. Lett. 101, 207202 (2008).

[2] Maksimov, A. et al. Phys. Rev. B 62, R7767 (2000), J. Seufert et al., Phys. Rev. Lett. 88, 027402 (2002).

[3] R. Beaulac et al., Science 325, 973 (2009).

[4] I. R. Sellers, et al., Phys. Rev. B 82, 195320 (2010).

[5] R. Oszwaldowski, et al., Phys. Rev. Lett. 106, 177201 (2011)

[6] P. Stano, R. Oszwaldowski, A. G. Petukhov, and I. Zutic, preprint.

[7] J. M. Pientka, R. Oszwaldowski, A. G. Petukhov, J. E. Han and I. Zutic, Reentrant Magnetic Polaron Formation in Quantum Dots, preprint.

¹Supported by DOE-BES, U.S. ONR, AFOSR-DCT, NSF-ECCS, and CAREER.

8:36AM P14.00002 Reentrant Magnetic Polaron Formation in Quantum Dots¹, JAMES PIENKA, RAFAL OSZWALDOWSKI, JONG HAN, IGOR ZUTIC, SUNY at Buffalo, ANDRE PETUKHOV, South Dakota School of Mines and Technology — Recently, there have been several theoretical studies that show multiple ways of manipulating magnetic ordering in Quantum Dots (QD) [1,2]. Experiments [3,4] display the formation of Magnetic Polarons in both colloidal and self-assembled QDs. We focus on a type-II QD band profile, where the electrons reside in the barrier, while the holes are localized in the QD interior, which contains the magnetic impurities. In our model, photo-excitation of carriers induces a quasi equilibrium. We consider various QD states to describe the carrier-mediated magnetic ordering in QDs. Allowing for different QD states changes the magnetic properties due to different carrier spin density [5], which affects the alignment of the magnetic impurities. [1] R. M. Abolfath, A. G. Petukhov, and I. Zutic, Phys. Rev. Lett. 101, 207202 (2008); [2] I. Zutic and A. G. Petukhov, Nature Mater. 4, 623 (2009). [3] R. Beaulac et al., Science 325, 973 (2009). [4] I. R. Sellers, R. Oszwaldowski, et al., Phys. Rev. B 82, 195320 (2010). [5] J. M. Pientka, R. Oszwaldowski, A. G. Petukhov, J. E. Han, and I. Zutic, Reentrant Magnetic Polaron Formation in Quantum Dots, preprint.

¹Supported by DOE-BES, AFOSR-DCT, US ONR, NSF-ECCS CAREER, NSF-DMR.

8:48AM P14.00003 Magnetic anisotropies of quantum dots¹, KAREL VYBORNÝ, University at Buffalo, SUNY, NY and Academy of Sciences of the Czech Republic, J.E. HAN, RAFAL OSZWALDOWSKI, IGOR ZUTIC, University at Buffalo, SUNY, NY, A.G. PETUKHOV, South Dakota School of Mines and Technology, Rapid City, SD — Magnetic anisotropies in quantum dots (QDs) doped by magnetic ions are discussed in terms of two frameworks: anisotropic g-factors and magnetocrystalline anisotropy energy [1]. Two examples, related to zinc-blende *p*-doped materials, are given of how these frameworks are utilized: four-level Hamiltonian of a flat QD and a cuboid infinite-well QD containing a single hole. The latter model, despite being an idealization of a real QD, displays a rich phenomenology of anisotropies. We quantify the anisotropy constants for ZnSe and CdTe QDs, confirming that the Ising-like effective Hamiltonians apply to magnetic QDs [2]. Compared to bulk systems, confinement tuning offers a new way to control easy axes in magnetic QDs. [1] K. Vyborný et al., preprint (2011). [2] C. Le Gall et al., Phys. Rev. Lett. 107, 057401 (2011).

¹The work is supported by DOE-BES, NSF-DMR, AFOSR-DCT, U.S. ONR, and NSF-ECCS.

9:00AM P14.00004 The Interplay of Electronic Properties and Magnetic Anisotropy in Quantum Dots, IGOR ZUTIC, JEONGSU LEE, SUNY at Buffalo, KAREL VYBORNÝ, SUNY at Buffalo / Institute of Physics, ASCR, JONG HAN, SUNY at Buffalo, ANDRE PETUKHOV, South Dakota School of Mines & Technology — Tunability of magnetic anisotropy (MA) in nanostructures is a fascinating topic, for both fundamental understanding of nanomagnetism and possible spintronic applications. While there have been preceding efforts to systematically study the MA in bulk [1], we still lack a fundamental understanding of that in magnetic quantum dots (QDs). We first explore electronic properties of nonmagnetic QDs that can be significantly altered from the bulk-state depending upon the material and geometry. Focusing on II-VI materials forming both cubic and non-cubic QDs, we confirm qualitatively different energy spectra between different materials [2]. These findings can guide the control of MA in magnetic QDs. Supported by DOE-BES, NSF-DMR, AFOSR-DCT, U.S. ONR, and NSF-ECCS.

[1] X. Liu, Y. Sasaki and J. K. Furdyna, Phys. Rev. B 67, 205204 (2004).

[2] K. Výborný, J.E. Han, R. Oszwaldowski, I. Žutić, and A. G. Petukhov, preprint (2011).

9:12AM P14.00005 Theory of collective quantum effects of the nuclear spin bath in a Ge/Si core/shell nanowire quantum dot, WILLIAM A. COISH, STEFANO CHESI, McGill University — We study a quantum-dot spin-valve setup with a uniform hyperfine coupling of the electron spin to the nuclear bath. We propose Ge/Si core/shell nanowire quantum dots as a promising platform in which, through engineering of the nuclear spin positions and of the radial and longitudinal electron confinement, a nearly uniform hyperfine interaction can be realized. The dynamics of this coupled system are exactly soluble in terms of collective nuclear states with fixed total angular momentum. We theoretically show that the quantum-mechanical properties of such collective states of the nuclear spins can be probed through electron transport in this spin-valve setup. The associated transport current shows an enhancement due to coupling to collective modes in the nuclear-spin system directly analogous to the problem of superradiance in quantum optics. This effect is robust to dephasing of the nuclear spins and would provide a demonstration of large-scale collective quantum effects in a nuclear-spin system.

9:24AM P14.00006 Magnetotransport in Ge/Si Quantum Dot Molecules Fabricated by Directed Self-Assembly¹, DONGYUE YANG, Department of Physics and Astronomy, University of Pittsburgh, CHRIS PETZ, Department of Materials Science and Engineering, University of Virginia, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh, JERROLD FLORO, Department of Materials Science and Engineering, University of Virginia — The electronic states of strained self-assembled Ge quantum dots embedded in silicon provide an attractive system for controlling electron spin interactions via direct exchange². Directed self-assembly of sub-10 nm Ge islands are fabricated to produce laterally coupled quantum dot molecules with geometrically-defined spin exchange couplings. Ge islands are coupled to the Si capping layer, and geometries can be defined that are suitable for either vertical or lateral transport. We describe low-temperature vertical magneto-transport measurements on individual and small arrays of Ge islands grown on SOI substrate. Characteristic features in the magnetotransport are observed that correspond to specific geometrical arrangements of the quantum dots.

¹This work is supported by DOE BES (DE-FG02-07ER46421).

²C. E. Pryor, M. E. Flatte, and J. Levy, Applied Physics Letter **95**, 232103 (2009)

9:36AM P14.00007 Singlet-triplet splitting in double dots due to spin orbit and hyperfine interactions, DIMITRIJE STEPANENKO, University of Basel, MARK RUDNER, BERTRAND I. HALPERIN, Harvard University, DANIEL LOSS, University of Basel — We analyze the low-energy spectrum of a detuned double quantum dot in the presence of magnetic fields, spin orbit interaction, and nuclear spins, and focus on the regime of spin blockade. Starting from a realistic model for two interacting electrons in a double dot, we derive perturbatively an effective two-level Hamiltonian in the vicinity of an avoided crossing between singlet and triplet levels, which are coupled by the spin-orbit and hyperfine interactions. We evaluate the level splitting at the anticrossing in various parameter regimes, and show that it depends on two controllable parameters: the angle between the external magnetic field and the internal spin orbit field, and on the detuning, as well as on the difference between nuclear fields in the two dots. We identify a parameter regime where spin orbit and hyperfine terms can become of equal strength and propose a protocol for tuning their relative sizes.

9:48AM P14.00008 Single-shot correlations and two-qubit gate of solid-state spins¹, LIEVEN VANDERSYPEN, Kavli Institute of Nanoscience, TU Delft — Recent advances in nanotechnology and quantum engineering have made it possible to probe single spins in the solid-state. Here we report independent single-shot read-out of two electron spins in a double quantum dot. The read-out method is all-electrical, cross-talk between the two measurements is negligible, and read-out fidelities are $\sim 86\%$ on average. This allows us to directly probe the anti-correlations between two spins prepared in a singlet state and to demonstrate the operation of the two-qubit exchange gate on a complete set of basis states. Ongoing work focuses on integration with single-spin rotations, scaling and extending coherence times.

K.C. Nowack, M. Shafiei, M. Laforest, G.E.D.K. Prawiroatmodjo, L.R. Schreiber, C. Reichl, W. Wegscheider and L. M. K. Vandersypen, Single-shot correlations and two-qubit gate of solid-state spins, Science 330, 1269 (2011)

¹Supported by IARPA, ERC, FOM, SOLID

10:24AM P14.00009 Spin-orbit effects on the full dynamics of double quantum dot qubit states¹, ERNESTO COTA, Centro de Nanociencias y Nanotecnología - UNAM, Ensenada, Mexico, JUAN E. ROLON, Department of Physics and Astronomy, Ohio University, Athens, OH 45701-2979 USA, GLORIA PLATERO, Instituto de Ciencia de Materiales de Madrid - CSIC, Cantoblanco 28049, Madrid, Spain, SERGIO E. ULLOA, Department of Physics and Astronomy, Ohio University, Athens, OH 45701-2979 USA — We study spin-orbit interaction (SOI) and relaxation effects on the measurement of the extended singlet state return probability $P(S)$ in a double quantum dot (DQD) system with two electrons, in the presence of hyperfine interaction (HFI) and weak external magnetic fields. Using appropriate pulse cycles to change the detuning between the two quantum dots, we describe the full dynamical behavior of the system taking into account the complete set of states. We find that the mixing of the $m_s = 1$ (T_+) triplet with the (0,2) local singlet, induced by SOI via non-spin-conserving tunneling transitions, has an important effect on the measurement of $P(S)$, and a clear experimental signature. The numerical results are also analyzed in terms of a Feshbach projection to the effective low-energy dynamics, which explain the role of SOI on the relaxation and overall dynamics relevant in experiments. We also explore the case of the Landau-Zener-Stückelberg interferometry realized via voltage sweeps through the $S - T_+$ anticrossing generated by HFI in the DQD energy spectrum [1]. We focus on studying the effects of SOI and relaxation on the interferometric properties of the system in this regime. [1] J.R. Petta, H. Lu and A.C. Gossard, Science 327, 669 (2010).

¹Supported by NSF-PIRE, NSF-MWN/CIAM and PAPIIT-DGAPA-UNAM

10:36AM P14.00010 Spin blockade in a triple silicon quantum dot in CMOS technology¹, E. PRATI, G. PETRETTO, M. BELL, Laboratorio MDM, CNR-IMM, G. MAZZEO, Laboratorio MDM, CNR-IMM and Università Milano Bicocca, S. COCCO, M. DE MICHELIS, Laboratorio MDM, CNR-IMM, M. FANCIULLI, Laboratorio MDM, CNR-IMM and Università Milano Bicocca, F. GUAGLIARDO, Politecnico di Milano, M. VINET, LETI-Minatec, CEA, R. WACQUEZ, CEA Grenoble and Université Joseph Fourier — We study the spin blockade (SB) phenomenon by quantum transport in a triple quantum dot made of two single electron transistors (SET) on a CMOS platform separated by an implanted multiple donor quantum dot [1]. Spin blockade condition [2] has been used in the past to realize single spin localization and manipulation in GaAs quantum dots [3]. Here, we reproduce the same physics in a CMOS preindustrial silicon quantum device. Single electron quantum dots are connected via an implanted quantum dot and exhibit SB in one current direction. We break the spin blockade by applying a magnetic field of few tesla. Our experimental results are explained by a theoretical microscopic scheme supported by simulations in which only some of the possible processes through the triple quantum dot are spin blocked, according to the asymmetry of the coupling capacitances with the control gates and the central dot. Depending on the spin state, the SB may be both lifted and induced. Spin control in CMOS quantum dots is a necessary condition to realize large fabrication of spin qubits in some solid state silicon quantum device architectures. [1] Pierre et al., Appl. Phys. Lett., 95, 24, 242107 (2009); [2] Liu et al., Phys. Rev. B 77, 073310 (2008); [3] Koppens et al., Nature 442, 766-771 (2006)

¹Work funded by the FPVII AFSID Project

10:48AM P14.00011 Spin-orbit effects in triple dot quantum shuttles, JORGE VILLAVICENCIO, Facultad de Ciencias-UABC, IRENE MALDONADO, Centro de Investigación Científica y de Educación Superior de Ensenada (CICESE), ERNESTO COTA, Centro de Nanociencias y Nanotecnología-UNAM, GLORIA PLATERO, Instituto de Ciencia de Materiales de Madrid (CSIC) — Within the framework of a fully quantum mechanical approach we use a generalized density matrix formalism to study the spin-orbit coupling effects in a triple dot quantum shuttle. An interesting feature of this type of nanoelectromechanical systems is that the interplay between the electronic, spin, and mechanical degrees of freedom give rise to novel transport phenomena that has attracted a great deal of interest in both the applied and basic research. In this work, the effect of spin-orbit coupling is incorporated into the system by introducing non spin-conserving tunneling elements between the quantum dots. We explore the features of spin-polarized current by changing the Zeeman-split levels of the dots, and the frequency of the oscillating central dot. We show that the spin-orbit effect manifests itself as sidebands in the spin-polarized current, and that the tunneling channels can be controlled by adequately tuning the relative energies of the Zeeman-split levels, and by manipulating the current contribution from the vibrational modes.

Wednesday, February 29, 2012 8:00AM - 11:00AM –
Session P15 DMP FIAP GMAG: Focus Session: Spins in Metals - Spin Current Generation and Spin Motive Force 213

8:00AM P15.00001 Slonczewski-like torque due to Rashba spin-orbit coupling in thin magnetic layers, HYUN-WOO LEE, KYOUNG-WHAN KIM, Department of Physics, POSTECH, SOO-MAN SEO, Department of Material Science and Engineering, Korea University, JISU RYU, Department of Physics, POSTECH, KYUNG-JIN LEE, Department of Material Science and Engineering, Korea University — Recent experiments report that large Rashba spin-orbit coupling (RSOC) can exist for ferromagnetic nanostructure with structural asymmetry. Previous theories of spin-transfer torque (STT) induced by RSOC addressed this problem by introducing an effective field due to RSOC. However, the Rashba field is not sufficient, and another STT perpendicular to the Rashba STT is required to explain experimental results. In this work, we propose the mechanism of such STT based on nonadiabaticity and examine the effect of the torque. By studying the domain wall (DW) motion, we demonstrate that the DW motion is significantly affected by our result. We show that the effect of the RSOC-induced torque on the DW velocity can be so large that the DW can move along the current direction without assuming negative nonadiabaticity or spin polarization. Our result is discussed in comparison with experimental results.

8:12AM P15.00002 Spin-orbit coupling of Pt studied by circular dichroism in soft x-ray ARPES¹, JUN MIYAWAKI, ASHISH CHAINANI, YASUTAKA TAKATA, MASAKI OURA, RIKEN SPring-8 Center, YASUNORI SENBA, HARUIHIKO OHASHI, JASRI/SPring-8, SHIK SHIN, RIKEN SPring-8 Center, ISSP Univ. Tokyo, GUANG-YU GUO, Taiwan Univ., SADAMICHI MAEKAWA, JAEA, NAOTO NAGAOSA, Univ. Tokyo — Pt has a large spin-orbit coupling (SOC) and is reported to exhibit the largest spin Hall conductivity among all materials studied to date [1,2]. To establish the role of SOC in the electronic structure, we investigate the bulk electronic structure of Pt(111) using circular dichroism (spin-orbit dichroism) in soft x-ray (SX)-ARPES. We have measured band dispersions along Γ -K-X, L-W and Γ -L and the complete set of Fermi surfaces of Pt. Calculated band dispersions including SOC gives a very good match with the experimental results [2,3], thus demonstrating the role of SOC. Our results also show a k -dependent suppression of spin-orbit dichroism, implying a k -dependent quenching of the spin polarization [3]. [1] T. Kimura *et al.*, Phys. Rev. Lett. **98**, 156601 (2007). [2] G. Y. Guo *et al.*, Phys. Rev. Lett. **100**, 096401 (2008). [3] M. Gradhand *et al.*, Phys. Rev. B **80**, 224413 (2009).

¹The present work has been performed under the approval of RIKEN (Proposal No. 20100055 and No. 20110021).

8:24AM P15.00003 Spin pumping with coherent elastic waves¹, M. WEILER, H. HUEBL, F.S. GOERG, F.D. CZESCHKA, R. GROSS, S.T.B. GOENNENWEIN, Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — The generation and detection of pure spin currents is an important topic for spintronic applications. Spin currents may be generated, e.g., via spin pumping. In this approach, a precessing magnetization relaxes via the emission of a spin current. Conventionally, electromagnetic waves, i.e. microwave photons, are used to drive the magnetization precession. We here show that a spin current can also be pumped by means of an acoustic wave, i.e. microwave phonons. In the experiments, coherent surface acoustic wave (SAW) phonons with a frequency of 1.55 GHz traverse a ferromagnetic thin film/normal metal (Co/Pt) bilayer. The SAW phonons drive the resonant magnetization precession via magnetoelastic coupling [1]. We use the inverse spin Hall voltage in the Pt film as a measure for the generated spin current and record its evolution as a function of time and external magnetic field magnitude and orientation. Our experiments show that a spin current is generated in the exclusive presence of a resonant elastic excitation. This establishes acoustic spin pumping as a resonant analogue to the spin Seebeck effect and opens intriguing perspectives for applications in, e.g., micromechanical resonators.

[1] M. Weiler *et al.*, Phys. Rev. Lett. **106**, 117601 (2011)

¹Financial support from the DFG via GO 944/4-1, SPP 1538 and the German Excellence Initiative via the “Nanosystems Initiative Munich (NIM)” is gratefully acknowledged.

8:36AM P15.00004 Giant spin accumulation and long-distance spin precession in metallic lateral spin valves, YASUHIRO FUKUMA, RIKEN — The non-local spin injection technique in lateral spin valves (LSVs) has provided not only scientific interests to study spin transport and relaxation in a nanowire but also potential spintronic device applications. The non-local method involves no charge-current flow but spin accumulation in the nonmagnetic wire. In order to increase the output signal, related to the spin accumulation splitting for electrochemical potential, efficient spin injection into nonmagnet from ferromagnet as well as high applied current are indispensable. The spin resistance mismatch between the ferromagnet and the nonmagnet needs to be overcome by using high interface resistance such as tunnel barrier for the efficient spin injection, while a low junction resistance is preferred for applying high current. In this talk, I will discuss a guideline to design metallic LSVs with high output signal. The interface resistance of around $0.1 \Omega \mu\text{m}^2$, several orders of magnitude smaller than that of a typical tunnel junction, could effectively overcome the spin resistance mismatch in the metallic system [1] and leads to the giant spin accumulation signal over $200 \mu\text{V}$ in LSVs with NiFe/MgO/Ag junctions [2,3]. The Hanle effect measurements demonstrate a long-distance collective 2π spin precession along the $10 \mu\text{m}$ long Ag wire. This result will accelerate the development of novel spintronic devices utilizing the pure spin current and the spin accumulation.

[1] Y. Fukuma, L. Wang, H. Idzuchi and Y. Otani, Appl. Phys. Lett. **97**, 012507(2010).

[2] Y. Fukuma, L. Wang, H. Idzuchi, S. Takahashi, S. Maekawa and Y. Otani, Nature Mater. **10**, 527(2011).

[3] L. Wang, Y. Fukuma, H. Idzuchi, G. Yu, Y. Jiang and Y. Otani, Appl. Phys. Exp. **4**, 093004(2011).

9:12AM P15.00005 Temperature and temporal evolution of nonlocal spin signals¹, HAN ZOU, YI JI, University of Delaware — An unusual non-monotonic temperature dependence of spin signals was previously observed for nanoscale metallic nonlocal spin valves (NLSV): The spin signal increases as the temperature decreases from room temperature, reaches a maximum value around 50 K, and then decreases as the temperature approaches 4 K. This has been interpreted as due to a high rate of surface spin-flip scattering in the nonmagnetic channel, but the origins of the high surface spin-flip rate are yet to be understood. In this work, we show that for an as fabricated Py-Cu NLSV device this temperature dependence is clearly observed. The device was then stored in the ambient environment for a period of 5 months. Afterwards, an increase of the spin signals was found, and more interestingly the temperature dependence became monotonic. From room temperature to 50 K the spin signal increases, but from 50 K to 4 K the spin signal levels off instead of decreasing further. We conclude that the surface spin-flip scattering originates from the magnetic impurities embedded in the Cu channel near the side surfaces. The impurities are introduced into the Cu during the fabrication procedure. Upon oxidizing the Cu in the ambient environment, the surface impurities are buried in copper oxide and become less accessible to the conduction electrons. Therefore the surface spin-flip rate is reduced over time, resulting in a larger spin signal and monotonic temperature dependence.

¹This work is supported by DOE Grant No. DE-FG02-07ER46374.

9:24AM P15.00006 Continuous dc Spinmotive Force in a Patterned Ferromagnetic Film, YUTA YAMANE, Advanced Science Research Center, Japan Atomic Energy Agency and Institute for Materials Research, Tohoku University, KOHEI SASAGE, TOSHU AN, KAZUYA HARIU, Institute for Materials Research, Tohoku University and CREST, Japan Science and Technology Agency, Japan, JUN-ICHIRO OHE, CREST, Japan Science and Technology Agency and Dept of Physics, Toho University, JUN'ICHI IEDA, Advanced Science Research Center, JAEA, and CREST, Japan Science and Technology Agency, STEWART BARNES, Physics Department, University of Miami, EIJI SAITOH, Advanced Science Research Center, JAEA; Institute for Materials Research, Tohoku University; and CREST, Japan Science and Technology Agency, SADAMICHI MAEKAWA, Advanced Science Research Center, Japan Atomic Energy Agency and CREST, Japan Science and Technology Agency — Recently, a motive force of spin origin, i.e., a “spinmotive force”, has been theoretically predicted[1] and experimentally observed[2,3]. A spinmotive force reflects the spin of electrons in an essential manner and is a new concept relevant to electronic devices. However, problems remain, one of which is the continuous generation of such a spinmotive force. In this study, we present experiment and theory that demonstrate the continuous generation of a dc spinmotive force by exciting a ferromagnetic resonance of a single comb-shaped ferromagnetic thin film[4]. Experimental results are well reproduced by theoretical calculations, offering a quantitative and microscopic understanding of this spinmotive force.
 [1] S. Barnes and S. Maekawa, PRL 98, 246601 (2007). [2] S. A. Yang et al. PRL 102, 067201 (2009). [3] P. N. Hai et al. Nature 458, 489 (2009). [4] Y. Yamane, K. Sasage et al., to appear in PRL.

9:36AM P15.00007 Theory of anomalous Hall and spin Hall effects in ferromagnetic metals, BO GU, Advanced Science Research Center, Japan Atomic Energy Agency, TIMOTHY ZIMAN, CNRS and Institut Laue Langevin, SADAMICHI MAEKAWA, Advanced Science Research Center, Japan Atomic Energy Agency — We give a unified theory of the anomalous Hall effect (AHE) and the spin Hall effect (SHE) in ferromagnetic metals (FM). We do this by extending Kondo's theory of the AHE in FM and including the short range spin-spin correlations. We find a novel relation between the SHE and the second order nonlinear spin fluctuation in FM near Curie temperature T_c , which has been hidden for about 50 years, since Kondo gave a relation between the AHE and the first order nonlinear spin fluctuation in pure FM near T_c in 1962. Our results show an essential difference between the AHE and SHE in terms of the symmetry. Our theory can be applied to the recent SHE experiment in FM near T_c by Y. Otani et al.

9:48AM P15.00008 Spin motive force in a Rashba system, KYOUNG-WHAN KIM, Department of Physics, POSTECH, JUNG-HWAN MOON, KYUNG-JIN LEE, Department of Material Science and Engineering, Korea University, HYUN-WOO LEE, Department of Physics, POSTECH — Spin motive force (SMF) is the nonconservative spin force induced by magnetization dynamics. In addition to spin-transfer torque (STT), SMF is considered as one of the representative interactions between magnetization and conduction electrons. It has been reported that large Rashba-type spin-orbit coupling (RSOC) can show up in magnetic nanostructures containing thin ferromagnetic layers with structural asymmetry. In this work, we investigate the effect of RSOC on SMF. The additional SMF induced by RSOC is proportional only to time variation of magnetization while the conventional SMF is proportional to both time and space variation of magnetization. This result indicates that SMF can be induced from even homogeneous magnetic structure. The resulting RSOC SMF has so large magnitude that the feedback effect on the magnetization dynamics can be significant. Combining RSOC SMF and the previously known Rashba STT effect, we derived that Gilbert damping is one or two orders of magnitude enhanced by RSOC. Lastly, we show that the symmetry breaking nature of RSOC and the induced SMF greatly help the electrical distinction of magnetization structure. It is expected that RSOC will play a key role in extending applicable area of SMF.

10:00AM P15.00009 Light-induced pure spin current¹, JINGZHE CHEN, YIBIN HU, HONG GUO, Physics department of McGill University, HONG GUO'S GROUP TEAM — We propose theoretically that a pure spin current without an accompanying charge current can be generated by light in magnetic tunneling junctions. The principle is based on a photovoltaic effect combined with the spin selectivity of the magnetic electrodes of the junction. We demonstrate this effect in graphene nanostructures by atomic first principles calculation. The results show that appreciable pure spin-currents and open circuit spin bias are generated in pure graphene nanostructures, and it can reach significant values if half metal with high spin polarization is used as the electrodes.

¹We gratefully acknowledge financial support by NSERC of Canada, FRQNT of Quebec and CIFAR (H.G.). We thank CLUMEQ and RQCHP for providing computation facilities.

10:12AM P15.00010 Perpendicular switching of a single ferromagnetic layer induced by in-plane current injection, KEVIN GARELLO, Catalan Institute of Nanotechnology (ICN-CIN2), E-08193 Barcelona, Spain, I.M. MIRON, G. GAUDIN, P.J. ZERMATTEN, SPINTEC, UMR-8191, CEA/CNRS/UJF/GINP, INAC, F-38054 Grenoble, France, M. COSTACHE, Catalan Institute of Nanotechnology (ICN-CIN2), E-08193 Barcelona, Spain, S. AUFFRET, SEBASTIEN BANDERA, B. RODMACQ, A. SCHUHL, SPINTEC, UMR-8191, CEA/CNRS/UJF/GINP, INAC, F-38054 Grenoble, France, P. GAMBARDELLA, Catalan Institute of Nanotechnology (ICN-CIN2); Universitat Autònoma de Barcelona; Institució Catalana de Recerca i Estudis Avançats (ICREA) — We demonstrate switching of a ferromagnetic Pt/Co/AIOx layer with perpendicular anisotropy through lateral current-injection. Magnetization reversal occurs as an unpolarized electric current is injected parallel to an in-plane magnetic field of moderate magnitude. The switching direction depends on the sign of the current with respect to that of the in-plane field. The critical switching current scales with the lateral dimensions of the layer and duration of the current pulse. Our measurements also indicate that the switching efficiency increases with the magnetic anisotropy of the Co layer and oxidation of the top Al layer. The symmetry of this effect corresponds to an in-plane torque perpendicular to the current. We will discuss possible contributions to this torque, including Rashba-induced spin accumulation and the spin Hall effect [1].
 [1] I. M. Miron, K. Garello, G. Gaudin, P.-J. Zermatten, M. V. Costache, S. Auffret, S. Bandera, B. Rodmacq, A. Schuhl, and P. Gambardella, Nature 476, 189 (2011).

10:24AM P15.00011 Current induced magnetization dynamics in spin-orbit coupled thin film ferromagnets¹, DMYTRO PESIN, ALLAN MACDONALD, The University of Texas at Austin, Austin, TX — We consider the effect of an in-plane current on the magnetization dynamics of a two-dimensional spin-orbit coupled nanoscale itinerant ferromagnet. By solving the appropriate kinetic equation for an itinerant electron ferromagnet, we show that Rashba spin-orbit interaction provides transport currents with a switching action, as observed in a recent experiment (I. M. Miron *et al.*, Nature 476, 189 (2011)). The dependence of the effective switching field on the magnitude and direction of an external magnetic field in our theory agrees well with experiment. We comment on the possibility of finding materials in which this spin-orbit switching effect can be achieved at moderate current densities

¹This work was supported by Welch Foundation grant TBF1473, and by the ARO MURI on bioassembled nanoparticle arrays.

10:36AM P15.00012 Spin-flipping at Sputtered Co/Ag Interfaces¹, HOANG NGUYEN, REZA LOLOEE, WILLIAM PRATT, JACK BASS, Department of Physics and Astronomy, Michigan State University — We measured at 4.2K the Current-Perpendicular-to-Plane Magnetoresistances (CPP-MRs) of sputtered ferromagnetically coupled $[\text{Co}(3\text{ nm})/\text{Ag}(1.8\text{ or }2.0\text{ nm})]_n\text{Co}(3\text{ nm})$ multilayers with $n = 0$ to 8 that were imbedded in the middle of symmetric, Py-based, double exchange-biased spin-valves. The measurements yielded the parameter for spin-flipping at the Co/Ag interface, $\delta_{\text{Co/Ag}} = 0.30^{+0.05}_{-0.1}$. δ is related to the probability P of spin-flipping at the Co/Ag interface by $P = [(1-\exp(-\delta))]$. Despite the expected larger lattice-mismatch-induced disorder at the Co/Ag interface, this value is similar to that reported earlier for the Co/Cu interface [1], suggesting that such disorder does not play a major role in $\delta_{F/N}$ at ferromagnetic/non-magnetic (F/N) interfaces.

[1] B. Dassonneville et al., Appl. Phys. Lett. 96, 022509 (2010).

¹Supported in part by NSF grant DMR 08-04126 and KIST.

10:48AM P15.00013 Large non-inverted and inverted spin signals in break-junction-based nonlocal spin valves¹, SHUHAN CHEN, HAN ZOU, SIU-TAT CHUI, YI JI, University of Delaware — A nonlocal spin valve (NLSV) is a lateral structure with a ferromagnetic (F) spin injector, an F spin detector and a nonmagnetic (N) channel. A pure spin current can be generated in the N channel by electrical injection through the injector, and can be detected as a spin signal between the spin detector and the N channel. For a typical metallic NLSV, one expects a regular spin signal meaning that the nonlocal resistance is high for the parallel (P) states of the injector and the detector and low for the antiparallel (AP) states. We investigate spin signals of NLSV's with a break junction formed between the detector and the copper N channel by electrostatic discharge. We observed both non-inverted and inverted spin signals with large magnitudes. An inverted spin signal has low nonlocal resistance values for the P states and high values for the AP states. The magnitude is up to 90 milliohms at 4 K and up to 30 milliohms at 300 K, larger than the typical metallic NLSV with similar dimensions. The large magnitude can be explained by the spin-charge coupling across the highly resistive break-junction. The signs of the spin signals (non-inverted vs. inverted) are determined by the local spin-dependent density of states near the break-junction.

¹This work was supported by US DOE grant No. DE-FG02-07ER46374

Wednesday, February 29, 2012 8:00AM - 11:00AM – Session P16 DCMP: Heavy Fermions- Mostly URu₂Si₂ 251

8:00AM P16.00001 Fano resonance and hybridization gap in the Kondo lattice URu₂Si₂^{*1}, WAN KYU PARK, University of Illinois at Urbana-Champaign, P.H. TOBASH, F. RONNING, E.D. BAUER, J.L. SARRAO, J.D. THOMPSON, Los Alamos National Laboratory, L.H. GREENE, University of Illinois at Urbana-Champaign — The nature of the 'hidden' order transition in URu₂Si₂ remains puzzling despite intensive research over the past two and half decades. A key question under debate is whether a hybridization gap between the renormalized bands can be identified as the long-sought hidden order parameter. We report on the measurement of a hybridization gap in URu₂Si₂ employing a spectroscopic technique based on quasiparticle scattering across a ballistic metallic junction [1]. The differential conductance data exhibit an asymmetric double-peak structure, a signature for a Fano resonance in a Kondo lattice [2]. The extracted hybridization gap opens well above the hidden order transition temperature, indicating that it is not the order parameter for the hidden order phase. Our results place constraints on the origin of the hidden order transition in URu₂Si₂.

[1] W. K. Park *et al.*, arXiv:1110.5541.

[2] M. Maltseva, M. Dzero, P. Coleman, PRL 103, 206402 (2009).

¹The work at UIUC is supported by the U.S. DOE under Award Nos. DE-FG02-07ER46453 (WKP) and DE-AC02-98CH10886 (EFRC, LHG), and the work at LANL is carried out under the auspices of the U.S. DOE, Office of Science.

8:12AM P16.00002 Tuning soft point-contact spectroscopy of URu₂Si₂ from hidden order to antiferromagnetic state through pressure¹, XIN LU, F. RONNING, P.H. TOBASH, K. GOFTRY, E.D. BAUER, J.D. THOMPSON, Los Alamos National Laboratory — We have extended the soft point-contact spectroscopy technique under nearly hydrostatic pressure to make charge-spectroscopy measurements of URu₂Si₂ in both hidden order (HO) and large-moment antiferromagnetic (LMAF) states. In the HO state at ambient pressure, the spectroscopy shows two asymmetric peaks around the Fermi energy that emerge below the hidden order temperature $T_{HO} \sim 17.5\text{ K}$. In the LMAF state at higher pressures, the spectra are remarkably similar to those in the HO state, indicating a similar Fermi surface gapping in the HO and LMAF states. The energy scale of this gap is, within experimental uncertainty, consistent with that of the incommensurate spin resonance at $Q_1 = (1 \pm 0.4, 0, 0)$, which also is present in both HO and LMAF states. Our results provide a new clue to unraveling the puzzling HO state.

¹Work at Los Alamos was performed under the auspices of the U. S. Department of Energy, Division of Materials Science and Engineering and supported in part by the Los Alamos LDRD program.

8:24AM P16.00003 Temperature-dependent phonon dispersions in URu₂Si₂, NICHOLAS BUTCH¹, JASON JEFFRIES, MICHAEL MANLEY, Lawrence Livermore National Laboratory, JEFFREY LYNN, NIST Center for Neutron Research, MARC JANOSCHEK², BRIAN MAPLE, University of California, San Diego — The acoustic and low-energy optical phonon modes of a single crystal of URu₂Si₂ were studied via inelastic neutron scattering. The temperature dependence of the phonon dispersions will be compared with results of prior studies of phonons in this material. Our measurements were also sensitive to the temperature evolution of magnetic excitations in the hidden order phase. We will reflect on implications for the nature of the hidden order parameter.

¹also University of Maryland, College Park

²current address: Los Alamos National Laboratory

8:36AM P16.00004 Hidden Order Transition in URu₂Si₂: Evidence for the Emergence of a Coherent Anderson Lattice from Scanning Tunneling Spectroscopy, JEREMY FIGGINS, TING YUAN, DIRK MORR, University of Illinois at Chicago — The heavy-fermion compound URu₂Si₂ exhibits an onset of Kondo screening around $T \approx 55\text{K}$ and undergoes a second order phase transition at $T_0 = 17.5\text{K}$ into a state with a still unknown hidden order parameter. Recent scanning tunneling spectroscopy experiments have provided insight into the temperature evolution of the electronic structure. Above the hidden order transition, the differential conductance, dI/dV , exhibits a characteristic Fano lineshape. In contrast, below T_0 , a soft gap opens up in dI/dV and a quasi-particle interference (QPI) analysis reveals a band structure similar to that expected in a screened Kondo lattice. We demonstrate that the experimental dI/dV and QPI results below T_0 are consistent with the formation of a coherent Anderson lattice (CAL). In particular, dI/dV exhibits characteristic signatures of the Anderson lattice band structure, such as an asymmetric gap and a peak inside the gap which arises from the van Hove singularity of the heavy f-electron band. We identify several branches of the QPI pattern arising from intra- and interband scattering. Finally, the temperature evolution of dI/dV suggests that the formation of the CAL below the HOT is primarily driven by a strong increase of the lifetime of the heavy quasi-particles.

8:48AM P16.00005 Nuclear Magnetic Resonance Study of the Paramagnetic State of URu₂Si₂, KENT SHIRER, ADAM DIOGUARDI, JOHN CROCKER, ABIGAIL SHOCKLEY, NICHOLAS APROBERTS-WARREN, PETER KLAVINS, NICHOLAS CURRO, UC Davis — URu₂Si₂ is a heavy fermion system that has challenged researchers for many years due to its transition into a hidden order (HO) state at 17.5K. We present new nuclear magnetic resonance (NMR) data in the paramagnetic phase near the HO phase transition. An analysis of the spin-lattice relaxation rate indicates a suppression of the spin fluctuations above the HO phase transition extending up to approximately 30 K. We analyze this data in the context of several different models for the spin lattice relaxation.

9:00AM P16.00006 Evidence of New Features in the c-axis Optical Conductivity of URu₂Si₂, JESSE HALL, McMaster University, TOOMAS RÕÕM, TAANIEL ULEKSIN, URMAS NAGEL, Estonian National Institute for Chemical Physics and Biophysics, TRAVIS WILLIAMS, GRAEME LUKE, TOM TIMUSK, McMaster University — The hidden order state of URu₂Si₂ remains mysterious despite many years of investigation. High quality, low noise optical data on both cleaved and cut-and-polished faces with in-plane c-axis of the tetragonal structure offer new insight into the electronic behavior at the ordering temperature. As the gap opens in the density of states, a new mode appears in the gap region that is visible in the conductivity only when reflectance is measured with light polarized along the crystal c-direction. A marked anisotropy in the gap energy seen in the optical conductivity between a-axis and c-axis provides further insight into the structure and magnitude of the energy gap and the behavior of the electrons near the greatly-reduced Fermi surface.

9:12AM P16.00007 Linear and Nonlinear Susceptibility Measurements in URu₂Si₂ and UPt₃¹, BELLAVE SHIVARAM, University of Virginia, PRADEEP KUMAR, University of Florida, DAVID HINKS, Argonne National Labs — We will discuss both DC and AC susceptibility measurements in single crystals of URu₂Si₂ and UPt₃. In URu₂Si₂ we detect a ferromagnetic signature separated only by $\sim 1\text{ K}$ from the well established antiferromagnetic signature due to the hidden order at 17.5 K. This ferromagnetic signature appears to be well pronounced only in those samples where a strong ferromagnetic anomaly (also observed by others previously) appears at 35 K. This new ferromagnetic signature is further apparent in AC measurements, with its fingerprint appearing in a pronounced manner in first order, third order and fifth order susceptibility measurements. In contrast at the hidden order transition signatures are seen only in the first order and the fifth order susceptibility with no apparent change in the third order susceptibility. In UPt₃, the DC third order susceptibility measurements reveal a broad peak at $\sim 10\text{ K}$ which is at half the temperature where a peak in the linear susceptibility is observed. This proportionality appears thus far to be universal across the f-electron based strongly correlated metals.

¹Supported by NSF DMR

9:24AM P16.00008 Small Angle Neutron Scattering Studies of the Vortex Lattice of UPt₃¹, W.J. GANNON, W.P. HALPERIN, Northwestern University, IL, USA, M.R. ESKILDSEN, University of Notre Dame, IN, USA, J. GAVILANO, Paul Scherrer Institute, Switzerland — Although a paradigm for unconventional superconductivity, the true nature of the superconducting order parameter in UPt₃ is still an open question. We present results from small angle neutron scattering (SANS) studies on the vortex lattice (VL) of UPt₃, for fields both perpendicular and parallel to the crystal c-axis, that have implications for the superconducting order parameter. For perpendicular fields, an unconventional temperature dependence of the VL form factor – and thus penetration depth – is seen, with different dependences in the A and B-phases. This bulk measurement of the penetration depth indicates the presence of nodes in the superconducting gap. For parallel fields, we report the first measurement of a rocking curve from the VL. This is an encouraging result for the viability of using SANS to detect signatures of time reversal symmetry breaking, as the c-axis is taken as the chiral axis in these order parameter theories.

¹Support from DOE/BES awards DE-FG02-10ER46783 and DE-FG02-05ER46248.

9:36AM P16.00009 Hidden order and unconventional superconductivity in URu₂Si₂, JEFFREY RAU, HAE-YOUNG KEE, University of Toronto — The nature of the so-called hidden order in URu₂Si₂ and the subsequent superconducting phase have remained a puzzle for over two decades. Motivated by evidence for rotational symmetry breaking seen in recent magnetic torque measurements [Okazaki et al. Science **331**, 439 (2011)], we derive a simple tight-binding model consistent with experimental Fermi surface probes and ab-initio calculations. From this model we use mean-field theory to examine the variety of hidden orders allowed by existing experimental results, including the torque measurements. We then construct a phase diagram in temperature and pressure and discuss relevant experimental consequences.

9:48AM P16.00010 Hastatic Order in URu₂Si₂, PREMALA CHANDRA, PIERS COLEMAN, Center for Materials Theory, Department of Physics and Astronomy, Rutgers University, REBECCA FLINT, Department of Physics, Massachusetts Institute of Technology — The hidden order that develops below 17.5K in URu₂Si₂ has eluded identification for twenty-five years. Here we show that the recent observation of Ising quasiparticles in URu₂Si₂ suggests a novel “hastatic order” (Latin: *spear*), with a two-component order parameter describing hybridization between electrons and the Ising $5f^2$ states of the uranium atoms. Hastatic order breaks time-reversal symmetry by mixing states of different Kramers parity; this accounts for the magnetic anomalies observed in torque magnetometry and the pseudo-Goldstone mode observed in neutron scattering. Hastatic order is predicted to induce a basal-plane magnetic moment of order $0.01\mu_B$, a gap to longitudinal spin fluctuations that vanishes continuously at the first-order antiferromagnetic transition and a narrow resonant nematic feature in the scanning tunneling spectra.

10:00AM P16.00011 Staggered spin-orbit coupling induced hidden order state in heavy-fermion metal URu₂Si₂, TANMOY DAS, LANL — The order parameter responsible for a second-order phase transition in the heavy fermion metal URu₂Si₂ at T = 17.5 K has remained a long-standing mystery. Here we show via ab-initio calculations that an incommensurate Fermi surface “nesting” in the partially-filled f-states causes a staggered spin-orbit coupling in the hidden-order state. In this cause neither the spin (S) nor the orbital (L) alone causes ordered state, rather a modulated spin-momentum locked density wave propagates along the unidirectional nesting direction with a polarized total angular momentum $m_J = \pm 2$, in excellent agreement with experiments. It breaks spontaneous rotational symmetry, but not the time-reversal symmetry and thus gives rise to the recently observed “nematic order” in this state. The hidden order state will be immune to any time-reversal invariant perturbation such as pressure, whereas magnetic field will destroy it. Remarkably, these are the hallmark properties of the hidden order state. We also compute the topological quantum number to show that the hidden-order gap opening can cause a trivial to non-trivial topological phase transition, and hence defines a novel “topological quantum critical point.” Work is supported by US DOE.

10:12AM P16.00012 Emergent Rank-5 “Nematic” Order in URu₂Si₂, HIROAKI IKEDA, Department of Physics, Kyoto University, MICHITO SUZUKI, CCSE, Japan Atomic Energy Agency, RYOTARO ARITA, Department of Applied Physics, University of Tokyo, TETSUYA TAKIMOTO, Asia Pacific Center for Theoretical Physics, POSTECH, TAKASADA SHIBAUCHI, YUJI MATSUDA, Department of Physics, Kyoto University — In the strongly correlated f-electron systems, novel electronic states often appear due to the interplay between electron correlations and entangled spin and orbital degrees of freedom. A spectacular example is the so-called “hidden-order” phase in the heavy-electron metal URu₂Si₂. The phase transition is characterized by the large amount of entropy loss observed at $T_{HO} = 17.5\text{K}$, however no evidence of magnetic/structural phase transition below T_{HO} have been reported so far. Despite efforts over a quarter century, the order parameter has remained unidentified. We show here that the hidden order is a rank-5 multipole (dotriacontapole) state with E^- symmetry, based on the first-principles theoretical approach. This novel electronic state provides natural explanations of the key features including anisotropic magnetic excitations, nearly degenerate antiferromagnetic state, and spontaneous fourfold symmetry breaking.

10:24AM P16.00013 Electronic Structure and Correlation Effects in PuCoIn₅ as Compared to PuCoGa₅¹, JIAN-XIN ZHU, P.H. TOBASH, E.D. BAUER, F. RONNING, B.L. SCOTT, Los Alamos National Laboratory, K. HAULE, G. KOTLIAR, Rutgers University, R.C. ALBERS, J.M. WILLS, Los Alamos National Laboratory — Since their discovery nearly a decade ago, plutonium-based superconductors have attracted considerable interest, which is now heightened by the latest discovery of superconductivity in PuCoIn₅. In the framework of density functional theory (DFT) within the generalized gradient approximation (GGA) together with dynamical mean-field theory (DMFT), we present a comparative study of the electronic structure of superconducting PuCoIn₅ with an expanded unit cell volume relative to its PuCoGa₅ cousin. Overall, a similar GGA-based electronic structure, including the density of states, energy dispersion, and Fermi surface topology, was found for both compounds. The GGA Pu 5f band was narrower in PuCoIn₅ than in PuCoGa₅ due to the expanded lattice, resulting in an effective reduction of Kondo screening in the former system, as also shown by our DMFT calculations.

¹This work was supported by U. S. DOE at LANL, Office of Basic Energy Sciences, and LANL LDRD Program.

10:36AM P16.00014 Upper critical field of p-wave superconductors with orthorhombic symmetry, CHRISTOPHER LÖRSCHER, RICHARD KLEMM, University of Central Florida — Recent experiments on exotic ferromagnetic superconducting materials such as UCoGe and topological superconductors such as Cu_xBi₂Se₃, have spawned renewed interest in p-wave superconductivity. We present an extension of the Scharnberg-Klemm theory of H_{c2} in p-wave superconductors to cases of partially broken symmetry in an orthorhombic crystal. Using a uniaxial anisotropic pairing interaction as is appropriate for the low-field regime of UCoGe, we have shown that a field induced crossover from one p-wave state to another can lead to kinks in $H_{c2}(T)$, which can mimic upward curvature in all three crystal axis directions. Reasonably good fits to the low-field UCoGe data are obtained. We have also investigated the angular dependence of the axial p-wave state, which might prove useful in identifying the p-wave state present in certain materials, and possibly suggest new experiments on well known p-wave superconductors.

10:48AM P16.00015 Time-resolved quasiparticle dynamics of the itinerant antiferromagnet UPtGa₅¹, ELBERT CHIA, Nanyang Technological University, JIAN-XIN ZHU, Los Alamos National Laboratory, DIYAR TALBAYEV, Tulane University, H.J. LEE, University of California at Berkeley, NAMJUNG HUR, Inha University, N.O. MORENO, Federal University of Sergipe, R.D. AVERITT, Boston University, J.L. SARRAO, A.J. TAYLOR, Los Alamos National Laboratory — Time-resolved photoinduced reflectivity is measured in the spin-density-wave phase of the itinerant antiferromagnet UPtGa₅. Two relaxation components were seen: (a) a slow component whose amplitude appears below T_N , and relaxation time τ_{slow} exhibits an upturn near T_N ; (b) the fast component persists at all temperatures, with the relaxation time τ_{fast} also exhibiting an upturn near T_N . Comparing with pump-probe data on UNiGa₅, the differences are explained in the context of UPtGa₅ having A-type, (rather than G-type) antiferromagnetism, resulting in partial Fermi surface nesting, partial gapping and consequently finite density of states, at the Fermi surface.

¹MOE AcRF Tier 1 (RG41/07), Tier 2 (ARC 23/08), and NRF-CRP4-2008-04

Wednesday, February 29, 2012 8:00AM - 11:00AM –

Session P17 DMP GERA FIAP: Focus Session: Thermoelectrics - TE and Thermal Conductivity

252A

8:00AM P17.00001 Skutterudite Thermoelectric Generator for Electrical Power Generation from Automotive Waste Heat¹, GREGORY MEISNER, GM Global Research and Development — Filled skutterudites are state-of-the-art thermoelectric (TE) materials for electrical power generation from waste heat. They have suitable intrinsic transport properties as measured by the thermoelectric figure of merit $ZT = S^2\sigma T/\kappa$ (S = Seebeck coefficient, σ = electrical conductivity, T = temperature, and κ = thermal conductivity) and good mechanical strength for operation at vehicle exhaust gas temperatures of $>550^\circ\text{C}$. We have demonstrated TE electrical power generation on a production test vehicle equipped with a fully functional prototype TE generator (TEG). It was assembled with TE modules fabricated from filled skutterudites synthesized at GM. Our results and analysis show that improvement in total power generated can be achieved by enhanced thermal and electrical interfaces and contacts. A substantial T decrease along the exhaust gas flow results in a large variation of voltage, current, and power output for each TE module depending on its position in the module array. Total TEG output power depends directly on the position-dependent T profile via the temperature dependence of both ZT and Carnot efficiency. Total TEG power output also depends on how the modules are connected in parallel or series combinations because mismatch in output voltage and/or internal resistance among the modules degrades the performance of the entire array. Uniform T profiles and consistent TE module internal resistances improve overall TEG performance.

¹Supported by the US DOE Vehicle Technologies Program

8:12AM P17.00002 Theoretical Study of the Properties of the Type II Clathrates $A_x\text{Si}_{136}$ and $A_x\text{Ge}_{136}$ ($A = \text{Na}, \text{K}$), CRAIG HIGGINS, Texas Tech University, CHARLEY MYLES, Professor, Texas Tech University, TEXAS TECH TEAM — Type II clathrate semiconductors have cage-like lattices where atoms are tetrahedrally coordinated and sp^3 bonded. An observed property of these materials is the variation of unit cell volume as different types of alkali metal atoms are placed in the clathrate cages. Experiments¹ on $\text{Na}_x\text{Si}_{136}$ reveal that, starting with Si_{136} , as x increases ($0 < x < 8$), the cell volume contracts; where ($8 < x < 24$), the cell volume expands. This variation with x has been explained² as due to preferential incorporation of Na into the Si_{28} cages for $x < 8$, followed by incorporation into the Si_{20} cages for $8 < x$ (when all Si_{28} cages are full). With this motivation, we have used density functional theory to explore the possibility Type II Si and Ge clathrates with alkali atom guests other than Na may exhibit a similar variation in cell volume with guest inclusion. We present results for the electronic and vibrational properties of the $\text{Na}_x\text{Si}_{136}$, $\text{Na}_x\text{Ge}_{136}$, $\text{K}_x\text{Si}_{136}$, and $\text{K}_x\text{Ge}_{136}$ clathrates. These results are compared with experiment and the properties of the materials are compared and contrasted.

¹M. Beekman, et al, *Inorganic Chem* **49**, 5338 (2010)

²Ibid.

8:24AM P17.00003 Enhanced Thermoelectric Property of Single Phase $\text{MnSi}_{1.75}$ through Non-equilibrium Synthesis Method, XIAOYA SHI, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, Upton, New York, 11973, IVO DIMITROV, Brookhaven National Lab, SU JUNG HAN, QIANG LI, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, Upton, New York, 11973, BROOKHAVEN NATIONAL LAB TEAM — We report thermoelectric properties of the single phase $\text{MnSi}_{1.75}$ using a one-step non-equilibrium synthesis method. Extremely high quenching speed of melt spinning prevents the formation of the second phase MnSi, which is usually found in this class of materials made by using the conventional solid state reaction methods. We found that the phase-pure $\text{MnSi}_{1.75}$ samples exhibit much higher electrical conductivity, as compared with the conventionally prepared samples. Thermal conductivity is measured and analyzed by introducing the Debye model. It is found that the reduced grain sizes after melt spinning play an important role on decreasing lattice thermal conductivity. The combination of enhanced electrical conductivity and reduced lattice thermal conductivity results in large increase of the thermoelectric figure of merit zT at room temperature.

8:36AM P17.00004 Investigation of phonon mass-difference scattering model by molecular dynamics, TAKUMA SHIGA, TAKUMA HORI, SHIGEO MARUYAMA, JUNICHIRO SHIOMI, Department of Mechanical Engineering, The University of Tokyo — While nanostructuring has been shown to be a promising approach to effectively reduce lattice thermal conductivity and enhance efficiency of thermoelectrics, alloying still remains to be a key process that determines the base material performance. Therefore, understanding lattice thermal conductivity of alloyed crystals, particularly from the viewpoint of mode-dependent phonon transport, holds importance. In this work, we have investigated phonon scattering rates in alloy crystals by focusing on the mass-difference scattering. The phonon mass-difference scattering rates were obtained through spectral analysis of phase-space molecular trajectories computed by molecular dynamics simulations. Obtained results for simple Lennard-Jones crystals show that the mass-difference scattering rates of long-wavelength phonons follow the frequency dependence of Rayleigh scattering regardless of isotope mass and concentration. Meanwhile we obtained the large deviation from scattering models based on the mass perturbation theory. We will report and discuss details of frequency-dependence of mass-difference scattering rates to clarify validity and limit of the models. Furthermore, the analysis will be extended to thermoelectric materials, such as lead telluride. This work is supported by Global COE Program, Global Center of Excellence for Mechanical System Innovation.

8:48AM P17.00005 Stronger phonon scattering by larger differences in atomic mass and size in p-type half-Heuslers $\text{Hf}_{1-x}\text{Ti}_x\text{CoSb}_{0.8}\text{Sn}_{0.2}$, XIAO YAN, WEISHU LIU, HUI WANG, SHUO CHEN, Boston College, JUNICHIRO SHIOMI, The University of Tokyo, HENGZHI WANG, DEZHI WANG, Boston College, GANG CHEN, MIT, ZHIFENG REN, Boston College, BOSTON COLLEGE TEAM, MIT COLLABORATION, THE UNIVERSITY OF TOKYO COLLABORATION — High lattice thermal conductivity has been the bottleneck for further improvement of thermoelectric figure-of-merit (ZT) of half-Heuslers (HHs) $\text{Hf}_{1-x}\text{Zr}_x\text{CoSb}_{0.8}\text{Sn}_{0.2}$. Theoretically the high lattice thermal conductivity can be reduced by exploring larger differences in atomic mass and size in the crystal structure. In this paper, we experimentally demonstrated that lower than ever reported thermal conductivity in p-type HHs can indeed be achieved when Ti is used to replace Zr, i.e., $\text{Hf}_{1-x}\text{Ti}_x\text{CoSb}_{0.8}\text{Sn}_{0.2}$, due to larger differences in atomic mass and size between Hf and Ti than Hf and Zr. The highest peak ZT of about 1.1 in the system $\text{Hf}_{1-x}\text{Ti}_x\text{CoSb}_{0.8}\text{Sn}_{0.2}$ ($x=0.1, 0.2, 0.3$, and 0.5) was achieved with $x=0.2$ at 800°C .

9:00AM P17.00006 Neutron Scattering Study of the Temperature-Dependent Phonon Spectra of AgSbTe_2 ¹, JIE MA, OLIVIER DELAIRE, ANDREW MAY, MICHAEL MCGUIRE, BRIAN SALES, OLIVIER GOURDON, ASHFIA HUQ, DOUGLAS ABERNATHY, MATTHEW STONE, Oak Ridge National Laboratory, PO Box 2008, Oak Ridge, TN 37831, USA, OAK RIDGE NATIONAL LABORATORY, PO BOX 2008, OAK RIDGE, TN 37831, USA COLLABORATION — The thermoelectric material AgSbTe_2 has attracted much attention due to its simple rocksalt structure, high thermoelectric figure-of-merit, and its extremely low thermal conductivity in bulk samples. Previous theoretical studies have suggested that phonons can be scattered by anharmonicity (phonon-phonon coupling) and nano-defects in AgSbTe_2 . However, systematic measurements of phonons in this compound have not been available. We report our results of detailed time-of-flight neutron scattering measurements, as a function of temperature, and departure from stoichiometry. The temperature dependence of the phonon density-of-states is discussed, and compared with the reported thermal conductivity in this system.

¹O.D. and J.M. acknowledge funding from US DOE, Office of Basic Energy Sciences as part of the S3TEC Energy Frontier Research Center, DOE DE-SC0001299.

9:12AM P17.00007 Inelastic Neutron Study of Phonon Lifetime Effects in Thermoelectric $\text{Bi}_2(\text{Se},\text{Te})_3$ Alloys¹, DILLON GARDNER, Massachusetts Institute of Technology, OLIVIER DELAIRE, MARK LUMSDEN, TAO HONG, Oak Ridge National Laboratory, DOYLE TEMPLE, Norfolk State University, YOUNG LEE, Massachusetts Institute of Technology — One important avenue of optimizing the thermoelectric figure of merit, ZT , is to reduce the thermal conductivity of phonons while preserving the electrical conductivity. Mass disorder caused by alloying provides an avenue of enhancing phonon scattering. In this work, the phonon spectra of different alloys of $\text{Bi}_2(\text{Se},\text{Te})_3$ are measured using inelastic neutron measurements. The temperature and composition dependence provide information on phonon softening and enhanced phonon scattering of acoustic phonon modes. Measurements on single crystals also reveal the dependence on the polarization of the modes. An additional low energy dispersing mode has been observed.

¹This work was supported by the US DOE, Office of Basic Energy Sciences as part of the S3TEC Energy Frontier Research Center, DOE DE-SC0001299

9:24AM P17.00008 Anomalous Lattice Dynamics in PbTe and Its Implications to Low Intrinsic Lattice Thermal Conductivity, YI ZHANG, Department of Physics and HiPSEC, University of Nevada, Las Vegas, XUEZHI KE, Department of Physics, East China Normal University, Shanghai, China, PAUL KENT, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, CHANGFENG CHEN, Department of Physics and HiPSEC, University of Nevada, Las Vegas, JIHUI YANG, Materials Science and Engineering Department, University of Washington — Recent experiments on PbTe-based high performance thermoelectric materials raise fundamental questions about the nature of low intrinsic lattice thermal conductivity and underlying lattice dynamics. We show by first-principles calculations that the reported results can be attributed to abnormally large-amplitude thermal vibrations that stem from a delicate competition of dual ionicity and covalency, which puts PbTe near ferroelectric instability. It produces anomalous properties such as partially localized low-frequency phonon modes, a soft transverse optical phonon mode, and a positive temperature coefficient for the band gap. These results account for experimental findings and resolve the underlying atomistic mechanisms. The relation between these anomalies and the low intrinsic lattice thermal conductivity will be discussed.

9:36AM P17.00009 Phonon Anharmonicity in PbTe Thermoelectrics¹, OLIVIER DELAIRE, JIE MA, KAROL MARTY, ANDREW MAY, MICHAEL MCGUIRE, MAO-HUA DU, DAVID SINGH, ANDREY PODLESNYAK, GEORG EHLERS, MARK LUMSDEN, BRIAN SALES, Oak Ridge National Laboratory — Achieving high thermoelectric conversion efficiency requires limiting the thermal conductivity, through the disruption of phonon propagation. A detailed understanding of phonon dispersions and linewidths is thus critical to develop accurate microscopic theories of thermal conductivity, and design efficient thermoelectric materials. We investigate the phonon dispersions and linewidths in the thermoelectric material PbTe with inelastic neutron scattering experiments. Our measurements indicate that the soft transverse optic mode in PbTe is strongly anharmonic, which could cause a lowering of thermal conductivity by scattering the heat-conducting acoustic modes [1]. We also present results on the effect of alloying.

[1] O. Delaire et al., Nature Materials 10, 614 (2011).

¹O.D. and J.M. acknowledge funding from US DOE, Office of Basic Energy Sciences as part of the S3TEC Energy Frontier Research Center, DOE DE-SC0001299.

9:48AM P17.00010 Anharmonic vibrational effects of thermoelectric Cu-Sb-Se ternary semiconductors: Density-functional theory studies, YONGSHENG ZHANG, Materials Science and Engineering, Northwestern University, ERIC SKOUG, JEFFREY CAIN, DONALD MORELLI, Chemical Engineering and Materials Science, Michigan State University, VIDVUDS OZOLINS, Materials Science and Engineering, University of California, Los Angeles, CHRISTOPHER WOLVERTON, Materials Science and Engineering, Northwestern University — Strong anharmonicity can lead to intrinsically minimal thermal conductivity even in defect-free single crystals. In an effort to understand this behavior, we have investigated two Cu-Sb-Se ternary semiconductors, Cu_3SbSe_4 and Cu_3SbSe_3 , by both experimental measurements and density functional theory (DFT) calculations. The experimental lattice thermal conductivity measurements show that while Cu_3SbSe_4 exhibits classical behavior, the lattice thermal conductivity in Cu_3SbSe_3 is anomalously low and nearly temperature independent. The vibrational properties of these two semiconductors are calculated by DFT phonon calculations within the quasi-harmonic approximation. The average of the Grüneisen parameters of the acoustic mode in Cu_3SbSe_3 is larger than that of Cu_3SbSe_4 , which theoretically confirms that Cu_3SbSe_3 has a stronger lattice anharmonicity than Cu_3SbSe_4 . Using our DFT-determined longitudinal and transverse Grüneisen parameters, Debye temperatures, and phonon velocities, we calculate the lattice thermal conductivity using the Debye-Callaway model (without the use of any adjustable parameters). The calculated thermal conductivity is in good agreement with the experimental measurements.

10:00AM P17.00011 First-principles calculation of anharmonicity induced phonon lifetimes in FeSi¹, MOSES NTAM, JIANJUN DONG, Auburn University, OLIVIER DELAIRE, PAUL R. KENT, Oak Ridge National Laboratory — FeSi has attracted a lot of interest as a promising thermoelectric material for refrigeration applications. We present a first principle calculation of phonon lifetimes of FeSi based on our newly developed computational technique which combines first-principles density functional theory (DFT) and quantum scattering theory. Phonon lifetimes are calculated within the Fermi's golden rule using third order lattice anharmonicity tensors and vibrational phonon frequencies as inputs. Second order force constant matrices and third order lattice anharmonicity tensors are extracted using a real space supercell technique within the local density approximation (LDA). We compare our calculated phonon spectrum and lifetimes with recent neutron scattering measurements of phonon dispersions and linewidths. Finally we use the calculated phonon lifetimes to estimate the thermal conductivity of FeSi using kinetic transport theory.

¹NSF (EAR-0757847)

10:12AM P17.00012 Resistivity and Specific Heat under Localized Anharmonic Motion in Type-I $\text{Ba}_8\text{Ga}_{16}\text{Sn}_{30}$ Clathrate, XIANG ZHENG, SERGIO Y. RODRIGUEZ, LAZIZ SARIBAEV, JOSEPH H. ROSS, JR, Department of Physics and Astronomy, Texas A&M University, College Station, TX, 77843, USA — Anharmonic guest atom oscillation has direct connection to the thermal transport and thermoelectric behavior of type-I $\text{Ba}_8\text{Ga}_{16}\text{Sn}_{30}$ clathrate. This behavior can be observed through several physical properties, with for example the heat capacity providing a measure of the overall excitation level structure. In addition the nuclear magnetic resonance (NMR) relaxation behavior provides a sensitive probe for the oscillator dynamics, as we have recently reported. Localized anharmonic excitations also influence the low-temperature resistivity, as we show in this paper. By combining heat capacity and transport measurements we address the distribution of local-oscillators in this material, as well as the shape of the confining potential for Ba ions in the cages. Analyzed along with NMR relaxation measurements for the same sample, a two phonon Raman process is used to extract information about the excitation energies, which along with a quantum computational solver we have used to address the potential structure. We also compare to the soft-potential model and other models used for this system. The results indicate that a single confining potential cannot describe the system properly, whereas a distribution of local oscillators provides a more reasonable fit to the data.

10:24AM P17.00013 The Debye-Waller factor and its application to anharmonic vibrations, DOUGLAS SAFARIK, ANNA LLOBET, JASON LASHLEY, Los Alamos National Laboratory — The Debye-Waller factor relates the intensities of the Bragg peaks to the mean square displacements of the atoms. In the structural refinement of diffraction data it is standard practice to use the harmonic expression for Debye-Waller factor. For most materials and conditions the phonons are only mildly anharmonic, thus the harmonic assumption is a good one. For some materials and conditions, however, the phonons can be strongly anharmonic, and thus the harmonic assumption is physically unrealistic. As examples we cite the rattling atoms in clathrates and skutterudites, and atoms participating in displacive phase transitions. In the present study we investigate the error associated with using the harmonic Debye-Waller factor to analyze anharmonic vibrations. We find that even for strongly anharmonic potentials, such as a double well, the mean square displacements deduced using the harmonic approximation are at most 15% larger than those deduced using a full anharmonic analysis. Furthermore, the quasi-harmonic and anharmonic values have nearly the same temperature dependences. We conclude that the error introduced by using the harmonic approximation is comparable to or smaller than the usual errors associated with measurement and refinement of diffraction patterns.

10:36AM P17.00014 Minimum thermal conductivity in superlattices: A first-principles formalism¹, JIVTESH GARG, GANG CHEN, Massachusetts Institute of Technology — In certain superlattice systems such as silicon-germanium superlattices a minimum in thermal conductivity with increase in period thickness has been observed. This minimum has been reported at a relatively short superlattice period of a few nanometers and cannot be explained by existing formalisms. An accurate prediction of this minimum thermal conductivity holds importance for thermoelectrics where low thermal conductivity is desired. We develop a first-principles formalism based on use of harmonic and anharmonic force-constants derived from density-functional perturbation theory and single-mode relaxation time approximation to predict the thermal conductivity of superlattices. The phonon relaxation times are computed based on scattering due to both anharmonicity and interface roughness. We show that the formalism leads to an excellent agreement between predicted and measured values and also explains the observed minimum in thermal conductivity.

¹This material is based upon work supported as part of the S3TEC, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-FG02-09ER46577

10:48AM P17.00015 Thermal transport across perovskite superlattices¹, JAYAKANTH RAVICHANDRAN, AJAY YADAV, University of California, Berkeley, RAMEZ CHEAITO, University of Virginia, Charlottesville, PIM ROSSEN, University of California, Berkeley, SIRIYARA SURESHA, Lawrence Berkeley National Lab, Berkeley, PATRICK HOPKINS, University of Virginia, Charlottesville, ARUN MAJUMDAR, Department of Energy, RAMAMOORTHY RAMESH, University of California, Berkeley — Understanding thermal transport across interfaces is useful for designing materials for thermal management, thermoelectricity etc. Despite years of investigation, there are several open questions on the nature of thermal transport across solid-solid interfaces. The ability to control materials synthesis down to a monolayer has enabled study of interface phonon scattering in systems such as superlattices, heterostructures etc. We chose perovskite oxides, which are excellent thermoelectric materials, as model systems to study interfacial thermal transport. Superlattices of SrTiO₃, CaTiO₃ and CaMnO₃, with period thicknesses ranging from 1-176 monolayers were grown using pulsed laser deposition, monitored by in-situ RHEED. We measured temperature dependent (100 - 400 K) cross plane thermal conductivity of these superlattices using the time domain thermoreflectance (TDTR). The lowest thermal conductivity measured is below the alloy limit at room temperature. The period thickness dependent thermal conductivity shows signs of zone folding for short period superlattices.

¹This research was supported by the Office of Basic Energy Sciences, Department of Energy. JR acknowledges support from Link Foundation.

Wednesday, February 29, 2012 8:00AM - 11:00AM –
Session P18 DMP: Focus Session: Electron, Ion, and Exciton Transport in Nanostructures - Quantum Transport I 252B

8:00AM P18.00001 Electrostatic tuning between 1-dimensional and 2-dimensional electron gases, DIGBIJOY NATH, PIL SUNG PARK, MICHELE ESPOSTO, The Ohio State University, DAVID BROWN, STACIA KELLER, UMESH MISHRA, University of California, Santa Barbara, SIDDHARTH RAJAN, The Ohio State University, THE OHIO STATE UNIVERSITY TEAM, UNIVERSITY OF CALIFORNIA, SANTA BARBARA TEAM — Although low dimensional systems such as 1-D and 2-D electron gases have been separately studied in details, a system enabling co-existence of both dimensions is still challenging to achieve. Such a system where the dimensionality can be tuned between 1-D and 2-D electrons can be an extremely promising platform to explore new phenomena. Here we investigate a novel system based on vicinal GaN-based heterostructure where we exploit its polarization charges to demonstrate for the first time, direct electrostatic tuning of the dimensionality of electrons between 1-D and 2-D. This tuning is achieved by adjusting the Fermi level with applied gate bias. A capacitance-voltage profiling to probe the Fermi occupation function of electron gas was used to demonstrate distinct signatures of the density of states for both the dimensions at room temperature. We developed a 2-sub-band model consisting of 1-D and 2-D sub-bands to describe the behavior of the electron gas, which is in excellent agreement with our experimental data, confirming the co-existence of electrons of both dimensions. This demonstration of co-existence of 1-D and 2-D electrons and the ability to tune between their dimensions at room temperature could open new research paths for low-dimensional physics besides enabling devices with added functionalities.

8:12AM P18.00002 Quantum coherence phenomena in bismuth thin film nanostructures, MARTIN RUDOLPH, J. J. HEREMANS, Virginia Tech — We present low temperature quantum magnetotransport measurements on bismuth nanostructures. The large spin-orbit interaction and prominent surface states in Bi films are expected to produce non trivial mesoscopic quantum transport. Bi thin films are grown by thermal evaporation onto SiO₂ with a two-step process to optimize the film mobility and ensure oriented growth along the [111] direction. The optimization leads to a minimum thickness of 25 nm for continuous films. Structures as small as 100 nm are subsequently patterned into the film via lithographic techniques. Phase and spin coherence lengths are obtained by analyzing electron interference phenomena in mesoscopic wires and rings. We show that the phase coherence shows a decreasing trend with decreasing channel width. The decrease in phase coherence in Bi wires ranging in width from 1200 nm to 100 nm cannot readily be accounted for by increased boundary scattering. A width dependence of the spin coherence is also detected. The observed confinement dependence of the phase and spin coherence in Bi nanostructures will be discussed (DOE DE-FG02-08ER46532).

8:24AM P18.00003 Resistance oscillations and dephasing in ring patterns on InGaAs/InAlAs two-dimensional electron systems, SHAOLA REN, J.J. HEREMANS, Virginia Tech, C.K. GASPE, S. VIJAYARAGUNATHAN, T.D. MISHIMA, M.B. SANTOS, University of Oklahoma — In InGaAs/InAlAs heterostructures with spin-orbit interaction, patterned into mesoscopic rings, we experimentally investigate low-temperature Aharonov-Bohm resistance oscillations. The oscillation amplitude was studied as function of applied current and temperature, to obtain the dependence of these parameters on dephasing. Previous results on mesoscopic quantum interferometers have shown a lobe structure in the dependence of the oscillation amplitude on measurement bias, in some models ascribed to Coulomb interaction, and have surmised a universal behavior with an energy scale dependent on interferometer size. The ring interferometers studied here were of typical radius of 700 nm, and lithographic arm width of 300 nm, similar-sized but of higher carrier density than in the previous studies, and used for similar bias- and temperature-induced dephasing studies. The measurements so far show the expected temperature dependence, but have not revealed the lobe structure in the bias dependence. We discuss the results in the light of dephasing phenomena expected in mesoscopic quantum interferometers (DOE DE-FG02-08ER46532, NSF DMR-0520550).

8:36AM P18.00004 Transport through double quantum dot with electron-LO-phonon interaction, AKIHIRO YAMADA, RIN OKUYAMA, MIKIO ETO, Keio University — We theoretically study the transport through a serial double quantum dot (DQD) in the presence of electron-LO-phonon interaction. In contrast to the case of acoustic phonon,¹ the coherent coupling between an electron and an optical phonon, so-called polaron formation, has a small dissipation, which influences the transport properties markedly. We calculate the current through the DQD using the Keldysh Green function, as a function of the tuning of energy levels between the quantum dots, when the bias voltage is sufficiently large. The electron-phonon interaction is considered by the perturbation expansion. We find a subpeak structure of the current due to the polaron formation and evaluate elastic and inelastic components of the current.

¹P. Roulleau *et al.*, Nat. Commun. **2**, 239 (2011).

8:48AM P18.00005 Imaging Spatial Current Eigenmodes in Nanoscopic Quantum Networks¹

, TANKUT CAN, University of Chicago, DIRK MORR, University of Illinois-Chicago — Using the Keldysh Green's function formalism, we study the non-equilibrium charge transport in nanoscopic quantum networks [1]. Due to quantum confinement, charge transport takes place via current eigenmodes that possess characteristic spatial patterns of current paths. In the ballistic limit, these patterns exhibit unexpected features such as current backflow and closed loops of circulating currents. These current eigenmodes are the non-equilibrium analogue of eigenmodes in the local density of states of confined systems [2]. Moreover, we demonstrate that dephasing leads to a smooth evolution of the current patterns, and ultimately reproduces the charge transport in a classical resistor network. Finally, we propose a new method using scanning tunneling spectroscopy to image the spatial current patterns associated with individual current eigenmodes in nanoscopic quantum networks.

[1] T. Can, H. Dai, and D.K. Morr, in preparation

[2] M. Crommie, C. Lutz, and D. Eigler. Confinement of electrons to quantum corrals on a metal surface. *Science*, 262, 1993.

¹This work is supported in part by the U.S. Department of Energy under Award No. DE-FG02-05ER46225. T.C. is supported by a Department of Education GAANN fellowship.

9:00AM P18.00006 Microscopic Theory for the 0.7 Anomaly in Quantum Point Contacts - the Role of Geometry- and Interaction-Enhanced Spin-Fluctuations

, JAN HEYDER, FLORIAN BAUER, ENRICO SCHUBERT, DAVID BOROWSKY, DANIELA TAUBERT, Ludwig-Maximilians University, DIETER SCHUH, University Regensburg, WERNER WEGSCHEIDER, ETH Zurich, JAN VON DELFT, STEFAN LUDWIG, Ludwig-Maximilians University — We present a detailed microscopic analysis of some local observables of a quantum point contact (QPC) to gain better understanding of the origin of the 0.7 conductance anomaly. We model the system by a one-dimensional tight binding model with local interactions, a smooth potential barrier and a homogeneous magnetic field. We calculate conductance G , local density n and local magnetization m as a function of magnetic field at zero temperature, using the functional Renormalization Group (fRG). Our potential can be tuned to describe the smooth crossover from a single barrier, representing a QPC, to a double barrier, modelling a quantum dot (QD) exhibiting the Kondo effect. We find that both geometries show interaction-enhanced spin-fluctuations, manifested via an enhanced local spin susceptibility, for gate voltages that lead to an anomalously large negative magnetoconductance, characterized by an anomalously small low-energy scale B_* . This finding explains why both the Kondo effect and the 0.7-anomaly exhibit a very similar conductance behavior at sufficiently low magnetic fields and temperatures ($T, B \ll T_*$), amenable to a similar Fermi-liquid description. We also show that at high fields ($B \gg B_*$) the analogy between Kondo effect and 0.7-anomaly breaks down.

9:12AM P18.00007 Towards a Fermi-Liquid description of the 0.7 Anomaly in Quantum Point Contacts

, FLORIAN BAUER, JAN HEYDER, ENRICO SUBERT, Ludwig-Maximilians-Universitaet Muenchen, DAVID BOROWSKI, None, DANIELA TAUBERT, Ludwig-Maximilians-Universitaet Muenchen, DIETER SCHUH, Universitaet Regensburg, WERNER WEGSCHEIDER, ETH Zuerich, JAN VON DELFT, STEFAN LUDWIG, Ludwig-Maximilians-Universitaet Muenchen — In addition to plateaus in integer values of $G_0 = \frac{2e^2}{h}$, the linear conductance of a quantum point contact (QPC) shows an anomalous shoulder at around $0.7G_0$ that evolves in a characteristic fashion with rising magnetic field and temperature. We present a microscopic theory for the 0.7 conductance anomaly, based on a one-dimensional tight binding model with a local interaction, a smooth potential barrier and a homogeneous magnetic Zeeman field. We calculate the conductance as a function of magnetic field and temperature using standard second order perturbation theory. Furthermore we use a more sophisticated method, the functional Renormalisation Group (fRG), to obtain a more reliable description at zero temperature and finite magnetic field. We analyze the leading temperature T and magnetic field B dependence of the conductance, which define, respectively, low-energy scales T_* and B_* and find that both T_* and B_* depend exponentially on gate voltage, whereas the ratio $\frac{B_*}{T_*}$ is almost independent of gate voltage. This result indicates that the low-energy behavior of the 0.7 anomaly displays Fermi-liquid behavior. We present new experimental data that corroborate this conclusion.

9:24AM P18.00008 Quantum Wires with Electrons and Cold Atoms

, LINEY HALLA KRISTINSDDOTTIR, JONAS C. CREMON, ANDREAS WACKER, STEPHANIE M. REIMANN, Lund University — Advances in atom trapping and atom chip techniques allow the controlled preparation and manipulation of clouds of cold, neutral atoms, in optical lattices as well as on lithographically patterned gate structures. This opens up many new possibilities to study quantum transport in systems other than semiconductor quantum dots or nanowires, with the exciting perspective of future "atomtronic" systems. Inspired by these developments, we study transport through two different interacting systems as a function of externally controllable parameters: Electrons in a nanowire, and cold atoms in a one-dimensional finite well. For a nanowire system we can demonstrate that Wigner crystallization occurs, when the length of the wire is changed in the experiment [1]. Distinct diamond patterns appear, when conductance is plotted against source-drain bias and the gate voltage, as common for quantum dot systems. The same holds for more general types of "interaction blockade," and we demonstrate that such phenomena can also be studied by cold atom systems.

[1] Kristinsdóttir, L.H., J. Cremon, H. Nilsson, H. Xu, H. Linke, L. Samuelson, A. Wacker and S.M. Reimann, *Phys. Rev. B* **83**, 041101, (2011).

9:36AM P18.00009 Functional dependence of the exact time-dependent Kohn-Sham potential for quantum transport

, JAMES RAMSDEN, REX GODBY, University of York — We present methods for determining exact steady-state and time-dependent Kohn-Sham potentials from known charge and current densities. Applying these methods to cases of a single electron added to the conduction band of a model semiconductor, we calculate the exact Kohn-Sham potentials and discuss their meaning in the context of describing quantum transport. We show that the inclusion of a longitudinal Kohn-Sham vector potential is quite unavoidable in describing steady-state current-carrying systems, whereas the addition of an electron in a wavepacket state necessitates, inter alia, the appearance of an exchange-correlation electric field. We also present our findings on the functional dependence of the exact Kohn-Sham scalar and vector potentials on the charge and current density.

9:48AM P18.00010 Waiting time distributions of mesoscopic conductors

, GERALDINE HAACK, University of Geneva, Switzerland, MATHIAS ALBERT, University of Paris Sud, Orsay, France, CHRISTIAN FLINDT, MARKUS BUETTIKER, University of Geneva, Switzerland — Electronic transport through mesoscopic structures is stochastic due to the quantum nature of the charge carriers. In full counting statistics the interest is in the number of particles that are detected in a given time interval. Another important and fundamental question concerns the waiting time between consecutive carriers. Recently, waiting time distributions (WTD) have been calculated for periodically driven systems described by master equations and shown to clearly distinguish random charge emissions from charge transfer processes which are frequency-locked to the period of the external drive [1]. In this work we investigate the WTD of a biased quantum point contact (QPC) with one channel [2]. The WTD clearly reflects the fermionic statistics of the elementary charges: with increasing transmission probability of the QPC, the WTD changes from that of a Poisson process for a nearly closed QPC to a Wigner-Dyson distribution, known from the analogous problem of free fermions described by random matrix theory. [1] M. Albert, C. Flindt and M. Buettiker, *Phys. Rev. Lett.* **107**, 086805 (2011). [2] M. Albert, G. Haack, C. Flindt and M. Buettiker, *in preparation*.

10:00AM P18.00011 Magnetic field induced mixed level Kondo effect in two-level quantum dots, ARTURO WONG, U of Florida, ANH NGO, SERGIO ULLOA, Ohio U — Semiconductor quantum dots provide an easily tunable environment in which to investigate the Kondo effect. As it is known, Kondo correlations are suppressed by magnetic fields, showing e.g. a drop in the conductance of a quantum dot device. However, certain systems may exhibit an increasing conductance as a function of an applied magnetic field [1]. In this work we use the numerical renormalization group method to study a two-level quantum dot system with on-level and interlevel Coulomb repulsion, coupled to a single channel. When there is a finite detuning between levels, and a local singlet develops in one of them, the linear conductance of the device shows a maximum structure as a function of an in-plane magnetic field, which depends on the temperature of the system. This maximum occurs at a magnetic field strength such that the spin up state of one of the levels and spin down of the other are degenerate, allowing a “mixed level” Kondo effect. The respective spectral functions feature a resonance at the Fermi energy, commensurate with the Kondo physics. We discuss the properties of this mixed level Kondo state in terms of the detuning and the other parameters of the system.

[1] R. Sakano and N. Kawakami, PRB 73, 155332 (2006)

10:12AM P18.00012 Time dependent quantum transport in a vibrating quantum dot in Kondo regime¹, ALI IHSAN GOKER, Department of Physics, Bilecik University — We employ the time dependent non-crossing approximation to investigate the effect of strong electron-phonon coupling on the instantaneous conductance and thermopower of a single electron transistor which is abruptly shifted into the Kondo regime via a gate voltage. We find that the instantaneous conductance exhibits decaying sinusoidal oscillations on the long timescale for infinitesimal bias [1]. The ambient temperature and electron-phonon coupling strength influence the amplitude of these oscillations and the frequency of oscillations is equal to the phonon frequency. We discuss the origin of these oscillations and the effect of finite bias on them. On the other hand, we argue that measurement of the decay time of thermopower to its steady state value in linear response might be an alternative tool in determination of the Kondo temperature and the actual value of the electron-phonon coupling strength in an experiment.

[1] A. Goker, J. Phys.: Condens. Matter, 23 (2011) 125302

¹Supported by Tubitak grant 111T303.

10:24AM P18.00013 Dynamic response of a single-electron transistor in the ac Kondo regime, THANH NGUYEN, CARLOS BOLECH, NAYANA SHAH, Department of Physics, University of Cincinnati — A single-electron transistor (SET) consisting of a small conducting island contacted by macroscopic conductors can be used to study strongly correlated electrons in artificial systems. SETs also provide possibilities of exploring non-equilibrium Kondo phenomena by applying source-drain voltage. In the context of recent measurements, we will discuss the non-trivial dynamics that emerges when externally imposed energy scales compete with the Kondo correlations. The response of the system to a simultaneous application of a magnetic field and a high-frequency modulation of the SET voltages will also be reported.

10:36AM P18.00014 Double Quantum Dot Kondo Effect in a Magnetic Field, SAMI AMASHA, ANDREW J. KELLER, ILEANA G. RAU, Stanford University, JORDAN A. KATINE, Hitachi Global Storage Technologies, HADAS SHTRIKMAN, Weizmann Institute, DAVID GOLDBERGER-GORDON, Stanford University — Conventionally the Kondo effect is thought of as describing how conduction electrons screen a localized spin. More generally, it describes how itinerant electrons screen a degenerate degree of freedom of a localized site. A double quantum dot (with negligible inter-dot tunneling) can have both spin degeneracy, as well as a degeneracy associated with an electron being on dot 1 or dot 2. The latter degeneracy corresponds to a pseudo-spin degree of freedom that can also be screened by the Kondo effect [A. Hübel, et al. PRL 101, 186804 (2008)]. Applying a finite magnetic field can split the spin degeneracy of the dots, which should allow the realization of a purely pseudo-spin Kondo effect. We present conductance measurements of this double dot Kondo effect in a magnetic field. We compare our measurements to theoretical predictions for SU(2) Kondo to check whether we have realized a purely pseudo-spin Kondo effect in a double dot.

10:48AM P18.00015 Theory of anomalous magnetotransport in triple quantum dots¹, BENJAMIN D'ANJOU, WILLIAM A. COISH, McGill University — Magneto-transport measurements on a triple quantum dot ring have recently shown anomalous quantum oscillations with dominant frequencies separated by a factor of three in magnetic flux [1]. Such oscillations, suggestive of a one-third periodicity in the flux quantum, are usually not observed in larger mesoscopic rings in which only larger periods are observed. We develop a microscopic transport model for the triple dot and show that the anomalous oscillations can dominate the transport behavior under certain conditions. Furthermore, we discuss the range of validity of our model by studying dephasing due to broadening and electric dipole interactions.

[1] L. Gaudreau et al., Phys. Rev. B 80, 075415 (2009)

¹This work was made possible with the support of the Canadian Institute CIFAR and of the Quebec provincial institutes INTRIQ and RQMP.

Wednesday, February 29, 2012 8:00AM - 11:00AM –
Session P19 DCMP GIMS: Invited Session: Dynamics of Strongly Correlated Systems: Control and Ultrafast X-Ray Probes 253AB

8:00AM P19.00001 Controlling Quantum Condensed Matter With Light, ANDREA CAVALLERI, Max Planck Department for the Structure and Dynamics of Matter, Hamburg; Department of Physics - University of Oxford — In this talk I will discuss some of our recent work aimed at controlling the properties of quantum condensed matter with light, for instance in High-Tc cuprates or in Mott Insulators. The focus is on the use of high-field THz radiation rather than near-visible excitations, thus using photon energies that do not destroy the broken symmetry state of the solid, for example by breaking Cooper pairs. Rather we study the non-linear electrodynamics of the solid, for example by manipulating low-lying lattice vibrations coherently or by driving the phase excitations in superconducting condensates. A straightforward conceptual analogy can be found with experiments that that study driven dynamics of strongly correlated atomic gases in optical lattices. Due to the short lengthscales and the fast timescales involved in condensed matter, femtosecond x-ray scattering and spectroscopy experiments with the LCLS Free Electron Laser are necessary to interrogate the microscopic non-equilibrium paths explored by the stimulated solid.

8:36AM P19.00002 Light induced meltdown of quasiparticles in high temperature superconductors, ALESSANDRA LANZARA, University California, Berkeley and Material Sciences Division, Lawrence Berkeley National Laboratory — Ultrafast time- and angle- resolved photoemission spectroscopy (tr-ARPES) is emerging as a powerful tool to access the non-equilibrium quasiparticles dynamics and Cooper pairs formation in unconventional superconductors. In a tr-ARPES experiment a non-equilibrium transient state is created by pumping with an infrared pulse and is then measured via photoemission with an ultraviolet probe pulse. By varying the time delay between pump and probe we can directly access the recovery of the superconducting gap and the non-equilibrium quasiparticles population decay. Here we present a detailed momentum, temperature, doping and density dependent study of the response of a high temperature Bi2212 superconductor to a femtosecond pump-probe. In particular, through systematic pump fluence dependence we have induced the meltdown of quasiparticles and have driven the system normal by inducing a collapse of the superconducting gap. Interestingly we observed that only quasiparticles beyond a particular boson mode respond to the pump laser excitations, while the others remain untouched and that both quasiparticles recombination and gap dynamics are a density, momentum and doping dependent process, showing a crossover from a weakly perturbed to a strongly perturbed regime. These results point to a new dichotomy between the ultrafast gap and quasiparticles response within and beyond the Fermi arc and reveal a new window into the nature of the pairing interaction in high T_c superconductors.

9:12AM P19.00003 Shooting the electronic structure movie: Femtosecond time-resolved photoemission of layered charge-density-wave systems, KAI ROSSNAGEL, University of Kiel — Charge-density waves (CDWs) are broken-symmetry states of low-dimensional materials that are brought about by strong electron-phonon interaction. Yet surprisingly, a universal microscopic understanding beyond this statement has not really evolved for this classical paradigm of condensed matter physics. In quasi-two-dimensional systems, for example, the common approaches based on ARPES band structure results—looking for nested sections of the Fermi surface or for a peak in the electronic susceptibility—have almost no predictive power. Apparently, more successful explanations have to take into account the delicate balance between several factors including not only electronic and phononic structure, but also electron-electron and electron-phonon interactions. Here, we will show that femtosecond time-resolved XPS and ARPES using pulsed extreme ultraviolet radiation generated by the free-electron laser FLASH [1] as well as by a table-top high-harmonic-generation source [2] can provide novel insights into the relative roles that the various factors play in CDW formation. We will focus on three conspicuous CDWs in prominent members of the family of layered transition-metal dichalcogenides: the $(\sqrt{13} \times \sqrt{13})$ CDW in the Mott insulator 1T-TaS₂, the $c(2\sqrt{3} \times 4)rect.$ CDW in the Peierls insulator Rb_xTaS₂, and the $(2 \times 2 \times 2)$ CDW in the possible excitonic insulator 1T'-TiSe₂. The specific program is to reveal the relative importance of electronic and phononic contributions to the various CDW transitions by relating measured melting and relaxation times of CDW-induced spectral features to typical elementary time scales in layered materials.

[1] S. Hellmann *et al.*, Phys. Rev. Lett. **105**, 187401 (2010).

[2] T. Rohwer *et al.*, Nature **471**, 490 (2011).

9:48AM P19.00004 Theoretical description of photo-doping in Mott and charge-transfer insulators, MARTIN ECKSTEIN, Max Planck Research Department for Structural Dynamics, University of Hamburg, Centre for Free Electron Laser Science, Hamburg, Germany — Many aspects of photo-excited insulator-to-metal transitions in Mott and charge-transfer systems are theoretically not well understood: How is the photo-doped state related to a chemically doped state? On what timescale do we expect the formation of quasiparticles? To describe the electronic dynamics of Mott insulators, we have used nonequilibrium dynamical mean-field theory (DMFT) in combination with Quantum Monte Carlo and various weak and strong-coupling [1] techniques. In the talk, I will briefly present the current status of this approach and of related cluster approaches for nonequilibrium. I will then discuss results for the photo-doping in the Hubbard model, and in a p-d model for charge-transfer insulators. When the onsite Coulomb repulsion U is much larger than the hopping, rapid thermalization of the pump-excited Mott insulator is inhibited by the energetic stabilization of doublon-hole pairs [2], and various types of non-thermal states can arise. Immediately after the excitation process, the system of doublons and holes is too hot to form quasiparticle states, but coupling to a heat-bath of phonons can drive the system into a metallic state with well developed doublon and hole bands. Close to the metal-insulator transition, on the other hand, when U is of the order as the hopping, doublons and holes rapidly thermalize due to the electron-electron interaction, which makes the system a bad metal rather than a Fermi liquid.

[1] M. Eckstein and Ph. Werner, Phys. Rev. B **82**, 115115 (2010).

[2] M. Eckstein and Ph. Werner, Phys. Rev. B **84**, 035122 (2011).

10:24AM P19.00005 High frequency properties of individual metallic carbon nanotubes¹, DANIEL SANTAVICCA, Department of Applied Physics, Yale University — We study the electrical and electrothermal dynamics of individual metallic single-walled carbon nanotubes (SWNT). Using Johnson noise thermometry, we characterize the dependence of the electron temperature on the dc bias current. This allows us to determine the thermal conductance associated with cooling of the nanotube electron system as a function of both temperature and nanotube length [1]. This thermal conductance can be used to predict the measured radio frequency (rf) bolometric response. At low temperatures and low bias current, an additional rf response is observed from the (non-thermal) electrical nonlinearity of the contacts [2]. Finally, we compare these rf measurements with measurements of terahertz (THz) detection. The THz measurements are used as a probe of plasmon standing wave resonances on the SWNT.

[1] D.F. Santavicca, J.D. Chudow, D.E. Prober, M.S. Purewal, and P. Kim, Nano Lett. **10**, 4538 (2010).

[2] D.F. Santavicca, J.D. Chudow, D.E. Prober, M.S. Purewal, and P. Kim, Appl. Phys. Lett. **98**, 223503 (2011).

¹In collaboration with Joel Chudow, Chris McKitterick, and Daniel Prober (Yale) and Philip Kim (Columbia). This work is supported by NSF-DMR and NSF-CHE.

Wednesday, February 29, 2012 8:00AM - 11:00AM – Session P20 FEd: Invited Session: Scientific Reasoning in a Physics Course 253C

8:00AM P20.00001 Empowering the crowd: faculty discourse strategies for facilitating student reasoning in large lecture, DEDRA DEMAREE, Oregon State University — Oregon State University (OSU) has restructured its introductory calculus-based sequence including reformed curriculum modeled after the Interactive Science Learning Environment (ISLE). ISLE is driven by an experimental cycle roughly summarized as: observe phenomena, find patterns and devise explanations, test explanations, develop a model, apply the model to new observations. In implementing ISLE at OSU we have chosen to focus on student scientific reasoning, specifically student ability to develop and test models, make explicit judgments on how to approach open-ended tasks, and take an authoritative role in knowledge development. In order to achieve these goals, the lecture course heavily utilizes social engagement. During large-lecture group work, emphasis is placed on facilitating student discourse about issues such as what systems to choose or how to define an open-ended problem. Instructional strategies are aimed at building off the group discourse to create a full-class community where knowledge is developed through collaboration with peers. We are achieving these goals along with an increase in measured student conceptual knowledge and traditional problem solving abilities, and no loss of content coverage. It is an ongoing effort to understand “best” instructional strategies and to facilitate new faculty when they teach the curriculum. Our research has focused on understanding how to facilitate activities that promote this form of discourse. We have quantitative analysis of engagement based on video data, qualitative analysis of dialogue from audio data, classroom observations by an external researcher, and survey data. In this session we share a subset of what we have learned about how to engage students in scientific reasoning discourse during large lecture, both at the group-work and full-class level.

8:36AM P20.00002 Designing and using multiple-possibility physics problems in physics courses, VAZGEN SHEKOYAN, Queensborough Community College, CUNY — One important aspect of physics instruction is helping students develop better problem solving expertise. Besides enhancing the content knowledge, problems help students develop different cognitive abilities and skills. This presentation focuses on multiple-possibility problems (alternatively called ill-structured problems). These problems are different from traditional “end of chapter” single-possibility problems. They do not have one right answer and thus the student has to examine different possibilities, assumptions and evaluate the outcomes. To solve such problems one has to engage in a cognitive monitoring called epistemic cognition. It is an important part of thinking in real life. Physicists routinely use epistemic cognition when they solve problems. I have explored the instructional value of using such problems in introductory physics courses.

9:12AM P20.00003 Assessing high-level scientific reasoning in a physics exam: Pipe-dream or reality?, DAVID BROOKES, Florida International University — What do we want students to be able to do when they have finished their introductory physics course? In addition to learning the physics content, we want students to learn to think like physicists. We want students to develop specific scientific reasoning abilities that are the hall-mark of scientific thinking. These include, analyzing and interpreting experimental data, designing an experiment to test different hypotheses, identifying assumptions in a physical model amongst many others. Physics courses such as the Investigative Science Learning Environment (ISLE) have been developed to focus specifically on developing students' scientific reasoning abilities. Research has shown that ISLE is successful in achieving its goal. We would like our assessments to directly reflect our learning goals for our students. In order to measure higher-level scientific reasoning, we can, for example, require students to participate in a laboratory practical exam in which they have to engage in experimental design and analysis. However, this assessment method could become very difficult to administer and grade in a large-enrollment class. Is it possible to assess scientific thinking abilities of students using traditional formats such as paper and pencil exams? In this talk I will present some of our latest ideas about how to re-design traditional exam questions to measure a range of scientific reasoning abilities.

9:48AM P20.00004 Using mathematics to make sense in undergraduate physics, SUZANNE BRAHMIA, Rutgers University — Physics courses involve the study of physical quantities constructed to facilitate the characterization of nature, and the study of the connections between these quantities. These connections are often ratios or products of more familiar quantities. Learning to use the predictive power these relationships provide is an important part of learning to make sense of the physical world. Mathematically inspired reasoning is foundational to the way physicists make sense of the natural world and math is often referred to as the language of physics. Students rarely understand the relationships between the physical quantities in the way their instructors hope they will. There is often a disconnect between the specialized way we use mathematics in physics and the broad spectrum of processes that students learn to master as they progress through the pre-college mathematics curriculum. We are often surprised by how little math our students are able to use in physics, despite successful performance in their previous math classes. Much of the reasoning used in introductory physics is borrowed from mathematics that is taught in middle school and early high school (facility and practice with integers, fractions and ratios, multiplication and division using symbolic representations, manipulation of linear equations, analyzing right triangles.) But physics is a very different context, with confounding factors that often render the mathematics opaque to the learner. In this talk, I will discuss the specific ways in which physicists' use of mathematics differs from what many students acquired in their math classes. I will discuss how a weak mastery of conceptualizing fundamental mathematical operations interferes with students' ability to make sense in physics, and can carry over into difficulties with subsequently more abstract reasoning at higher levels. I will also offer suggestions for ways in which instructors can be more cognizant of (and transparent about) their specialized use of mathematics, thereby helping their students to effectively use mathematics for making sense of the physics they are learning.

10:24AM P20.00005 Student reasoning about ratio and proportion in introductory physics¹, ANDREW BOUDREAUX, Western Washington University — To many students, introductory physics must seem a fast-moving parade of abstract and somewhat mysterious quantities. Most such quantities are rooted in proportional reasoning. Using ratio, physicists construct the force experienced by a unit charge, and attach the name electric field, or characterize a motion with the velocity change that occurs in a unit time. While physicists reason about these ratios without conscious effort, students tend to resort to memorized algorithms, and at times struggle to match the appropriate algorithm to the situation encountered. Although the term “proportional reasoning” is prevalent, skill in reasoning with these ratio quantities is neither acquired nor applied as a single cognitive entity. Expert ability seems to be characterized by the intentional use of a variety of components, or elements of proportional reasoning, by a fluency in shifting from one component to another, and by a skill in selecting from among these components. Based on this perspective, it is natural to expect students to develop proportional reasoning ability in fits and starts as various facets are acquired and integrated into existing understandings. In an ongoing collaboration between Western Washington University, New Mexico State University, and Rutgers, we are attempting to map the rich cognitive terrain of proportional reasoning, and to use our findings to guide the design of instruction that develops fluency. This talk will present a provisional set of proportional reasoning components, along with research tasks that have been developed to measure student ability along these components. Student responses will be presented as evidence of specific modes of thinking. The talk will conclude with a brief outline of our approach to improving student understanding.

¹Supported by NSF grants DUE-1045227, DUE-1045231, & DUE-1045250.

Wednesday, February 29, 2012 8:00AM - 11:00AM — Session P21 DCMP: Superconductivity: Electronic Structure of Cuprates 254A

8:00AM P21.00001 Co-existence of spin fluctuation and superconductivity in electron doped cuprate $\text{Pr}_{1-x}\text{LaCe}_x\text{CuO}_4$, DONGJOON SONG, S.R. PARK, CHUL KIM, S.K. CHOI, W.S. JUNG, Y.Y. KOH, Y.K. KIM, Yonsei University, Rep. of Korea, H. EISAKI, Y. YOSHIDA, AIST, Japan, C. KIM, Yonsei University, Rep. of Korea — Even though spin fluctuation has been proposed to be as the pairing glue in the cuprate high temperature superconductivity, there is lack of a clear evidence for its coupling to electron. One of the reasons is that, for hole doped cuprates, both anti-ferromagnetism (AFM) and recently proposed charge ordering effects due to Fermi surface nesting occur in the same region of the momentum space (anti-nodal region). On the other hand, electron doped cuprates are known to have the pseudo gap effect at hot spots from AFM band renormalization. This fact makes it advantageous to investigate electron doped cuprates for the spin fluctuation issue. We performed ARPES studies on superconducting electron doped cuprates PLCCO ($x=0.1, 0.15, 0.18$) to investigate the relation between the spin fluctuation and superconductivity. We observe pseudo gap for all the dopings, which indicates that the short range AFM ordering survives far away from the AFM phase boundary. This coincidence of the short range AFM and superconductivity even in the over doped state may support the spin fluctuation scenarios at least in the electron doped side.

8:12AM P21.00002 Evidence for the coexistence of antiferromagnetism and superconductivity in the electron-doped infinite-layer cuprate $\text{Sr}_{1-x}\text{La}_x\text{CuO}_2$ from ARPES, JOHN HARTE, DANIEL SHAI, ERIC MONKMAN, YUEFENG NIE, DARRELL SCHLOM, Cornell University, LUIGI MARITATO, University of Salerno, KYLE SHEN, Cornell University — The asymmetry between hole doping and electron doping of cuprates has major implications for theories of high- T_c superconductivity, yet the vast majority of our knowledge of electron-doped cuprates originates from the $\text{Re}_{2-x}\text{Ce}_x\text{CuO}_4$ (RCCO) materials. One salient feature of electron doping is the robustness of antiferromagnetism, but at present it has not been established whether this is intrinsic to the electron-doped CuO_2 plane or idiosyncratic to the RCCO family. Here we report high-resolution *in situ* angle-resolved photoemission spectroscopy measurements of superconducting $\text{Sr}_{1-x}\text{La}_x\text{CuO}_2$ (SLCO) thin films grown by molecular beam epitaxy. The observed electronic structure exhibits many features consistent with (π, π) scattering, and the clear observation of such scattering in this material demonstrates that strong antiferromagnetism is generic to the electron-doped CuO_2 plane. Furthermore, the (π, π) order in SLCO is sufficiently strong to fully gap the nodal portion of the Fermi surface, leaving only electron pockets at $(\pi, 0)$; these pockets are gapped by the coexisting (presumably d-wave) superconductivity. This offers a simple explanation for the many reports of s-wave superconductivity in this material.

8:24AM P21.00003 Electronic structure modulations in the stripe phase of $\text{La}_{1.475}\text{Nd}_{0.4}\text{Sr}_{0.125}\text{CuO}_4$, ANDREW ACHKAR, University of Waterloo, FEIZHOU HE, Canadian Light Source, RONNY SUTARTO, University of British Columbia, JOCHEN GECK, Leibniz Institute for Solid State and Materials Research IFW Dresden, HARRY ZHANG, YOUNG-JUNE KIM, University of Toronto, DAVID HAWTHORN, University of Waterloo — A prevailing description of the stripe phase in underdoped cuprate superconductors is that the charge carriers (holes) phase segregate into hole rich regions that form anti-phase boundaries between regions of anti-ferromagnetic order. I will present resonant elastic x-ray scattering measurements of stripe-ordered $\text{La}_{1.475}\text{Nd}_{0.4}\text{Sr}_{0.125}\text{CuO}_4$ at the Cu $L_{3,2}$ and O K absorption edges that point to an alternate interpretation of the stripe phase. Analysis of the energy dependence of the scattering intensity reveals that the dominant feature of the charge density wave state is a spatial modulation in the energies of Cu $3d$ and O $2p$ states rather than the large modulation of the valence (charge density) envisioned in the common stripe paradigm. These energy shifts are interpreted as a spatial modulation of the electronic structure, possibly involving a modulation of the Cu $3d$ – O $2p$ hopping, t_{pd} , the onsite Coulomb repulsion, U_{dd} , and other local electronic structure parameters. This result may point towards a valence-bond-solid interpretation of the stripe phase, where translational symmetry can be broken with minimal modulation of the charge density.

8:36AM P21.00004 Quantum Oscillations in a π -Striped Superconductor, MIRSAEED ZELLI, CATHERINE KALLIN, McMaster University, JOHN BERLINSKY, McMaster University and Perimeter Institute for Theoretical Physics — Within Bogoliubov-de Gennes theory, a semiclassical approximation is used to calculate the Fermi surface area associated with quantum oscillations in a model of a π -striped superconductor, where the d-wave superconducting order parameter oscillates spatially with zero average value. This system has a non-zero density of particle-hole states at the Fermi energy, which form Landau-like levels in the presence of a magnetic field. The oscillation frequency found for large pairing interaction, for π -stripes with period 8, is close to that reported for experimental measurements in the cuprates. A comparison is made of this theory to data for quantum oscillations in the specific heat measured by Riggs et al.

8:48AM P21.00005 Density-functional theory calculation of Fermi surface in stripe ordered $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$, SIMON BLACKBURN, MICHEL COTE, University of Montreal — High temperature superconductors (HTSC) attract a lot of interests since their discovery in 1986. More recently, observations of quantum oscillations in underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$ (YBCO6.5) at a low frequency suggested a small pocket constitute the Fermi surface (Doiron-Leyraud et al. Nature 447, 565 (2007)). In this work, we present results of density-functional theory (DFT) calculations of YBCO electronic structure. In order to better represent the electron-electron interaction, we add an on-site repulsion term (Hubbard term) on the copper d-orbitals (DFT+U). This method is known to improve DFT calculations for Mott insulators like La_2CuO_4 and $\text{YBCO}_{6.0}$ since the Hubbard term favors an anti-ferromagnetic ground state. Using this method, we compare various magnetic states calculated with different values of the Hubbard term U. Our results suggest that an atom-centered stripe, similar to the one found in $\text{La}_{1.875}\text{Sr}_{0.125}\text{CuO}_4$ (Tranquada et al. Nature 375 561 (1995)), is consistent with the presence of a Fermi pocket of the size reported in the experiments. We further show that the size of the pocket and the nature of the carriers (electrons or holes) can be varied with pressure suggesting a way to test this hypothesis.

9:00AM P21.00006 Kinetics-Driven Superconducting Gap in Underdoped Cuprate Superconductors Within the Strong-Coupling Limit¹, WEI KU, YUCEL YILDIRIM, CMPMSD, Brookhaven National Laboratory — A generic theory [1] of the quasiparticle superconducting gap in underdoped cuprates is derived in the strong-coupling limit, and found to describe the experimental “second gap” in absolute scale. In drastic contrast to the standard pairing gap associated with Bogoliubov quasiparticle excitations, the quasiparticle gap is shown to originate from anomalous kinetic (scattering) processes, with a size unrelated to the pairing strength. Consequently, the k dependence of the gap deviates significantly from the pure $d_{x^2-y^2}$ wave of the order parameter. Our study reveals a new paradigm for the nature of the superconducting gap, and is expected to reconcile numerous apparent contradictions among existing experiments and point toward a more coherent understanding of high-temperature superconductivity.

[1] Y. Yildirim and Wei Ku, PRX 1, 011011 (2011).

¹Work supported by DOE DE-AC02-98CH10886

9:12AM P21.00007 Recent ARPES study on extremely underdoped LSCO system, YU HE, Department of Applied Physics, Stanford University, MAKOTO HASHIMOTO, SLAC National Accelerator Laboratory, SUNG-KWAN MO, RUIHUA HE, Advanced Light Source, LBNL, YOICHI ANDO, Department of Quantum Functional Materials, Institute of Scientific and Industrial Research, SEIKI KOMIYA, Central Research Institute of Electric Power Industry, ZHI-XUN SHEN, Department of Applied Physics, Stanford University — It has been widely accepted that Mott physics plays an important role in how superconductivity develops in high T_c cuprates. However, only a few in the family can reach to deeply underdoped region where Mott physics truly dominates, where the “pseudogap” is entirely disentangled from superconducting gap. Being an important compound to tackle this issue, extremely underdoped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ samples were systematically investigated through ARPES experiments. The doping dependence of Gaussian envelope at higher binding energy suggests strong polaronic contribution to the near Fermi level coherent feature. In complementary to previous observation of nodal gap in semiconducting LSCO, we found the Fermi surface to be fully gapped over wide range in the phase diagram in accordance with transport measurements. By comparing the marginal Fermi liquid model with momentum/temperature dependent MDC width analysis, we will extend our discussion on the intriguing connections between the nodal gap, polaronic excitation and “pseudogap” in this system.

9:24AM P21.00008 One gap, two gaps, and universality in high temperature superconductors, JUNJING ZHAO, University of Illinois at Chicago, UTPAL CHATTERJEE, MIKE NORMAN, Argonne National Lab, MOHIT RANDERIA, Ohio State University, JUAN CARLOS CAMPUZANO, University of Illinois at Chicago — A dramatic change in energy gap anisotropy upon reducing carrier concentration has often been observed in the cuprate high temperature superconductors (HTSC). A simple d-wave gap in materials with the optimal T_c evolves with underdoping into a ?two-gap? structure, with different dependences in different regions of momentum space. It is tempting to associate the large antinodal gap with a second order parameter distinct from d-wave superconductivity. We use angle-resolved photoemission spectroscopy (ARPES) to show that this two-gap behavior, and the concomitant destruction of well defined electronic excitations, are not universal features of HTSC, and depend sensitively on how the underdoped materials are prepared. Depending on cation substitution, underdoped crystals either show two-gap behavior or not. In contrast, many characteristics of HTSC like the superconducting dome (T_c versus doping), nodal quasiparticles, antinodal gap that decreases monotonically with doping, and the pseudogap, are present in all samples, irrespective of whether they exhibit two-gap behavior or not. Our results imply that universal aspects of high T_c superconductivity are insensitive to differences in the electronic states in the antinodal region of the Brillouin zone.

9:36AM P21.00009 Imaging Doped Holes in a Cuprate Superconductor with High-Resolution Compton Scattering, B. BARBIELLINI, Northeastern U. (NU), Y. SAKURAI, M. ITOU, JASRI, SPring-8, P.E. MIJNAREND, NU and Delft University of Technology, R.S. MARKIEWICZ, NU, S. KAPRZYK, NU and AGH Krakow, J.-M. GILLET, Ecole Centrale Paris, S. WAKIMOTO, Quantum Beam Science Directorate, Japan Atomic Energy Agency, M. FUJITA, Tohoku University, S. BASAK, Y.J. WANG, W. AL-SAWAI, H. LIN, A. BANSIL, NU, K. YAMADA, Tohoku University — The high-temperature superconducting cuprate $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) shows several phases ranging from antiferromagnetic insulator to metal with increasing hole doping. To understand how the nature of the hole state evolves with doping, we have carried out high-resolution Compton scattering measurements at room temperature together with first-principles electronic structure computations on a series of LSCO single crystals in which the hole doping level varies from the underdoped (UD) to the overdoped (OD) regime [1]. Holes in the UD system are found to primarily populate the O 2p_x/p_y orbitals. In contrast, the character of holes in the OD system is very different in that these holes mostly enter Cu d orbitals. High-resolution Compton scattering provides a bulk-sensitive method for imaging the orbital character of dopants in complex materials.

[1] Y. Sakurai *et al.* Science **332**, 698 (2011).

9:48AM P21.00010 Anisotropic quasiparticle scattering in overdoped La-based cuprate superconductors: An angle resolved photoemission study, JOHAN CHANG, EPFL Lausanne and Paul Scherrer Institut, Switzerland, MARTIN MAANSSON, YASMINE SASSA, CHRISTIAN MATT, ETH Zurich, Switzerland, OLOF GOTBERG, OSCAR TJERNBERG, KTH, Sweden, STEFAN PAILHES, University of Lyon, France, OLIVER LIPSCOMPE, STEPHEN HAYDEN, Bristol University, UK, MING SHI, LUC PATTHEY, Swiss light source, Paul Scherrer Institut, Switzerland, JOEL MESOT, EPFL Lausanne and Paul Scherrer Institut, Switzerland — High-temperature superconductivity remains one of the outstanding unresolved problems of condensed matter physics. In the cuprate superconductors, a central part of the problem is to understand the unusual normal state properties. Here we present a new angle resolved photoemission spectroscopy (ARPES) study on the normal state of overdoped La-based cuprates. The pseudogap phase is found to vanish in a quantum critical point x_c inside the superconducting dome. Momentum dependent quasiparticle scattering has been studied for doping concentrations larger than x_c . Comparison to angle-integrated bulk probes such as electrical transport measurements will be made.

10:00AM P21.00011 ARPES evidence for a unidirectional bond-direction order in La-based cuprates, RUI-HUA HE, ALS-Stanford, M. HASHIMOTO, Stanford, K. TANAKA, S.-K. MO, ALS, T. SASAGAWA, TIT, M. FUJITA, T. ADACHI, K. YAMADA, Y. KOIKE, Tohoku, Z. HUSSAIN, ALS, Z.-X. SHEN, Stanford — Lattice translational symmetry breaking has wide implications with a variety of emergent quantum phases of condensed matters. In cuprate superconductors, various types of shadow bands have been observed in ARPES as band replicas that are displaced from the main bands by specific wave vectors in momentum space, suggestive of the breaking of lattice translational symmetry in different forms. Shadow bands associated with a wave vector along the Cu-O bond direction, were recently observed in a Y-based cuprate, which are ascribed to the unique occurrence of oxygen ordering in the CuO chains of the material. In contrast, the shadow bands reported so far in other cuprates without CuO chains in their crystal structures are associated with some wave vectors all along the bond-diagonal direction and it remains controversial, in most cases, whether they are due to some orderings of primarily structural or electronic origins. Here we report the first clear observation of shadow bands in ARPES associated with a bond-direction wave vector in the La-based cuprates (without CuO chains). These shadow bands were observed under various polarization conditions over a wide doping range in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and are associated with a unidirectional order. We will present a doping and temperature dependence study of this order and discuss the results in relation to the complementary bulk-sensitive scattering experiments on the same system.

10:12AM P21.00012 Synchrotron X-ray study reveals oxygen chains in $\text{HgBa}_2\text{CuO}_{4+\delta}$ ¹, WOJCIECH TABIS, University of Minnesota — X-ray scattering work shows that the double-layer high- T_c superconductors $\text{YBa}_2\text{Cu}_3\text{O}_{8+\delta}$ and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{6+\delta}$ are intrinsically inhomogeneous [1-3], with short-range lattice modulations driven by oxygen dopants. $\text{HgBa}_2\text{CuO}_{4+\delta}$ (Hg1201) has a simpler (tetragonal) structure and the highest T_c (at optimal doping) among all single-layer cuprates. It is thus a very good candidate system to address the issue of charge modulations. Using synchrotron X-ray scattering and high-quality single crystals, we have observed a short-range lattice modulations in Hg1201. Careful analysis of the diffuse intensity pattern, and a study of the doping and temperature dependence, point toward the formation of local one-dimensional order in the form of uncorrelated oxygen chains in the charge-reservoir layer. The chains exist at intermediate and high doping, form along [100], and have typical lengths of 15-30 lattice constants [4].

1. Z. Islam *et al.* PRL **93** 157008 (2004)
2. J. Strempfer *et al.* PRL **93**, 157007 (2004)
3. J. P. Castellan *et al.* PRB **73**, 174505 (2006)
4. G. Chabot-Couture, W. Tabis, J. N. Hancock Z. Islam, L. Lu, G. Yu, Y. Li, X. Zhao, Y. Ren, A. Mehta, M. Greven, (unpublished)

¹This work was supported by DOE Basic Energy Sciences

10:24AM P21.00013 Doping dependent intrinsic line width of the Cu-O bond-stretching phonon with $\mathbf{q}=(0.25\ 0\ 0)$ in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, S.R. PARK, University of Colorado at Boulder, A. HAMANN, L. PINTSCHOVUS, KIT, D. LAMAGO, KIT; Laboratoire Leon Brillouin, CEA-Saclay, G. KHALIULLIN, MPI, M. FUJITA, K. YAMADA, Tohoku University, G.D. GU, J.M. TRAN-QUADA, Brookhaven National Laboratory, D. REZNIK, University of Colorado at Boulder — We have recently found that the charge inhomogeneities provide significant broadening in the Cu-O bond stretching phonon of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, and the line shape of the phonon at zone boundary is well reproduced by the simple model which takes charge inhomogeneous effect into account [1]. The question is, now, how large intrinsic line width of the phonon at $\mathbf{q}=(0.25\ 0\ 0)$, where the giant phonon softening and broadening exist [2], is apart from the charge inhomogeneous effect on the line width. In this talk, we will show the doping dependence of the intrinsic line width of the phonon from $x=0.05$ to $x=0.30$. Interestingly, the intrinsic line width as a function of doping follows the superconducting transition temperature. We will discuss relationship between the phonon and the superconductivity in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$.

- [1] S. R. Park *et al.*, accepted for publication in PRB (2011).
- [2] D. Reznik *et al.*, Nature **440**, 1170 (2006).

10:36AM P21.00014 Investigation of Fermi & Luttinger surfaces in $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$ using ARPES, SIMON BELL, San Jose State University, GEY-HONG GWEON, JIANQIAO MENG, UC Santa Cruz, K.H. KIM, H G LEE, Pohang University of Science & Technology, S.I. LEE, Seogang University — The electronic structure & occupancy of doped cuprate superconductors $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$ of various doping levels is probed using angle-resolved photoemission spectroscopy (ARPES). The Fermi surface investigated shows that the Luttinger sum rule involving only the Fermi surface fails to account for the particle sum rule. Instead, the Luttinger sum rule that involves both the Fermi surface and the Luttinger surface seems necessary. We argue that such a generalized sum rule indicates the importance of very strong electron correlations.

10:48AM P21.00015 The electronic structure of tetragonal CuO, SIMON MOSER, Ecole Polytechnique Federale de Lausanne, Advanced Light Source, LUCA MORESCHINI, Advanced Light Source, DAVIDE INNOCENTI, University of Rome Tor Vergata, YOUNG JUN CHANG, AARON BOSTWICK, ELI ROTENBERG, Advanced Light Source, MARCO GRIONI, Ecole Polytechnique Federale de Lausanne — The cupric oxide CuO exhibits an insulating ground state with a correlation-induced charge-transfer gap and antiferromagnetism. It is, in principle, the most straightforward parent compound of the doped cuprates, and therefore has been theoretically studied as a model material for high temperature superconductivity. Bulk CuO crystallizes in a low-symmetry monoclinic form, in contrast to the rocksalt structure typical of late 3d transition metal monoxides. It was recently synthesized by epitaxial growth on SrTiO_3 substrates in a higher symmetry tetragonal structure with elongated c-axis (Siemons et al. PRB 79, 2009). Extrapolating the behavior of other 3d transition metal monoxides, this phase of CuO is predicted to have a much higher Neel temperature than its bulk counterpart. At beamline 7 of the Advanced Light Source, we have grown tetragonal CuO thin films by pulsed laser deposition and investigated their electronic structure by angle-resolved photoelectron spectroscopy (ARPES). These measurements represent the first mapping of the band structure of this new material, not available in bulk phase, and will serve as a reference point for future doping experiments.

Wednesday, February 29, 2012 8:00AM - 10:48AM – Session P22 DMP DCOMP: Focus Session: Fe-based Superconductivity - Fe(Te,Se) 254B

8:00AM P22.00001 Electronic disorder and magnetic-field-induced superconductivity enhancement in $\text{Fe}_{1+y}(\text{Te}_{1-x}\text{Se}_x)$, JIN HU, TIJIANG LIU, BIN QIAN, ZHIQIANG MAO, Department of Physics and Engineering Physics, Tulane University — The iron chalcogenide $\text{Fe}_{1+y}(\text{Te}_{1-x}\text{Se}_x)$ superconductor system exhibits a unique electronic and magnetic phase diagram distinct from those seen in iron pnictides: bulk superconductivity does not appear immediately following the suppression of long-range $(\pi,0)$ AFM order. Instead, an intermediate phase with weak charge carrier localization appears between AFM order and bulk superconductivity (Liu et al., Nat. Mater. 9, 719 (2010)). In this talk, we report our recent studies on the relationship between the normal state and superconducting properties in $\text{Fe}_{1+y}(\text{Te}_{1-x}\text{Se}_x)$. We show that the superconducting volume fraction V_{SC} and normal state metallicity significantly increase while the normal state Sommerfeld coefficient γ and Hall coefficient R_H drop drastically with increasing Se content in the underdoped superconducting region. Additionally, V_{SC} is surprisingly enhanced by magnetic field in heavily underdoped superconducting samples. The implications of these results will be discussed. Our analyses suggest that the suppression of superconductivity in the underdoped region is associated with electronic disorder caused by incoherent magnetic scattering arising from $(\pi,0)$ magnetic fluctuations.

8:12AM P22.00002 The structure of the oxygen-annealed $\text{Fe}_{1.08}\text{Te}_{0.55}\text{Se}_{0.45}\text{O}_x$ superconductor, HEFEI HU, JIAN-MIN ZUO, MAO ZHENG, JAMES N. ECKSTEIN, WAN KYU PARK, LAURA H. GREENE, University of Illinois at Urbana-Champaign, JINSHENG WEN, ZHIJUN XU, ZHIWEI LIN, QIANG LI, GENDA GU, Brookhaven National Laboratory — Effect of oxygen annealing on the iron chalcogenide superconductor with excess Fe is studied and structure change is investigated by using electron microscopy. The as-grown single crystal $\text{Fe}_{1.08}\text{Te}_{0.55}\text{Se}_{0.45}$ with the tetragonal PbO-type structure is non-superconducting owing to the excess Fe. Superconductivity is induced after oxygen annealing with an onset and zero resistance transition temperature around 14.5 K and 11.5 K, respectively. The oxygen doping is evidenced by electron energy loss spectroscopy, and accompanied by improved homogeneity in the remaining PbO-type phase as well as an increase in the $L_{3/2}$ intensity ratio of the Fe- $L_{2,3}$ edge, indicating an increase in Fe valence. Local phase transformation from the tetragonal PbO-type phase to the hexagonal NiAs-type phase is also observed after oxygen annealing.

8:24AM P22.00003 Unusual Persistence of Superconductivity Against High Magnetic Fields in the Strongly-Correlated Iron-Chalcogenide Film FeTe:O_x , IVO DIMITROV, WEIDONG SI, WEI KU, SU-JUNG HAN, QIANG LI, Brookhaven National Laboratory — We report an unusual persistence of superconductivity against high magnetic fields in the iron chalcogenide film FeTe:O_x below 2.52 K. Instead of saturating like a mean-field behavior with a single order parameter, the measured low-temperature upper critical field increases progressively, suggesting a large supply of superconducting states accessible via magnetic field or low-energy thermal fluctuations. We demonstrate that superconducting states of finite momenta can be realized within the conventional theory, despite its questionable applicability. Our findings reveal a fundamental characteristic of superconductivity and electronic structure in the iron-based superconductors.

8:36AM P22.00004 Growth conditions for pulsed laser deposited FeTeO_y superconducting thin films and observation of a low temperature structural transition¹, LAHIRU NARANGAMMANA, University of Connecticut, Storrs, CT, YUEFENG NIE, Cornell University, Ithaca, NY, JOSEPH BUDNICK, University of Connecticut, Storrs, CT, XUERONG LIU, JOHN HILL, GENDA GU, Brookhaven National Laboratory, Upton, NY, CHRISTOF NIEDERMAYER, Paul Scherrer Institut Villigen, PSI, Switzerland, BARRETT WELLS, University of Connecticut, Storrs, CT — FeTe thin films were grown by pulsed laser deposition and oxygen was incorporated to make superconducting FeTeO_y . The Te concentration of the films was highly dependent on growth temperature, due to the evaporation of Te at higher temperatures. Films grown using a porous, unreacted Fe/Te target showed islanding, an open structure, and a strong c axis texture. Oxygen could be easily added or removed by low temperature anneals. Films grown using a dense, polycrystalline conglomerate for a target and a short target-substrate distance had better epitaxy, and were dense, continuous and smooth. Post processing of oxygen on these films was difficult, but we were able to control oxygen concentration during growth using a small oxygen partial pressure. Initial low temperature diffraction studies of these films using both x-rays and neutrons indicate a sudden change in c axis lattice parameter at the superconducting T_C , but continued exposure of the beam drives out oxygen. Dense epitaxial films should allow for studying this phase change.

¹Supported by DOE through contact # DE-FG02-00ER45801(Uconn).

8:48AM P22.00005 Growth and oxygen doping of thin film FeTe by Molecular Beam Epitaxy¹, MAO ZHENG, CAN ZHANG, HEFEI HU, JIAN-MIN ZUO, JAMES ECKSTEIN, University of Illinois Urbana-Champaign — FeTe is isomorphic to FeSe , a representative of the 11 family of iron based superconductors. While not a superconductor itself, FeTe , particularly in thin film form, undergoes a superconducting transition when doped with oxygen. In this presentation, we will discuss the growth of FeTe by MBE and various schemes we used to dope the samples. Evidence from our investigation suggests that FeTe films are doped via an oxygen diffusion process which is strongly activated by temperature.

¹This material is based upon work supported as part of the Center of Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-AC0298CH10

9:00AM P22.00006 Suppression of superconductivity in Fe chalcogenides by annealing: A reverse effect to pressure, PENG TONG, DESPINA LOUCA, Department of Physics, University of Virginia, ANNA LLOBET, Lujan Neutron Scattering Center, Los Alamos National Laboratory, JIAQIANG YAN, Department of Materials Science and Engineering, University of Tennessee, RYOTARO ARITA, Department of Applied Physics, University of Tokyo, and JST TRIP — Superconductivity in $\text{FeTe}_{1-x}\text{Se}_x$ can be controlled by annealing, in the absence of extrinsic influences. Using neutron diffraction, we show that T_C sensitively depends on the atomic configurations of the Te and Se ions. Low temperature annealing not only homogenizes the Te and Se ion distribution as previously observed, it suppresses T_C because of changes in the chalcogen ions' z-parameter. In particular, the height of Te from the Fe basal plane is much reduced while that for Se shows a modest increase. These trends are reverse of the effects induced by pressure.

9:12AM P22.00007 Phase diagram and oxygen annealing effect of $\text{FeTe}_{1-x}\text{Se}_x$ iron-based superconductor, YASUNA KAWASAKI, KEITA DEGUCHI, SATOSHI DEMURA, HIROYUKI OKAZAKI, TOSHINORI OZAKI, TAKAHIDE YAMAGUCHI, HIROYUKI TAKEYA, YOSHIHIKO TAKANO, National Institute for Materials Science — Phase diagrams of as-grown and O_2 -annealed $\text{FeTe}_{1-x}\text{Se}_x$ decided by magnetic susceptibility measurement were obtained. For as-grown samples, the antiferromagnetic order was fully suppressed in the region of $x \geq 0.15$ and superconductivity appeared at $x \geq 0.1$. However, bulk superconductivity emerged at only $x = 0.5$. Interestingly, for O_2 -annealed samples, complete suppression of the magnetic order and bulk superconductivity was observed at $x \geq 0.1$. We found that O_2 annealing induces the bulk superconductivity for $\text{FeTe}_{1-x}\text{Se}_x$. The O_2 probably play a key role of a suppression of the magnetic order and appearance of bulk superconductivity.

9:24AM P22.00008 Magnetism and superconductivity in $\text{Pd}_{1-x}\text{Fe}_x\text{Te}$, AMAR KARKI, SHANE STADLER, DANA BROWNE, JIANNENG LI, RONGYING JIN, Louisiana State University — PdTe is a long-known superconductor but its physical properties are almost unknown. We have recently studied its basic physical properties in both normal and superconducting states. While FeTe forms different crystallographic structure and is known to form spin density wave below $T_N = 70$ K, we have successfully synthesized $\text{Pd}_{1-x}\text{Fe}_x\text{Te}$ with x from 0 to 1. By measuring its electrical and magnetic properties, we establish the phase diagram of $\text{Pd}_{1-x}\text{Fe}_x\text{Te}$ for the first time. With increasing x, we found that T_C is quickly suppressed. Ferromagnetism appears for the samples with $x \geq 0.02$. For $0.25 \leq x \leq 1.0$, the system exhibits antiferromagnetic ordering with T_N increasing with x. This is a prototype system for studying the interplay between superconductivity and magnetism.

9:36AM P22.00009 $\text{FeSe}_{0.5}\text{Te}_{0.5}$ thin films with critical current density above $1\text{MA}/\text{cm}^2$, WEIDONG SI, SU JUNG HAN, IVO DIMITROV, QIANG LI, Brookhaven National Laboratory — High quality $\text{FeSe}_{0.5}\text{Te}_{0.5}$ thin films have been prepared on various substrates, such as SrTiO_3 , LaAlO_3 and YSZ, some with buffer layers. T_C 's as high as 20K with superconducting transition widths of about 1K were obtained. These T_C 's are much higher than those of bulk $\text{FeSe}_{0.5}\text{Te}_{0.5}$ ($\sim 15\text{K}$). Our films carry high critical current densities J_c 's (above $1\text{MA}/\text{cm}^2$) at liquid helium temperature. These films hold J_c 's above $1 \times 10^5 \text{A}/\text{cm}^2$ and very low J_c anisotropies (< 3) under magnetic fields as high as 30T at 4.2K. We have also prepared textured $\text{FeSe}_{0.5}\text{Te}_{0.5}$ thin films on a buffered metal template with results similar to the ones mentioned above. This shows that iron chalcogenides have a very promising future for high-field applications at liquid helium temperatures. Pinning force analysis indicates the presence of a point defect flux-pinning mechanism, suggesting a straightforward approach to conductor optimization.

9:48AM P22.00010 London penetration depth measurements of $\text{Fe}_{1+y}(\text{Te}_{1-x}\text{Se}_x)$ single-crystals at ultra-low temperatures¹, ANDREI DIACONU, Department of Physics, AMRI, University of New Orleans, New Orleans, Louisiana 70148, USA, JIN HU, TIJIANG LIU, BIN QIAN, ZHIQIANG MAO, Department of Physics and Engineering Physics, Tulane University, New Orleans, Louisiana 70118, USA, LEONARD SPINU, Department of Physics, AMRI, University of New Orleans, New Orleans, Louisiana 70148, USA — The evolution of the superconducting properties as derived from the in-plane penetration depth measurements as a function of temperature in single crystals of $\text{Fe}_{1.02}(\text{Te}_{1-x}\text{Se}_x)$, with Se concentration spanning from 25% to 45%, was studied using a tunnel diode oscillator technique in a dilution refrigerator down to a temperature of 30mK. By using a set of two mutually coupled planar inductors parallel to the ab plane of the samples, the probing ac field is uniform across the sample along the c axis making the variation in susceptibility solely due to in-plane currents while significantly increasing the signal to noise ratio compared to usual inductors used in similar experiments. The evolution of the topology of the superconducting gap from underdoped to optimally doped samples, as derived from exponential and power law behavior of λ_{ab} at low temperatures, is presented.

¹Work supported by the DOD ARO under Grant No. W911NF0910530

10:00AM P22.00011 Electron-phonon coupling in layered FeSe compounds¹, TIMUR BAZHIROV, MARVIN L. COHEN, University of California, Berkeley — Iron-chalcogenide superconductors, showing many characteristic physical properties, can serve as a model materials to study the electron-pairing mechanism for all iron-based superconductivity. Layered iron-chalcogenide systems including single layer FeSe, bulk FeSe, K-intercalated FeSe, were studied using first principle pseudopotential density functional based approach. Electronic structure, vibrational properties and electron-phonon coupling strength were studied for the cases with and without iron magnetic moment ordering. The latter is incorporated using local spin density approximation. Our results show significant changes to electronic structure resulting in much higher electron-phonon coupling for spin-resolved configurations. Electron-phonon matrix elements for particular phonon mode of A_{1g} symmetry are showing dramatic increase. Superconducting transition temperature estimates based on McMillan's equation are showing values significantly higher than previously reported, but still not high enough to account for the experimental results.

¹This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by the Lawrence Berkeley National Laboratory

10:12AM P22.00012 Magnetism and superconductivity in modulated FeTe systems., KALUM PALANDAGE, Trinity College, Hartford, CT, GAYANATH FERNANDO, University of Connecticut, Storrs, CT, ARMEN KOCHARIAN, California State University, Los Angeles, CA — We examined the interplay between magnetism and superconductivity by monitoring the non-superconducting chalcogenide FeTe. We studied its transitions under insertion of oxygen, iron and vacancies of iron using spin-polarized band structure methods (LSDA with GGA) starting from the collinear and bicollinear magnetic arrangements. A supercell with 8-Fe and 8-Te atoms was used so that it can capture local changes in magnetic moments. The calculated values of magnetic moments agree well with available experimental data while some of the modulations lead to significant changes in the bicollinear or collinear magnetic moments/arrangements. The total energies of these systems indicate that the collinear-derived structure is more favorable prior to a possible superconducting transition.

10:24AM P22.00013 Revealing the dual nature of magnetism in iron pnictides and iron chalcogenides using x-ray emission spectroscopy, HLYNUR GRETTARSSON, ANDREEA LUPASCU, YOUNG-JUNE KIM, WENLONG WU, STEPHEN R. JULIAN, University of Toronto, JUNGHO KIM, DIEGO CASA, THOMAS GOG, Argonne National Laboratory, ZHI JUN XU, JIN SHENG WEN, GENDA GU, Brookhaven National Laboratory, R.H. YUAN, Z.G. CHEN, NAN-LIN WANG, Chinese Academy of Sciences, SEUNGHYUN KHIM, KEE HOON KIM, Seoul National University, IGNACE JARRIGE, SHINICHI SHAMOTO, M. ISHIKADO, Japan Atomic Energy Agency, JIUN-HAW CHU, IAN RANDAL FISHER, Stanford University — We present a Fe $K\beta$ x-ray emission spectroscopy study of local magnetic moments in various iron-based superconductors in their paramagnetic phases. Our findings show that a local magnetic moments exists in all samples studied: PrFeAsO , $\text{Ba}(\text{Fe}, \text{Co})_2\text{As}_2$, LiFeAs , $\text{Fe}_{1+x}(\text{Te}, \text{Se})$, and $\text{A}_2\text{Fe}_4\text{Se}_5$ (where $\text{A} = \text{K}, \text{Rb}, \text{and Cs}$). The moment size is independent of temperature or carrier concentration, but varies significantly across different families. Specifically, all iron pnictides samples have local moments of about $1\mu_B/\text{Fe}$, while FeTe and $\text{K}_2\text{Fe}_4\text{Se}_5$ families have much larger local moments of $\sim 2\mu_B/\text{Fe}$ and $\sim 3.3\mu_B/\text{Fe}$, respectively. Our results illustrate the importance of multi-orbital physics in describing magnetism of these compounds.

10:36AM P22.00014 Electronic Structure of $\text{A}_y\text{Fe}_{2-x}\text{Se}_2$ from First Principles¹, CHAO CAO, JIANHUI DAI, Hangzhou Normal University — The newly discovered $\text{A}_y\text{Fe}_{2-x}\text{Se}_2$ iron-selenide material family was studied in a series of first-principles simulations. The electronic structure and magnetic properties of possible vacancy-superstructure phases $\text{A}_2\text{Fe}_3\text{Se}_4$ and $\text{A}_2\text{Fe}_4\text{Se}_5$, as well as the possible parental phase of superconductivity AFe_2Se_2 were examined. It was discovered that AFe_2Se_2 ground state is a SDW-AFM metal without hole Fermi-surface, thus FS-nesting is absent and its magnetism is very likely to be local moment; $\text{A}_2\text{Fe}_3\text{Se}_4$ is a Mott insulator with SDW-AFM magnetism; $\text{A}_2\text{Fe}_4\text{Se}_5$ shows block-spin AFM ground state with $400\sim 600$ meV band gap. Under high pressure, the $\text{A}_2\text{Fe}_4\text{Se}_5$ phase exhibits rich and exotic physical properties.

[1] Chao Cao and Jianhui Dai, Block Spin Ground State and Three-Dimensionality of $(\text{K}, \text{Ti})_y\text{Fe}_{1.6}\text{Se}_2$, *Phys. Rev. Lett.* **107**, 056401 (2011)

[2] Chao Cao and Jianhui Dai, Electronic structure and Mott localization of iron-deficient $\text{TiFe}_{1.5}\text{Se}_2$ with superstructures, *Phys. Rev. B* **83**, 193104 (2011)

[3] Chao Cao and Jianhui Dai, Electronic Structure of KFe_2Se_2 from First-Principles Calculations, *Chin. Phys. Lett.* **28**, 057402 (2011)

¹NSFC and NSF Zhejiang Province

Wednesday, February 29, 2012 8:00AM - 11:00AM – Session P23 DCMP: Superconductivity Theory II: p-wave, chiral, and topological 255

8:00AM P23.00001 Spin-orbit induced mixed-parity pairing in Sr_2RuO_4 : a self-consistent quantum many-body analysis, JOHN DEISZ, TIM KIDD, University of Northern Iowa — The unusual superconducting state in Sr_2RuO_4 has long been viewed as being analogous to a superfluid state in liquid ^3He . Nevertheless, calculations based on a pure odd-parity state are presently unable to completely reconcile the properties of Sr_2RuO_4 . Using a self-consistent quantum many-body scheme that employs realistic parameters, we are able to model several signature properties of the normal and superconducting states of Sr_2RuO_4 such as the weak temperature dependence of the spin susceptibility below T_c . However, we find that the dominant component of the model superconducting state is of even parity and closely related to superconducting state for the high- T_c cuprates although a smaller odd-parity component is induced by spin-orbit coupling. This mixed parity pairing state provides an alternative scenario for understanding the complex phenomena measured in Sr_2RuO_4 .

8:12AM P23.00002 Spin and charge collective excitations in the multiband superconductivity of Sr_2RuO_4 , SUK BUM CHUNG, SRINIVAS RAGHU, STEVE KIVELSON, Stanford University — Multiband superconductors with weak interband pair scattering can support soft collective modes. In the case of spin-singlet superconductivity, interband pair scattering leads to fluctuations of the relative phase of the order parameter on the different bands. However, when the superconductivity is spin-triplet, the interband pair scattering gives rise to fluctuations of both the relative phase and the relative spin on the different bands. One possible example of a multiband triplet superconductor is a recently proposed model [1] of the superconductivity in Sr_2RuO_4 in which the pairing occurs primarily on the two quasi-1D bands. We show that the collective excitations arising from relative spin fluctuations can lead to a double resonance peak in the presence of an oscillating magnetic field. We discuss how the presence or absence of such collective modes can yield clear information concerning the precise microscopic structure of the order parameter.

[1] S. Raghu, A. Kapitulnik, and S. Kivelson, *Phys. Rev. Lett.* **105**, 136401 (2010)

8:24AM P23.00003 Dynamics of domain walls in chiral p-wave superconductors¹, KIRILL SAMOKHIN, Brock University — Two-fold degeneracy of the ground state of chiral p-wave superconductors or superfluids with $k_x \pm ik_y$ order parameter makes it possible for domain walls separating regions of opposite chirality to exist. In addition to affecting the scattering spectrum in the bulk, the domain walls also carry localized low-energy fermionic quasiparticles, whose energy essentially depends on the Josephson phase difference between the domains. Dynamical properties of the domain walls are determined by the transitions between different quasiparticle states induced by the domain wall motion. We present a microscopic calculation of the viscous friction coefficient and the effective mass of the domain walls.

¹Supported by NSERC, Canada

8:36AM P23.00004 Stability of topological defects in chiral superconductors: London theory¹, VICTOR VAKARYUK, Argonne National Lab — We examine thermodynamic stability of chiral domain walls and vortices – topological defects which can exist in chiral superconductors. Using London theory it is demonstrated that at sufficiently small applied and chiral fields the existence of domain walls and vortices in the sample is not favored and the sample's configuration is a single domain. The particular chirality of the single-domain configuration is neither favored nor disfavored by the applied field. Increasing the field leads to an entry of a domain wall loop or a vortex into the sample. Formation of a straight domain wall is never preferred in equilibrium. Values of the entry (critical) fields for both types of defects, as well as the equilibrium size of the domain wall loop, are calculated. The applicability of these results to Sr_2RuO_4 – a tentative chiral superconductor – is discussed.

¹Supported by CES-EFRC DoE Award No. DE-AC0298CH1088.

8:48AM P23.00005 Intrinsic Hall effect in a multiband chiral superconductor¹, EDWARD TAYLOR, CATHERINE KALLIN, McMaster University — We identify an intrinsic, dissipationless Hall effect in multiband chiral superconductors in the absence of a magnetic field (i.e., an *anomalous* quantum Hall effect). Similarly to its analog in ferromagnets, this effect arises from inter-band transitions when time-reversal symmetry is spontaneously broken. We discuss the implications of this effect for the putative chiral p-wave superconductor, Sr_2RuO_4 , and show that it can be of the right order of magnitude to contribute significantly to the polar Kerr rotation observed in experiments, depending on the structure of the order parameter across the bands.

¹Supported by NSERC and the Canadian Institute for Advanced Research.

9:00AM P23.00006 Topologically protected surface Majorana arcs and bulk Weyl fermions in ferromagnetic superconductors¹, SUMANTA TEWARI, Department of Physics and Astronomy, Clemson University, Clemson, SC 29634, JAY SAU, Department of Physics, Harvard University, Cambridge, MA 02138 — A number of ferromagnetic superconductors have been recently discovered which are believed to be in the so-called “equal spin pairing” (ESP) state. In the ESP state the Cooper pairs condense forming order parameters $\Delta_{\uparrow\uparrow}, \Delta_{\downarrow\downarrow}$, which are decoupled in the spin-sector. We show that these 3D systems generically support topologically protected surface Majorana arcs and bulk Weyl fermions as gapless excitations. Similar protected low-energy exotic quasiparticles should also appear in the recently discovered non-centrosymmetric superconductors in the presence of a Zeeman field. The protected surface arcs can be probed by angle-resolved photoemission (ARPES) as well as fourier transform scanning tunneling spectroscopy (FT-STs) experiments.

¹Work Supported by DARPA-MTO, NSF, and Harvard Quantum Optics Center

9:12AM P23.00007 Thermodynamic signatures of half-quantum vortices in $p + ip$ Josephson junction arrays¹, GRAHAM KRAHN, UC Riverside, KIRILL SHTENGEL, Associate Professor of Physics, UC Riverside — A very interesting type of excitation in a chiral p-wave superconductor is a half-quantum vortex. As the name suggests, they carry half of a superconducting flux quantum, and are only possible in superconductors with spin-triplet pairing. An astonishing feature of these excitations is the presence of topologically protected Majorana zero modes. Single half-quantum vortices were recently discovered (J. Jang et al, Science **331**(6014): 186-188) in superconducting mesoscopic rings made of Sr_2RuO_4 , yet to this date they have not been observed in macroscopic samples. We propose a method for detecting half-quantum vortices in Josephson junction arrays, which could host a large number of these vortices. Contrary to a 3D setting, we argue that half-quantum vortices can be energetically preferable in quasi-2D chiral spin-triplet superconductors. As a result, half-quantum vortices rather than full vortices could drive a Berezinskii-Kosterlitz-Thouless transition (which manifests itself as a resistive transition). We propose to look for their signatures by comparing transition temperatures in $p + ip$ Josephson junction arrays in a transverse magnetic field in both unfrustrated and frustrated cases.

¹NSF DMR-0748925

9:24AM P23.00008 Scattering theory of chiral Majorana fermion interferometry¹, JIAN LI, Department of Theoretical Physics, University of Geneva, Switzerland, GENEVIÈVE FLEURY, CEA-Saclay, France, MARKUS BUTTIKER, Department of Theoretical Physics, University of Geneva, Switzerland — Using scattering theory, we investigate interferometers composed of chiral Majorana fermion modes coupled to normal metal leads. We advance an approach in which also the basis states in the normal leads are written in terms of Majorana modes. As a consequence the scattering at the junctions of the lead to the Majorana mode couples modes effectively only pair-wise irrespective of the number of normal scattering modes. We demonstrate that the charge current can also be expressed in terms of interference between pairs of Majorana modes. These two basic facts permit a treatment and understanding of current and noise signatures of chiral Majorana fermion interferometry in an especially elegant way. As a particular example of applications, in Fabry-Perot-type interferometers where chiral Majorana modes form loops, resonances (anti-resonances) upon such loops always lead to peaked (suppressed) Andreev differential conductances and negative (positive) cross-correlations originate purely from two-Majorana-fermion exchange. These investigations are intimately related to current and noise signatures of Majorana bound states.

¹Swiss NSF and the NCCR Quantum Science and Technology

9:36AM P23.00009 Probing Majorana fermions in one-dimensional topological superconductors using non-equilibrium transport: an open-quantum-system study, DIBYENDU ROY, CARLOS J. BOLECH, NAYANA SHAH, Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221 — We study one-dimensional topological superconductors using an open-quantum-system approach based on Langevin equations. We go beyond a low-energy effective model of Majorana fermions, to derive different non-equilibrium transport properties exactly in these systems. The role of the coupling between the superconducting wire and metallic leads in physical experiments to detect Majorana bound states is also examined.

9:48AM P23.00010 Majorana End States of Au Wires in Proximity to $d_{x^2-y^2}$ -wave Superconductors, KAM TUEN LAW, LOK MAN WONG, Hong Kong University of Science & Technology — We propose a one dimensional DIII class Hamiltonian which respects time-reversal symmetry and supports zero-energy double Majorana end states. Single Majorana end states can appear if time-reversal symmetry is broken. Majorana fermions survive in the quasi-1D regime when multiple transverse sub-bands of the wire are occupied. More importantly, this model can be realized by inducing $d_{x^2-y^2}$ -wave superconductivity on a quantum wire with strong spin-orbit coupling. We suggest Au wires deposited on doped LSCO realize this topological superconducting phase. The energy scales of this set-up, an induced proximity gap of 10meV and the Rashba energy of 60meV, are two orders of magnitude larger than the corresponding energy scales in semiconductor-based proposals.

10:00AM P23.00011 Topological Josephson effect for arbitrary values of the tunnel coupling in the Kitaev model¹, FLAVIO NOGUEIRA, ILYA EREMIN, Institut für Theoretische Physik III, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany — We investigate the Josephson effect for a setup with two lattice quantum wires featuring fused Majorana boundary modes at the tunnel junction. We show exactly that additional degeneracies occur when the size of the Josephson coupling attains a certain critical value, thus introducing additional energy level crossings. The physical consequences of these additional level crossings are discussed. It is shown that for this critical coupling the Andreev levels can be cast in the form $E_{m\sigma} = 2\sigma\sqrt{2}w \cos(\phi/6 - \pi m/3)$, where $m = -1, 0, 1$ and $\sigma = \pm 1$. The exact Josephson current exhibits the characteristic 4π periodicity along with additional features related to the extra crossings of Andreev levels at the critical value of the tunnel coupling.

¹Supported by SFB TR12 via the Deutsche Forschungsgemeinschaft

10:12AM P23.00012 ABSTRACT WITHDRAWN —

10:24AM P23.00013 Single-particle off-diagonal long range order in $|Pf\rangle$ wave function for topological superconductors, OLEXEI MOTRUNICH, California Institute of Technology — We ask what can be glimpsed about a fermion system from a boson wave function obtained as the absolute value of the fermion wave function in the particle number basis. We consider examples of spinless p -wave superconductors in one and two dimensions and find that thus constructed wave function shows single-boson off-diagonal long range order when the fermion system is in the weak-coupling topological phase, but only pair-boson order in the strong-coupling non-topological phase. We discuss implications when such fermion states are used as factors in trial wave functions e.g. from slave-fermion construction.

10:36AM P23.00014 Topological Superconductivity in Spin-Orbit Coupled Bands, AARON FARRELL, TAMI PEREG-BARNEA, McGill University — Topological superconductors have nontrivial winding of their order parameter phase and are expected to support Majorana Fermions in their vortex cores. For this reason they have been sought after in the past couple of decades. Over the past few years, a new and promising route for realizing topological superconductors has opened due to recent advances in the field of topological insulators. The current proposals are based on semiconductor heterostructures. In the proposed devices, spin-orbit coupled bands are Zeeman split by a magnetic field and superconductivity is induced by proximity to a conventional superconductor. This leads to heterostructures of two or three layers. This talk will focus on the prospect of realizing a topological superconductor in materials with inherent spin-orbital coupling and an intrinsic tendency for superconductivity. The proposed device will allow simplification of recently suggested devices as the need for a superconducting layer will be eliminated.

10:48AM P23.00015 Theory of Superconductivity in Mesoscopic Systems¹, JIAWEI HUO, WEIQIANG CHEN, Department of Physics, The University of Hong Kong, Hong Kong, China, SRINIVAS RAGHU, Department of Physics, Stanford University, Stanford, CA, 94305, FUCHUN ZHANG, Department of Physics, The University of Hong Kong, Hong Kong, China — By using Bogoliubov-de Gennes (BdG) equations, we study superconducting (SC) states in a quasi 2-dimensional system of radius R . It is shown that no vortices exist in s -wave SC samples with $R < R_c \sim \xi(0)$, the $T = 0$ coherence length. We predict that chiral p -wave states exhibit superconductivity for $R < R_c$ only in the presence of a vortex with opposite chirality. This *reentrant* SC phase is a consequence of non-zero chirality of the pairing order parameter and implies the presence of chiral edge currents. Our study may be applied to sharply probing the pairing symmetry of unconventional superconductors.

¹This work is partially supported by Hong Kong RGC Grant GRF HKU707211, HKUST3/CRF/09 and start-up funds at Stanford University (S.R.).

Wednesday, February 29, 2012 8:00AM - 11:00AM – Session P24 FIAP: Fractional Quantum Hall Effect I 256

8:00AM P24.00001 Exploring the possibility of Universal Edge Physics in the Fractional Quantum Hall States¹, ZI-XIANG HU, RAVIN BHATT, XIN WAN, Princeton University, KUN YANG, Florida State University — The edge of a fractional quantum Hall (FQH) droplet is described by the chiral Luttinger liquid theory which predicts a universal power-law behavior in the current-voltage (I - V) characteristics when electrons tunneling into the FQH edge through a barrier, e.g., from a three-dimensional Fermi liquid. However, this universality has not been unambiguously observed in transport experiments in two-dimensional electron gases based on GaAs/GaAlAs heterostructures or quantum wells. One plausible cause is reconstruction of the fractional quantum Hall edge, which introduces non-chiral edge modes. The coupling between counterpropagating edge modes can modify the exponent of the I - V characteristics. By comparing the fractional quantum Hall states at the filling factor $\nu = 1/3$ in modulation-doped semiconductor devices and in graphene devices, we show that the GaAs-based FQH experiments are always in the edge reconstruction regime, whereas graphene-based systems have an experimental accessible parameter region where edge reconstruction can be avoided. This regime offers the possibility of the exploration of the universal edge tunneling exponent predicted by the chiral Luttinger liquid theory.

¹This work is supported by DOE grant No. DE-SC0002140

8:12AM P24.00002 Exploration of the Limits to Mobility in Two-Dimensional Hole Systems in C-Doped (001) GaAs/AlGaAs Quantum Wells¹, JOHN WATSON, Dept. of Physics and Birck Nano Center, Purdue University, W. Lafayette, IN, SUMIT MONDAL, Dept. of Physics, Purdue University, GEOFF GARDNER, Birck Nano Center and School of Materials Engineering, Purdue University, MICHAEL MANFRA, Dept. of Physics, Birck Nano Center, and Schools of Materials Engineering and Electrical and Computer Engineering, Purdue University — We report on the growth of a series of high mobility two-dimensional hole systems (2DHSs) in 20 nm (001) oriented GaAs/AlGaAs quantum wells and the analysis of possible scattering mechanisms. The hole density was controlled by changing the delta-doping setback and Al mole fraction and was measured at low temperature ($T = 300$ mK) after illumination with a red LED. We varied the density over a range from $2.0 \times 10^{10} \text{ cm}^{-2}$ to $1.9 \times 10^{11} \text{ cm}^{-2}$, and the mobility was observed to peak at an intermediate density of $6.5 \times 10^{10} \text{ cm}^{-2}$ where we report a new record $T = 300$ mK mobility of $2.3 \times 10^6 \text{ cm}^2/\text{Vs}$. We find that even when the density dependent effective mass is taken into account, remote and background impurity scattering cannot qualitatively explain the behavior of the mobility, in contrast with comparable 2DEGs. We discuss possible mechanisms leading to the observed non-monotonic density dependence of the mobility and the factors leading to our new record mobility.

¹JW is supported by the Sandia Nat'l Lab, Purdue Univ. Excellence in Science and Engineering Fellowship. MM acknowledges support from the Miller Family Foundation

8:24AM P24.00003 Effective Field Theory of Fractional Quantized Hall Nematics, MICHAEL MULLIGAN, Massachusetts Institute of Technology, CHETAN NAYAK, University of California at Santa Barbara and Station Q, SHAMIT KACHRU, Stanford University — We present a Landau-Ginzburg theory for a fractional quantized Hall nematic state and the transition to it from an isotropic fractional quantum Hall state. This justifies Lifshitz-Chern-Simons theory – which is shown to be its dual – on a more microscopic basis and enables us to compute a ground state wave function in the symmetry-broken phase. In such a state of matter, the Hall resistance remains quantized while the longitudinal DC resistivity due to thermally-excited quasiparticles is anisotropic. We interpret recent experiments by Xia et al. (cond-mat/1109.3219) at Landau level filling factor $\nu = 7/3$ in terms of our theory.

8:36AM P24.00004 Dipolar Bogolons: From Superfluids to Pfaffians, SIDDHARTH PARAMESWARAN, UC Berkeley, STEVEN KIVELSON, Stanford University, R. SHANKAR, Yale University, SHIVAJI SONDHI, Princeton University, BORIS SPIVAK, University of Washington — We study neutral fermionic ‘Bogolons’ which are quasiparticle excitations of gapped phases that arise due to fermion (BCS) pairing, such as superfluids, superconductors, and paired quantum Hall states. As we demonstrate, a naïve construction of a quasiparticle wavepacket by solving the mean-field BCS equations leads to a contradiction: there is a net electrical current *even when the group velocity vanishes*. Resolution of this paradox requires the computation of supercurrents in the wavepacket state, typically a complicated exercise in self-consistency. In this Letter we demonstrate that these corrections may be approximately calculated from correlations in the mean-field ground state, and lead to a divergence-free, dipolar current pattern associated with the quasiparticle. When Maxwell electrodynamics is included, as appropriate to a superconductor, this pattern is confined over a penetration depth. For paired quantum Hall states of composite fermions, the Maxwell term is replaced by a Chern-Simons term, which leads to a dipolar *charge* distribution, paralleling Read’s observation that composite fermions are neutral dipoles.

8:48AM P24.00005 Coulomb Oscillations in Antidots in the Integer and Fractional Quantum Hall Regimes¹, A. KOU, C.M. MARCUS, Harvard University, L.N. PFEIFFER, K.W. WEST, Princeton University — We present measurements of Coulomb oscillations as a function of both top gate and magnetic field in gate-defined, micron-scale antidots in the integer and fractional quantum Hall regimes. We find resistance oscillations at filling factors $\nu = 2, \nu = 1, \nu = 2/3$, and $\nu = 1/3$. At $\nu = 1$, we find the tunneling charge to be e and the presence of one edge. At $\nu = 2$, we also find the tunneling charge to be e and the presence of two edges. A generalized picture of Coulomb oscillations in the fractional quantum Hall regime suggests the presence of one charged edge at both $\nu = 1/3$ and $\nu = 2/3$. We find the tunneling charge at $\nu = 1/3$ to be $e/3$ but unexpectedly find the tunneling charge at $\nu = 2/3$ to be $(2/3)e$.

¹Research funded by Microsoft Corporation Project Q, NSF (DMR-0501796), the Department of Energy Office of Science Graduate Fellowship Program, and Harvard University. Device fabrication at Harvard's Center for Nanoscale Systems.

9:00AM P24.00006 Lande's g values and the quantum Hall effect, KESHAV SHRIVASTAVA, University of Hyderabad — It is reported that the Lande's formula for the g values of the electron as a function of L, S and J does not have the particle-hole symmetry needed for the understanding of high magnetic field data of quantum Hall effect. Hence it is modified to yield the particle-hole symmetry by means of the two signs before S in $J = L \pm S$. The correct g value is then given by $g = (2J+1)/(2L+1)$. Since the Bohr magneton involves the charge of the particles, the corrected g value formula explains the data of quantum Hall effect. The value $L/2L+1$ gives $1/3$ and $(L+1)/(2L+1)$ gives $2/3$. The consideration of Landau levels gives many values in agreement with the data. In electron clusters the spin need not be $1/2$. Hence a lot of data is explained by means of spin greater than $1/2$. Some of the clusters show the formation of spin waves so that there is a finite spin deviation which is characteristic of electron lattices. It is found that Laughlin's wave function is the ground state of $\nabla^2 \delta(r_i - r_j)$ type Hamiltonian which is not equivalent to Coulomb's Hamiltonian. K. N. Shrivastava, Intl. J. Mod. Phys. B 25, 1301-1357(2011).

9:12AM P24.00007 Numerical Study of Realistic Models of the $\nu = 5/2, 7/3, 8/3$ Hamiltonians: Effects of Landau-level mixing and Finite Well-width¹, MICHAEL PETERSON, California State University Long Beach, University of California Santa Barbara, CHETAN NAYAK, Microsoft Research, University of California Santa Barbara — We construct a realistic effective Hamiltonian for electrons in the first excited Landau level, taking into account the effects of both Landau-level mixing and the finite width of the GaAs quantum well. The latter includes both short-distance softening of the Coulomb interaction as well as sub-band mixing. Through exact diagonalization, we find a rich phase diagram as a function of the Landau level mixing parameter κ and quantum well width d . In particular, small changes in either parameter can drive phase transitions between states in the universality classes of the Moore-Read Pfaffian, anti-Pfaffian, and exotic compressible metallic states.

¹We acknowledge support from DARPA and Microsoft Station Q

9:24AM P24.00008 Thermopower and the Fractional Quantized Hall Effect in the N=1 Landau Level¹, W.E. CHICKERING, J.P. EISENSTEIN, Caltech, L.N. PFEIFFER, K.W. WEST, Princeton — Having recently eliminated an issue involving long thermal time constants [1], we are now able to resolve diffusion thermopower deep into the fractional quantized Hall effect (FQHE) regime. In this talk we report measurements of thermopower in the first excited (N=1) Landau level as a continuous function of magnetic field down to temperatures as low as 30mK. Above 50mK we can clearly resolve the $\nu = 5/2$ as well as $\nu = 7/3, 8/3$, and $14/5$ FQHEs in both the electrical and thermoelectrical transport. Below 50mK a prominent feature of the electrical transport in the first excited Landau level is the Re-entrant Integer Quantized Hall Effect (RIQHE) which is associated with insulating collective phases [2]. In this temperature regime the thermopower exhibits a series of intriguing sign reversals that are as yet not fully understood. We will conclude with a brief discussion of the connection between thermopower and the entropy of the 2D electron system. This connection is invoked by a recent prediction [3] of the thermopower at $\nu = 5/2$, which assumes the ground state is the non-Abelian Moore-Read paired composite fermion state.

[1] Chickering, Phys. Rev. B 81, 245319 (2010)

[2] Eisenstein, Phys. Rev. Lett. 88, 076801 (2002)

[3] Yang, Phys. Rev. B 79, 115317 (2009)

¹This work is supported by Microsoft Project Q and DOE grant DE-FG03-99ER45766.

9:36AM P24.00009 Tilt Magnetic Field Dependence of the 12/5 Fractional Quantum Hall State, CHI ZHANG, Princeton University, Sandia National Labs, CHAO HUAN, JIAN-SHENG XIA, NEIL S. SULLIVAN, University of Florida and NHMFL, WEI PAN, Sandia National Labs, K.W. BALDWIN, K.W. WEST, L.N. PFEIFFER, D.C. TSUI, Princeton University — The 12/5 state has attracted growing interest due to its superior potential in performing universal topological quantum computation. Up to date, except for the observation of a well developed quantum Hall plateau at this filling, much less experimental work has been carried out and there is no experimental evidence to support this state being a parafermionic or non-Abelian state. Here, we present our tilt magnetic field dependence results in examining its spin-polarization. It was observed that the diagonal resistance R_{xx} at $\nu=12/5$ shows a non-monotonic dependence on tilt angle (θ). It first increases sharply with increasing θ , reaches a maximal value of $\sim 60 \Omega$ around $\theta \sim 14^\circ$, and then decreases with θ further increased. Correlated with this R_{xx} dependence, the 12/5 activation energy gap ($\Delta_{12/5}$) also shows a non-monotonic θ dependence. $\Delta_{12/5}$ first decreases. Around 14° , R_{xx} becomes non-activated and a true activation energy gap is not obtainable. With further increasing θ , R_{xx} becomes activated again and $\Delta_{12/5}$ increases with θ . This tilt dependence in R_{xx} and $\Delta_{12/5}$ is similar to the composite fermion states at $\nu=2/5$ and $8/5$ in the lowest Landau level, which was interpreted as a spin transition. Our results thus call for more investigations on the nature of the 12/5 ground state.

9:48AM P24.00010 The temperature-dependences of the dissipative conductance in quantum Hall states, N. D'AMBRUMENIL, University of Warwick, Coventry, CV4 7AL, UK, B.I. HALPERIN, Harvard University, Cambridge, Massachusetts 02138, USA, RUDOLF H. MORF, Paul Scherrer Institute, CH-5232 Villigen, Switzerland — We discuss how to estimate the saddle point gap of quantized Hall states from the temperature dependence of the longitudinal response, $\log \sigma_{xx}$. The dissipative response is assumed to be the result of thermally activated quantum tunneling through saddle points in the long-range impurity potential set up by the ionized donors (see Phys. Rev. Lett. 106, 126804 (2011)). We apply the method to published data on states at $\nu = 5/2$, as well data at other integer and fractional filling fractions, and compare the gap estimates and the typical parameters of the saddle points with expectation from microscopic calculations. Even in the case of very weak quantum Hall states, we find that the analysis suggests saddle point gaps which are consistently around 50% of the gap predicted for the homogeneous system.

10:00AM P24.00011 Fractionalization in spontaneous integer quantum Hall systems¹ , ARMIN RAHMANI, RODRIGO MUNIZ, IVAR MARTIN, Los Alamos National Laboratory — We show that electron fractionalization can occur in quantum Hall liquids even in the absence of strong correlations. Focusing on a Kondo lattice model that exhibits spontaneous integer Hall effect due to non-coplanar magnetic ordering, we find that Z_2 vortices in the magnetic order parameter can bind fractional quantum numbers. The vortices have anyonic exchange statistics.

¹LANL DE-AC52-06NA25396

10:12AM P24.00012 Exact soliton solutions in a many-body system in non-trivial background¹ , ANDREY GROMOV, ALEXANDER ABANOV, Stony Brook University, MANAS KULKARNI, University of Toronto — Soliton solutions are usually described as lumps of density propagating without changing their shape. They usually occur in integrable systems. We consider the classical Calogero model in an external harmonic potential. Due to the presence of the external potential, momentum in the system is not conserved and the aforementioned description of solitons is inapplicable, nevertheless the system remains integrable. Naturally, the question about the existence and the form of soliton solutions arises. I will explain what a soliton solution of this model is and I will show how to find these solutions in the case of finite number of particles and in the hydrodynamic limit. In the latter limit the model is described by hydrodynamic equations on continuous density and velocity fields. Soliton solutions in this case are finite dimensional reductions of the hydrodynamic model and describe the propagation of lumps of density and velocity in the nontrivial background. These solutions of Calogero model were previously qualitatively described by A. Polychronakos in the context of the quantum Hall effect.

¹The work was supported by the NSF under grant no DMR-0906866

10:24AM P24.00013 On the hydrodynamic description of FQHE fluid¹ , ALEXANDER ABANOV, Stony Brook University — A simple classical two-dimensional hydrodynamic model for FQHE fluid has been constructed. Hydrodynamics of this model is Hamiltonian, nonlinear and has many features of fractional quantum Hall states. The effective classical fluid is incompressible and has a correct static structure factor. The model incorporates FQHE relation between the density and the vorticity of the fluid, gives the correct value for the Hall viscosity and for the Hall conductivity at finite wavevectors. The model can serve as a starting point in deriving the boundary theory of FQHE states beyond chiral Luttinger liquid. Indeed, in the leading approximation the model is reduced to chiral waves with nonlinearities defined by a curvature of the confining potential.

¹The work was supported by the NSF under grant no DMR-0906866

10:36AM P24.00014 Anomalous resistance across a quantum point contact in the integer and fraction quantum Hall regimes , COLIN DILLARD, XI LIN, MARC KASTNER, MIT, LOREN PFEIFFER, KEN WEST, Princeton University — A ~ 600 nm quantum point contact (QPC) is studied in various integer and fractional quantum Hall states. An anomalous increase of the differential resistance across the QPC from the expected quantized value is observed at nonzero DC bias. The onset of this increased differential resistance occurs sharply at DC bias values which vary continuously with magnetic field and gate voltage. Dependence of the increased resistance on filling factor, magnetic field, gate voltage, and temperature is presented. Of particular interest is the observation that the onset DC bias shows opposite gate voltage dependence for integer and fractional quantum Hall states.

10:48AM P24.00015 Improved Measurements of Quasi-Particle Tunneling in the $\nu = 5/2$ Fractional Quantum Hall State¹ , XI LIN, COLIN DILLARD, MARC KASTNER, MIT, LOREN PFEIFFER, KEN WEST, Princeton University — It is predicted that the $\nu = 5/2$ fractional quantum Hall state may potentially exhibit novel non-abelian quasi-particle statistics, which would make it a candidate for implementation of topological quantum computation. We present measurements of quasi-particle tunneling between edge channels, which provide information about the wave function of the $\nu = 5/2$ state. Weak tunneling is investigated as a function of temperature and DC bias and fit to the theoretical tunneling conductance. We improve on previous quasi-particle tunneling measurements by reducing measurement noise and studying two different quantum point contact (QPC) geometries. For both QPCs the best fits give e^* , the quasi-particle effective charge, close to the expected value of $e/4$ and g , the strength of the interaction between quasi-particles, close to $3/8$. Here we show that fits corresponding to the various proposed wave functions, along with qualitative features of the data, strongly favor the abelian 331 state.

¹Supported by: National Science Foundation under Grant No. DMR-1104394, Gordon and Betty Moore Foundation, National Science Foundation MRSEC Program through the Princeton Center for Complex Materials (DMR-0819860).

Wednesday, February 29, 2012 8:00AM - 11:00AM –
Session P25 DCOMP GSCCM DMP: Focus Session: Simulation of Matter at Extreme Conditions - Static Pressure 257A

8:00AM P25.00001 A new metastable phase of silicon in the *Ibam* structure , BRAD D. MALONE, MARVIN L. COHEN, Department of Physics, University of California, Berkeley, and Materials Science Division, Lawrence Berkeley National Laboratory — In a study aimed at finding new useful forms of silicon, we use an *ab initio* random structure searching (AIRSS) method to identify a new phase of silicon in the *Ibam* structure. The *Ibam* phase is found to be semimetallic within density functional theory with a small band overlap, and it is expected that quasiparticle corrections using the GW approximation would yield a semiconducting state with a small band gap. Calculation of the lattice dynamics reveals that the structure is locally stable. Enthalpy-pressure relations are calculated for the *Ibam* structure as well as all other known Si structures, including the previously predicted phases *st12* and *bct*. These results indicate that *Ibam* silicon is metastable over the pressure range considered. Calculated coexistence pressures of the other known phase transitions are in good agreement with experimental observation.

8:12AM P25.00002 Ultra-incompressible Three Dimensional Long-range Ordered Amorphous Carbon Clusters¹ , LIN WANG, Carnegie Institution of Washington, 1HPSYNC, GEOPHYSICAL LABORATORY, CARNEGIE INSTITUTION OF WASHINGTON, ARGONNE, IL 60439, USA TEAM — Here we report the synthesis of a long range ordered material constructed from units of amorphous carbon clusters and solvent molecular. This material has super-incompressibility which can make indents on diamonds. It was synthesized by crushing the fullerenes cages at high pressure. Using high pressure x-ray diffraction and Raman spectroscopy, we observed that the fullerenes cages collapse as the pressure higher but the sample remains in crystalline phase even at 60 GPa. The high pressure phase is ultraincompressible, quenchable and much denser than the starting material. The discovery of the existence of such a unique phase should lead to a great deal of interest for design and synthesis of materials with this characteristic.

¹This work was supported as part of the EFree, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science under Award Number DE-SC0001057.

8:24AM P25.00003 Anharmonicity and bonding electrons in silicon under high pressures, GUOYIN SHEN, DAIJO IKUTA, HPCAT, Carnegie Institution of Washington — Electron density distributions have been measured for silicon at high pressures by single crystal diffraction using a diamond anvil cell. An abrupt change in charge density distribution is observed at 10.1 GPa, a pressure close to a phase transition from diamond structure to beta-tin structure at 12.5 GPa. Our results show a strong anharmonicity effect in silicon in a pressure range of 2.5 GPa before the phase transition to beta-tin.

8:36AM P25.00004 Formation of superconducting platinum hydride under pressure: an *ab initio* approach, DUCK YOUNG KIM, Geophysical laboratory, Carnegie institution of Washington, RALPH SCHEICHER, Uppsala University, Uppsala, Sweden, CHRIS PICKARD, University College London, London, UK, RICHARD NEEDS, University of Cambridge, Cambridge, UK, RAJEEV AHUJA, Uppsala University, Uppsala, Sweden — Noble metals such as Pt, Au, or Re are commonly used for electrodes and gaskets in diamond anvil cells for high-pressure research because they are expected to rarely undergo structural transformation and possess simple equation of states. Specifically Pt has been used widely for high-pressure experiments and has been considered to resist hydride formation under pressure. Pressure-induced reactions of metals with hydrogen are in fact quite likely because hydrogen atoms can occupy interstitial positions in the metal lattice, which can lead to unexpected effects in experiments. In our study, PRL 107 117002 (2011), we investigated crystal structures using *ab initio* random structure searching (AIRSS) and predicted the formation of platinum mono-hydride above 22 GPa and superconductivity T_c was estimated to be 10 – 25 K above around 80 GPa. Furthermore, we showed that the formation of fcc noble metal hydrides under pressure is common and examined the possibility of superconductivity in these materials.

8:48AM P25.00005 New ultrahigh pressure phases of H₂O ice predicted using an adaptive genetic algorithm¹, MIN JI, CAI-ZHUANG WANG, Iowa State University, KOICHIRO UMEMOTO, University of Minnesota, KAI-MING HO, Iowa State University, RENATA WENTZCOVITCH, University of Minnesota — We propose three new phases of H₂O under ultrahigh pressure. Our structural search was performed using an adaptive genetic algorithm which allows an extensive exploration of crystal structure at density functional theory(DFT) accuracy. The new sequence of pressure-induced transitions beyond ice X at 0 K should be ice X → Pbcm → Pbca → Pmc2₁ → P2₁ → P2₁/c phases. Across the Pmc2₁-P2₁ transition, the coordination number of oxygen increases from 4 to 5 with a significant increase of density. All stable crystalline phases have nonmetallic band structures up to 7 TPa.

¹MJ,CZW, and KMH were supported by the US Department of Energy, Basic Energy Sciences, Division of Materials Science and Engineering, under Contract No. DE-AC02-07CH11358. KU and RMW were supported by EAR-0757903, 0810272, 1047629, and ATM-0426757 (VLab).

9:00AM P25.00006 Quantum Monte Carlo applied to Solids under Pressure, LUKE SHULENBURGER, T.R. MATTSSON, Sandia National Laboratories — Diffusion quantum Monte Carlo (DMC) has been applied to solids under pressure in several different contexts a high degree of success.¹ All of these calculations must address three errors present in DMC calculations of solids: the fixed node approximation, the pseudopotential approximation and the finite size approximation. Due to the varying approximations to address these errors, these calculations suffer from an uncertainty that is almost comparable to that introduced by the choice of functional in density functional theory (DFT). In this presentation, we present lattice constants and bulk moduli of more than fifteen solids under compression performed with a consistent approach to these three approximations. These results help establish the general accuracy that may be expected from DMC calculations of solids under pressure and also provide a reference from which improvements to DMC methods may be judged.

Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

¹J. Kolorenc and L. Mitas. Rep. Prog. Phys. 74 026502 (2011)

9:12AM P25.00007 First-principles simulations on bonding pathways of chemical transformations under hydrostatic compression, ANGUANG HU, FAN ZHANG, DRDC Suffield — High pressure as a thermodynamic parameter provides a strong structural constraint to lead chemical transformations with selective ways. Thus, chemical transformations under pressure can create novel materials which may not be accessible by covalent synthesis. However, bonding evolution toward high pressure chemical transformations can be a complex process and may happen over widely different pressures. To understand bonding evolution pathways of high pressure chemical transformations, first-principles simulations were performed following hydrostatic compression enthalpy minimization paths to obtain experimentally and theoretically established phase transitions of carbon. The results showed that the chemical transformations from hydrostatic compression carbon to single-bonded phases were characterized by a sudden decrease in principal stress components, indicating the onset of chemical transformation. On this basis, a number of hydrostatic compression chemical transformations from molecular precursors to novel materials were predicted, such as hydrocarbon graphane, a hydrogenated carbon nitride sheet, and carbon nitrides. All predicted hydrostatic compression transformations are featured as a sudden change in principal stress components, representing chemical bonding destruction and formation reactions with a cell volume collapse.

9:24AM P25.00008 Dielectric constant of water under deep Earth pressures and temperature conditions¹, DING PAN, LEONARDO SPANU, Department of Chemistry, University of California, Davis, FRANCOIS GYGI, Department of Computer Science, University of California, Davis, GIULIA GALLI, Department of Chemistry, University of California, Davis; Department of Physics, University of California, Davis — The knowledge of the dielectric constant of water as a function of pressure (P) and temperature (T) plays a critical role in understanding the chemistry of aqueous systems, and in particular of fluids in the Earth mantle, where water is stored in hydrous minerals. By using first-principles molecular dynamics, we have computed the dielectric constant of water at T = 1000 K, between 1 and 10 GPa, under conditions of the Earth upper mantle. We present a detailed comparison of our results with available experimental data and empirical models, and we discuss how the liquid dielectric constant is affected by the changes in the hydrogen-bond network and molecular dipole moment observed upon compression.

¹DOE/SciDAC-e: DE-FC02-06ER25777

9:36AM P25.00009 Hydrogen-Helium Mixtures at High Pressures, MIGUEL A. MORALES, SEBASTIEN HAMEL, KYLE CASPERSEN, ERIC SCHWEGLER, LLNL — We extend our previous work on hydrogen-helium mixtures (Morales, M. A., et. al. PNAS 106, 1324 (2009).) to lower pressures and lower temperatures, across the molecular dissociation regime in hydrogen, to the low pressure molecular liquid. Using density functional theory-based molecular dynamics together with thermodynamic integration techniques, we calculate the Gibbs free energy of the dense liquid as a function of pressure, temperature, and composition. Our work focuses on the mixing properties of the liquid, the optical properties including conductivity and reflectivity, and the creation of accurate mixing models for thermodynamic properties, including pressure and entropy. The resulting models will provide the basis for accurate first-principles equations of state for planetary modeling. Prepared by LLNL under Contract DE-AC52-07NA27344.

9:48AM P25.00010 Pressure makes mercury a transition metal: a first-principles study of HgF₄ solid phases, XIAOLI WANG, HAIQING LIN, Beijing Computational Science Research Center, YANMING MA, State Key Lab of Superhard Materials, Jilin University, MAOSHENG MIAO, Materials Research Lab, University of California Santa Barbara — Mercury is considered as a post-transition metal, because its d shell is filled and does not involve in forming chemical bonds. Yet, because the large relativistic effect pushes up the outmost d level, there is a high expectation that Hg can be stabilized in a higher oxidation state. The HgF₄ molecule has been predicted by calculations, and an evidence of such molecule is shown by IR absorption recently. However, there is neither computation nor experiment report on possible high oxidation state of Hg in solid. By using first-principles density functional theory and a structure-searching method, we studied the structural change of a solid system of Hg and F under pressures from 0 to 300 GPa. We found that at lower pressure, the stable structure consists of HgF₂ and F₂ molecules. At about 25 GPa, the system undergoes a structural change and forms HgF₄ planar molecules featuring d₈ configuration. The calculations show that the d orbitals of Hg involve in chemical bonding, which is the signature of a transition metal.

10:00AM P25.00011 Ab-initio parametrization of a fully polarizable and dissociable force field for water¹, C. PINILLA, A. IRANI, N. SERIANI, S. SCANDOLO, The Abdus Salam International Centre for Theoretical Physics Trieste, 34151, Italy — A novel all-atom, dissociative, and polarizable force field for water is presented. The force field is parameterized based on forces, stresses and energies obtained from ab-initio calculations of liquid water at ambient conditions. The accuracy of the force field is tested by calculating structural and dynamical properties of liquid water and the energetics of small water clusters. The transferability of the force field to dissociated states is studied by considering the solvation a proton and the ionization of water at extreme conditions of pressure and temperature. In the case of the solvated proton the force field properly describes the presence of both Eigen and Zundel configurations. In the case of the pressure-induced ice VIII / ice X transition and the temperature-induced transition to a superionic phase, the force field is found to describe accurately the proton symmetrization and the melting of the proton sublattice,

¹ EU-FP7-NMP 229205

10:12AM P25.00012 ABSTRACT WITHDRAWN —

10:24AM P25.00013 Spin states and hyperfine interactions of iron incorporated in MgSiO₃ post-perovskite¹, YONGGANG YU, HAN HSU, MATTEO COCCIONI, RENATA WENTZCOVITCH, University of Minnesota — Using density functional theory + Hubbard *U* (DFT+*U*) calculations, we investigate the spin states and nuclear hyperfine interactions of iron incorporated in magnesium silicate (MgSiO₃) post-perovskite (Ppv), a major mineral phase in the Earth's D'' layer, where the pressure ranges from about 120 to 135 GPa. In this pressure range, ferrous iron (Fe²⁺) substituting for magnesium at the dodecahedral (A) site remains in the high-spin (HS) state; intermediate-spin (IS) and low-spin (LS) states are highly unfavorable. As to ferric iron (Fe³⁺), which substitutes magnesium at the A site and silicon at the octahedral (B) site to form (Mg,Fe)(Si,Fe)O₃ Ppv, we find the combination of HS Fe³⁺ at the A site and LS Fe³⁺ at the B site the most favorable. Neither A-site nor B-site Fe³⁺ undergoes a spin-state crossover in the D'' pressure range. The computed iron quadrupole splittings are consistent with those observed in Mössbauer spectra. The effects of Fe²⁺ and Fe³⁺ on the equation of state of Ppv are found nearly identical, expanding the unit cell volume while barely affecting the bulk modulus.

¹This work was supported by EAR-081272, EAR-1047629, and by the MRSEC Program of NSF grants DMR 0212302 and DMR-0819885. Calculations were performed at the Minnesota Supercomputing Institute (MSI).

10:36AM P25.00014 Effects of aluminum on spin-state crossover of iron in the Earth's lower mantle¹, RENATA WENTZCOVITCH, HAN HSU, YONGGANG YU, University of Minnesota — Using density functional theory + Hubbard *U* (DFT+*U*) calculations, we investigate how aluminum affects the spin-state crossover of iron in MgSiO₃ perovskite and post-perovskite, the major mineral phases in and at the bottom of the Earth's lower mantle. We find that aluminum does not change the response of iron spin state to the increasing pressure, namely, only the ferric iron (Fe³⁺) residing the octahedral (B) site undergoes a crossover from high-spin to low-spin state, same as aluminum-free iron-bearing MgSiO₃. The presence of aluminum, however, does affect the population of B-site ferric iron significantly — the majority of Fe³⁺ reside the dodecahedral (A) site at lower pressures, and the population of B-site Fe³⁺ increases with pressure at higher pressure range. Therefore, in the Earth's lower mantle, the amount of B-site Fe³⁺ and the degree of elastic anomalies (and thus the possible seismic anomalies) associated with spin-state crossover is directly affected by the concentration and configuration of aluminum.

¹This work was supported by the MRSEC Program of NSF grants DMR 0212302, DMR-0819885, EAR-081272, and EAR-1047629. Calculations were performed at the Minnesota Supercomputing Institute (MSI).

10:48AM P25.00015 Phase stability of mixtures at extreme conditions: implications for the interior structure of the Outer Planets, SEBASTIEN HAMEL, Lawrence Livermore National Lab — The unusual magnetic fields of the planets Uranus and Neptune represent important observables for constraining and developing deep interior models. Models suggests that the non-dipolar and non-axial magnetic fields of these planets originate from a thin convective and conducting shell of material around a stratified fluid core. We present a computational study of the physical properties of a fluid compositionally similar to what is expected in the interior of Uranus and Neptune. Our diffusivity and conductivity results suggest that the core cannot be well mixed if it is to generate non-axisymmetric magnetic fields. The simulations highlight the importance of chemistry on the properties of this complex mixture, including the possible formation of carbon and nitrogen clusters. We present results concerning the overall phase stability of the mixture under conditions relevant to the planetary interiors.

Wednesday, February 29, 2012 8:00AM - 10:48AM —

Session P26 DCOMP GSNP: Focus Session: Friction, Fracture and Deformation Across Length Scales - Friction and Geometric Effects 257B

8:00AM P26.00001 Effect of Atomic Scale Geometry on Contact and Friction Between Rough Solids¹, TRISTAN A. SHARP, MARK O. ROBBINS, Johns Hopkins University — Microscopic roughness on real surfaces is known to have a profound influence on macroscopic contact mechanics. It has previously been reported that surfaces that differ only at the atomic level can show different relationships between load, stiffness, and friction. Here we use molecular dynamics simulations to study contact properties of self-affine rough surfaces that are identical at continuum scales, but differ at the atomic scale. We compare surfaces that have atomic positions displaced to a self affine surface to "stepped" surfaces that have been cut from a lattice. The stepped surfaces exhibit more plasticity, contributing to a larger contacting area at a given load. A unified framework captures the relation between roughness, system size, surface separation, stiffness, and contact area.

¹ AFOSR FA9550-0910232

8:12AM P26.00002 Breakdown of Amontons' Law of Friction in Sheared-Elastomer with Local Amontons' Friction, HIROSHI MATSUKAWA, Department of Physics and Mathematics, Aoyama Gakuin University, 5-10-1 Fuchinobe, Sagamihara 252-5258, MICHIO OTSUKI, Retired — It is well known that Amontons' law of friction i.e. the frictional force against the sliding motion of solid object is proportional to the loading force and not dependent on the contact area, holds well for various systems. Here we show, however, the breakdown of the Amontons' law for the elastic object which have local friction obeying Amontons' law and is under uniform pressure by FEM calculation. The external shearing force applied to the trailing edge of the sample induces local slip. The range of the slip increases with the increasing external force adiabatically at first. When the range reaches the critical magnitude, the slips moves rapidly and reaches the leading edge of the sample then the whole system slides. These behaviors are consistent with the experiment by Rubinstein et.al. (Phys. Rev. Lett. 98, 226103). The static frictional coefficient, the ratio between the static frictional force for the whole system and the loading force, decreases with the increasing pressure. This means the breakdown of Amontons' law. The pressure dependence of the frictional coefficient is caused by the change of the critical length of the local slip. The behaviors of the local slip and the frictional coefficient are well explained by the 1 dimensional model analytically.

8:24AM P26.00003 Geometry and elasticity for detachment fronts in friction, ALESSANDRO TALONI, ANDREA BENASSI, STEFANO ZAPPERI, CNR-IENI istituto per l'energetica e le interfaci — Mesoscale friction bridges nanoscale contact mechanics to the macroscopic Amontons laws and is relevant for several mechanical problems including seismology. Recent experiments on polymeric blocks show that the onset of friction occurs by nucleation of detachment fronts and that frictional properties vary along the sample surface. The earthquake-like dynamics found at the millimeter scale is in contrast with the usual assumption of uniform detachment without a coherent pattern in the front formation. Simulating the quasi-equilibrium dynamics of an elastic sample sliding on a rough surface under a shear force, we show that the dynamics of detachment fronts depends on the sample geometry. In particular, we study the effect of the sample aspect ratio by computing the elastic Green function for a finite three-dimensional slider. Our model allows to study the onset of friction in different geometries, from the thin slabs used in the aforementioned experiments to more general samples shapes.

8:36AM P26.00004 Local friction at a rubber/glass multicontact interface, ANTOINE CHATEAUMINOIS, DANH TOAN NGUYEN, CHRISTIAN FRETIGNY, ESPCI - PPMD Laboratory, YOHAN LE CHENADEC, MAUDE PORTIGLIATTI, Manufacture Francaise des Pneumatiques Michelin — When rubber is squeezed against a hard, rough surface contact only occurs at localized spots between surface asperities. Friction thus involves the shearing of a myriad of micro-contacts which are distributed over length scales ranging from micrometers down to nanometers. In order to get more insights into this widely debated problem, spatially resolved measurements of frictional stresses are much needed. We recently proposed a method to measure local friction of rubbers by means of a contact imaging approach. Silicon rubber substrates marked on their surface are prepared in order to measure the displacement field induced by the steady state friction of a glass lens. Then, the deconvolution of this displacement field provides a spatially resolved measurement of the actual shear stress and contact pressure distributions within the contact interface. As a result, the local friction law, i.e. the relationship between the actual shear stress and normal pressure, is obtained. The effect of roughness are analyzed from experiments using statistically rough surfaces differing in their roughness power density spectrum. Experimental results are discussed in the light of theoretical contact models for the friction of multi-contact interfaces.

8:48AM P26.00005 Adhesive contact of randomly rough surfaces, LARS PASTEWKA, MARK ROBBINS, Johns Hopkins University — The contact area, stiffness and adhesion between rigid, randomly rough surfaces and elastic substrates is studied using molecular statics and continuum simulations. The surfaces are self-affine with Hurst exponent 0.3 to 0.8 and different short λ_s and long λ_L wavelength cutoffs. The rms surface slope and the range and strength of the adhesive potential are also varied. For parameters typical of most solids, the effect of adhesion decreases as the ratio λ_L/λ_s increases. In particular, the pull-off force decreases to zero and the area of contact A_c becomes linear in the applied load L . A simple scaling argument is developed that describes the increase in the ratio A_c/L with increasing adhesion and a corresponding increase in the contact stiffness [1]. The argument also predicts a crossover to finite contact area at zero load when surfaces are exceptionally smooth or the ratio of surface tension to bulk modulus is unusually large, as for elastomers. Results that test this prediction will be presented and related to the Maugis-Dugdale [2] theories for individual asperities and the more recent scaling theory of Persson [3]. [1] Akarapu, Sharp, Robbins, Phys. Rev. Lett. 106, 204301 (2011) [2] Maugis, J. Colloid Interface Sci. 150, 243 (1992) [3] Persson, Phys. Rev. Lett. 74, 75420 (2006)

9:00AM P26.00006 The Effect of Surface Topography on Interface Stresses During Peeling, YE XU, ERIC DUFRESNE, Yale University — Surface topography can have a large impact on the adhesive strength of soft interfaces. While previous experiments have revealed some of the underlying mechanisms, there has been no direct measurement of interface stresses during adhesive failure. We use traction force microscopy to measure the microscopic distribution of interface stresses during peeling. We focus on the relationship between local stresses and topography near the peeling front.

9:12AM P26.00007 Direction dependence of static friction for commensurate and moderately incommensurate surfaces, MICHAEL WOLLOCH, Vienna University of Technology / Austrian Center of Competence for Tribology, PETER MOHN, JOSEF REDINGER, Vienna University of Technology, ANDRAS VERNES, Austrian Center of Competence for Tribology — We present results from our calculations of quasi-static sliding of two atomically flat surfaces in dry, wearless contact using the Density Functional Theory package VASP. The main focus of our work was to determine to which extent commensurability of the surfaces and the sliding direction effects the friction force. The examined systems include commensurate fcc (111) Aluminium slabs and moderately incommensurate surfaces like bcc (110) Titanium on hcp (001) Titanium. A model consistent with stick-slip friction was devised to calculate the friction forces along sliding paths of up to $1\ \mu\text{m}$ on a quantum mechanical basis. To map all forces and energies for rigid and relaxed atomic positions the top slab was scanned over the bottom one on a properly fine grid, which covers the entire unit cell. In this manner, it is shown that the mean friction force depends on the sliding direction and that due to relaxations incommensurate paths may result, counter-intuitively, in higher friction than commensurate ones.

9:24AM P26.00008 Laser induced projectile impact test (LIPIT): A micron-scale ballistic test for high-strain rate mechanical study of nano-structures, JAE-HWANG LEE, Department of Mechanical Engineering and Materials Science, Rice University, DAVID VEYSSET, KEITH NELSON, Department of Chemistry, MIT, EDWIN THOMAS, Department of Mechanical Engineering and Materials Science, Rice University — We present a method to apply a highly localized deformation at a high-strain-rate for the study of mechanical characteristics of micro- and nano-structures. In the technique, Laser Induced Projectile Impact Test (LIPIT), micro-projectiles (solid silica spheres of $3.7\ \mu\text{m}$ diameter) are accelerated to a supersonic speed (up to 4 km/s) in air by a micro-explosion created by laser ablation of polystyrene and impact a sample target. The velocity information of the micro-projectiles is explicitly determined by two consecutive high-speed images during the flight of the projectiles. For demonstration, a glassy-rubbery nanocomposite consisting of a periodic self-assembled stack of 20 nm thick layers of polystyrene and polydimethylsiloxane blocks (PS-b-PDMS) is tested by LIPIT at the extremely high-strain rate of $10^8\ \text{s}^{-1}$. The polymer nanocomposite demonstrates new orientation dependent deformation and failure mechanisms including a surprising order to disorder transition fluidization, and the energy absorbing ability of a layered nanocomposite through plastic deformation leading to a melting of the layered structure.

9:36AM P26.00009 Probing the sliding interactions between bundled actin filaments, ANDY WARD, ZVONIMIR DOGIC, Brandeis University — Assemblies of filamentous biopolymers are hierarchical materials in which the properties of the overall assemblage are determined by structure and interactions between constituent particles at all hierarchical levels. For example, the overall bending rigidity of a two bundled filaments greatly depends on the bending rigidity of, and the adhesion strength between individual filaments. However, another property of importance is the ability for the filaments to slide freely against one another. Everyday experience indicates that it is much easier to bend a stack of papers in which individual sheets freely slide past each other than the same stack of papers in which all the sheets are irreversibly glued together. Similarly, in filamentous structures the ability for local re-arrangement is of the utmost importance in determining the properties of the structures observed. We have developed a method to directly measure the frictional interactions between a pair of aligned filaments in a well-defined and controllable configuration. This enables us to systematically investigate the role of adhesion strength, filament orientation, length, and surface structure.

9:48AM P26.00010 Harnessing polymer gels to regulate friction between sliding surfaces¹, HASSAN MASOUD, ALEXANDER ALEXEEV, Georgia Institute of Technology, George W. Woodruff School of Mechanical Engineering — We examine the microscale tribological behavior of a pair of gel coated surfaces separated by a thin layer of lubricant. The soft, elastic gel is modeled using a bond-bending lattice spring model that captures the micromechanics of a random network of interconnected filaments. We couple this model with the dissipative particle dynamics that explicitly models the hydrodynamics of a viscous fluid. We probe how elasticity and internal structure of compliant gels affect the tribological behavior and examine how gel elasticity can be harnessed to regulate friction between sliding surfaces. We also study the effect of lubricant composition and the inclusion of nanoscopic particles of different shapes on the friction forces between wet compliant surfaces. Our findings could be useful for developing new methods for regulating friction and reducing wear of lubricated surfaces and also for understanding the micro-mechanics of friction in biological systems.

¹Financial support from the Donors of the Petroleum Research Fund, administered by the ACS, is gratefully acknowledged.

10:00AM P26.00011 On the Equilibrium of an Heavy Elastic Cylinder on Horizontal Nondeformable Plane, LAVRENT SHEKYAN, SERGEY VERLINSKI, Dr. — The plane static contact problem of the equilibrium of a homogeneous heavy elastic cylinder on fixed non-deformable horizontal plane is discussed. In the vicinity of the initial contact between these bodies, there is some contact area, which covers the central angle and which are unknown contact stresses. The elastic equilibrium of a cylinder under the influence of its gravity and some unknown contact stress is discussed. To determine the distribution of contact stress, the size of the contact area of the cylinder and immersion in the horizontal plane is required.

10:12AM P26.00012 Internal friction peak in silicon revealed by moderate temperature annealing¹, THOMAS METCALF, XIAO LIU, JEREMY ROBINSON, Naval Research Laboratory — In order to maximize of the quality factor of a mechanical resonator, one must minimize energy loss mechanisms. We have identified a new internal friction (IF) peak that is present in as-fabricated ultra-high Q silicon resonators known as Double Paddle Oscillators. The IF peak can be removed (and thus its presence revealed) by annealing at moderate (300 °C) temperatures in both inert (Argon) and reactive (H₂) atmospheres, and does not re-appear after aging for 10⁷ s. The success of a relatively low temperature operation in eliminating this mechanism indicates that the phenomenon is surface-, as opposed to bulk- related. We compare this loss mechanism to other known loss mechanisms in silicon.

¹Work supported by the Office of Naval Research

10:24AM P26.00013 ABSTRACT WITHDRAWN —

10:36AM P26.00014 Investigation of stability for an electrostatically actuated flexible electrode, CORY HINTON, MATTHEW MCFARLAND, THOMAS WARD, North Carolina State University — An argument for employing dimensional analysis to explore stability in an electrostatically actuated flexible electrode is presented theoretically and experimentally. The electrode is configured as a cantilever beam, as many applications in MEMs, medical devices, and sensing devices have been studied for years. This study investigates a macro scale beam (length = 100mm - 150mm), for applications in cooling fan and flapping micro air vehicle devices. The influence of scale is validated, voltage potential and frequency contributions are quantitatively measured, and a comparison of input signal (analog versus digital) is discussed using dynamical systems analysis. Based on experimental data and numerical models, characteristics of stability are presented that could influence design considerations for various micro- and macro-scale devices.

Wednesday, February 29, 2012 8:00AM - 11:00AM —
Session P27 DCMP: Invited Session: Transport Studies of Topological Insulators 258AB

8:00AM P27.00001 Towards the quantum anomalous Hall effect in HgMnTe, HARTMUT BUHMANN, Physikalisches Institut, Universität Würzburg — Although there are plenty of theoretical and experimental studies of the anomalous Hall effect in the ferromagnetic materials, the quantum version, namely “quantum anomalous Hall effect”, has never been observed in the realistic materials. In this work, we report the experimental evidence of the quantum anomalous Hall effect in the Mn doped HgTe quantum wells. We observe a long quantized Hall plateau from 0.2 T to > 25 T with the Hall conductance e^2/h in the p-doped regime. By carefully analyzing the gate voltage and temperature dependence of the experimental data, we find the long plateau originates from the fact that the two zero Landau levels in HgMnTe doped system have the same slope, which is exactly the required condition for the quantum anomalous Hall effect. Theoretical $\mathbf{k}\cdot\mathbf{p}$ calculation is carefully compared with the experimental data to identify the influence from the magnetic impurities. A HgMnTe-ferromagnet hybrid structure is proposed for the possible future device applications.

8:36AM P27.00002 Quantum Spin Hall Insulator Made of InAs/GaSb, IVAN KNEZ, Rice University — Quantum Spin Hall Insulator (QSHI) is a two-dimensional variant of a novel class of materials characterized by topological order, whose unique properties have recently triggered much interest and excitement in the condensed matter community. Most notably, topological properties of these systems hold a great promise in mitigating the difficult problem of decoherence in implementations of quantum computers. Although QSHI has been theoretically predicted in a few different materials, so far only the semiconductor systems of HgTe/CdTe and, more recently, inverted InAs/GaSb, have shown direct evidence for the existence of this phase. Ideally insulating in the bulk, QSHI is characterized by one-dimensional channels at the sample perimeter, which have helical property, with carrier spin tied to the carrier direction of motion, and protected from back-scattering by time-reversal symmetry. Here we present low temperature transport measurements of inverted InAs/GaSb quantum wells, showing strong evidence for the existence of proposed helical edge channels. Edge modes persist in spite of conductive bulk, which is of non-trivial origin but highly tunable via electrostatic gates, and show only a weak magnetic field dependence. This is a direct consequence of a gap opening away from the zone center leading to effective decoupling of edge to bulk states due to the Fermi velocity mismatch. Low Schottky barrier of this material system and good interface to superconductors allows us to further probe topological properties of helical channels in Andreev reflection measurements and opens a promising route in realization of exotic Majorana modes.

9:12AM P27.00003 Transport Studies of Topological Insulators and Superconductors¹, YOICHI ANDO, Institute of Scientific and Industrial Research, Osaka University — A topological state of matter is characterized by a topological feature of the quantum-mechanical wavefunction in the Hilbert space. In 3D topological insulators (TIs), a non-trivial Z_2 topology of the bulk valence band leads to the emergence of Dirac fermions on the surface. Similarly, in 3D topological superconductors (TSCs), a non-trivial winding number of the superconducting wavefunction leads to the appearance of Majorana fermions on the surface. The Dirac or Majorana fermions in those topological states of matter are of fundamental interest, but there have been significant materials problems that hindered their experimental studies so far: In the case of TIs, most of the materials identified as such are poor insulators in the bulk, making it difficult to probe the peculiar surface transport properties; in the case of TSCs, no concrete example has yet been discovered. In this talk, I will present our recent contributions to address these issues. For TIs, we discovered that the chalcogen-ordered tetradymite TI material $\text{Bi}_2\text{Te}_2\text{Se}$ presents a high bulk resistivity, allowing one to observe clear surface quantum oscillations [Z. Ren *et al.*, PRB **82**, 241306(R) (2010)]; more recently, we discovered that the bulk-insulating nature can be further improved in the solid-solution system $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_{3-y}\text{Se}_y$, making it possible to achieve the surface-dominated transport in a bulk crystal and observe both Dirac holes and electrons via Shubnikov-de Haas oscillations [A. A. Taskin *et al.*, PRL **107**, 016801 (2011)]. For TSCs, we developed a new synthesis technique for a candidate TSC, $\text{Cu}_x\text{Bi}_2\text{Se}_3$, to obtain single-crystal samples with a high shielding fraction [M. Kriener *et al.*, PRL **106**, 127004 (2011); PRB **84**, 054513 (2011)]. Using these crystals, we have recently succeeded in observing the surface Andreev bound state which gives evidence for an unconventional superconductivity; since the unconventional superconductivity in $\text{Cu}_x\text{Bi}_2\text{Se}_3$ can only be topological (thanks to the simple and peculiar band structure), one can conclude with confidence that this material is the first concrete example of a TSC [S. Sasaki *et al.*, PRL **107** (2011)]. Work in collaboration with A. A. Taskin, Z. Ren, S. Sasaki, and K. Segawa.

¹Supported by JSPS (NEXT Program) and AFOSR (AOARD 10-4103).

9:48AM P27.00004 Quantum anomalous Hall effect in the thin film of magnetic topological insulators and semimetals¹, XI DAI, Institute of Physics, Chinese Academy of Sciences — The great interests on Hall effects come with their quantization under certain conditions. By now all five types of the Hall effects have been discovered, and the only remaining one is the quantized anomalous Hall effect, which is the quantized Hall effect without external magnetic field and the formation of Landau levels. In the present talk, I will summarize two possible ways proposed by our group to reach such an effect, which are thin films of magnetically doped topological insulators and topological semimetals. I will mainly focus on the latter proposal, which is important in the following sense. First the proposal is based on the stoichiometric material, which is very good for obtaining large mobility. Second, the exchange coupling energy between the magnetization and the valence electrons is of the order of eV, which makes QAHE more easy to be realized.

¹This work has been supported by NSF of China and the 973 program of China

10:24AM P27.00005 Crossover between weak localization and weak antilocalization in magnetically doped topological insulator, QIKUN XUE, Tsinghua University — No abstract available.

Wednesday, February 29, 2012 8:00AM - 10:48AM –
Session P28 FIAP: Optical Applications: Nonlinear Optics, Waveguides, and Novel Structures
 258C

8:00AM P28.00001 An optical antenna for high-count-rate single-photon-sensitive superconducting transition edge sensors¹, FAUSTIN CARTER, DANIEL SANTAVICCA, DANIEL PROBER, Yale University — There are number of promising applications for a GHz count-rate, energy-resolving single-photon detector in the near-infrared. However, such a detector has not yet been perfected. For thermal detectors, this is partly due to the difficulty of coupling relatively large (~ 1 micron) photons into the necessarily small (~ 100 nm) thermal sensor element. We report on the simulation, fabrication, and preliminary measurements of an antenna-coupled superconducting transition edge sensor. The optical antenna is designed to directly couple incident near-infrared photons into much shorter wavelength surface plasmons, which are then delivered to a nanoscale superconducting niobium detector element at the antenna feed. This detector is inherently energy resolving, unlike the superconducting nanowire single-photon detector (SNSPD) or the single-photon avalanche photodiode (SPAD), and it operates at the relatively convenient temperature of 4 K.

¹This work is supported by the NASA CT Space Grant Consortium and NSF-CHE.

8:12AM P28.00002 Nanocrystal-based Optoelectronic Devices¹, KENNETH EVANS, Applied Physics Ph.D. Program, Rice University, JOSEPH HERZOG, DANIEL WARD, DOUGLAS NATELSON, Department of Physics & Astronomy, Rice University — Optoelectronic devices capable of detecting and emitting light on a scale well below its wavelength could have a profound impact on basic and applied experimental research in light-based electronics, on-demand photon generation, and for studying poorly understood quantum phenomena such as blinking and spectral wandering. We present a fabrication procedure for ultrasmall, nanocrystal optoelectronic devices based on self-assembled layers of quantum dots in plasmonically-active gold nanogaps. We provide preliminary experimental results which examine the possibility for surfaced-enhanced fluorescence, subwavelength detection and emission of light as well as plasmon-based optical trapping in these systems.

¹Funding provided by The II-VI Foundation.

8:24AM P28.00003 Frequency and Intensity Stabilization of Planar Waveguide-External Cavity Lasers, GREGORIO TELLEZ, STEVEN SHOEN, VOLKER QUETSCHKE, University of Texas at Brownsville — Planar Waveguide External Cavity Lasers (PW-ECL) show an immense potential for use in precision measurement tasks and space missions because of its compactness and simple design. We show the techniques used to frequency and intensity stabilize a PW-ECL 1550nm laser system with the goal of achieving a frequency stability of 30 Hz/sqrt(Hz) and a RIN of less than 10^{-6} . These PW-ECL systems are a potential replacement for Non-Planar Ring Oscillator (NPRO) laser systems, which have become a standard for low-noise interferometric applications, if the PW-ECL can meet the required stability. We present the initial experimental results of the intensity and frequency stabilization setup and we show a comparison between PW-ECL lasers and NPRO lasers with respect to measurements and applications requiring a high frequency and intensity stability.

8:36AM P28.00004 Experimental setup to demonstrate low-frequency high-precision frequency stabilization of 1550 nm ECL Lasers, STEVEN SHOEN, GREGORIO TÉLLEZ, VOLKER QUETSCHKE, University of Texas at Brownsville — Advances in fiber and waveguide technologies have brought about a new type of laser: the Planar Waveguide External Cavity Laser (PW-ECL) that shows a great potential for precision interferometric measurements. We show an experimental setup based on a 1550nm PW-ECL which was designed to achieve a frequency stabilization of $30 \text{ Hz}/\sqrt{\text{Hz}}$ or less at 10 mHz. The presented design makes use of thermal shielding to suppress temperature fluctuations at low frequencies as well as a vacuum system, high finesse cavity and low-noise electronics to reduce the frequency noise. A description of the components used in the design is given and initial results are presented.

8:48AM P28.00005 Experimental demonstration waveguide with arbitrary bending angles in hyperuniform disordered photonics materials, WEINING MAN, San Francisco State University, MARIAN FLORESCU, University of Surrey, SEYED HASHEMIZAD, ERIC WILLIAMSON, DEVIN LINER, YINGQUAN HE, BRIAN LEUNG, San Francisco State University, PAUL CHAIKIN, New York University — Contradicting to the long standing intuition that long-range translational order is required in photonic band gap formation, recently a new class of disordered hyperuniform materials was predicted to possess sizeable photonic band gaps. We report the first experimental demonstration of complete and isotropic photonic band gap for all polarizations in such disordered hyperuniform structures made of alumina with a dielectric constant of 8.7. In periodic structures there are only a limited number of allowed rotational symmetries; hence bending angles of waveguiding channels are greatly limited. In isotropic hyperuniform disordered structures there are no preferential symmetry directions and waveguiding channels can be constructed with arbitrary bending angles. In our study, near 100 percent transmission of electromagnetic waves around sharp corners of arbitrary angles with bending radii smaller than one wavelength are observed experimentally. The hyperuniform disordered structures also enable the realization of isotropic confinement of radiation in cavities and can be used as flexible optical insulator platforms.

9:00AM P28.00006 Kerr Nonlinear Modes in Photonic Crystal Waveguide with Off-channel Features¹, BUDDHI RAI, Western Michigan University, GULAY BIRKOK, Gebze Institute of Technology, ARTHUR MCGURN, Western Michigan University — A theoretical method using nonlinear difference equation approach has been developed for investigating guided modes of photonic crystal waveguide for cases in which the guided modes interact with multiple bound electromagnetic modes localized on off-channel impurity features of Kerr nonlinear media. The interest is on the properties of resonant scattering of the modes exhibited by the system formed of both linear and nonlinear media sites in the photonic crystal lattice. The scattering is treated and compared with results of the scattering of the modes in the linear limit of the Kerr media, i.e. in the absence of intensity $|E|^2$ term in the Kerr dielectrics derived in recursive difference equation formulation. The equations of the system are simple and can be quickly solved to demonstrate the wide and interesting varieties of behavior present in the system, including among others, optical bistability and induced transparency. Additionally, the method is applied for a case in which the field dependence of Kerr dielectric properties allows two different frequency waveguide modes to interact with one another by a modulation of the off-channel site dielectric properties. In this interaction, the one mode is used to model numerically the transmission characteristics of the other.

¹Western Michigan University

9:12AM P28.00007 The Phase Effect in perturbative nonlinear optics, CI-LING PAN, National Tsing Hua University, RUEI-YIN LIN, National Chiao Tung University, WEI-JAN CHANG, National Tsing Hua University, CHAO-KUEI LEE, National Sun yat-sen University — Waveform control is essential for ultrafast nonlinear optical processes such as high-order harmonic generation (HHG). For example, a sawtooth-like waveform can enhance the kinetic energies of the electrons such that the cutoff of HHG is extended. In this work, we show that relative phase of the two-color driving laser can affect the outcome of perturbative nonlinear optical processes such as lower-order harmonic generation. Consider the third-harmonic signal generated in argon by the fundamental and second-harmonics of a pump laser with frequencies of ω_1 , and ω_2 . A cross-term emerges due to interference of four-wave mixing signals of $(\omega_1 + \omega_1 + \omega_1)$ and $(\omega_2 + \omega_2 - \omega_1)$. When the intensities of two-color pump at ω_1 and ω_2 are equal, the modulation in the third-harmonic signal by the cross-term is about 30% of the DC term. As the relative phase between ω_1 and ω_2 varies, a sinusoidal modulation in output intensity at $3\omega_1$ is expected. We have also calculated the phase effects for fifth, seventh and ninth harmonic generation, which show more complicated behavior.

9:24AM P28.00008 Micro-Photoluminescence for Optoelectronic Material Characterization, EMIR MAGDEN, VICTOR MINDEN, COREY SHEMELYA, THOMAS VANDERVELDE, Tufts University — A hardware environment and software bundle have been developed for measuring the absolute value of and the variance in photoluminescence (PL) intensity across samples of optoelectrical materials. The fully automated assembly uses a dual-axis translation stage to allow for “micro-PL” measurements of the sample surface with a resolution of 10 microns on either axis. The user is given the option to digitally adjust the boundaries of the area being mapped, and set the measurement resolution to produce coarse or fine detailed PL maps of the sample surface. By using a monochromator, the system can perform preliminary measurements of PL at wavelengths ranging from 400nm to 1.7um, and determine the optimal spectral operation settings for detailed mapping. Since the system is a modular design, components can be switched to operate in other spectra ranges as well. As all components are digitally controlled by a PC, a universal user interface and integration module has been created to allow for simultaneous operation of all components with minimal user interaction, and intuitive representations of final data for material quality assessment. Various materials are characterized and discussed to demonstrate the utility.

9:36AM P28.00009 Rapid adiabatic passage in nonlinear optics for complete power transfer between ultrabroadband optical pulses, JEFFREY MOSES, Massachusetts Institute of Technology, FRANZ KÄRTNER, Massachusetts Institute of Technology and DESY-Center for Free-Electron Laser Science, Hamburg, Germany, HAIM SUCHOWSKI, Weizmann Institute of Science and UC Berkeley — Rapid adiabatic passage is a central tool for full transfer of level populations in an atomic system. Recent work showed the equation of motions describing three-optical-wave mixing in a dielectric medium through a nonlinear electric susceptibility are isomorphic to the optical Bloch equations for a two-level atom (neglecting radiative losses) when the middle frequency wave is strong. We have exploited this analogy for the first time to prove the principle of complete Landau-Zener adiabatic transfer in nonlinear wave mixing. Using intense laser pulses and a specially designed poled potassium titanyl phosphate nonlinear crystal with an adiabatic longitudinal variation of the poling period, we demonstrate complete energy transfer of a near-IR pulse to the mid-IR. Moreover, we find the principle is upheld for huge laser bandwidths. In our experiment the power transfer covers two-thirds of an octave of bandwidth with preservation of the power spectral density profile. Control of optical power transfer through rapid adiabatic passage thus can serve to optimize sources for coherent control and strong-field physics.

9:48AM P28.00010 Nano-Gap Embedded Plasmonic Gratings for Surface Plasmon Enhanced Fluorescence, KUNAL BHATNAGAR, SANGHO BOK, VENUMADHAV KORAMPALLY, SHUBHRA GANGOPADHYAY, University of Missouri - Columbia, CENTER FOR NANO/MICRO SYSTEMS AND NANOTECHNOLOGY TEAM — Plasmonic nanostructures have been extensively used in the past few decades for applications in sub-wavelength optics, data storage, optoelectronic circuits, microscopy and bio-photonics. The enhanced electromagnetic field produced at the metal/dielectric interface by the excitation of surface plasmons via incident radiation can be used for signal enhancement in fluorescence and surface enhanced Raman scattering studies. Novel plasmonic structures on the sub wavelength scale have been shown to provide very efficient and extreme light concentration at the nano-scale. The enhanced electric field produced within a few hundred nanometers of these structures can be used to excite fluorophores in the surrounding environment. Fluorescence based bio-detection and bio-imaging are two of the most important tools in the life sciences. Improving the qualities and capabilities of fluorescence based detectors and imaging equipment has been a big challenge to the industry manufacturers. We report the novel fabrication of nano-gap embedded periodic grating substrates on the nanoscale using micro-contact printing and polymethylsilsequioxane (PMSSQ) polymer. Fluorescence enhancement of up to 118 times was observed with these silver nanostructures in conjugation with Rhodamine-590 fluorescent dye. These substrates are ideal candidates for low-level fluorescence detection and single molecule imaging.

10:00AM P28.00011 Micro-manufacturing with Three-dimensional Intensity Patterns: Practical Limits and Considerations¹, DANIEL MCADAMS, DANIEL COLE, University of Pittsburgh — It is possible to generate 3D intensity patterns for micro-manufacturing using a phase hologram displayed on a liquid-crystal spatial light modulator (SLM). Knowledge of the phase and amplitude of a field in a single plane (the SLM plane) allows for calculation of the phase and amplitude in any set of subsequent planes. Iterative phase retrieval algorithms can take a 3D target intensity pattern and generate a hologram for display on the SLM; however, arbitrary 3D intensity patterns are not necessarily achievable because the light field must obey the wave equation. Furthermore, these algorithms have not been discussed from the point of view of lithographic micro-manufacturing. This paper presents one method for making a 3D intensity pattern that can be used to cure resist in a single-shot, and discusses the limits to patterning due to power, resolution, and SLM-related issues. The relationship between the resolution in the patterning volume and physical specifications of the SLM is more restrictive than if the patterning were being done in a single plane, but with sufficient laser power, this algorithm could be used in high-throughput 3D micro-manufacturing.

¹This work was funded by NSF Grant No. CMMI-0928353

10:12AM P28.00012 High Finesse Microcavity for Gas Sensing, BENJAMIN PETRAK, KUMARASIRI KONTHAS-INGHE, ANDREAS MULLER, University of South Florida — We report our progress in using optical Fabry-Perot microcavities for multiatomic gas sensing. The microcavities consist of one micromirror at a fiber tip and another micromirror on a planar silica substrate, each with a diameter near 50 microns. The micromirrors were fabricated by an improved CO₂ laser ablation process that uses feedback from the light emitted during ablation to control the mirror dimensions. A cavity finesse in excess of 50 000 was obtained in the near-infrared. Our goal is to make use of the Purcell effect of cavity quantum electrodynamics to obtain an enhancement of Raman scattering when a double resonance condition is achieved.

10:24AM P28.00013 Control of transverse optical patterns in semiconductor quantum well microcavities¹, M.H. LUK, Y.C. TSE, Physics Department, Chinese University of Hong Kong, N.H. KWONG, College of Optical Sciences, University of Arizona, P.T. LEUNG, Physics Department, Chinese University of Hong Kong, S. SCHUMACHER, Physics Department, University of Paderborn, R. BINDER, College of Optical Sciences and Department of Physics, University of Arizona — Recently, a low intensity all optical switching scheme exploiting directional optical instabilities in a semiconductor quantum well microcavity was proposed. It was demonstrated numerically that a sufficiently strong laser (pump) beam normally incident on the microcavity can suffer directional instabilities, generating new beams in oblique directions. These off-axis beams form a pattern when projected onto a plane in the far field placed transverse to the pump. Furthermore, the numerical results showed that the azimuthal orientation of the transverse optical pattern can be reversibly switched by applying a control beam much weaker than the pattern intensity. These phenomena are mediated by the nonlinear interactions among elementary excitations of the microcavity — polaritons formed from strong coupling between the quantum well excitons and photons in a cavity mode. In this Contribution, we provide an overview of the rich parametric dependencies of pattern selection, the time scale of pattern formation, and the switching process. We also present an analysis of system's dynamics based on the contributing polariton wave-mixing processes.

¹S. S. acknowledges financial support from the Deutsche Forschungsgemeinschaft.

10:36AM P28.00014 MEMS Fabricated MM-Wave Slow Wave Structure¹, MARK FIELD, ROBERT BORWICK, Teledyne Scientific & Imaging LLC, 1049 Camino Dos Rios, Thousand Oaks CA 91360, YOUNG-MIN SHIN, Department of Physics, Northern Illinois University, DeKalb, IL 60115 & Fermi National Accelerator Laboratory, Batavia, IL 60510, LARRY BARNETT, NEVILLE LUHMANN, Department of Electrical Engineering, University of California Davis, Davis, CA 95616, TAKUJI KIMURA, JOHN ATKINSON, Communications and Power Industries, 811 Hansen Way, Palo Alto, CA 94304 — We report on the fabrication and test of a MEMS slow wave structure designed for a > 40 GHz bandwidth centered on 220 GHz operation, that slows radiation down to group velocity of $8.16 \times 10^7 \text{ ms}^{-1}$ where the velocity matches the speed of electrons from a 20 keV source. The slow wave device uses a 40 mm long staggered interdigitated vane structure within a waveguide [1]. Ultimately, such a device will be integrated with an electron beam to become part of a sheet beam travelling wave tube (SBTWT) amplifier. A gold coated deep reactive ion etched (DRIE) silicon test structure was fabricated to test the RF properties of the design. This MEMS structure was coupled to WR-4 waveguide in a metal fixture and the S-parameters measured using a vector network analyzer, allowing extraction of the insertion loss and signal delay as a function of frequency. A further MEMS structure with just 10 cells of the vane structure within a cavity were fabricated which allows points on the dispersion curve to be directly measured as resonances of the structure. Extraction of the dispersion curve verifies the group velocity measurement of the device.

[1] Y-M. Shin & L.R. Barnett, *Appl.Phys. Lett.* 2008, 92 pp. 091501.

¹Supported under the DARPA HiFIVE Program, Contract W911NF-08-C-0050

Wednesday, February 29, 2012 8:00AM - 11:00AM —

Session P29 GQI: Focus Session: Superconducting Qubits: Multiple Qubits and Entanglement

8:00AM P29.00001 Prospects for a prototype quantum processor based on three-dimensional superconducting cavities and qubits, CHAD RIGETTI, IBM T. J. Watson Research Center — Superconducting qubits embedded in three-dimensional waveguide resonators (recently pioneered by Paik, et al., arXiv:1105.4652) have shown excellent coherence properties and an ease of implementation that make them an enticing core component for small prototype quantum processors. The relatively large physical dimensions of the microwave modes of these 3D-cQED systems may lead one to discount their prospects for scaling. We argue that the larger characteristic dimensions, among others factors, in fact facilitate scaling for currently practicable prototype systems of ~ 10 to 1,000 qubits. This emerges from significantly reduced fabrication complexity and costs, larger tolerances to parameter deviations, a more prevalent role for off-the-shelf components, and greater amenability to full-device electromagnetic simulation. At IBM we are working towards a modular quantum processor prototype based on 3D-cQED. Multi-qubit cavities, each implementing an artificial NMR molecule, are to be connected in an array by non-linear elements which double as tunable couplers between qubits in adjacent cavities and as single-shot readout circuitry. The resulting lattice of physical qubits provides a fabric on which surface code error correction can take place, implying a fault-tolerant threshold error rate for this architecture of $\sim 1\%$. We describe recent experiments demonstrating a two-qubit gate with a two qubit/one cavity device and progress toward tunable coupling of qubits in adjacent cavities.

8:36AM P29.00002 Prime factoring using a Josephson phase-qubit architecture: $15 = 3 * 5$, ERIK LUCERO, R. BARENDs, J. BOCHMANN, Y. CHEN, B. CHIARO, J. KELLY, M. LENANDER, M. MARIANTONI, A. MEGRANT, C. NEILL, P. O'MALLEY, P. ROUSHAN, D. SANK, A. VAINSENER, University of California, Santa Barbara, H. WANG, Zhejiang University, J. WENNER, T. WHITE, Y. YIN, A.N. CLELAND, JOHN M. MARTINIS, University of California, Santa Barbara — We demonstrate a compiled version of Shor's algorithm using a quantum processor. The processor consists of "off-the-shelf" components: qubits and resonators arranged in the ReZQu architecture. We have performed the algorithm for $N=15$ and the period $r=2$. The required two and three qubit entanglement is observed during the computation, which exemplifies the quantum nature of the algorithm.

8:48AM P29.00003 Building Transmon Qubits in the ReZQu Architecture, JULIAN KELLY, R. BARENDs, J. BOCHMANN, B. CHIARO, Y. CHEN, M. LENANDER, E. LUCERO, M. MARIANTONI, A. MEGRANT, C. NEILL, P. O'MALLEY, P. ROUSHAN, D. SANK, A. VAINSENER, J. WENNER, T. WHITE, Y. YIN, ANDREW CLELAND, JOHN M. MARTINIS, UC Santa Barbara — Transmon qubits are promising candidates for use in a superconducting quantum computer because of their long coherence times, but traditionally involve a difficult measurement scheme. By reading out each transmon through a phase qubit, we are able to take advantage of the single shot and multiplexed readout technologies already in use. This allows us to drop transmons into the ReZQu architecture. However, fabricating a transmon and phase qubit on the same chip comes with its own set of challenges. We present fabrication techniques and preliminary data as we move toward our next generation of qubits.

9:00AM P29.00004 High-fidelity CZ gate for the quantum Von Neumann architecture¹, JOYDIP GHOSH, University of Georgia, Athens, ANDREI GALIAUTDINOV, ALEXANDER KOROTKOV, University of California, Riverside, ZHONGYUAN ZHOU, MICHAEL GELLER, University of Georgia, Athens, JOHN MARTINIS, University of California, Santa Barbara — The building block of a scalable superconducting quantum computer has recently been demonstrated [M. Mariantoni et al., Science 334, 61 (2011)]. This architecture consists of superconducting phase qubits capacitively coupled both to individual memory resonators as well as a common bus. In this work we investigate the fidelity of a CZ logic gate between a qubit and bus in a multi-qubit device. Our results show that it is possible to implement the CZ gate with 99.99% intrinsic fidelity in 30ns with a simple two-parameter pulse profile (plus two Z rotations). An analytical error model is also developed to explain and extend this result.

¹IARPA

9:12AM P29.00005 High-fidelity gates towards a scalable superconducting quantum processor, JERRY M. CHOW, ANTONIO D. CORCOLES, JAY M. GAMBETTA, CHAD RIGETTI, IBM TJ Watson Research Center, BLAKE R. JOHNSON, BBN Raytheon Technologies, JOHN A. SMOLIN, SETH MERKEL, STEFANO POLETO, JIM ROZEN, MARY BETH ROTHWELL, GEORGE A. KEEFE, MARK B. KETCHEN, MATTHIAS STEFFEN, IBM TJ Watson Research Center — We experimentally explore the implementation of high-fidelity gates on multiple superconducting qubits coupled to multiple resonators. Having demonstrated all-microwave single and two qubit gates with fidelities $> 90\%$ on multi-qubit single-resonator systems, we expand the application to qubits across two resonators and investigate qubit coupling in this circuit. The coupled qubit-resonators are building blocks towards two-dimensional lattice networks for the application of surface code quantum error correction algorithms.

9:24AM P29.00006 Driving two-qubit entanglement with an enhanced ZZ interaction in circuit QED¹, BLAKE R. JOHNSON, C.A. RYAN, M.P. DA SILVA, Raytheon BBN Technologies, J.M. CHOW, J.M. GAMBETTA, S. MERKEL, IBM T.J. Watson Research, T. OHKI, Raytheon BBN Technologies — The quantum bus architecture is fast becoming a popular approach for coupling superconducting qubits [1,2]. With two fixed-frequency qubits coupled by a resonator, it is possible to engineer the system's frequencies such that the qubits experience a strong ZZ interaction. This interaction can be used as a resource for creating entanglement when needed, but can also be suppressed at will using appropriate decoupling sequences. We will show measurements of a device where this ZZ interaction is enhanced by interactions with higher-levels of superconducting transmon qubits. To achieve high-fidelity control in this regime, we employ robust composite pulses and optimal control methods to decouple the two-qubit interaction during single-qubit operations. The resulting system serves as a testbed for adapting control techniques from liquid-state NMR to fixed-frequency superconducting qubits.

[1] L. DiCarlo *et al.* Nature **460**, 240-244 (2009).

[2] Matteo Mariantoni *et al.* Science **334**, 61-65 (2011).

¹We acknowledge support from IARPA under contract W911NF-10-1-0324.

9:36AM P29.00007 Controlling superconducting qubits in the presence of a strong, constant ZZ interaction, SETH MERKEL, IBM, IBM QUANTUM COMPUTING TEAM — We look at the problem of optimal gate design in a system of two superconducting qubits coupled by a cavity. The system is designed to have a strong "always on" ZZ interaction, which is essential for two-qubit entangling gates, but presents a challenge for single qubit manipulation. Using pulse shaping ideas from NMR we are able to analytically derive single qubit gates that remove this unwanted coupling to 3rd order in the Magnus expansion, and applying DRAG corrections prevents leakage to higher oscillator levels. In the limit of strong cross-talk these pulses break down when the qubit being manipulated has a resonance close to the higher transition frequencies of the other, however we are still able to find high fidelity pulses numerically.

9:48AM P29.00008 Implementation of a Toffoli Gate with Superconducting Circuits, ARKADY FEDOROV, LARS STEFFEN, MATTHIAS BAUR, ETH Zurich, MARCUS DA SILVA, Raytheon BBN Technologies, ANDREAS WALLRAFF, ETH Zurich — The Toffoli gate is an important primitive in many quantum circuits and quantum error correction schemes. Here we demonstrate the implementation of a Toffoli gate with three superconducting transmon qubits coupled to a microwave resonator [1]. Following Ralph *et al.* [2] we used the third energy level of the transmon qubit to significantly reduce the number of elementary gates needed to implement the Toffoli gate in comparison to approaches using two-level systems only. A similar scheme to realize a Toffoli-class gate has independently been devised on a system of three logical qubits encoded in the states of two qubits and a resonator [3]. Our gate fidelity evaluated by both full process tomography and Monte Carlo process certification is $68.5 \pm 0.5\%$. The results reinforce the potential of macroscopic superconducting qubits for implementation of complex quantum operations and point at the possibility to implement quantum error correction schemes [4].

[1] A. Fedorov *et al.*, arXiv:1108.3966.

[2] T. C. Ralph, K. J. Resch, A. Gilchrist, Phys. Rev. A **75**, 022313 (2007).

[3] M. Mariantoni, *et al.* Science **334**, 61 (2011).

[4] M. D. Reed, *et al.*, arXiv:1109.4948.

10:00AM P29.00009 Multiple photon effects in coupled anharmonic oscillators for circuit QED architectures, JAY GAMBETTA, IBM T.J. Watson Research Center, Yorktown Heights, New York 10598, USA, IBM QUANTUM COMPUTING TEAM — In recent years many superconducting qubits have emerged that are essentially weak anharmonic oscillators. When these systems are coupled, due to the weak anharmonicity the major source of error in this system is leakage. In this talk I will present a method for reducing leakage when implementing a two qubit gate. I will also show that due to this weak anharmonicity new multi-photon transitions emerge that can be used for implementing new types of two qubit gates.

10:12AM P29.00010 Observing Resonant Entanglement Dynamics in Circuit QED, J.A. MLYNEK, A.A. ABDUMALIKOV, J.M. FINK, L. STEFFEN, C. LANG, A.F. VAN LOO, A. WALLRAFF, ETH Zurich — We study the resonant interaction of up to three two-level systems and a single mode of an electromagnetic field in a circuit QED setup. Our investigation is focused on how a single excitation is dynamically shared in this fourpartite system. The underlying theory of the experiment is governed by the Tavis-Cummings-model, which on resonance predicts dynamics known as vacuum Rabi oscillations. The resonant situation has already been studied spectroscopically with three qubits [1] and time resolved measurements have been carried out in a tripartite system [2]. Here we are able to observe the coherent oscillations and their $\sqrt{N}$ -enhancement by tracking the populations of all three qubits and the resonator. Full quantum state tomography is used to verify that the dynamics generates the maximally entangled 3-qubit W-state when the cavity state factorizes. The $\sqrt{N}$ -speed-up offers the possibility to create W-states within a few ns with a fidelity of 75%. We compare the resonant collective method to an approach, which achieves entanglement by sequentially tuning qubits into resonance with the cavity.

[1] J. M. Fink, Physical Review Letters **103**, 083601 (2009)

[2] F. Altomare, Nature Physics **6**, 777–781 (2010)

10:24AM P29.00011 Benchmarking a Teleportation Protocol realized in Circuit QED, MATTHIAS BAUR, ARKADY FEDOROV, LARS STEFFEN, ETH Zurich, MARCUS DA SILVA, Raytheon BBN Technologies, ANDREAS WALLRAFF, ETH Zurich — Teleportation of a quantum state may be used for distributing entanglement between distant qubits in quantum communication and for realizing universal and fault-tolerant quantum computation. Here we demonstrate the implementation of a teleportation protocol, up to the single-shot measurement step, with superconducting qubits coupled to a microwave resonator [1]. Using full quantum state tomography and evaluating an entanglement witness, we show that the protocol generates a genuine tripartite entangled state of all three-qubits. Calculating the projection of the measured density matrix onto the basis states of two qubits allows us to reconstruct the teleported state. Repeating this procedure for a complete set of input states we find an average output state fidelity of 86% for the teleported state.

[1] M. Baur, A. Fedorov, L. Steffen, S. Filipp, M.P. da Silva, and A. Wallraff, arXiv:1107.4774.

10:36AM P29.00012 Characterization of a two-transmon processor with individual single-shot qubit readout¹, DENIS VION, FLORIAN ONG, VIVIEN SCHMITT, ROMAIN LAURO, NICOLAS BOULANT, PATRICE BERTET, ANDREAS DEWES, DANIEL ESTEVE, CEA-Saclay, France — We report the characterization of a two-qubit processor implemented with two capacitively coupled tunable superconducting qubits of the transmon type, each qubit having its own non-destructive single-shot readout. The fixed capacitive coupling yields the $\sqrt{i}$ SWAP two-qubit gate for a suitable interaction time. We reconstruct by state tomography the coherent dynamics of the two-bit register as a function of the interaction time, observe a violation of the Bell inequality by 22 standard deviations after correcting readout errors, and measure by quantum process tomography a gate fidelity of 90%.

¹We acknowledge support from the European research contracts MIDAS and SOLID, from ANR Masquelspec and C’Nano.

10:48AM P29.00013 Demonstrating quantum speed-up in a superconducting two-qubit processor¹, ANDREAS DEWES, ROMAIN LAURO, FLORIAN ONG, VIVIEN SCHMITT, DANIEL ESTEVE, PATRICE BERTET, DENIS VION, CEA Saclay, PEROLA MILMAN, Laboratoire Matériaux et Phénomènes Quantiques, Université Paris Diderot — We operate a superconducting quantum processor consisting of two tunable transmon qubits coupled by a swapping interaction, and equipped with non destructive single-shot readout of the two qubits [1]. With this processor, we run the Grover search algorithm among four objects and find that the correct answer is retrieved after a single run with a success probability between 0.52 and 0.67, significantly larger than the 0.25 achieved with a classical algorithm. This constitutes a proof-of-concept for the quantum speed-up of electrical quantum processors [2].

[1] arXiv:1109.6735v1

[2] arXiv:1110.5170v1

¹We gratefully acknowledge financial support from the European research contracts MIDAS and SOLID, from ANR Masquelspec and C’Nano and from the German Ministry of Education and Research.

Wednesday, February 29, 2012 8:00AM - 11:00AM –
Session P30 GQI: Semiconductor Qubits - Communication and Hybridization 259B

8:00AM P30.00001 Circuit Quantum Electrodynamics with Semiconductor Quantum Dots ,

ANDREAS WALLRAFF, TOBIAS FREY, PETER J. LEEK, MATTHIAS BECK, ETH Zurich, ALEXANDRE BLAIS, Université de Sherbrooke, THOMAS IHN, KLAUS ENSSLIN, ETH Zurich — Research on semiconductor quantum dots has tremendously contributed to the understanding of the physics of individual charges and spins in a solid state environment. Typically, quantum dots are investigated by direct current transport measurements or using quantum point contacts for charge sensing. Instead, we have realized a novel device in which a semiconductor double quantum dot is dipole coupled to a GHz-frequency high-quality transmission line resonator. This approach allows us to characterize the properties of the double dot by measuring both its dispersive and dissipative interaction with the resonator [1]. In addition to providing a new readout mechanism, this architecture has the potential to isolate the dots from the environment and to provide long distance coupling between spatially separated dots. These features are expected to improve the potential for realizing a quantum information processor with quantum dots as previously demonstrated for superconducting circuits making use of circuit quantum electrodynamics.

[1] T. Frey et al., arXiv:1108.5378v1 (2011)

8:12AM P30.00002 Dispersive microwave readout of a silicon double quantum dot¹ ,

ANDREW SCHMIDT, EDWARD HENRY, U.C. Berkeley, QNL, M.G. HOUSE, UCLA, Y.T. WANG, C.C. LO, H. LI, L. GREENMAN, U.C. Berkeley, H. PAN, M. XIAO, UCLA, K.B. WHALEY, U.C. Berkeley, H.W. JIANG, UCLA, E. YABLONOVITCH, J. BOKOR, U.C. Berkeley, I. SIDDIQI, U.C. Berkeley, QNL — Microwave resonators coupled to quantum systems have been used for fast dispersive measurement in several different architectures in solid state and atomic physics. The electronic states of a semiconductor quantum dot represent a promising candidate for quantum information processing. Our work is geared toward developing a fast, non-demolition readout of a semiconductor qubit as realized in silicon by coupling to a superconducting resonant circuit. We report progress on a novel design of a lateral double quantum dot with a unique accumulation gate that allows for control of the spatial location of the 2DEG on the device, allowing the lossy 2DEG to be decoupled from the resonator.

¹This work is supported by the DARPA-QuEST program.

8:24AM P30.00003 Coupling a single charge in a nanowire double quantum dot to a high-Q superconducting microwave resonator¹ ,

K.D. PETERSSON, M.D. SCHROER, L.W. MCFAUL, M. JUNG, J.R. PETTA, Department of Physics, Princeton University, Princeton, New Jersey 08544 — In the field of circuit quantum electrodynamics (cQED), superconducting microwave cavities have provided an important tool with which to probe single superconducting qubits and mediate interactions between distant qubits [1,2]. In view of applying the cQED architecture to semiconductor qubits [3,4], we have integrated a tunable InAs nanowire double quantum dot (DQD) into a high-Q (> 2000), high frequency (~ 6 GHz) niobium microwave resonator. Our design enables a dipole coupling of ~ 40 MHz between the DQD and cavity. We will present experimental results demonstrating how the microwave cavity can be used to explore coherence in nanowire DQDs and discuss prospects for achieving the strong coupling regime.

[1] A. Wallraff et al., Nature 431, 162 (2004)

[2] L. DiCarlo et al., Nature 467, 574 (2010)

[3] J.R. Petta et al., Science 309, 2180 (2005)

[4] K.D. Petersson et al., Phys. Rev. Lett. 105, 246804 (2010)

¹Research supported by the Sloan and Packard Foundations, Army Research Office, and DARPA QuEST.

8:36AM P30.00004 Communication between spin qubits with microwave photons ,

RUSKO RUSKOV, CHARLES TAHAN, Laboratory for Physical Sciences, College Park, MD 20740, U.S.A. — We consider possibilities of quantum state transfer between spin qubits (e.g. electrons in quantum dots) utilizing a microwave transmission line and a tunable coupler. We outline the possibility for optimal quantum transfer between qubit nodes depending on qubit-resonator coupling strengths and tunability, and in the presence of imperfections. Implications of such systems to practical quantum computing in silicon and/or GaAs quantum dots are considered.

8:48AM P30.00005 Spin echo measurements for hybrid qubit systems ,

HANS MALISSA, Department of Electrical Engineering, Princeton University, DAVID SCHUSTER, Department of Physics, University of Chicago, ALEXEI TYRYSKHIN, ANDREW HOUCK, STEPHEN LYON, Department of Electrical Engineering, Princeton University — We have performed electron spin echo measurements on donor spins in silicon samples using micro resonator structures fabricated in thin superconducting niobium films on sapphire substrates. The ability to implement refocusing pulses is an important constituent towards the realization of spin memories for hybrid superconducting/spin qubit applications. The resonators consist of quarter wavelength sections of coplanar waveguide with one end shorted and the other end capacitively coupled to a common feed line. These devices are suitable for pulsed ESR experiments on a commercial spectrometer at microwave frequencies between 9 and 10GHz, and in-plane magnetic fields of about 0.35T, which is well below the critical field of the thin film superconductor. Samples are flip-chip mounted on the resonator, and the magnetic component of the microwave radiation that extends into the sample is used for ESR excitation and detection. The high filling factor due to the small resonator size and the high quality factors that can be obtained with superconductors lead to high sensitivity to small numbers of spins, making our devices an attractive alternative to conventional resonators for certain ESR applications. The low microwave power requirements are appealing for low temperature measurements.

9:00AM P30.00006 Long-distance spin-spin coupling via floating gates ,

LUKA TRIFUNOVIC, University of Basel, OLIVER DIAL, Harvard University, MIRCEA TRIF, JAMES WOOTTON, University of Basel, REDJET ABEBE, AMIR YACOBY, Harvard University, DANIEL LOSS, University of Basel — The electron spin is a natural two level system that allows a qubit to be encoded. When localized in a gate defined quantum dot, the electron spin provides a promising platform for a future functional quantum computer. The essential ingredient of any quantum computer is entanglement—between electron spin qubits—commonly achieved via the exchange interaction. Nevertheless, there is an immense challenge as to how to scale the system up to include many qubits. Here we propose a novel architecture of a large scale quantum computer based on a realization of long-distance quantum gates between electron spins localized in quantum dots. The crucial ingredients of such a long-distance coupling are floating metallic gates that mediate electrostatic coupling over large distances. We show, both analytically and numerically, that distant electron spins in an array of quantum dots can be coupled selectively, with coupling strengths that are larger than the electron spin decay and with switching times on the order of nanoseconds.

9:12AM P30.00007 Quantum gates between non-neighboring spin qubits¹ ,

JIANJIA FEI, YUN-PIL SHIM, University of Wisconsin-Madison, SANGCHUL OH, XUEDONG HU, University at Buffalo, SUNY, MARK FRIESEN, University of Wisconsin-Madison — In quantum circuits involving many qubits, we usually need to perform gates such as CNOT between qubits that are not proximal. For spin qubits, this requires intermediate gate operations because the exchange interaction is very short ranged. Here, we consider three quantum dots in a linear array. We explore the effective coupling between the two outer spins mediated by the central spin. By using the central spin as a “bus”, we show how to efficiently perform gates such as CNOT between the outer spins. We find that arbitrary two-qubit gates can be achieved by applying the bus operations repetitively, with additional single-qubit rotations.

¹Work supported by DARPA-QuEST

9:24AM P30.00008 Resonant Adiabatic Passages of Spin Qubits¹, SANGCHUL OH, Department of Physics, University at Buffalo, The State University of New York, YUN-PIL SHIM, MARK FRIESEN, Department of Physics, University of Wisconsin-Madison, XUEDONG HU, Department of Physics, University at Buffalo, The State University of New York — We study adiabatic quantum teleportation through a spin chain with XX and Heisenberg couplings. We show that an adiabatic quantum teleportation protocol on a three-spin chain can be mapped exactly onto two parallel and coherent adiabatic passage channels, one for each spin orientation. When the time evolution is non-adiabatic, the information transfer displays a series of resonances where perfect transmission fidelity is achieved. This resonant operation is both fast and robust, indicating a possible new route for implementing robust quantum gates between spin qubits.

¹This work was supported by the DARPA QuEST through AFOSR and NSA/LPS through ARO.

9:36AM P30.00009 Quantum phase transitions in a spin bus system, YUN-PIL SHIM, Department of Physics, University of Wisconsin-Madison, SANGCHUL OH, XUEDONG HU, Department of Physics, University at Buffalo, State University of New York, MARK FRIESEN, Department of Physics, University of Wisconsin-Madison — A spin chain can be used as a quantum data bus to enable long distance interactions and to create multi-qubit entanglement between spin qubits. The operation of the spin bus strongly depends on its ground state properties. When the ground state changes abruptly, quantum phase transitions (QPTs) occur and affect the bus operation. Here, we describe the theory of QPTs induced by an external magnetic field in a Heisenberg spin chain which acts as a spin bus. We study the non-analytic behavior of the entanglement between qubits connected to the spin bus and its scaling properties near a quantum critical point. In some cases, we find the entangling properties actually grow with the length of the chain. We also analyze the magnetically induced anisotropy and disorder effects on the effective interactions between qubits.

9:48AM P30.00010 Coupling semiconductor qubits to phonons via a nanomechanical phoniton system, CHARLES TAHAN, RUSKO RUSKOV, Laboratory for Physical Sciences — We explore the possibility of strongly coupling semiconductor qubit states to nanomechanical resonators (phonons) in silicon. These systems may be relevant to qubit transduction schemes, as supporting technology for quantum information processing, for qubit characterization, and for quantum-enabled devices. Specifically, we consider systems where cavity phonons can interact with suitable qubit states in the 1-10 GHz (and higher) regime (tunable using strain, electric and/or magnetic fields). These results may be useful for several solid-state devices as well as being of interest to the optomechanics community.

10:00AM P30.00011 Phonon Mediated Off-resonant Quantum Dot-Cavity Interaction, ARKA MAJUMDAR, ERIK KIM, MICHAL BAJCSY, ARMAND RUNDQUIST, JELENA VUCKOVIC, E. L. Ginzton Lab, Stanford, CA-94305 — Optically controlled quantum dot (QD) spins coupled to semiconductor microcavities constitute a promising platform for robust and scalable quantum information processing devices. In recent experiments on coupled QD optical cavity systems a pronounced interaction between the dot and the cavity has been observed even for detunings of many cavity linewidths. This interaction has been attributed to an incoherent cavity enhanced phonon-mediated scattering process and is absent in atomic systems. We demonstrate that despite its incoherent nature, this process preserves the signatures of coherent interaction between a QD and a strong driving laser, which may be observed via the optical emission from the off-resonant cavity. Under bichromatic driving of the QD, the cavity emission exhibits spectral features consistent with optical dressing of the QD transition, namely Rabi side-bands. These cavity emission measurements are more akin to absorption measurements of a strongly driven QD rather than resonance fluorescence measurements. In addition to revealing new aspects of the off-resonant QD-cavity interaction, this result provides a new, simpler means of coherently probing QDs and opens the possibility of employing off-resonant cavities to optically interface QD-nodes in quantum networks.

10:12AM P30.00012 Rabi-Vibronic resonance at large number of vibrational quanta¹, MIKHAIL RAIKH, RACHEL GLENN, University of Utah — Rabi oscillations of a resonantly driven two-level system (qubit) which is linearly coupled to a cavity (vibrational mode) with frequency, ω_0 , much smaller than the driving frequency, are studied theoretically. We show that, for small coupling constant $\lambda \ll 1$, Rabi oscillations are strongly modified in the vicinity of the *Rabi-vibronic resonance* $\Omega_R = \omega_0$, where Ω_R is the Rabi frequency proportional to the amplitude of the driving field. The width of the resonance is shown to be $(\Omega_R - \omega_0) \sim \lambda^{4/3} \omega_0$, and is much larger than the polaronic frequency shift, $\lambda^2 \omega_0$. We show that within the resonant domain of Ω_R the actual frequency of the Rabi oscillations exhibits bistable behavior as a function of Ω_R . Most importantly, within the resonant domain, the oscillator is highly excited, which allows one to treat it classically. Decay of the Rabi oscillations due to losses in the cavity and spontaneous emission of two-level system are also studied.

¹Supported by NSF DMR-0808842 and MRSEC DMR-1121252.

10:24AM P30.00013 Photon heralded entanglement between radiatively mismatched matter qubits, ZHEXUAN GONG, LUMING DUAN, Department of Physics and MCTP, University of Michigan — Photon heralded entanglement usually requires well matched radiative characteristics of two matter-based qubits. In practice, we may want to entangle two solid-state or atomic qubits with different radiative lifetime, or to entangle a solid-state qubit with an atomic qubit that has significant mismatch in lifetime and transition frequency. We propose a protocol that can effectively shape the emitted photon pulses of two matter qubits to a common analytically known function by simply tuning the classical laser fields applied to each qubit. Entanglement fidelity and success rates are found to be promising under current experimental conditions.

10:36AM P30.00014 Fast optically-controlled two-qubit operation for cavity-coupled semiconductor quantum dots, DMITRY SOLENOV, SOPHIA E. ECONOMOU, THOMAS L. REINECKE, Naval Research Laboratory — Electron spin qubit systems based on charged InAs/GaAs quantum dots have demonstrated long coherence times and the capability of ultra fast single- and two-qubit operations in a configuration when two dots are tunnel-coupled. Designing fast two- and multi-qubit gates for spatially-separated quantum dots is currently an important challenge. We propose fast optically controlled design where a two-qubit gate is mediated by a photonic crystal cavity mode. The design addresses the challenge of scalability and does not require quantum dots to have the same energies. The proposed gate scheme is also compatible with available optically induced single qubit rotations.

10:48AM P30.00015 H1 Photonic Crystal Microcavities for Quantum Information, JENNA HAGE-MEIER, Physics Department, University of California Santa Barbara, USA, CRISTIAN BONATO, Huygens Laboratory, Leiden University, The Netherlands, TUAN-ANH TRUONG, Materials Department, University of California Santa Barbara, USA, HYOCHUL KIM¹, Physics Department, University of California Santa Barbara, USA, PIERRE PETROFF, Materials Department, University of California Santa Barbara, USA, DIRK BOUWMEESTER, Physics Department, University of California Santa Barbara, USA and Huygens Laboratory, Leiden University, The Netherlands — Semiconductor quantum dots coupled to photonic crystal microcavities show promise for quantum information processing in solid-state systems. For many applications, the cavity mode needs to have high extraction efficiency and unpolarized emission. Here we describe a possible implementation using the two orthogonally-polarized, spectrally-degenerate dipole modes of the H1 photonic crystal microcavity. By modifying the shape of the far-field profile, high collection efficiency from the H1 cavity modes can be achieved while maintaining a high cavity quality factor. We optimize and experimentally measure the far-field profiles of our cavities, which show good agreement with simulations. We also implement techniques to minimize the energy splitting of the two dipole modes due to fabrication imperfections, which are compatible with the far-field optimization.

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Wednesday, February 29, 2012 8:00AM - 10:36AM – Session P31 DCMP: Topological Insulators: Disorder 260

8:00AM P31.00001 Disordered topological conductor, KUN WOO KIM, California Institute of Technology, ALEXANDRA JUNCK, Freie Universitt Berlin & California Institute of Technology, DORON BERGMAN, California Institute of Technology, TAMI PEREG-BARNEA, McGill University & California Institute of Technology, GIL REFAEL, California Institute of Technology, FELIX VON OPPEN, Freie Universitt Berlin — A topological conductor, like a topological insulator is a system in which the bands are characterized by non-trivial topological invariants such as the Chern numbers. However, unlike a topological insulator, in this system the Fermi energy does not lie in an energy gap but instead intersects at least one of the bulk bands. Although not an insulator the topological conductor supports chiral edge modes. In this work we consider a disordered topological conductor and analyze its properties. In particular we find that moderate disorder reduces the edge conductivity from its quantum value and stronger disorder increases it before the whole system is localized and the conductivity drops to zero. This effect is seen numerically on a lattice system and analytically in a disorder averaged continuum model.

8:12AM P31.00002 Dislocations and their braiding in topological insulators, ANDREJ MESAROS, Department of Physics, Boston College, VLADIMIR JURICIC, JAN ZAAENEN, Instituut-Lorentz, Leiden University — We demonstrate the fundamental importance of crystal lattice dislocations in two-dimensional topological insulators. These defects characterize the topological state through the appearance of electronic localized midgap states. The states turn out to be robust even for the class of materials where they are not protected. At the same time, these localized electronic states have interesting quantum properties. We show that adiabatic braiding of dislocations, which can be achieved using lattice shear induced dislocation glide, brings out the quantum statistics of the electronic bound states.

8:24AM P31.00003 Study of the robustness of two dimensional topological insulators, DANIEL GOSALBEZ-MARTINEZ, Departamento de Fisica Aplicada, Universidad de Alicante, JOAQUIN FERNANDEZ-ROSSIER, International Iberian Nanotechnology Laboratory and Departamento de Fisica Aplicada, Universidad de Alicante, JUAN JOSE PALACIOS, Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid — Two dimensional topological insulators present gapless spin filtered edge states which are topologically protected against backscattering. As long as disorder does not mix the states of opposite edges or with bulk ones, these states contribute to the two terminal conductance as a single quantum channel regardless of the amount of non-magnetic disorder present in the sample. We address this problem studying the effect of different types of disorder: constrictions and Anderson disorder, for two different materials that have been predicted to present the quantum spin Hall insulator phase, graphene and a bilayer of Bi(111). We also study the effect of the zigzag edge reconstruction of graphene over the robust behavior of the edge states. We describe their electronic structure using an orthogonal tight-binding model in the Slater-Koster approximation including the intra-atomic spin-orbit interaction. The conductance is computed using the Landauer formula making use of the ALACANT transport package.

8:36AM P31.00004 Investigating Impurities on 3D Topological Insulators with Multiple Scattering Theory, ROBERT VAN WESEP, University of Tennessee - Knoxville/Oak Ridge National Lab — Recently a new class of materials, three-dimensional topological insulators (3DTI), have generated significant theoretical and experimental interest due to surface states (SS) exhibiting linear dispersion at a Dirac point that are protected by time-reversal symmetry (TRS). Using magnetism to break TRS is of particular interest, especially via the deposition of magnetic impurities (MI) on the 3DTI surface. Experimental studies are in the early stages and consensus on the effect of MI of 3DTI SS has yet to be reached. Multiple scattering theory (MST) has proven useful in investigating surfaces, impurities and disordered systems and provides an ideal framework for first-principles, computational study. This presentation will report on progress in adapting MST to 3DTI systems with impurities.

8:48AM P31.00005 LDOS Multifractal Hunter's Guide to Dirty Topological Insulators, MATTHEW FOSTER, Rutgers, the State University of New Jersey — We compute the multifractal spectra associated to local density of states (LDOS) fluctuations due to weak quenched disorder, for a single Dirac fermion in two spatial dimensions. Our results are relevant to the surfaces of Z_2 topological insulators such as Bi_2Se_3 and Bi_2Te_3 , where LDOS modulations can be directly probed via scanning tunneling microscopy. We find a qualitative difference in spectra obtained for magnetic versus non-magnetic disorder. Randomly polarized magnetic impurities induce quadratic multifractality at first order in the impurity density; by contrast, no operator exhibits multifractal scaling at this order for a non-magnetic impurity profile. For the time-reversal invariant case, we compute the first non-trivial multifractal correction, which appears at two loops (impurity density squared). We discuss spectral enhancement approaching the Dirac point due to renormalization, and we survey known results for the opposite limit of strong disorder.

9:00AM P31.00006 Effects of Strong Disorder in a 3-Dimensional Topological Insulators: Phase Diagram and Mapping of the Z_2 Invariant, BRYAN LEUNG, Rutgers University, EMIL PRODAN, Yeshiva University — We study the effect of strong disorder in a 3-dimensional topological insulators with time-reversal symmetry and broken inversion symmetry. Using level statistics analysis, we demonstrate first the persistence of delocalized bulk states even at large disorder. The delocalized spectrum displays the levitation and pair annihilation effect, indicating that the delocalized states continue to carry the Z_2 invariant after the onset of disorder. The Z_2 invariant is computed via twisted boundary conditions using a novel and efficient numerical algorithm. We demonstrate that the Z_2 invariant remains well defined and quantized even after the spectral gap closes and becomes filled with dense localized states. In fact, our results indicate that the Z_2 remains quantized until the mobility gap closes or until the Fermi level touches the mobility edge. Based on such data, we compute the phase diagram as function of disorder strength and position of the Fermi level.

9:12AM P31.00007 Strong potential impurities on the surface of a three-dimensional topological insulator, ANNICA M. BLACK-SCHAFFER, Uppsala University, ALEXANDER V. BALATSKY, Los Alamos National Laboratory — Topological insulators (TIs) are said to be stable against non-magnetic impurity scattering due to suppressed backscattering in the Dirac surface states. We solve a lattice model of a three-dimensional TI in the presence of strong potential impurities on the surface and find that both the Dirac point and low-energy states are significantly modified: low-energy impurity resonances are formed that produce a peak in the density of states near the Dirac point, which is destroyed and split into two nodes that move off-center. The impurity-induced states penetrate up to 10 layers into the bulk of the TI. These findings demonstrate the importance of bulk states for the stability of TIs and how they can destroy the topological protection of the surface. Extensions to sub-surface and extended defects, as well as direct comparisons to recent experimental results are also made.

9:24AM P31.00008 Disorder induced quantized conductance with fractional value and universal conductance fluctuation in three-dimensional topological insulators, LEI ZHANG, JIANING ZHUANG, Department of Physics, The University of Hong Kong, YANXIA XING, Department of Physics, The University of Hong Kong; Department of Physics, Beijing Institute of Technology, JIAN WANG, Department of Physics, The University of Hong Kong, DEPARTMENT OF PHYSICS, THE UNIVERSITY OF HONG KONG TEAM, DEPARTMENT OF PHYSICS, BEIJING INSTITUTE OF TECHNOLOGY COLLABORATION — We report a theoretical investigation on the conductance and its fluctuation of three-dimensional topological insulators (3D TI) in Bi_2Se_3 and Sb_2Te_3 in the presence of disorders. Extensive numerical simulations are carried out. We find that in the diffusive regime the conductance is quantized with fractional value. Importantly, the conductance fluctuation is also quantized with a universal value. For 3D TI connected by two terminals, three independent conductances G_{zz} , G_{xx} and G_{zx} are identified where z is the normal direction of quintuple layer of 3D TI. The quantized conductance are found to be $\langle G_{zz} \rangle = 1$, $\langle G_{xx} \rangle = 4/3$ and $\langle G_{zx} \rangle = 6/5$ with corresponding quantized conductance fluctuation 0.54, 0.47, and 0.50. The quantization of average conductance and its fluctuation can be understood by theory of mode mixing. The experimental realization that can observe the quantization of average conductance is discussed.

9:36AM P31.00009 Conducting state of GeTe by defect-induced topological insulating order, JINWOONG KIM, Department of Physics, Pohang University of Science and Technology, SEUNG-HOON JHI, Department of Physics and Division of Advanced Materials Science, Pohang University of Science and Technology — Topological insulating order protected by time-reversal symmetry is robust under structural disorder. Interestingly, recent studies on phase change materials like GeSbTe showed that their topological insulating order is sensitive to atomic stacking sequences. It was also shown that their structural phase transition is correlated with topological insulating order. GeTe, a well-known phase change material, is trivial insulator in its equilibrium structure. In this study, we discuss how atomic defects such as Ge tetrahedral defect observed in amorphous GeTe can change its topological insulating order based on first-principles calculations and model Hamiltonian. We also investigated the critical density of such tetrahedral defects to induce topological insulating order in GeTe. Our study will help explore hidden orders in GeTe.

9:48AM P31.00010 Mapping the conductivity tensor of disordered topological insulators in the presence of magnetic fields¹, EMIL PRODAN, YU XUE, Department of Physics, Yeshiva University — Transport measurements on topological insulators revealed extremely interesting effects and generated data that contain extremely valuable information. It is now possible to control the carriers' concentration using finely tuned gate voltages and to do the transport measurements under controlled applied magnetic fields. As such, accurate maps of the conductivity tensor are now available, as function of the Fermi level and the magnetic field strength. To extract useful information, we need a quantitative theory of charge transport for aperiodic systems in presence of magnetic fields. Such theory has been developed in the past using C^* -Algebras and Non-Commutative calculus, the result being closed and exact formulas for the conductivity tensor. In this talk we explain how to manipulate the algebras and how to implement the non-commutative calculus on a computer, in order to compute the conductivity tensor of topological insulating materials in the presence of disorder and magnetic fields. Quantitative simulations of the transport experiments on 2D (and possibly 3D) topological insulators will be presented. Since the methodology can treat disorder and magnetic fields in the same time, it enable us to reproduce, for example, the quantization and the plateaus of the Hall conductance.

¹Research supported by the U.S. NSF grants DMS-1066045 and DMR-1056168

10:00AM P31.00011 Magnetic field induced Quasi Helical Liquid state in a disordered 1D electron system with strong spin-orbit interaction, ANDERS STRÖM, University of Gothenburg, Sweden, BERND BRAUNECKER, Universidad Autónoma de Madrid, Spain, G.I. JAPARIDZE, Andronikashvili Institute of Physics, Georgia and Ilia State University, Georgia — We study the crossover from a Luttinger liquid to a quasi-helical liquid state in a one-dimensional system of interacting electrons with strong spin-orbit interaction in the presence of a transverse magnetic field, which leads to a gap for one-half of the conducting modes. In particular, we study the effect of gap opening by electron localization in the presence of non-magnetic disorder. We show that the localization length has a nonuniform behavior as a function of the magnetic field. With increasing field, the localization length grows from its zero-field Luttinger-liquid value to a maximum, after which it crosses over to again smaller values corresponding to the localization length of spinless fermions.

10:12AM P31.00012 Delocalized States and Topological Edge States of Quantum Walks in Random Environment, HIDEAKI OBUSE, Karlsruhe Institute of Technology, Germany, NORIO KAWAKAMI, Kyoto University, Japan — The quantum walk (QWs) describe quantum mechanical time evolution of particles, which is identified as random walks when systems are brought to classical limit. QWs can be applied for efficient algorithms of quantum computation and have been realized in experiments. Remarkably, QWs realized by many experiments possess chiral symmetry. Thereby, QWs in a one dimensional (1D) space possibly have non-trivial topological phases and show edge states near boundaries of the system. In this work, we consider QWs interacting with spatial and temporal disorders and study how the edge states of QWs are influenced. Even by introducing the weak spatial disorder to the QWs, the edge states are robust. However, in the strong disorder limit, the energy gap vanishes and the edge states disappear. We found that critical states due to the Anderson transition in the 1D chiral class alternatively appear at energy $\omega = 0$ in this case. Significantly, these critical states also appear at $\omega = \pm\pi/2$ for any strength of static disorder, since the extra sublattice symmetry of the time-evolution operator U makes $\omega = \pm\pi/2$ singular. Consequently, for the QWs with relatively weak spatial disorder, the edge states, critical states, and Anderson localized states are coexist.

10:24AM P31.00013 The strong side of weak topological insulators, YAACOV KRAUS, ZOHAR RINGEL, ADY STERN, Weizmann Institute of Science — Three-dimensional topological insulators are classified into "strong" (STI) and "weak" (WTI) according to the nature of their surface states. While the surface states of the STI are topologically protected, in the WTI they are believed to be very fragile to disorder. In this work we show that the WTI surface states are actually protected from any random perturbation which does not break time-reversal symmetry, and does not close the bulk energy gap. Consequently, the conductivity of metallic surfaces in the clean system will remain finite even in the presence of strong disorder of this type. In the weak disorder limit the surfaces are perfect metals, and strong surface disorder only acts to push them inwards. We find that WTI's differ from STI's primarily in their anisotropy, and that the anisotropy is not a sign of their weakness but rather of their richness.

Wednesday, February 29, 2012 8:00AM - 11:00AM –
Session P32 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides - BiFeO₃ 261

8:00AM P32.00001 Inelastic neutron scattering study of spin-wave from single crystal BiFeO₃

, GUANGYONG XU, ZHIJUN XU, Brookhaven National Laboratory, JINSHENG WEN, UC Berkeley, MATTHEW STONE, Oak Ridge National Laboratory, GENDA GU, STEPHEN SHAPIRO, Brookhaven National Laboratory, R.J. BIRGENEAU, UC Berkeley, CHRIS STOCK, PETER GEHRING, NIST Center for Neutron Research — BiFeO₃ is one of the most promising multiferroic materials for device applications in spintronics and memory devices. There have been a number of studies on electric field tuning of antiferromagnetic domains, as well as possible E-field control of spin-waves in this material. The potential of controlling spin dynamics using electric field is extremely appealing. However, so far there have been very limited work on the direct measurements of spin-waves in BiFeO₃, mostly due to lack of large size single crystals. We will present our recent inelastic neutron scattering studies on a single crystal BiFeO₃, showing the full spin-wave spectrum in three-dimensions. A classical spin-wave model can be used to describe the results in details. The coupling parameters and spin-wave velocities have been obtained, and are in good agreements with those obtained in Raman measurements.

8:12AM P32.00002 Local Raman spectroscopic study of BiFeO₃ strained states

, YEN-CHIN HUANG, YI-CHUN CHEN, FENG-NAN CHU, Department of Physics, National Cheng Kung University, WEN-I LIANG, HSIANG-JUNG CHEN, YING-HAO CHU, Department of Materials Science and Engineering, National Chiao Tung University — Among single-phase multiferroic materials, BiFeO₃ (BFO) has relatively high Curie and Néel temperatures, which possesses ferroelectric and antiferromagnetic couplings at room temperature, so is motivated for novel device applications. Recent studies had shown piezoelectric and magnetic properties of BFO in strained states varied significantly. For BFO epitaxial films grown on LaAlO₃ substrate, high piezoelectric coefficient and spontaneous ferromagnetic moments had been demonstrated in a new kind of morphotropic tetragonal-rhombohedral phase boundary driven by substrate strain. In this study, we used Raman spectrum to investigate the local BFO distorted structure under substrate strain or strain caused by external electric fields. The crystal structure of BFO under compressive substrate strain is monoclinically distorted. The ordering of the monoclinic structures could also be controlled by electric field. These two kinds of strained states were locally studied by atomic force microscopy (AFM) equipped with on-axis Raman measurement. This study provided the basic physical insight of unique physical properties depended on distorted structures.

8:24AM P32.00003 Unambiguous phonon mode assignment in multiferroic BiFeO₃ single crystals

, CHRISTIANNE BEEKMAN, University of Toronto, SANG-WOOK CHEONG, Rutgers University, KENNETH BURCH, University of Toronto — In Bismuth ferrite (BiFeO₃) antiferromagnetic and ferroelectric order parameters coexist at room temperature, making this material an excellent candidate for new functionalities, such as electrical control of magnetism. Despite extensive reports on Raman scattering experiments on single crystals and thin films, controversy still remains in the observation and assignment of the phonon mode symmetries. We present polarized micro-Raman spectroscopy of single crystals ((1 0 0)_{cubic} surface) with uniform ferroelectric polarization. Careful examination of the Raman spectra upon crystal rotation enables us to unambiguously assign the (A_1 , E_x and E_y) modes. We will show that ambiguity is easily introduced by slight misalignment of the crystal and that the crystal rotation is necessary to reach unambiguous mode assignment. Our method not only results in proper Raman mode assignment, which is necessary to describe the phonons critical for the multiferroic behavior, it also allows study of symmetry breaking and may provide a way to non-invasively check the ferroelectric polarization direction.

8:36AM P32.00004 Multiple Phase Transitions in the model multiferroic BiFeO₃

, JENS KREISEL, CNRS - Grenoble Institute of Technology — Bismuth ferrite BiFeO₃ (BFO) is commonly considered a model system for multiferroics, and is perhaps the only material that is both magnetic and a ferroelectric with a strong electric polarization at 300K [1]. Despite numerous investigations, the crystal structures of BFO as a function of temperature and pressure are still not established and lead to ongoing controversial reports in the literature [1,3]. Besides being a model multiferroic, BFO is also one of the very few materials that present both octahedra tilts and strong cation displacements at room temperature. Here we report the high-pressure phase transitions in BFO by both synchrotron x-ray diffraction and Raman spectroscopy, namely a surprising richness of six phase transitions in the 0–60 GPa range [2-3]. At low pressures, 4 transitions are evidenced at 4, 6, 7 and 11 GPa. In this range, the crystals display in that range unusual large unit cells and complex domain structures, which suggests a competition between complex tilt systems and possibly off-center cation displacements. The non polar Pnma phase remains stable over a large pressure range between 11 and 38 GPa. The two high pressure phase transitions at 38 and 48 GPa are marked by the occurrence of larger unit cells and an increase of the distortion away from the cubic parent perovskite cell. The previously reported insulator-to-metal transition appears to be symmetry breaking. Finally, we will present a new schematic P-T phase diagram for BFO and discuss the recently reported phase transition in highly strained BFO films [4,5] in the light of our high-pressure findings.

[1] G. Catalan, J. F. Scott, Advanced Materials 21, 1 (2009).

[2] R. Haumont et al., Phys. Rev. B 79, 184110 (2009).

[3] M. Guennou et al., Phys. Rev. B 2011, accepted <http://arxiv.org/abs/1108.0704>.2011

[4] J. Kreisel et al. J. Phys.: Cond. Matt. 23, 342202 (2011).

[5] W. Siemons et al. Appl. Phys. Express 4 (2011).

9:12AM P32.00005 Phase Transitions in Epitaxial (-110) BiFeO₃ Films from First Principles*¹

, SERGEY PROSANDEEV, University of Arkansas, IGOR KORNEV, Ecole Centrale Paris, LAURENT BELLAICHE, University of Arkansas — The effect of misfit strain on properties of epitaxial BiFeO₃ films that are grown along the pseudo-cubic $\bar{1}10$ direction, rather than along the “usual” [001] direction, is predicted from density functional theory. These films adopt the monoclinic Cc space group for compressive misfit strains smaller in magnitude than $\approx 1.6\%$ and for any investigated tensile strain. In this Cc phase, both polarization and the axis about which antiphase oxygen octahedra tilt rotate *within* the epitaxial plane as the strain varies. Surprisingly and unlike in (001) films, for compressive strain larger in magnitude than $\approx 1.6\%$, the polarization vanishes and two orthorhombic phases of $Pnma$ and $P2_12_12_1$ symmetry successively emerge via strain-induced transitions. The $Pnma$ -to- $P2_12_12_1$ transition is a rare example of a so-called pure “gyrotropic” phase transition, and the $P2_12_12_1$ phase exhibits original interpenetrated arrays of ferroelectric vortices and antivortices. This work is mostly supported by ONR Grants N00014-08-1-0915 and N00014-07-1-0825 (DURIP). *S. Prosandeev, Igor A. Kornev, and L. Bellaiche, Phys. Rev. Lett. 107, 117602 (2011).

¹DOE, contract ER-46612, and NSF DMR-0701558 and DMR-0080054 (C-SPIN). Computations were possible thanks to the MRI NSF grant 0722625 and Challenge grant from HPCMO of DOD.

9:24AM P32.00006 Nonlinearity in the high-electric-field piezoelectric response of epitaxial BiFeO₃¹, PICE CHEN, REBECCA SICHEL², JIYOUNG JO³, RYAN SMITH, CHANG-BEOM EOM, University of Wisconsin-Madison, OSAMI SAKATA, SPRING-8, ERIC DUFRESNE, Argonne National Laboratory, PAUL EVANS, University of Wisconsin-Madison — The multiferroic material BiFeO₃ provides the means to understand the piezoelectric coupling between lattice strain and ferroelectric polarization. Little is known about the piezoelectric properties of BiFeO₃ under high electric fields. In our study, the transient high-electric-field piezoelectricity of BiFeO₃ was measured at electric fields up to about 300 MV/m using time-resolved x-ray microdiffraction. A linear strain-electric field response with a piezoelectric coefficient of 55 pm/V was observed at electric fields up to 150 MV/m. At higher electric fields, the strain is larger than the value anticipated from the low-field regime, reaching 0.02 at 281 MV/cm. The integrated intensity near the BiFeO₃ (002) Bragg reflection is unchanged in large electric fields, showing that the enhanced piezoelectricity occurs without producing a field-induced phase transition. We also observe a relative increase of diffuse x-ray intensity at high electric fields. We will discuss a model in which the increase of piezoelectricity and diffuse scattering originates from the softening of phonon modes at high electric fields.

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9:36AM P32.00007 Ultrafast photostriction in BiFeO₃ thin films, L.Y. CHEN, C.W. LUO, Department of Electrophysics, National Chiao Tung University, Hsinchu 300, Taiwan, Y.H. CHU, Department of Materials Science and Engineering, National Chiao Tung University, Hsinchu 300, Taiwan, T. KOBAYASHI, Department of Electrophysics, National Chiao Tung University, Hsinchu 300, Taiwan — The ultrafast dynamics of BiFeO₃ (BFO) thin films was studied by dual-color transient reflectivity measurements ($\Delta R/R$) from 80 K to room temperature. Based on the thickness-dependent propagating time of the photoinduced strain pulse, the sound velocity along [110] direction of BFO is 4.76 km/s. Anisotropic photostriction effect in BFO generated within short time scale of 5 ps is enhanced by the optical rectification effect. Furthermore, the anomalous changes of the temperature-dependent $\Delta R/R$ at 130 K and 210 K may reveal the spin-orbital coupling and magnetoelastic effect in BFO.

9:48AM P32.00008 Photoinduced structural dynamics in BiFeO₃ thin films studied by ultrafast x-ray diffraction¹, D.A. WALKO, E.M. DUFRESNE, J.H. LEE, J.W. FREELAND, Y. LI, H. WEN, Advanced Photon Source, Argonne National Laboratory, P. CHEN, P.G. EVANS, University of Wisconsin-Madison, C. ADAMO, D.G. SCHLOM, Cornell University, J. IHLEFELD, Sandia National Laboratories — We have used time-resolved x-ray diffraction to study the temporal response of multiferroic BiFeO₃ to laser excitation. Above-bandgap light pulses, with 400 nm central wavelength and 50 fs duration, were used to photoexcite 35-nm thick BiFeO₃ films grown by molecular beam epitaxy on SrTiO₃ (001) substrates. The angular shifts of BiFeO₃ Bragg peaks vs. time were recorded with ~100 ps resolution and used to determine the out-of-plane strain in the film. Observed strains range up to several tenths of a percent after excitation and relax on a several-ns timescale. Strains of such magnitude are too large to be explained by thermal expansion alone, but rather appear to be due to screening of the depolarization field by photoexcited carriers. At higher laser fluences, the integrated intensity of the Bragg peak decreases due to transient rearrangement of the atomic lattice on the scale of ~0.1 Å.

¹Supported by US Department Of Energy under contract No. DE-AC02-06CH11357.

10:00AM P32.00009 The valence electronic structure of multiferroic BiFeO₃ from high energy X-ray photo-electron spectroscopy and first principles theory, R. KNUT, Department of Physics and astronomy, Uppsala University, Uppsala, Sweden, S. FALIEV, DIPANJAN MAZUMDAR, O. MRYASOV, ARUNAVA GUPTA, Center for Materials for Information Technology, University of Alabama, O. KARIS, Department of Physics and astronomy, Uppsala University, Uppsala, Sweden, U ALABAMA TEAM, UPPSALA TEAM — BiFeO₃ (BFO) is a multi-functional material with high ferroelectric and magnetic ordering temperature. Here we have investigated the electronic structure of (001) oriented 100nm rhombohedral BFO thin films using high energy X-ray photoelectron spectroscopy (XPS). By making use of the energy dependence of the relative cross sections for different states, we were able to selectively probe the elemental contributions to the valence band. At high energies, states with high main quantum number will have a higher relative probability for photo-ionization, i.e., the Bi 6s and 6p contributions in the valence region are enhanced relative to the Fe 3d and O 2p. We find that the Bi 6p states hybridize strongly with the valence band dominated by the Fe 3d and O 2p states, resulting in a splitting of the 3d states due to bonding and anti-bonding combinations with the Bi 6p. Our results thus suggest that a previously relatively ignored electronic interaction needs to be considered for BFO and related Bi-TMOs. Ab initio calculations indicate the importance of screened Coulomb correlations to describe Bi and Fe electronic states.

10:12AM P32.00010 Direct characterization of the surface layer of BiFeO₃ Single Crystals, NEUS DOMINGO, JACKELINE NARVAEZ, Centre d'Investigació en Nanociència i Nanotecnologia CIN2, CSIC-ICN, Campus Bellaterra, 08193 Barcelona, Spain, XAVI MARTÍ, Charles University in Prague, Faculty of Mathematics and Physics, Czech Republic, MARIN ALEXE, Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany, GUSTAU CATALAN, Centre d'Investigació en Nanociència i Nanotecnologia CIN2, CSIC-ICN, Campus Bellaterra, 08193 Barcelona, Spain — A surface layer different from the bulk was found in single crystals of BiFeO₃, and was analyzed with different techniques such as surface impedance and grazing incidence x-ray diffraction, showing an specific phase transition at T* ~ 275 °C. Local physical characterization studies have been performed with different AFM techniques, such as Piezoelectric Force Microscopy (PFM), Scanning Kelvin Probe Microscopy (SKPM) and Force Modulated Microscopy (FMM) at different temperatures up to 300°C. The thin superficial skin layer is found to be an electrically "dead" layer with a thickness of 6 +/- 1 nm and different thermal expansion coefficient with respect to the bulk. The sharp thermal expansion of the surface layer at T* facilitates its mechanical decoupling from the underlying crystal at the transition temperature, enabling direct access to the sub-surface region using scanning probe microscopy techniques. A distribution of near-surface ferroelectric domains is found in a region of less than 200 nanometers depth under the surface. These nanodomains organize in a hierarchical metastructure on top of the existing bulk domains. The symmetry and properties of these sub-surface nanodomains will be discussed.

10:24AM P32.00011 First-principles investigation of phase-change effects in multiferroics¹, OSWALDO DIÉGUEZ, OTTO E. GONZÁLEZ-VÁZQUEZ, JACEK C. WOJDEŁ, JORGE ÍÑIGUEZ, ICMAB-CSIC, Campus de la UAB, 08193 Bellaterra — Using first-principles calculations we have characterized new phases of bulk multiferroic materials that are close in energy to the ground state, but that display very different properties. This suggests that the application of electric fields could induce phase changes that would involve large effects of different kinds. In particular, (i) we have found stable supertetragonal bulk phases for the prototype multiferroic bismuth ferrite [Diéguez *et al*, Phys. Rev. B **83**, 094105 (2011)], and (ii) we propose to use a solid solution of bismuth ferrite and bismuth cobaltite to create a material where it is possible to switch between two very different phases in a way that involves strong piezoelectric, electric, and magnetoelectric effects [Diéguez and Íñiguez, Phys. Rev. Lett. **107**, 057601 (2011)].

¹Supported by MICINN-Spain [Grants No. MAT2010-18113, No. MAT2010-10093-E, and No. CSD2007-00041; Ramón y Cajal program (OD)].

10:36AM P32.00012 Magnetic and structural properties of BiFeO₃ thin films grown epitaxially on SrTiO₃/Si substrates¹, DANIEL CURRIE, RYAN LAUGHLIN, GOKUL RADHAKRISHNAN, WEERASINGHE PRIYANTHA, ROCIO CONTRERAS-GUERERRO, RAVINDRANATH DROOPAD, NIKOLETA THEODOROPOULOU, Texas State University, San Marcos — Commensurate growth of SrTiO₃ (STO) on Si using molecular beam epitaxy (MBE) has been achieved. STO on Si is used as a virtual substrate to enable the growth of BiFeO₃ (BFO). Having a crystalline oxide surface on Si is an enabler for deposition of various functional oxides that would not have been possible directly on silicon. A systematic study of the dependence of the magnetic and structural properties of BFO on the growth conditions, such as O₂ plasma pressure and film thickness, is performed. The crystalline nature of the BFO film has been confirmed by X-Ray diffraction showing the expected peak positions for (100) oriented oxide films with no additional, unidentified peaks. The BFO/STO/Si films exhibit antiferromagnetic behavior with high transition temperatures, thus leading to the possibility of room temperature magnetoelectric coupling-based devices integrated onto Si CMOS circuitry. Thinner films at lower O₂ plasma pressures exhibit stronger magnetic characteristics.

¹This work was supported by AFOSR under grant FA 9550-10-0133.

10:48AM P32.00013 Magnetoelectric and Ferroelectric Properties of BiFeO₃/Ni film Deposited by Pulsed Laser Deposition, LI YAN, MUJIN ZHUO, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, ZHIGUANG WANG, JIANJUN YAO, JIEFANG LI, DWIGHT VIEHLAND, Dept. of Materials Science and Engineering, Virginia Tech, QUANXI JIA, Center for Integrated Nanotechnologies, Los Alamos National Laboratory — To fabricate a layer by layer (2-2) magnetoelectric (ME) sensor, ferroelectric (FE) BiFeO₃ film was directly deposited on ferromagnetic (FM) nickel foil by pulsed laser deposition (PLD) without oxide or noble metal buffer layer, which significantly lowers the cost of ME and FE devices, and makes it possible to deposit longer ME and FE bendable band by PLD. X-ray diffraction and transmission electron microscopy analysis confirmed that the BiFeO₃ film was successfully deposited on the top of nickel foil. The BiFeO₃ film had a saturation polarization and a piezoelectric d33 coefficient of 69 $\mu\text{C}/\text{cm}^2$ and 52 pm/V respectively. The ME coefficient of the sample was 4mV/cmOe which was measured under 1 Oe AC magnetic field at 1 kHz frequency.

Wednesday, February 29, 2012 8:00AM - 10:48AM – Session P33 GERA: Physics of Photovoltaics and other Electricity Production 106

8:00AM P33.00001 Light Reflection and Absorption by Free Standing Titania Nanotube Arrays¹, ABDELMOULA MOHAMED, JEFFREY SOKOLOFF, MENON LATIKA, Northeastern University, Boston, MA 02115 — Newly discovered titania nanotube arrays fabricated by anodization have become the main interest of many research groups around the world, mainly due to their potential use for solar energy harvesting. Light conversion to electron-hole pairs can occur in the surface area of these nanotubes, resulting from their very high aspect ratio and the low recombination probability in the titania surface. In our work we have investigated the transmission of light through the nanotubes for different tube lengths, to explore the penetration depth for various wavelengths in the nanotube array. Specifically, we have investigated the reflection and transmission of light incident from both the open and closed sides of the nanotubes. We find that the reflectivity is generally noticeably smaller for light incident on the open end, but the transmission is about the same, implying greater absorption for light incident on the open side, although for wavelengths close to 400nm, the reflectivity from the open side becomes larger than that from the closed side. We will present a theoretical model to explain our experimental results. The model treats wave propagation along the tubes in the eikonal approximation, and wave propagation transverse to the tubes as Bloch waves.

¹NSF ECCS Grant # 0925285 is acknowledged.

8:12AM P33.00002 A quantum-mechanical study of ZnO and TiO₂ based DSC, FRANCESCA RISPLENDI, GIANCARLO CICERO, Material Science and Chemical Engineering Department, Politecnico of Torino, C.so Duca degli Abruzzi 24, 10129, Torino, Italy, GIUSEPPE MALLIA, Thomas Young Centre, Department of Chemistry, Imperial College London SW7 2AZ, UK, LEONARDO BERNASCONI, Rutherford Appleton Laboratory, Oxfordshire OX11 0QX, UK, NICHOLAS HARRISON, Thomas Young Centre, Department of Chemistry, Imperial College London SW7 2AZ, UK; Daresbury Laboratory, Cheshire, WA4 4AD, UK — Since the pioneering work of Graetzel, Dye Sensitized Cells (DSCs) have attracted great attention as cheap and effective solar power devices based on wide bandgap metal oxide electrode. Optimization of the DSC is a challenging task as it is a highly complex interacting molecular system. Surface properties of the metal-oxide and proper sensitization with dyes may strongly affect the efficiency. Optimized DSCs based on TiO₂ photoanodes and organic dye have reached conversion efficiency of about 10% whereas the efficiency of ZnO based DSC has been found to be much lower, although this material has photochemical properties similar to TiO₂, in general due to the nature of the binding between sensitizer and semiconductor. For this reason understanding how anchoring groups interact with the metal-oxide is fundamental to shed light on the different behaviour of these materials in DSC. Aim of this work is to address the binding of small organic sensitizers, such as catechol and isonicotinic acid molecules, to TiO₂ and ZnO surfaces, in terms of geometry, stability, electronic structure and absorption properties. To this end, we employed quantum-mechanical simulations based on hybrid DFT and hybrid TDDFT.

8:24AM P33.00003 Band gap engineering and optical properties of tungsten trioxide¹, YUAN PING, Department of Chemistry, University of California, Davis, YAN LI, Computational Science Center, Brookhaven National Laboratory, DARIO ROCCA, Department of Chemistry, University of California, Davis, FRANCOIS GYGI, Department of Applied Science and Department of Computer Science, University of California, Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis — Tungsten trioxide (WO₃) is a good photoanode material for water oxidation but it is not an efficient absorber of sunlight because of its large band gap (2.6 eV). Recently, stable clathrates of WO₃ with interstitial N₂ molecules were synthesized [1], which are isostructural to monoclinic WO₃ but have a substantially smaller band gap, 1.8 eV. We have studied the structural, electronic, an vibrational properties of N₂-WO₃ clathrates using ab-initio calculations and analyzed the physical origin of their gap reduction. We also studied the effect of atomic dopants, in particular rare gases. Substantial band gap reduction has been observed, especially in the case of doping with Xe, due to both electronic and structural effects. Absorption spectra have been computed by solving the Bethe-Salpeter Equation [2] to gain a thorough insight into the optical properties of pure and doped tungsten trioxide. [1] Q. Mi, Y. Ping, Y. Li., B.S. Brunschwig, G. Galli, H B. Gray, N S. Lewis (preprint) [2]D. Rocca, D. Lu and G. Galli, J. Chem. Phys. 133, 164109 (2010)

¹NSF-Chem CALTECH 68D-1086057 and DOE-BES DE-FG02- 06ER46262

8:36AM P33.00004 Aluminum nanoparticles for plasmonic enhancement of light absorption in organic semiconductors¹, HANS ROBINSON, Virginia Tech, LAUREN NEELY, MicroXact, Inc., CHIH-YU JAO, Virginia Tech, VLADIMIR KOCHERGIN, MicroXact, Inc. — The energy conversion efficiency in organic photovoltaic (OPV) devices is low, primarily due to the short exciton diffusion length (10 nm) in organic semiconductors. Much effort is currently devoted to improving the optical absorptivities in OPVs by incorporating plasmonic nanostructures in or near the active layer, which would allow for significantly thinner absorption layers. We suggest that aluminum nanoparticles are a better choice than gold or silver particles for embedded plasmonic structures in OPV active layers. This is due to the high plasmon frequency of Al, which makes it easy to create good overlap between plasmon resonance and semiconductor absorption band in a random mixture of polymer and nanoparticles. We will present both modeling and experimental data to support this hypothesis.

¹Funding: AFOSR contract No. FA9550-10-C-0059

8:48AM P33.00005 Si-SiGe hetero-structure thin-film solar cells using integrated electro-optical modeling, MUHAMMAD KHIZAR, DONGMING MEI, Department of Physics, University of South Dakota, Vermillion, SD 57069 — Heterostructure Si-SiGe thin film solar cells have been designed and optimized using advanced electro-optical theoretical modeling and simulation. Some of the key characteristics such as short-circuit current density (J_{sc}), open circuit voltage (V_{oc}), and fill factor (FF) have been studied for varying concentration of Ge in SiGe buffer layer. The effect of thickness variation of alloyed layer for varying Ge composition ~ 0.1 –10% has been performed. The improvement in the conversion efficiency of these cells was calculated by tailoring the thickness of p+ doped layer. An approach relying on phenomena of improved absorption of the alloys which leads to a gain in the current was explored. Improved infrared response with higher short circuit current has been obtained for about 25 μm thick structures. With the optimized Ge concentration, and the incorporated structure design parameters, as much as 4–6% enhancement in the overall efficiency of the solar cells has been calculated compared to that of the conventional single crystal Si solar cells. Moreover, the efficiency of these cells can further be improved because Si-SiGe based solar cells have improved absorption characteristics and offer minimum operating temperature sensitivity. It is believed that with better understanding of the band-gap engineering of SiGe when used as buffer and junction layers, the overall conversion efficiency of such devices can further be improved and could play a critical role to develop low cost and high efficiency solar cells technology. This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota.

9:00AM P33.00006 Multiscale Simulation on a Light-Harvesting Molecular Triad¹, GUOXIONG SU, ARKADIUSZ CZADER, University of Houston, DIRAR HOMOUI, Khalifa University, Abu Dhabi, UAE, GABRIELA BERNARDES, SANA MATEEN, MARGARET CHEUNG, University of Houston — We have investigated the effect of solvation and confinement on an artificial photosynthetic material, carotenoid-porphyrin- C_{60} molecular triad, by a multiscale approach and an enhanced sampling technique (Replica Exchange Method). We have developed a combined approach of quantum chemistry, statistical physics, and all-atomistic molecular dynamics simulation to determine the partial atomic charges of the ground-state triad. The confinement effects on the triad were modeled by imposing three sizes of spherocylindrical nanocapsules. The triad is structurally flexible under ambient conditions and its conformation distribution is manipulated by the choice of water models and confinement. Two types of water models (SPC/E and TIP3P) are used for solvation. We have shown that a slight structural difference in the two water models with the same dipole moment can have great distinction in water density, water orientation and the number of hydrogen bonds in the proximity of a large flexible compound such as the triad. Subsequently, it has direct impact on the position of the triad in a confinement as well as the distribution of conformations at the interface of liquid and solid in a finite-size system.

¹Department of Energy (DOE) Basic Energy Sciences grant DE-FG02-10ER16175

9:12AM P33.00007 The Potential for Hot Carrier Collection from an Amorphous Semiconductor¹, REUBEN COLLINS, Colorado School of Mines, KRISTIN KIRILUK, Abengoa Solar, JEREMY FIELDS, BRIAN SIMONDS, LEVI MILLER, YU-PAN PAI, Colorado School of Mines, TING SU, BAOJIE YAN, JEFFREY YANG, SUBHENDU GUHA, United Solar Ovonic, LLC, ARUN MADAN, MVS Systems, Inc., CRAIG TAYLOR, Colorado School of Mines — The quest for clean, inexpensive sources of energy has produced intense interest in low-cost methods for dramatically increasing the efficiencies of solar cells. One such method is to collect carriers before they lose energy to heat. Here we present strong evidence for such hot carrier transfer in an unlikely place, between the amorphous and crystalline regions of nanocrystalline Si. Nanocrystalline Si is a thin film photovoltaic material formed of Si nanocrystallites imbedded in a hydrogenated amorphous Si matrix. Using a combination of photoluminescence quenching and electron spin resonance measurements as a function of nanocrystalline fraction, we observe clear evidence that above a critical fraction carriers excited in the amorphous region transfer to the nanocrystals rather than relaxing to band tail states of the amorphous silicon matrix. The average nanocrystallite spacing is consistent with estimates of the distance hot carriers can transfer in amorphous silicon before thermalization. This result has implications that extend from improving the stability of amorphous silicon under optical illumination to the development of a new paradigm in solar cell design using nanostructured amorphous absorbers.

¹This material is based upon work supported by the NSF through the Renewable Energy Materials Research Science and Engineering Center

9:24AM P33.00008 Enhanced photocatalytic H_2 production by sub-nanometer Au nanoparticles, SHEN ZHAO, Department of Materials Science and Engineering, Stony Brook University, YAN LI, Computational Science Center, Brookhaven National Laboratory, PEICHUAN SHEN, Department of Materials Science and Engineering, Stony Brook University, DONG SU, Center for Functional Nanomaterials, Brookhaven National Laboratory, ALEXANDER ORLOV, Department of Materials Science and Engineering, Stony Brook University — CdS surfaces were found to exhibit a dramatically enhanced photo-catalytic activity for the water splitting process when loaded with sub-nanometer Au particles, compared to that of bare CdS or CdS modified with other noble metal particles (Pt, Ru, Rh, Pd) with similar co-catalyst loading. As a first step towards understanding the striking photocatalytic activity of Au/CdS, we conducted a detailed characterization of the Au particle samples by combining mass spectroscopy, (scanning) transmission electron microscopy, UV-vis spectroscopy and first-principle calculations. In particular, we carried out systematic studies of the influence of particle size, surface termination and charge state on the structural, electronic and spectroscopic properties of ligand-protected Au nanoparticles using density functional theory and time-dependent density functional theory. The structural and electronic stability of diphosphine-protected Au_9 and Au_{11} cations with composition determined from mass spectroscopy, were confirmed from total energy and electronic structure calculations, while the computed optical absorption spectra were found to be in excellent agreement with UV-vis data. Work is underway to study the interaction between Au particles and Cds.

9:36AM P33.00009 First-principles study of III-V electrode interfaces for photoelectrochemical hydrogen production¹, BRANDON WOOD, TADASHI OGITSU, WOON CHOI, ERIC SCHWEGLER, LLNL — Photoelectrochemical (PEC) cells promise clean, sustainable production of hydrogen fuel using water and sunlight. However, combining solar conversion efficiency with durability in electrolyte solution has proven difficult, in part because the complex chemistry active at the electrode-electrolyte interface remains poorly understood. We use first-principles molecular dynamics simulations and model density-functional calculations to study the structure, stability, and chemical activity of GaP/InP semiconductor electrodes in contact with water. We find that a local bond-topological model is able to capture much of the basic surface chemistry. Interpretation of our results points to the particular importance of surface-adsorbed oxygen in determining the available reaction pathways for photocorrosion and water dissociation. Electronic signatures of the local bond topologies are compared to data from X-ray absorption and emission spectroscopy for insight into actual electrode structure.

¹Prepared by LLNL under Contract DE-AC52-07NA27344.

9:48AM P33.00010 ABSTRACT WITHDRAWN —

10:00AM P33.00011 Photoresistance of $\text{Li}_{0.2}\text{Zn}_{0.8}\text{O}$ thin films and $\text{Li}_{0.2}\text{Zn}_{0.8}\text{O}/\text{Al}_{0.15}\text{Zn}_{0.85}\text{O}$ multilayers, TIANJING LI, RENZHONG DU, Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA, GONGPING LI, School of Nuclear Science and Technology, Lanzhou University, Lanzhou 730000, China, QI LI, Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA — Thin films of $\text{Li}_{0.2}\text{Zn}_{0.8}\text{O}$ and $\text{Li}_{0.2}\text{Zn}_{0.8}\text{O}/\text{Al}_{0.15}\text{Zn}_{0.85}\text{O}$ multilayers have been grown on sapphire substrates by pulsed-laser deposition. P-type $\text{Li}_{0.2}\text{Zn}_{0.8}\text{O}$ is an insulator with the band gap of 3.26eV and n-type $\text{Al}_{0.15}\text{Zn}_{0.85}\text{O}$ is a transparent conductor. Under the ultraviolet light irradiation, the $\text{Li}_{0.2}\text{Zn}_{0.8}\text{O}$ films show photoresistance (PR) ($\text{PR}=(R_{\text{dark}}-R_{\text{irradiation}})/R_{\text{irradiation}}$) effect of $\sim 340\%$ at room temperature. In bilayers of $\text{Li}_{0.2}\text{Zn}_{0.8}\text{O}(\sim 110\text{nm})/\text{Al}_{0.15}\text{Zn}_{0.85}\text{O}(\sim 90\text{nm})$ where a p-n junction is formed, the photoresistance increases to $\sim 8600\%$. The photoresistance dependence on wavelength (300-700nm) measurement shows that the photoresistance effect is observed when the light wavelength is below $\sim 380\text{nm}$. The dependence of the light intensity and the response time of the resistance switching have also been measured and will be discussed. The largely enhanced PR effect in bilayers is probably due to the enhancement of the PR effect in p-n junctions. The increased photosensitivity indicates that the $\text{Li}_{0.2}\text{Zn}_{0.8}\text{O}/\text{Al}_{0.15}\text{Zn}_{0.85}\text{O}$ multilayers are promising for UV photodetection applications.

10:12AM P33.00012 Materials considerations for the efficiency of photon-enhanced thermionic emission, JARED SCHWEDE, DANIEL RILEY, KUNAL SAHASRABUDDHE, NICHOLAS MELOSH, ZHI-XUN SHEN, Stanford University — Photon-Enhanced Thermionic Emission (PETE) is a promising method of solar energy conversion that is based on thermal emission of photoexcited electrons from a high-temperature semiconductor, making it attractive for use in tandem with solar thermal systems. Theoretical efficiencies of PETE devices can exceed those of single junction photovoltaics, but experimental tests of the PETE process have displayed low efficiencies.[1] Here we examine this disconnect between experimental results and theoretical promise. We analyze the effects of real semiconductor parameters on the PETE process and relate them to the ultimate performance of a PETE device, directly translating non-idealities of practical materials into constraints on conversion efficiency. The analysis identifies fundamental challenges to efficient conversion based on PETE and establishes design rules that direct the search for semiconductor systems to form the basis of real devices. We also review experimental work guided by these insights that shows increased emission efficiency due to reduced surface recombination, one of the key challenges for realistic solar energy conversion based on PETE.
[1] J.W. Schwede, *et al.*, Nat. Mater. 9, 762-767 (2010)

10:24AM P33.00013 Designing long wavelength barrier based thermophotovoltaic cells, DANTE DEMEO, THOMAS VANDERVELDE, Tufts University Dept. of Electrical and Computer Engineering — This work describes the process of designing low source-temperature thermophotovoltaic cells to harvest energy from thermal sources in the 7-10 micron range. Simulations of the bandstructure are performed for strained layer superlattices (SLS) to act as the p, B, and n regions in a TPV barrier diode. Simulations of the band-alignment of these regions are then performed to ensure a high enough barrier in one band, and a smooth transition in the other. The process is performed iteratively to find an ideal match of specific SLS material and doping concentration in each region. Both conduction band barriers and valence band barriers have been investigated. The balance of system and test apparatuses will also be discussed, as well as preliminary results from samples grown via MBE.

10:36AM P33.00014 Thought waves remotely affect the performance (output voltage) of photoelectric cells, DAYONG CAO, DAQING CAO, Beijing Natural Providence Science & Technology Development Co., Ltd — In our experiments, thought waves have been shown to be capable of changing (affecting) the output voltage of photovoltaic cells located from as far away as 1-3 meters. There are no wires between brain and photoelectric cell and so it is presumed only the thought waves act on the photoelectric cell. In continual rotations, the experiments tested different solar cells, measuring devices and lamps, and the experiments were done in different labs. The first experiment was conducted on Oct 2002. Tests are ongoing. Conclusions and assumptions include: 1) the slow thought wave has the energy of space-time as defined by C1.00007: The mass, energy, space and time systemic theory- MEST. Every process releases a field effect electrical vibration which be transmitted and focussed in particular paths; 2) it has a information of order of tester; 3) the brain (with the physical system of MEST which like a hardware) and consciousness (with the spirit system of the mind, consciousness, emotion and desire-MECD! which like a software) build up a life-informational computer, through some algorithms of DNA and RNA, produce the life-information (include the Genetic code). The Life-Information is a female parent of any information; 4) human can optimize the information. This function is the intelligence; 5) In our experiments, not only thought waves can affect the voltage of the output photoelectric signals by its energy, but they can also selectively increase or decrease those photoelectric currents through remote consciousness interface by a life-information technology.

Wednesday, February 29, 2012 8:00AM - 10:48AM —

Session P34 DCP: Focus Session: Nano III: New Nanoscale Fabrication and Sensing 107A

8:00AM P34.00001 Direct imaging of colloidal nanoparticle growth, structure, and assembly in a transmission electron microscope, PAUL ALIVISATOS, University of California, Berkeley — No abstract available.

8:36AM P34.00002 Computational nanomaterials for novel desalination membrane design: Nanoporous graphene, DAVID COHEN-TANUGI, MIT, JEFFREY C. GROSSMAN, Department of Materials Science & Engineering, MIT — We describe a novel approach for desalination based on nanoporous graphene. Our molecular dynamics calculations show that freestanding graphene patterned with nanometer-sized pores can act as an ultra-thin filtration membrane. Due to size exclusion and chemical interactions with the confining pores, salt ions can be blocked from permeating the membrane at sufficiently small pore diameters. Notably, the pore diameter and the chemical interactions at the water-membrane interface are most important criteria for this system's desalination performance. We will share insights from Molecular Dynamics calculations regarding the theoretical performance of this membrane system and the effects of chemical passivation of the graphene pores on the filtration dynamics. Although the narrow range of acceptable pore sizes suggests that further design innovations will be necessary at the molecular scale before large-scale applications are possible, our existing results predict that pressure requirements for this system can be made roughly competitive with commercial Reverse Osmosis.

8:48AM P34.00003 Structural and electronic properties of bare and capped CdnSen/CdnTen nanoparticles (n = 6, 9), ALEKSEY KUZNETSOV, Department of Chemistry, Duke University, D. BALAMURUGAN, Department of Chemistry, Indiana University, SPIROS S. SKOURTIS, Department of Physics, University of Cyprus, DAVID N. BERATAN, Department of Chemistry, Biochemistry & Physics, Duke University — Relationships between structures and properties (energy gaps, vertical ionization potentials (IP_v), vertical electron affinities (EA_v), and ligand binding energies) in small capped CdSe/CdTe nanoparticles (NPs) are poorly understood. We have performed the first systematic density functional theory study of the structures and electronic properties of Cd_nSe_n/Cd_nTe_n NPs (n = 6, 9), both bare and capped with NH_3^- , SCH_3 , and OPH_3 -ligands. NH_3^- and OPH_3 -ligands cause HOMO/LUMO energy *destabilization* in capped NPs, more pronounced for the LUMOs than for the HOMOs. Orbital destabilization drastically reduces both the IP_v and EA_v of the NPs compared with the bare NPs. For SCH_3 -capped Cd_6X_6 NPs, formation of expanded structures was found to be preferable to crystal-like structures. SCH_3 -groups cause *destabilization* of the HOMOs of the capped NPs and *stabilization* of their LUMOs, which indicates a reduction of the IP_v of the capped NPs compared with the bare NPs. For the Cd_9X_9 NPs, similar trends in stabilization/destabilization of frontier orbitals were observed.

9:00AM P34.00004 New Directions in Plasmonics: Pushing the Space-Time Limit, RICHARD VAN DUYN, Chemistry Department Northwestern University — The lecture will begin with the discussion of our efforts to provide a robust existence proof for SMSERS (Single Molecule Surface Enhanced Raman Spectroscopy). Further, fundamental questions such as: (1) what is the largest possible enhancement factor (EF) and (2) what nanostructure produces the largest EF, will be addressed. Our approach to answering these questions involved the development of new tools such as single nanoparticle SERS and single nanoparticle LSPR spectroscopy spatially correlated with high resolution transmission electron microscopy (HRTEM). Recent results using LSPR biosensors to detect molecular binding events and conformation changes will be presented, including discussions of: (1) pushing the sensitivity of plasmonic biosensors towards the single-molecule detection limit, (2) combining LSPR with complementary molecular identification techniques such as matrix assisted laser desorption/ionization mass spectrometry (MALDI-MS), and (3) the development of new instrumentation for high throughput plasmonic biosensing, and gas sensing with plasmonic nanosensors. Finally, recent developments showing that for the first time, the revolutionary techniques of surface enhanced Raman spectroscopy and femtosecond stimulated Raman spectroscopy (FSRS) can be combined and substantial progress in tip-enhanced Raman spectroscopy (TERS) will be presented. A UHV-TERS instrument has been constructed with atomic resolution of the surface and sub-molecular resolution of the adsorbate, as illustrated with the copper phthalocyanine (CuPc)/Ag(111) system. We can now foresee the day when it will be possible to combine UHV-TERS and surface enhanced FSRS to enable single-molecule spectroscopy with simultaneous nanometer spatial resolution and femtosecond time resolution.

9:36AM P34.00005 Charge Distributions in Polar Semiconductor Nanorods explored with Linear-Scaling DFT Calculations, NICHOLAS HINE, PHILIP AVRAAM, PAUL TANGNEY, PETER HAYNES, Thomas Young Centre, Imperial College London, United Kingdom — Binary polar semiconductors in the wurtzite structure can be grown as nanorods along $\pm[0001]$. In such structures, large dipole moments have been observed. We have studied the distribution of charge in GaAs and ZnO nanorods to elucidate the origin of the dipole moments. To make contact with realistic experiments, rods containing thousands of atoms are simulated using Linear-Scaling DFT calculations with ONETEP [1]. From our calculations we show that both the direction and magnitude of the dipole moment of a nanorod, and its electric field, depend sensitively on how its surfaces are terminated, not on the spontaneous polarization of the underlying lattice. Furthermore, we observe that the Fermi level for an isolated nanorod always coincides with significant density of electronic surface states on its polar surfaces (either mid-gap states or band-edge states). These states pin the Fermi level, and therefore fix the potential difference along the rod. We provide evidence that this effect has a determining influence on the polarity of nanorods, with consequences for the response to changes in surface chemistry, scaling of dipole moment with size, and dependence of polarity on composition.

[1] C. Skylaris et al, JCP 122, 084119 (2005).

[2] P. Avraam et al, PRB 83 241402(R) (2011).

9:48AM P34.00006 Reduction of graphene oxide to graphene, A study of changes in the atomic structure¹, A. MITTAL, A. WAGNER, Univ. of Minnesota, C. MATTEVI, Rutgers Univ., A. CHOV, K. LIAO, C. MACOSKO, Univ. of Minnesota, M. CHHOWALLA, Imperial College, K. A. MKHOYAN, Univ. of Minnesota — An economic method for large scale production of graphene is based on exfoliation of graphite into 1-atom thick sheets by oxidation, creating graphene oxide (GO) and subsequent reduction of GO into graphene. Reduced GO sheets approach the highly desired properties of graphene, such as electrical conductivity and mechanical strength, to various degrees, but not completely. To understand why, we must understand the nanostructure of the sheets. Different methods of reduction result in products that are similar to graphene, but these products retain some oxidized areas or contain regions with sp^3 bonded carbon. The concentration and distribution of these defects on the reduced GO sheet affect the properties of the 2D material. Here, we have characterized the atomic structure of GO and reduced GO via high resolution transmission electron microscopy, electron diffraction, and electron energy loss spectroscopy. Spectroscopic data taken during thermal reduction of GO shows changes in the fine structure of carbon K-edge as the carbon changes from an oxidized form to elemental amorphous carbon to graphite like form, clearly delineating the process of reduction of GO to graphene. Products of several other reduction methods are also characterized revealing information on electronic environment surrounding carbon atoms, distribution of crystalline areas, and oxygen removal from GO.

¹Support from NSF, ADMIRE, and UMN Characterization Facility.

10:00AM P34.00007 Atomic-scale mapping of cerium valence in ceria-zirconia-supported Pd model planar catalysts¹, SHUYI ZHANG, MICHAEL KATZ, KAI SUN, University of Michigan, OBIEFUNE EZEKOYE, McKinsey & Company, MANJULA NANDASIRI, Pacific Northwest National Laboratory, HUNGWEN JEN, Ford Motor Company, GEORGE GRAHAM, XIAOQING PAN, University of Michigan, UNIVERSITY OF MICHIGAN TEAM, PACIFIC NORTHWEST NATIONAL LABORATORY COLLABORATION, FORD MOTOR COMPANY COLLABORATION — Cerium-based oxides have long been regarded as an important class of catalyst support materials. It is also recognized that the interaction between precious metal and ceria-based support material enhances the reducibility of the ceria. The combination of scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) can provide an atomic-scale picture of the interaction between precious metal particles and their support material. In our work, aberration corrected STEM-EELS is used to study the valence of cerium in the vicinity of palladium nanoparticles supported on a ceria-zirconia (CZO) thin film. A monolayer-equivalent of Pd was deposited onto a 50nm-thick CZO thin film, which was then subjected to different thermal treatments. The EELS spectra extracted from the top several atomic layers of the CZO film exhibit typical 3+ character following a low-temperature reduction treatment, indicating the formation of oxygen vacancies. A variety of control experiments have also been performed to exclude possible artifacts caused by electron beam irradiation.

¹DMR-0907191, CBET- 0933239, and DMR-0723032

10:12AM P34.00008 Correlated Percolation Model of Graphene Hydrogenation, ALEJANDRO SUAREZ, Department of Physics, Penn State University, TYLER MAUNU, School of Physics & Astronomy, University of Minnesota, JORGE O. SOFO, Department of Physics, Penn State University — Hydrogenation of graphene by exposure to an atomic hydrogen plasma is a random process. However, the presence of hydrogen already attached to the plane increases the sticking probability of incoming adatoms. We simulate this process as a correlated percolation model where the hydrogen occupation probability of a carbon site is increased or decreased depending on the hydrogenation of the nearest neighboring carbon atoms. This enhancement modifies the cluster distribution on the surface and consequently the electronic structure of the system. We study these effects with a tight binding model and find that, although the density of states at the Fermi level is greatly increased by hydrogenation, the inverse participation ratio shows that not all of these states will contribute to conduction. In fact, for hydrogenation levels of greater than 40% of the lattice, localized states begin to dominate at the Fermi level. A realistic set of values for the sticking probabilities is determined by analysis of the STM images of this system. Through the modeling of this mesoscopic process, we gain a better understanding of how chemically modified graphene is produced and what its transport properties are.

10:24AM P34.00009 Effect of charged impurities and morphology on oxidation reactivity of graphene, MAHITO YAMAMOTO, WILLIAM CULLEN, THEODORE EINSTEIN, MICHAEL FUHRER, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742-4111 — Chemical reactivity of single layer graphene supported on a substrate is observed to be enhanced over thicker graphene. Possible mechanisms for the enhancement are Fermi level fluctuations due to ionized impurities on the substrate, and structural deformation of graphene induced by coupling to the substrate geometry. Here, we study the substrate-dependent oxidation reactivity of graphene, employing various substrates such as SiO₂, mica, SiO₂ nanoparticle thin film, and hexagonal boron nitride, which exhibit different charged impurity concentrations and surface roughness. Graphene is prepared on each substrate via mechanical exfoliation and oxidized in Ar/O₂ mixture at temperatures from 400-600 °C. After oxidation, the Raman spectrum of graphene is measured, and the Raman D to G peak ratio is used to quantify the density of point defects introduced by oxidation. We will discuss the correlations among the defect density in oxidized graphene, substrate charge inhomogeneity, substrate corrugations, and graphene layer thickness. This work has been supported by the University of Maryland NSF-MRSEC under Grant No. DMR 05-20471 with supplemental funding from NRI, and NSF-DMR 08-04976.

10:36AM P34.00010 Numerical Study of Carrier Multiplication in Nanocrystalline form of PbSe and PbS and the bulk, ANDREI PIRYATINSKI, KIRILL VELIZHANIN, Theoretical Division, Los Alamos National Lab — Using previously developed Exciton Scattering Model, we report on systematic numerical study of the carrier multiplication (CM) dynamics in spherically symmetric PbSe and PbS nanocrystals (NCs) and bulk. The quantum efficiency (QE) associated with the photogeneration and population relaxation processes are calculated. It is found that the photogeneration event provides small, about 5%, contribution to the total QE compared to the contribution from the population relaxation process. The analysis shows that the impact ionization dynamics is the main mechanism responsible for the CM during *both* the photogeneration and the population relaxation events. Furthermore, the calculated photogeneration and total QEs for various size NCs are found never to exceed the calculated limiting values for bulk. This observation is explained in terms of the quantum-confinement induced weak effective Coulomb enhancement whose contribution to the impact ionization rate is fully suppressed by the reduction in the biexciton density of states. We also find weak dependence of the total QE on the transform limited pump pulse duration. Comparison of the calculated QEs to published experimental data shows that our calculations well reproduce the experimentally observed trends.

Wednesday, February 29, 2012 8:00AM - 11:00AM –
Session P35 DCP: Focus Session: DFT V: Partitioning and Embedding Theories; Finite-Temperature 107B

8:00AM P35.00001 Exactly Embedded Density Functional Theory for Modeling Chemical Reactions, THOMAS MILLER, California Institute of Technology — We will describe embedded density functional theory methods for performing accurate and scalable electronic structure theory calculations in large molecular systems [1,2], with application to clusters, liquids, and electrode interfaces.

[1] Goodpaster JD, Ananth N, Manby FR, and Miller TF, J. Chem. Phys., 133 (2010) 084103.

[2] Goodpaster JD, Barnes TA, and Miller TF, J. Chem. Phys., 134 (2011) 164108.

8:36AM P35.00002 Exactly embedded DFT for the efficient simulation of large systems, TAYLOR BARNES, JASON GOODPASTER, THOMAS MILLER, California Institute of Technology — Although standard wavefunction-based approaches to electronic structure problems have experienced great success in the study of small systems, their poor size scaling prohibits their application to larger systems. One promising technique for overcoming this scaling problem is embedded Density Functional Theory (e-DFT), in which a large system is divided into many smaller subsystems, with individual wavefunction-based calculations being performed on each subsystem. Using our newly developed Exactly Embedded (EE) technique, we demonstrate highly accurate e-DFT calculations on aqueous systems consisting of hundreds of atoms. Furthermore, these calculations are shown to exhibit excellent size scaling and to be massively parallelizable, allowing for efficient calculations of condensed-phase systems.

8:48AM P35.00003 A unified quantum mechanics embedding theory for materials and molecules¹, CHEN HUANG, Department of Physics, Princeton University, Princeton, New Jersey 08544, USA, MICHELE PAVONE, EMILY CARTER², Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544-5263, USA — It is essentially impossible to apply highly accurate quantum mechanics methods to large material samples, creating a need for a sophisticated embedding theory that can locally refine the accuracy of predicted properties. Here, we present a new ab-initio embedding theory that can treat different regions in the material with quantum mechanics methods of appropriately varying levels of accuracy in a seamless way. We first remove the non-uniqueness of embedding potential definitions that exists in most previous embedding theories by introducing a physical constraint that all regions share a common embedding (interaction) potential. We then introduce a key step to achieve seamless embedding: reformulating the system's total energy solely in terms of the embedding potential, i.e., we construct a potential-functional embedding theory (PFET). We demonstrate how to efficiently solve PFET for molecules and materials and give an outlook for how to perform seamless "multi-physics" material simulations with PFET.

¹We acknowledge the Office of Naval Research and the National Science Foundation for the support

²Both Pavone and Carter are also affiliated with the Program in Applied and Computational Mathematics, and the Andlinger Center for Energy and the Environment, Princeton University

9:00AM P35.00004 Multi-level partitioning using embedded density functional theory, JASON GOODPASTER, TAYLOR BARNES, THOMAS MILLER, California Institute of Technology — Embedded density functional theory (e-DFT) methods are typically limited to the description of weakly interacting systems, because an exact form of the kinetic energy (KE) density functional is unknown. We have developed a method that avoids approximations to the KE functional and provides a formally exact approach to performing electronic structure calculations in the e-DFT framework. This framework allows systems to be divided into smaller subsystems which can be treated at different levels of theory with the inter-subsystem potential calculated using our e-DFT protocol. Therefore, in regions of large systems where DFT is known to perform poorly, such as van der Waals interactions and strongly correlated electrons, wavefunction calculations can be used. We discuss density partitioning strategies for embedded density functional theory and the accuracy of this multi-level method.

9:12AM P35.00005 Partition Density Functional Theory, ADAM WASSERMAN, Purdue University — Partition Density Functional Theory (PDFT) is a formally exact method for obtaining molecular properties from self-consistent calculations on isolated fragments [1,2]. For a given choice of fragmentation, PDFT outputs the (in principle exact) molecular energy and density, as well as fragment densities that sum to the correct molecular density. I describe our progress understanding the behavior of the fragment energies as a function of fragment occupations, derivative discontinuities, practical implementation, and applications of PDFT to small molecules. I also discuss implications for ground-state Density Functional Theory, such as the promise of PDFT to circumvent the delocalization error of approximate density functionals.

[1] M.H. Cohen and A. Wasserman, J. Phys. Chem. A, 111, 2229(2007).

[2] P. Elliott, K. Burke, M.H. Cohen, and A. Wasserman, Phys. Rev. A 82, 024501 (2010).

9:48AM P35.00006 Finding Partition Potentials, JONATHAN NAFZIGER, Department of Physics, Purdue University, MORREL COHEN, Department of Physics and Astronomy, Rutgers University and Department of Chemistry, Princeton University, ADAM WASSERMAN, Department of Chemistry, Purdue University — Partition Density Functional Theory is a formally exact approach to partitioning molecules into fragments via functional minimization and constraints on fragment densities. Cohen and Car proposed a Dynamical Optimization Algorithm for Partition Theory inspired by the Car-Parrinello Method of electronic structure [1]. We modify this algorithm to incorporate a reference HOMO wave-function calculation as a guide to obtain the partition potential, a global quantity arising as the Lagrange multiplier that guarantees satisfaction of the density constraint. We report on the implementation of this procedure for one-dimensional systems, and possible implications for linear-scaling electronic-structure calculations.

[1] M. H. Cohen, and R. Car, J. Phys. Chem. A 2008, 112, 571-575

10:00AM P35.00007 Temperature dependence of Thomas-Fermi errors¹, AURORA PRIBRAM-JONES, Department of Chemistry, University of California, Irvine, KIERON BURKE, Departments of Physics and Chemistry, University of California, Irvine — Finite temperature Thomas-Fermi theory, in addition to its success in systems dominated by classical behavior, can also form the basis for development of a finite temperature local density approximation and its leading corrections. It is therefore imperative that we fully understand its limitations and strengths. To this end, the temperature dependence of Thomas-Fermi errors in densities and integrated quantities for simple models is explored. Behavior of finite-temperature Thomas-Fermi theory in limiting cases will be discussed in the contexts of traditional DFT and its semiclassical foundations. Analysis of finite temperature Thomas-Fermi as a potential functional will be presented.

¹Supported by DOE Grant No. NRF-2010-220-C00017 and NSF Grant No. CHE-0809859.

10:12AM P35.00008 Exact Conditions in Finite-Temperature Density-Functional Theory¹, S. PITTALIS, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA, C.R. PROETTO, Centro Atomico Bariloche and Instituto Balseiro, 8400 S. C. de Bariloche, Argentina, A. FLORIS, Department of Physics, King's College London, London, Strand WC2R 2LS, United Kingdom, A. SANNA, C. BERSIER, Max-Planck-Institut fuer Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany, K. BURKE, Department of Chemistry, University of California, Irvine, CA 92697, USA, E.K.U. GROSS, Max-Planck-Institut fuer Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — Density-Functional Theory (DFT) for electrons at finite-temperature is increasingly important in condensed matter and chemistry. The exact conditions that have proven crucial in constraining and constructing accurate approximations for ground-state DFT are generalized to finite-temperature, including the adiabatic connection formula [1]. We discuss consequences for functional construction.

[1] S. Pittalis, C. R. Proetto, A. Floris, A. Sanna, C. Bersier, K. Burke, and E. K. U. Gross, Phys. Rev. Lett, 107, 163001 (2011)

¹This work was supported by the Deutsche Forschungsgemeinschaft. C.R.P. was supported by a Marie Curie IIF (Grant No. MIF1-CT-2006-040222). S.P. was supported by DOE Grant No. DE-FG02-05ER46203. K.B. was supported by DOE Grant No. DE-FG02-08ER46496.

10:24AM P35.00009 Systematic Results in Finite Temperature DFT¹, TAMAS GAL, JAMES DUFTY, Department of Physics, University of Florida — An exact representation for the non-interacting free energy density functional is identified from the thermodynamics of a non-uniform, finite temperature system of particles in an external potential. A formally exact functional density expansion whose leading term is the Thomas-Fermi approximation is described to second order in the density non-uniformity. The familiar Perrot form [Phys. Rev. A 20, 586 (1979)] is recovered from a subsequent smooth gradient expansion. A related formal expansion about the Thomas-Fermi plus von Weizsacker functional to second order is also described and discussed.

¹Work supported under US DOE Grant DE-SC0002139.

10:36AM P35.00010 Finite Temperature Scaling of the Free Energy Density Functional¹, JAMES DUFTY, VALENTINE KARASIEV, SAMUEL TRICKEY, Department of Physics, University of Florida — Recently, we reported exact scaling relations and related bounds and inequalities for the non-interacting ("Kohn-Sham") free-energy density functional [Phys. Rev. B 84, 125118 (2011)]. Here we extend the analysis to obtain similar results for the full, interacting functional. The extension is obtained by dimensionless analysis for the case of v -representable densities. Connection with the corresponding ground-state scaling is made.

¹Work supported under US DOE Grant DE-SC0002139.

10:48AM P35.00011 Construction of Generalized Gradient Approximation Free Energy Density Functionals¹, SAM TRICKEY, VALENTIN KARASIEV, TRAVIS SJOSTROM, QTP, Physics and Chemistry, U. Florida — By analysis of the second-order gradient approximation (SGA) for the non-interacting electron free energy density, we propose a finite-temperature generalized gradient approximation (ftGGA) for the noninteracting free energy density (both kinetic and entropic contributions). By analogy we also introduce a ftGGA for the exchange free energy density functional. We have implemented the finite-temperature Thomas-Fermi (ftTF), SGA, and a new finite-temperature GGA free-energy functional in the orbital-free density functional theory (OFDFT) code PROFESS. We compare self-consistent OFDFT results with standard Kohn-Sham data. The local pseudopotentials used in the OFDFT calculations are validated by comparison between Kohn-Sham results obtained with standard non-local pseudopotentials and with the same local pseudopotentials.

¹Supported in part under US DoE Grant DE-SC0002139

Wednesday, February 29, 2012 8:00AM - 11:00AM —
Session P36 DCP: Focus Session: Environment III: Nanoparticles, Surfaces and Catalysis 107C

8:00AM P36.00001 Nanominerals, Mineral Nanoparticles, and Earth Processes: Details on How Nanoparticles Work in the Environment, MICHAEL HOHELLA, Virginia Polytechnic Institute and State University — Naturally occurring inorganic nanoparticles have been one of the principal catalytic components of Earth throughout its history. Yet these ubiquitous materials have largely escaped our close scrutiny until very recently. They are illusive and difficult to study. They have properties that change significantly with their exact size, shape, aggregation state, and surrounding environment. In the past, it has not even been clear how they accumulate, disperse, and move around the planet, nor even for sure what their major sources and sinks are. We have now compiled and derived a global budget for naturally occurring inorganic nanoparticles, including an assessment of their sources and sinks, as well as their fluxes between various Earth compartments (atmosphere, continents, continental shelves, and open oceans). In addition, these kinds of budgets provide a basis for fundamental understanding such as residence and transfer times between compartments. Specific findings include the following: 1) The primary producer of Earth's inorganic nanoparticles is soil through terrestrial weathering processes; 2) rivers, and to a lesser extent glaciers, bring 0.1% to 0.01% of the Earth's continental nanomaterial reservoir to the continental edge/ocean margins each year; 3) only about 1.5% of this material makes it to the deep oceans due to aggregation and settling in saline ocean margins; and 4) the airborne and waterborne inputs of nanominerals and mineral nanoparticles to the open oceans are very similar. These kinds of results, along with a much better understanding of the characteristics of naturally occurring inorganic nanoparticles via direct observation in the field coupled with laboratory studies, provide a useful foundation upon which to predict the behavior and fate of manufactured nanoparticles, many of which are very similar to naturally occurring varieties. Even when specific correlations between naturally occurring and manufactured nanoparticles cannot be made, important clues in manufactured nanoparticle behavior in complex environments can be obtained by observing natural systems.

8:36AM P36.00002 Surface Reactivity of Core Shell Iron-Iron Oxide Nanoclusters towards Breakdown of Carbon Tetrachloride, MANINDER K. TARSEM S., YOU QIANG, Department of Physics, University of Idaho, Moscow, ID 83844, HONGSEOK KIM, Pusan National University, Korea, 609-735, JAMES E. AMONETTE, DONALD R. BAER, Pacific Northwest National Laboratory, Richland, WA 99352 — Zero-valent iron (ZVI) is one of the technologies for groundwater remediation to reduce contaminants by removal of mobile chlorinated hydrocarbons. Iron-Iron oxide ($\text{Fe}/\text{Fe}_3\text{O}_4$) nanoclusters (NCs) made in our laboratory using cluster deposition technique have enhanced reactivity towards targeted contaminants due to the presence of ZVI protected by a passivated oxide shell. Here, we investigate the effectiveness of the $\text{Fe}/\text{Fe}_3\text{O}_4$ NCs in reducing carbon tetrachloride (CT) under laboratory conditions. The reactivity of the NCs was investigated by conducting unbuffered aqueous batch experiments to reduce CT at room temperature. Initial results show that 80% of the degradation of CT resulted in the formation of dichloromethane (DCM) and chloroform (CF); the remainder likely followed a competing pathway to yield nonhazardous products such as CO. The production of undesirable hydrogenated products such as DCM and CF suggests that the dominant reaction pathway occurs through hydrogen (H) atom transfer via H atoms generated by corrosion of the iron. Comparative experiments with ZVI NCs prepared by other methods are underway and the results will be reported. Future work is to analyze and understand factors that control the reaction pathways between desirable and undesirable products.

8:48AM P36.00003 Environmental Catalysis at the Boundary between Metals and Metal Oxides, WILLIAM F. SCHNEIDER, University of Notre Dame — Growing theoretical and computational evidence points to the participation of partially to completely oxidized catalyst surfaces during catalytic oxidations under realistic conditions. These catalytic oxidations are of both fundamental scientific interest and of practical importance in a variety of contexts, including in particular environmental NO_x remediation, yet fundamental understanding of the coupling between surface structure and composition, reactive environment, particle size, and catalytic reactivity is still in its infancy. In this work we use density functional theory (DFT) models to consider the coupling between catalytic oxidation activity and the transformation of metal to oxide surface, taking as our model CO and NO oxidation on oxygen-covered to oxidized Pt surfaces. We describe DFT-parameterized cluster expansions (CEs) of O on Pt that capture the transition from metal to oxide, spectroscopic signatures of these transformations, and the incorporation of the metal-to-oxide transition into kinetic models of surface reactivity.

9:24AM P36.00004 Effect of substrate-catalyst interaction on Spin-dependent chemical reactions: CO oxidation¹, SHUNFANG LI, Department of Materials Science and Engineering, University of Tennessee; School of Physics, Zhengzhou University, China, YANFEI GAO, Department of Materials Science and Engineering, University of Tennessee; Materials Science and Technology Division, ORNL, ZHENYU ZHANG, Department of Physics and Astronomy, University of Tennessee; ICQD, University of Science and Technology of China, Hefei, Anhui, China — First-principles calculations have been performed to investigate and compare the catalytic reactivity of $\text{Ni}(\text{Pd})_1/\text{TiO}_2(110)$ and $\text{Ni}(\text{Pd})_2/\text{TiO}_2$, for CO oxidation. A recent experiment showed that the catalysis of small $\text{Ni}(\text{Pd})_2$ clusters deposited on rutile $\text{TiO}_2(110)$ surface exhibit very different performance for CO oxidation, compared with the single atom cases, $\text{Ni}(\text{Pd})/\text{TiO}_2(110)$. However, the underlying mechanism of this interesting phenomenon is still unclear. Our calculations show that the catalyst-substrate interaction plays a key role in both the thermodynamic and kinetic process of the catalytic reactions. Particularly, the spin degree of freedom of the complex oxide is found to dominate the reaction rate. Essentially, the oxidation of CO on the single atom cases is a spin-forbidden reaction, while it is spin-permitting for the dimer cases. This work provides valuable guidance for high efficient catalyst design at the atomic scale.

¹Research sponsored by the U.S. National Science Foundation and the Natural Science Foundation of China.

9:36AM P36.00005 Assessing Actinide-Oxygen Covalency by K-edge X-ray Absorption Spectroscopy. , DAVID SHUH, Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — The development of many essential nuclear technologies requires a comprehensive grasp of the electronic ground and valence states of molecular actinide bonding interactions. Identifying itinerant or delocalized electrons – in molecular nomenclature, ionic or covalent bonds – is a longstanding problem in actinide science. Recent advances have shown that the transition intensities measured by ligand K-edge X-ray absorption spectroscopy (XAS) directly relate to coefficients of covalent orbital mixing. Ligand K-edge XAS has been employed successfully to describe the valence states of materials containing predominantly ionic metal–Cl and metal–S bonds, however, it remains experimentally challenging to obtain quantitative intensity information at the K-edge for light atoms such as C, O, N, and F. Insights regarding the nature and extent of orbital mixing in actinide–O bonds are now within reach through a combination of XAS with a scanning transmission X-ray microscope (STXM) and hybrid density functional theory calculations (DFT). A new effort to employ these techniques for non-conducting molecular systems containing interactions between actinide and oxygen-based ligands will be discussed. Oxygen K-edge XAS measurements and DFT for a series of six structurally related transition metal oxides suggest that metal nd and O 2p orbital mixing increases with increasing Z. The actinyl ions were chosen for the first O K-edge XAS measurements with actinides because they represent the most important high-valent actinide species in the environment. Features in the polarized XAS of the actinyls follow anticipated trends based on the 5f and 6d orbital energies and occupancies. Results from an ongoing collaboration with theorists ties these experimental trends in actinide–O orbital mixing to changes in 3d, 4d, 5d, and 6d/5f valence orbital occupancies.

10:12AM P36.00006 Submonolayers of Au/Pd on the hematite (0001) and magnetite (111) surfaces¹ , ADAM KIEJNA, TOMASZ PABISIAK, TOMASZ OSSOWSKI, Institute of Experimental Physics, University of Wrocław, Poland — Ultra-thin films and nanostructures formed by noble metals on oxide surfaces exhibit enhanced catalytic activity for CO oxidation. We used the spin-polarized density functional theory (DFT) and the DFT+U method, accounting for the strong on-site Coulomb correlations, to study the submonolayer adsorption of Au/Pd atoms on two stable iron-oxide surfaces: hematite (0001) and a magnetite (111). For each surface, adsorption on two terminations has been studied: one terminated with iron and the other with oxygen. Both Au and Pd bind strongly to hematite and magnetite surfaces and induce large changes in their geometry. DFT and DFT+U provide qualitatively similar surface geometries but they differ much in the prediction of the surface energetics and the electronic and magnetic properties of the oxides. Pd binds stronger than Au both to hematite and magnetite surfaces and the Au/Pd bonding to the O-terminated surface is distinctly stronger than that to the Fe-terminated one. For hematite, the DFT+U bonding is by 0.3–0.6 eV weaker than DFT on the Fe-terminated surface and about 2 eV stronger on the O-terminated one. For magnetite, in each case, DFT+U gives stronger bonding than DFT. The differences between DFT and DFT+U results are discussed based on the calculated electronic structure.

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10:24AM P36.00007 ABSTRACT WITHDRAWN —

Wednesday, February 29, 2012 8:00AM - 11:00AM —
Session P37 DCMP: CDW Materials - Chalcogenides and other 108

8:00AM P37.00001 Temperature- and pressure-dependent Raman scattering study of phase transitions in ZrTe_3 ¹ , S. GLEASON, S. YUAN, T. BYRUM, S.L. COOPER, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, IL 61801, C. PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973 — Pressure-induced superconductivity has been discovered in many classes of materials, such as the iron pnictides and transition metal chalcogenides. ZrTe_3 is a representative member of the latter whose ground state can be tuned between charge density wave and superconducting phases via pressure or intercalation. Microscopic information about the structural evolution of ZrTe_3 in response to applied pressure is lacking at present. In this talk, we describe a temperature- and pressure-dependent Raman scattering study of the structural evolution of ZrTe_3 through its temperature- and pressure-dependent phase transitions.

¹Work supported by the U.S. Department of Energy under Award No. DE-FG02-07ER46453. T.B. supported by an NSF Graduate Fellowship.

8:12AM P37.00002 Ultrafast Dynamics of a Charge Density Wave via Time-Resolved Resonant Diffraction , R.G. MOORE¹, SLAC National Accelerator Laboratory — Understanding the emergence of collective behavior in correlated electron systems remains at the forefront of modern condensed matter physics. The key to such an understanding is unraveling the contributions from the coupling degrees of freedom in exotic many body states. Density waves, both of charge and spin, have been studied for decades and a wealth of information and insight has been gained. However, there are still open questions that need to be solved for a complete description of the phenomena as there are several existing density wave systems that exhibit prototypical behavior while violating traditional theory. Ultrafast dynamics of such a system, TbTe_3 , has been investigated via time-resolved resonant diffraction at the SXR endstation at LCLS. Oscillations of the amplitude mode and coherent phonons have been observed previously in time resolved photoemission and reflectivity measurement but, here we reveal a direct observation of the lattice response via resonant diffraction. Watching dynamics of the two dimensional Te plane density wave diffraction peak at a resonant energy of a bystander Tb atom reveals new insights into the coupling responsible for the formation of the state. Results and comparison with previous time resolved measurements will be discussed.

¹This work represents the efforts of more than 20 authors who will be acknowledged during the presentation.

8:24AM P37.00003 Experimental Observation of Chiral Order in TiSe_2 ¹ , RAYMOND OSBORN, JOHN-PAUL CASTELLAN, STEPHAN ROSENKRANZ, JASPER VAN WEZEL, JACOB RUFF, UTPAL CHATTERJEE, Argonne National Laboratory, GORAN KARAPETROV, Drexel University — Recent STM measurements on TiSe_2 were interpreted as evidence of chirality in the charge-density-wave order parameter, i.e., a rotation in the phase of the three in-plane components of the CDW order from one layer to the next. Recently, J. van Wezel has shown theoretically how a chiral state can arise from the onset of orbital order of the Ti 3d and Se 4p states in conjunction with the charge order at a temperature at or below the CDW transition temperature [arXiv:1106.1930v1 (2011)]. This theory predicts a lowering of the symmetry of the ordered phase from $P3c1$ to $P2$. We present the results of synchrotron x-ray diffraction measurements on a single crystal of TiSe_2 that provide evidence of a second structural phase transition 15K below the CDW transition, consistent with the proposed space group.

¹Supported by U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under contract No. DE-AC02-06CH11357.

8:36AM P37.00004 Pressure-induced CDW suppression in 1T-TiSe₂¹, YOUNG IL JOE, University of Illinois, K. FINKELSTEIN, CHESS, S. YUAN, S.L. COOPER, PETER ABBAMONTE, University of Illinois — 1T-TiSe₂ is a prototypical transition-metal dichalcogenide showing a commensurate CDW phase transition. It has been shown that hydrostatic pressure suppresses the CDW order and induces superconductivity. Here we present a high-pressure x-ray scattering study of the CDW order parameter and its fluctuations in TiSe₂. The integrated intensity at the base temperature as a function of pressure shows a positive curvature, indicating deviation from mean-field behavior. The ratio between the lattice distortion and the critical temperature is pressure-dependent, indicating a cross-over from strong to weak coupling limits. Using a Monte Carlo simulation of the three-component Potts model, we argue that the amount of anisotropy and the effective dimension must be taken into account to explain the properties of the phase transition.

¹This work was supported by DOE grant DE-FG02-07ER46453

8:48AM P37.00005 Chiral charge and orbital order in 1T-TiSe₂¹, JASPER VAN WEZEL, Argonne National Laboratory — Helical arrangements of spins are common among magnetic materials. The first material to harbor a corkscrew pattern of charge density on the other hand, was discovered only very recently [1,2]. The nature of the order parameter is of key relevance, since rotating a magnetic vector around any propagation vector trivially yields a helical pattern. In contrast, the purely scalar charge density cannot straightforwardly support a chiral state. Here we resolve this paradox by identifying the microscopic mechanism underlying the formation of the chiral charge density wave in 1T-TiSe₂. It is shown that the emergence of chirality is accompanied by the simultaneous formation of orbital order [3]. We show that this type of combined orbital and charge order may in fact be expected to be a generic property of a broad class of charge ordered materials and discuss the prerequisites for finding chiral charge order in other materials.

[1] J. Ishioka, Y. H. Liu, K. Shimatake, T. Kurosawa, K. Ichimura, Y. Toda, M. Oda and S. Tanda, *Phys. Rev. Lett.* **105**, 176401 (2010).

[2] J. van Wezel and P. B. Littlewood, *Physics* **3**, 87 (2010).

[3] J. van Wezel, arXiv:1106.1930v1 (2011).

¹This research was supported by the US DOE, Office of Science, under Contract No. DE-AC02-06CH11357

9:00AM P37.00006 Evolution of the Charge Density Wave state in Cu_xTiSe₂¹, MARIA IAVARONE, ROBERTO DI CAPUA², XIN ZHANG, MARYAM GOLALIKHANI, STEVEN MOORE, Physics Department, Temple University, Philadelphia, PA 19122, USA, GORAN KARAPETROV, Physics Department, Drexel University, Philadelphia PA 19104, USA — 1T-TiSe₂ is a quasi two-dimensional CDW material showing a 2x2x2 superlattice modulation below 200 K. Upon Cu doping the CDW is suppressed and superconductivity is induced. We present scanning tunneling microscopy and spectroscopy measurements of the charge-density wave state in 1T-TiSe₂, Cu_{0.05}TiSe₂ and Cu_{0.06}TiSe₂ single crystals. Topography images at 4.2 K reveal that the charge density waves are present in all samples studied, although the amplitude of the charge modulation decreases with the Cu-doping. Moreover, the chiral phase of the charge density wave is preserved also in Cu-doped samples. Tunneling spectroscopy shows that there is only a partial gap in the pure compound, with bands crossing the Fermi surface. In the Cu-doped samples the system becomes more metallic due to the increase of the chemical potential.

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9:12AM P37.00007 Effect of dimensionality on charge density wave instabilities in TaS₂ and TaSe₂, YIZHI GE, AMY Y. LIU, Physics Department, Georgetown University — Recent successes in making exfoliated single-layer transition-metal dichalcogenides has brought new interest to these materials, particularly with respect to the effects of dimensionality. As layered bulk materials, the 1T and 2H polymorphs of TaS₂ and TaSe₂ undergo a number of charge-density-wave (CDW) transitions. However, recent experiments have found that the CDW instability does not survive in nanopatches of 2H-TaS₂. Here we present a density-functional theory investigation of the CDW instability in single- and few-layer TaS₂ and TaSe₂, focusing on the role of the interlayer interactions. The effects of dimensionality on structure, electronic structure, and electronic-phonon coupling will be discussed.

9:24AM P37.00008 Disorder Induced Melting of Charge Density Wave Order in doped 2H-NbSe₂ systems, UTPAL CHATTERJEE, STEPHAN ROSENKRANZ, JOHN CASTELLAN, JASPER VAN WEZEL, RAY OSBORN, Argonne National Laboratory, MARIA IAVARONE, Temple University, GORAN KARAPETROV, Drexel University — Using a combination of Angle Resolved Photoemission Spectroscopy (ARPES), X-ray diffraction, transport and Scanning Tunneling Microscopy (STM) measurements on pristine as well as disordered 2H-NbSe₂ samples, we have found that the onset Temperature T_{cdw} for Long Ranged Charge Density Wave (CDW) order gets quickly suppressed with concentration of disorder ions (X) and at certain critical concentration (X_c) it undergoes a quantum melting. Our STM measurements provide the evidence for local CDW ordering in doped samples for temperatures way above T_{cdw}. On the other hand, our ARPES measurements have found evidences for the presence of energy gap for both T > T_{cdw} & X > X_c. We argue, all these experimental observations from completely different probes hint towards phase fluctuations of the order parameter as the mechanism behind the destruction of CDW order in quasi 2-d systems, such as 2H-NbSe₂.

9:36AM P37.00009 Spectroscopic imaging of the charge density wave in 2H-NbSe₂¹, ANJAN SOUMYANARAYANAN, Massachusetts Institute of Technology, MICHAEL M. YEE, YANG HE, Harvard University, DIRK RAHN, KAI ROSSNAGEL, Kiel University, ERIC W. HUDSON, Pennsylvania State University, JENNIFER E. HOFFMAN, Harvard University — Transition metal dichalcogenides are an ideal playground to study the interplay between charge density waves (CDWs) and superconductivity. We perform atomically resolved scanning tunneling microscopy and spectroscopy at cryogenic temperatures on the chalcogenide polytype 2H-NbSe₂ to study the energy, temperature and spatial dependence of the CDW. By comparing our results with a tight-binding model, we disentangle the spectral behavior of the CDW phase in the material.

¹NSF (DMR-0847433), A*STAR, NSERC

9:48AM P37.00010 Strong Periodic Lattice Distortion in Transition Metal Dichalcogenides, JIXIA DAI, EDUARDO CALLEJA, YUE CAO, DANIEL DESSAU, KYLE MCELROY, Department of Physics, University of Colorado at Boulder, Boulder, Colorado 80309, USA, HELMUTH BERGER, Department de Physique, EPF Lausanne, CH-1015 Lausanne, Switzerland, XIANGDE ZHU, LIJUN LI, YUPING SUN, Key Laboratory of Materials Physics, Institute of Solid State Physics, CAS, Hefei 230031, China, T. WOLF, Karlsruher Institut für Technologie, Institut für Festkörperphysik, P.O.B. 3640, D-76021 Karlsruhe, Germany — The charge density wave (CDW) instability was initially proposed to be the result of the Peierls mechanism in which a divergence in electronic response function results in a periodic charge redistribution; i.e. the electron gas itself is unstable with respect to the formation of a periodically varying electron charge density. However, the mechanism of CDW in many 2D Transition Metal Dichalcogenide (TMD) is still under debate. Fermi surface nesting was originally believed to act as the driving mechanism of CDW transitions in these materials; however, recent reports from both theoretical and experimental studies are not quite within this simple model. We use Spectroscopic Imaging Scanning Tunneling Microscope (SI-STM) to study the surfaces of 2H-TaSe₂, 2H-TaS₂, and 2H-NbSe₂ at various temperatures from 6K to above 100K. Topographic images and differential conductance data were recorded and analyzed in order to help understanding the underlying physics of CDW phases. Our results shows that Periodic Lattice Distortion (PLD) likely plays a more important role than the charge modulation in 2D TMD.

10:00AM P37.00011 Low frequency resistance fluctuations in nanoribbons of charge density wave (CDW) conductor NbSe₃, ZHENZHONG SHI, ADAM STABILE, Department of Physics, PETER MARLEY, Department of Chemistry, SUJAY SINGH, Department of Physics, SARBAJIT BANERJEE, Department of Chemistry, GANAPATHY SAMBANDAMURTHY, Department of Physics, University at Buffalo, Buffalo, NY 14260. — We investigate finite size effects in the low-frequency ($1 \text{ mHz} < f < 10 \text{ Hz}$) resistance fluctuations of individual nanoribbons of single-crystalline NbSe₃ (cross sections of 10^4 nm^2) across the two CDW transitions ($\sim 59 \text{ K}$ and $\sim 141 \text{ K}$). This ultra sensitive frequency-dependent study of the electrical noise is crucial in improving our understanding of the mechanisms that generate noise around CDW transitions. The power spectral density, S_R , of the resistance noise has a generic form, $S_R \sim 1/f^\alpha$, typical of a diffusive metallic conductor. Below the CDW transition at 59 K , where the CDW is pinned by disorder, S_R (at 1 Hz) shows a non-monotonic behavior with a maximum magnitude around 45 K . A similar peak in S_R is also observed at 125 K , below the second CDW transition. Also, it is well known that the CDW state can be depinned by an application of a high bias voltage or current and S_R is measured as a function of current across the pinning-depinning of CDW. S_R shows a complex, non-monotonic dependence and is extremely sensitive to temperature below the CDW transition. In contrast, S_R is bias independent above the CDW transitions as expected from a metal. The implications of these noise behaviors in understanding the pinning and depinning of CDW in NbSe₃ will be discussed.

10:12AM P37.00012 Extrinsic control of collective transport in quasi-1D materials with end contacts geometry¹, A.F. ISAKOVIC, A. BELKADI, Khalifa University - KUSTAR, Abu Dhabi, UAE, K. EVANS-LUTTERODT, BNL-NSLS, NY, USA — End contacts to mesowires of NbSe₃ and TaS₃ were nanofabricated and tested with transport, noise and X-ray microdiffraction measurements. We measured unusual and unexpected weak dependence of collective current on temperature in the $[70\text{K}, 90\text{K}]$ range, close to $2/3T_{P1}$ point, indicating a modification of CDW condensate transport due to the end contact geometry. This is accompanied with modifications to the temperature dependence of the phase slip voltage. We also report a partial control of the threshold field (E_T) for CDW sliding, below T_{P2} , with the decrease in E_T by as much as one order of magnitude in a limited temperature range below $2/3T_{P2}$. These changes can be also seen in electric field modified X-ray topography images performed with sub-micron focused synchrotron X-rays (X13B beamline at NSLS). The most likely causes of these phenomena when end contacts are applied, are in modifications of: (a) carrier injection efficiency and, (b) the phase loop formation mechanism.

¹The work at BNL-NSLS was supported by US DOE, contract DE-AC02-98CH10886; the sample growth was done in Prof. R. E. Thorne laboratory at Cornell University. A.B. and A.F.I. also acknowledge recent support from ATIC-SRC (2011-KJ-2190) and KUSTAR.

10:24AM P37.00013 Spectroscopic evidence of the Peierls transition in three-dimensional charge density wave solids, BARBARA MANSART, MATHIEU COTTET, THOMAS J. PENFOLD, Ecole Polytechnique Federale de Lausanne, STEPHEN B. DUGDALE, University of Bristol, RICCARDO TEDIOSI, universite de Geneve, MAJED CHERGUI, FABRIZIO CARBONE, Ecole Polytechnique Federale de Lausanne — We studied the ultrafast photoinduced charge-density-wave to metal phase transition in a complex solid, namely Lu₅Ir₄Si₁₀. After melting the charge ordering using infrared laser pulses, the consequent charge redistribution is probed with fs time resolution through the spectral weight analysis of the transient optical response over a broad energy range. The time-dependent spectral weight reveals a signature of the CDW melting and the time-scale of this photo-induced phase transition. This new kind of analysis allows us to show that the charge order remains preserved until the lattice distorts sufficiently to induce the phase transition. These results are completed by ab-initio modeling of the electronic band structure, identifying the orbitals involved in the CDW and the electronic transitions leading to the photo-induced melting of the charge order. This allows us to reveal the Peierls origin of multiple CDW in this three-dimensional solid.

10:36AM P37.00014 Gapped sliding phononic modes in the incommensurate structure of the ladder-chain system Sr₁₄Cu₂₄O₄₁, ADRIAN GOZAR, CHRISTOPHER HOMES, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA, GIRSH BLUMBERG, Department of Physics and Astronomy, Rutgers, The State University of New Jersey, Piscataway, New Jersey 08854, USA, VERNER THORSMOLLE¹, HENRIK RONNOW, Laboratory for Quantum Magnetism, Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015, Switzerland — We report on low energy Raman and infra-red (IR) excitations in Sr₁₄Cu₂₄O₄₁. Two modes are observed starting from room temperature in the 1-2 meV range. One is a fully symmetric Raman mode and the other, observed in c-axis reflectance, is an excitation carrying a dipole moment along the chain/ladder direction. We associate these modes with the gapped c-axis sliding motions of the charged, incommensurate CuO₂ chains and Sr₂Cu₂O₃ ladder layers. This approach is able to quantitatively explain the range and relative energies of these excitations which are sensitive probes of the charge and spin density-wave ordering in the "14-24-41" systems.

¹also at: Departement de Physique de la Matiere Condensee, Universite de Geneve, CH-1211 Geneve 4, Switzerland

10:48AM P37.00015 Dynamics of Sr₁₄Cu₂₄O₄₁ in a transient high intensity THz field, ELSA ABREU, Boston University, Department of Physics, 590 Commonwealth Avenue, Boston MA, USA, RAVI SINGH, University of Warwick, Department of Physics, Coventry CV4 7AL, UK, VERNER THORSMOLLE, Departement de Physique de la matiere condensee, Universite de Geneve, CH-1211 Geneve 4, Switzerland, GEETHA BALAKRISHNAN, University of Warwick, Department of Physics, Coventry CV4 7AL, UK, RICHARD AVERITT, Boston University, Department of Physics, 590 Commonwealth Avenue, Boston MA, USA — Over the past few years new techniques have become available to generate electromagnetic radiation with high electric field values in the THz range [1], allowing the dynamic study of materials whose excitations lie in the far infrared frequency range. This is the case of many charge density wave compounds, which exhibit a collective response due to pinning. Sr₁₄Cu₂₄O₄₁ is a charge density wave compound of particular interest, given its quasi one-dimensional structure consisting of alternating layers of Cu₂O₃ chains and CuO₂ ladders [2]. Understanding the dynamics of Sr₁₄Cu₂₄O₄₁ excitations in the far infrared has the potential not only to shed light onto the complex nature of charge ordering in this material, but also to help provide a better understanding of the nature of superconducting behavior in two-dimensional high temperature superconducting cuprates. In our work, THz pulses generated using a LiNbO₃ crystal interact with single crystal Sr₁₄Cu₂₄O₄₁ samples grown by the traveling solvent floating zone method. We will present preliminary results of a high field THz study of the dynamics of Sr₁₄Cu₂₄O₄₁. [1] Jepsen et al., Laser Phot Rev 5 124 (2011) [2] Gorshunov et al., Phys Rev B 66 060508 (2002)

Wednesday, February 29, 2012 8:00AM - 10:36AM — Session P40 DBIO: Protein Fluctuations and Conformation Changes 156A

8:00AM P40.00001 Atomistic simulations of the MS2 coat protein conformational transition, MATTHEW PERKETT, FRANCESCO PONTIGGIA, MICHAEL HAGAN, Brandeis University — During the replication of many viruses, hundreds to thousands of proteins self-assemble to form a protective protein coat, called a capsid, around the viral nucleic acid. Often these proteins have identical amino acid sequences with slightly different, or quasi-equivalent, conformations, which join in precise spatial arrangements. Although the structure of completed capsids is known to atomic resolution, little is known about the assembly intermediates and how protein conformations are selected during assembly. In this talk, we will use all-atom simulations to investigate how protein-RNA interactions guide conformational transitions of capsid proteins from the single-stranded RNA bacteriophage MS2. Since conformational changes occur on timescales which are not accessible to all-atom simulations, we use enhanced sampling methods to sample probable transition pathways and corresponding free energy profiles. Specifically, we will present free energy profiles associated with the MS2 capsid protein conformation in the presence and absence of RNA.

8:12AM P40.00002 Conformational changes of surface immobilized proteins studied by combined Atomic Force Microscopy and Fluorescence Spectroscopy, DANIEL RIZZO, CRISTIAN STAIL, Physics and Astronomy, Tufts University — Atomic Force Microscopy (AFM) and Fluorescence Spectroscopy techniques have provided unique methods for characterizing conformational changes in proteins. Here we are using a technique called nanografting to immobilize proteins at well defined locations on atomically flat surfaces. In nanografting the AFM tip is used to shave alkanethiol molecules from a prescribed patch on a surface coated with an alkanethiol monolayer. Thiol-linked proteins in the surrounding solution are then able to self assemble on the newly exposed surface patch in a highly ordered array of the order of 100nm. Stable and meta-stable conformations of fluorescently tagged proteins and other molecules assembled in this manner can then be characterized using a combination of AFM and Fluorescent Resonance Energy Transfer (FRET). Due to the high spatial, temporal and force resolution provided by both AFM and FRET, a free energy landscape of the protein may be determined using this technique.

8:24AM P40.00003 The Glassy State of Crambin and the THz Time Scale Fluctuations Related to Protein Function, KRISTINA WOODS, BEDIHA BESER, Carnegie Mellon University — THz experiments have been used to characterize the picosecond time scale fluctuations taking place in the model protein crambin. Using both hydration and temperature as an experimental parameter, we have successfully identified the collective fluctuations ($\leq 200 \text{ cm}^{-1}$) in the protein (Figure 1). Observation of the transition of the protein dynamics in the THz spectrum from both below and above the glass transition temperature (T_g) provides unique insight into microscopic interactions and modes that allow the solvent to couple with the protein dynamics (Figure 2). Our findings suggest that the solvent dynamics on the picosecond time scale not only contribute to the flexibility of the protein but also provides a dynamical parameter that allows the protein to modulate local regions of its structure that are distinct from the protein whole. These distinct dynamical regions of the protein may be important for energy transport and hence, linked with protein function.

8:36AM P40.00004 Stabilization of peptide helices by length and vibrational free energies: *Ab initio* case study of polyalanine, MARIANA ROSSI, VOLKER BLUM, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin — Helices are one of the most abundant secondary structure “building blocks” of polypeptides and proteins. Here, we explore helix stabilization as a function of peptide length and temperature [harmonic approximation to the vibrational free energy (FE)], for the alanine-based peptide, Ac-Ala_n-LysH⁺ $n=4-15$, in the gas phase. For $n=4-8$, we predict the lowest energy structures in density-functional theory, using the van der Waals (vdW) corrected[1] PBE exchange-correlation potential. α -helices become the lowest energy structures at $n \approx 7-8$ on the potential energy surface, but only barely and if including vdW interactions. At finite temperatures, the helices are further stabilized over compact conformers. While the vibrational entropy is the leading stabilizing term at 300 K, also the zero-point-energies favor the helical structures. For $n \geq 8$, the α -helix should be the only accessible conformer in the FE surface at 300 K, in agreement with experiment[2] and with our own comparison[3] of calculated *ab initio* anharmonic IR spectra to experimental IR multiple photon dissociation data for $n=5, 10$, and 15. [1] Tkatchenko and Scheffler, PRL 102, 073055 (2009); [2] Kohtani and Jarrold, JACS 108, 8454 (2004); [3] Rossi et al., JPCL 1, 3465 (2010).

8:48AM P40.00005 A Physics-based Approach of Coarse-graining the cytoplasm of *E. coli*¹, QIAN WANG, MARGARET CHEUNG, University of Houston — We have investigated protein stability in an environment of *E. coli* cytoplasm using coarse-grained computer simulations. To coarse-grain a small slide of *E. coli*'s cytoplasm consisting of over 16 million atoms, we developed a self-assembled clustering algorithm (CGCYTO). CGCYTO uses a tunable resolution parameter (λ , ranging from 0 to 1) to justify the resolution of a cytoplasm, depending on the size of a test protein for the computation of covolumes and the volume of a macromolecule in the cytoplasm. We compared the results from a polydisperse cytoplasm model (PD model) from CGCYTO with two other coarse-grained hard-sphere cytoplasm models: (1) F70 model, macromolecules in the cytoplasm were modeled by homogeneous hard spheres with a radius of 55Å and (2) HS model, each macromolecule in the cytoplasm is modeled by hard spheres of various sizes. It was found that the folding temperature T_f of a test protein (apoazurin) is ~ 5 degrees higher in a PD model than that in a F70 model. In addition, there is a deviation of 1.7 degrees on T_f when an apoazurin is randomly placed at different voids formed by particle fluctuations in a PD model, 0.7 degrees higher than that in a HS model.

¹Supported by NSF, Molecular & Cellular Biosciences (MCB0919974).

9:00AM P40.00006 Investigation of flexibility in Myosin V using a new 3D mechanical model, MAHDI HAGHSHEENAS-JARYANI, Department of Mechanical Engineering, University of Texas at Arlington — This paper presents the development of a three dimensional rigid multibody model for the simulation and analysis of motor protein locomotion. The interesting aspect of this model is that it retains the mass properties, in contrast to the commonly used models which omit mass properties at the nano scale. The disproportionate size of the small mass of Myosin V relative to the large viscous friction forces requires a small integration step size that leads to a long simulation run time; however, the proposed model can be numerically integrated in a reasonable amount of time. This paper discusses modeling flexibility in the protein as an extension of the original rigid body model. Empirical studies have shown that Myosin V's neck domain can be considered as three pairs of tandem elements called IQ motifs which can bending at junctures between them. Therefore, each neck is modeled by three rigid bodies connected by ball-and-socket joints together, rather than single rigid body has been used in the previous works. Euler parameters are used to model the orientation of bodies in order to eliminate singularities in the description of orientation. In order to accomplish this, the equations of motion are reduced to minimal form using changing holonomic and non-holonomic constraints applied to the model which represent the normalization of the Euler parameters as well as contact and impact non-penetration conditions. The differences between the dynamic behavior of the new mechanical model, with flexible neck domains, and the original rigid body model are compared using simulation results.

9:12AM P40.00007 Barrel fluctuation and oxygen diffusion pathways in the monomeric fluorescent proteins, CHOLA REGMI, PREM CHAPAGAIN, YUBA BHANDARI, ILAN CHEMMAMA, BERNARD GERSTMAN, Florida International University — Fluorescent proteins are valuable tools as biochemical markers for studying cellular processes. Improving the photostability of the FPs is highly desirable in biochemical, biomedical and cell biology. Oxygen is necessary for the proper maturation of the chromophore in fluorescent proteins (FPs), but photobleaching of FPs is also oxygen sensitive. The photobleaching of the monomeric variant of RFPs has been attributed to the lack of proper shielding against oxygen or other small molecules, ions or halides. We use molecular dynamics simulation to investigate the protein barrel fluctuations in mCherry, one of the most useful monomeric mFruit variant of RFPs. We also employ oxygen diffusion simulations to search for possible pathways of oxygen to the chromophore. The ultimate goal is to use the results of these calculations to propose amino acid substitutions that will block the oxygen pathways and prevent photobleaching in the engineered proteins.

9:24AM P40.00008 Protein Dynamics Studied by Quasi-elastic Neutron Scattering¹, XIANG-QIANG (ROSIE) CHU, EUGENE MAMONTOV, Oak Ridge National Lab, MARCO LAGI, SOW-HSIN CHEN, MIT, MANAVALAN GAJAPATHY, JOSEPH NG, University of Alabama in Huntsville, KEVIN WEISS, LEIGHTON COATES, Oak Ridge National Lab, EMILIANO FRATINI, PIERO BAGLIONI, University of Florence — The biological function and activities of proteins are intimately related to their structures and dynamics. Nowadays, neutron scattering is one of the most powerful tools to study the protein dynamics. In this study, we use quasielastic neutron scattering (QENS) at the Spallation Neutron Source, ORNL, to study relaxational dynamics of two structurally different proteins — hen egg white lysozyme and an inorganic pyrophosphatase from a hyperthermophile, in the time range of 10ps to 1ns. We experimentally prove that the slow dynamics of globular proteins can be described by the mode-coupling theory (MCT) that was originally developed for glass-forming molecular liquids. The MCT predicts the appearance of a logarithmic decay for a glass-forming liquid. Such dynamic behavior is also observed by recent molecular dynamics (MD) simulations on protein molecules. In addition, we compare the temperature dependence of the dynamics of the two proteins with completely different activity profiles. Our results greatly help understanding the relation between protein dynamics and their biological functions.

¹This research is supported by the U.S. Department of Energy, managed by UT-Battelle, LLC, under contract no. DE-AC05-00OR22725.

9:36AM P40.00009 Intrinsic Mean Square Displacement in Proteins, DERYA VURAL, HENRY R. GLYDE, Department of Physics and Astronomy, University of Delaware — The dynamics of biological molecules is investigated in neutron scattering experiments, in molecular dynamics simulations, and using analytical theory. Specifically, the mean square displacement (MSD), $\langle r^2 \rangle_{exp}$, of hydrogen in proteins is determined from measurements of the incoherent elastic neutron scattering intensity (ENSI). The MSD, $\langle r^2 \rangle_{exp}$, is usually obtained from the dependence of the ENSI on the scattering wave vector Q . The MSD increases with increasing temperature reaching large values at room temperature. Large MSD is often associated with and used as an indicator of protein function. The observed MSD, however, depends on the energy resolution of the neutron spectrometer employed. We present a method, a first attempt, to extract the intrinsic MSD of hydrogen in protein from measurements, one that is independent of the instrument resolution. The method consists of a model of the ENSI that contains (1) the intrinsic MSD, (2) the instrument resolution width and (3) a parameter describing the motional processes that contribute to the MSD. Several examples of intrinsic MSDs $\langle r^2 \rangle$ in proteins obtained from fitting to data in the existing literature will be presented.

9:48AM P40.00010 Scaling Behavior in Twisted, Helical and Undulating Lysozyme Amyloid Fibrils, RAFFAELE MEZZENGA, CECILE LARA, JOZEF ADAMCIK, IVAN USOV, SOPHIA JORDENS, ETH Zurich — We combine atomic force microscopy single-molecule statistical analysis with polymer physics concepts to study the molecular conformations of lysozyme amyloid fibrils. We use different denaturation conditions to yield amyloid fibrils of different types. At 90 °C and pH2, highly laminated twisted and helical ribbons are found, in which as many as 17 protofilaments pack laterally for a total width approaching 180 nm. In the case of 60 °C and pH2, we find thin, wavy fibrils, in which the scaling behavior varies at multiple length scales. We use bond and pair correlation functions, end-to-end distribution and worm-like chain model to identify 3 characteristic length scales. At short length scales there is a first bending transition of the fibrils, corresponding to a bending length L_b . At slightly larger length scales ($>2L_b$), the fibrils become pseudoperiodic and start to undulate. Finally, at length scales larger than the persistence length L_p , the fibrils become flexible and are well described by a 2D self-avoiding random walk. We interpret these results in terms of the periodic fluctuations of the cross-section orientation of the fibrils (twisting) and the impact these have on the area moment of inertia and the corresponding propensity of the fibrils to bend.

10:00AM P40.00011 Probing Volume Changes and the Intracellular Water in Single Erythrocytes, SANGHOON PARK, SILKI ARORA, JENNIFER MAUSER, DEBOPAM CHAKRABARTI, ALFONS SCHULTE, University of Central Florida — In the living cell, water is one of the most abundant substances, and cells have developed very efficient machinery for transporting water in and out. Erythrocytes can undergo large, but reversible, volume changes under hydrostatic pressure and a possible mechanism may involve transport of water. We employ confocal micro-Raman spectroscopy over the frequency range from 150 to 4000 cm^{-1} to probe both the intracellular hemoglobin and water in individual red blood cells under physiological conditions. We investigate changes in the OH stretch bands near 3400 cm^{-1} due to the cellular water. Results of experiments that employ variations in external parameters such as pressure will be presented.

10:12AM P40.00012 Effects of pressure on the protein barrel and the chromophore interactions in mCherry, YUBA BHANDARI, PREM CHAPAGAIN, CHOLA REGMI, BERNARD GERSTMAN, Florida International University — Fluorescent proteins (FP) can be attached to proteins of interest, which makes it possible to study the movement, localization and many other physiological processes of the tagged proteins. A number of fluorescent proteins have been genetically engineered to enhance their intensity, photo-stability, pH-stability etc. The structural fluctuations of FPs determine the ease of access of small molecules like oxygen and may be an important consideration for their fluorescence spectrum and stability. A protein's response to pressure perturbations provides useful insights for understanding their folding and dynamics. Experiments have shown that application of pressure affects both the fluorescence peak as well as the quantum yield of the protein. We report on molecular dynamics computational investigations of the effect of pressure on the fluctuations of the beta barrel and the structure of the chromophore of a well characterized Red Fluorescent Protein, mCherry. We discuss our results on how pressure affects the ability of water and other ions to penetrate the barrel to reach the chromophore, as well as the effect on the time dependent hydrogen bonding network in the chromophore's cavity region.

10:24AM P40.00013 Thermal response of proteins (histone H2AX, H3.1) by a coarse-grained Monte Carlo simulation with a knowledge-based phenomenological potential¹, MIRIAM FRITSCHKE, DIETER HEERMANN, University of Heidelberg, Germany, RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — Using a coarse-grained bond fluctuating model, we investigate structure and dynamics of two histones, H2AX (143 residues) and H3.1 (136 residues) as a function of temperature (T). A knowledge based contact matrix is used as an input for a phenomenological residue-residue interaction in a generalized Lennard-Jones potential. Metropolis algorithm is used to execute stochastic movement of each residue. A number of local and global physical quantities are analyzed. Despite unique energy and mobility profiles of its residues in a specific sequence, the histone H3.1 appears to undergo a structural transformation from a random coil to a globular conformation on reducing the temperature. The radius of gyration of the histone H2AX, in contrast, exhibits a non-monotonic dependence on temperature with a maximum at a characteristic temperature (T_c) where crossover occurs from a positive (stretching below T_c) to negative (contraction above T_c) thermal response on increasing T . Multi-scale structures of the proteins are examined by a detailed analysis of their structure functions.

¹This work is supported by the Air Force Research Laboratory.

Wednesday, February 29, 2012 8:00AM - 10:48AM —
Session P41 DFD: Drops, Bubbles and Interfacial Fluid Mechanics 156B

8:00AM P41.00001 The Life and Death of the Air Film Beneath an Impacting Drop , JOHN KOLINSKI, Harvard School of Engineering and Applied Sciences, Cambridge, MA, USA, SHMUEL RUBINSTEIN, Weizmann Institute of Science, Physics of Complex Systems, Rehovot, Israel, L. MAHADEVAN, Harvard School of Engineering and Applied Sciences, Cambridge, MA, USA — Droplet impact is ubiquitous in our everyday experience; yet many mysteries associated with the phenomenon remain, including the role played by air during the impact process. When a liquid meets a solid surface in an atmosphere, it must drain the air beneath it before initiating contact. In spite of the relatively low viscosity of the air, recent experiments and simulations suggest that this drainage dominates the dynamics of drop impact. Here I present recent experimental work, wherein Total Internal Reflection (TIR) microscopy is used to directly observe the thin air films that develop above the impact surface. We find that the formation of the thin air film is insensitive to liquid viscosity over a range of impact velocities, confirming prior theoretical predictions of thin air film formation. Going beyond this, the viscous response of the drop is also found to be important - high viscosity liquids maintain a steep front that progresses outward as the breadth of the air film increases, whereas lower viscosity liquids broaden without a steep front, suggesting a transition in the kinematics of the air liquid interface.

8:12AM P41.00002 Manipulating Leidenfrost temperature with surface modification , HYUK-MIN KWON, Massachusetts Institute of Technology, JACY BIRD, Boston University, KRIPA VARANASI, Massachusetts Institute of Technology — When a drop contacts a surface that is at a sufficiently high temperature, the drop can float on it's own vapor in a process known as the Leidenfrost effect. Although it is known that the critical temperature needed to achieve this effect depends on the properties of the drop and its vapor, often these parameters are fixed for a particular process. Here, we demonstrate a new way to control the critical temperature through the surface structure.

8:24AM P41.00003 Reducing contact time of drops on superhydrophobic surfaces , R. DHIMAN, J.C. BIRD, H. KWON, K.K. VARANASI, Massachusetts Institute of Technology — When water drops impact on to a superhydrophobic surface, the drops can recoil to such an extent that they completely bounce off the solid material. The time it takes for the drop to spread and recoil the contact time scales with the hydrodynamic inertial-capillary timescale. However, there is evidence that the coefficient of this scaling depends on surface-structure interactions, such as pinning. Here we investigate how surface interactions can influence droplet contact time, and we compare our results to existing models. We highlight an assumption in the current theory that imposes a lower-bound on the contact time. By designing around this constraint, we demonstrate novel superhydrophobic surfaces on which water droplets impact with shorter contact times than previously thought possible.

8:36AM P41.00004 Hydrodynamic self-rectification: A novel mechanism for generating uniform static droplet arrays , SIVA VANAPALLI, SWASTIKA BITHI, MENG SUN, Texas Tech University — Microfluidic static droplet arrays are a powerful means to simultaneously monitor many biochemical reactions in individual drops. We report a new mechanism for generating exceptionally monodisperse microfluidic droplet arrays. When a train of surfactant-free confined droplets are introduced into a fluidic network with hydrodynamic traps, the droplets are immobilized in the traps due to collective hydrodynamic resistive interactions. In the event, that an immobilized drop either under-fills or overfills the trap, we find that subsequent drops rectify its volume through coalescence, followed by break-up. This self-rectification mechanism thus yields highly monodisperse static droplet arrays. We map the phase space in terms of drop size, spacing and capillary number and find a broad window where this mechanism operates. Because this mechanism alleviates the need to control drop size and spacing in the train to create arrays, we demonstrate its capability to create static arrays with tuneable drop volumes and variable composition.

8:48AM P41.00005 In Situ Observation of Liquid Capillary Bridges on Superhydrophobic Surfaces , ADAM PAXSON, SUSHANT ANAND, KRIPA VARANASI, MIT — We describe a new technique for observing the dynamic behavior of the contact line of a liquid droplet on a superhydrophobic surface using environmental scanning electron microscopy. We find that on a surface patterned with an array of superhydrophobic micropillars, the receding contact line exhibits discrete hierarchical de-pinning events. As the macroscopic contact line recedes across the pillars, capillary bridges are formed along with microscale contact lines, thus perpetuating a self-similar wetting condition. We are able to measure the local receding angle and find that it follows the Gibbs criterion of depinning. By considering the line density of the microscale features and the pinning strength of each of those features, we relate the macroscopic adhesion force to that derived from a model based on pinning of the capillary bridges.

9:00AM P41.00006 Two particle microrheology of quasi-2D viscous systems in the limit of shallow bulk layer , THIBAUT DIVOUX, Ecole Normale Supérieure de Lyon, 46 allée d'Italie, 69007 Lyon, France, KENNETH DESMOND, JAMES SEBEL, ERIC WEEKS, Department of Physics, Emory University, Atlanta, Georgia 30322, USA — Human serum albumin (HSA) protein molecules at an air-water interface is a model system for which it is difficult to decouple the properties of the 2D interfacial film from those of the 3D fluid. Here we focus on the influence of the bulk confinement (i.e. the thickness of the layer of water) on the dynamics of HSA at an air-water interface. To do so, we have developed a setup which allows us to control the depth of the water layer over which HSA protein molecules are dispersed. In particular, we investigate the limit of shallow layers, for which we report measurements of the spatially correlated motion of colloidal particles embedded at the interface, for different surface viscosities. We describe the influence of the bulk finite size on the behaviour of the spatial correlation functions of the particle motion, and extend the description of the correlation functions in terms of a master curve first obtained for large bulk volumes, to the limit of shallow layers.

9:12AM P41.00007 Measuring interfacial viscosity using macro- and micro-rheology , JAMES SEBEL, KENNETH DESMOND, ERIC R. WEEKS, THIBAUT DIVOUX, Emory University — We measure the viscous moduli of thin films using two different methods. First, we use a magnetic needle viscometer. Our apparatus employs Helmholtz coils to control the position and orientation of the needle in the film. By driving the needle we can produce a response in the film which allows us to probe the bulk viscous properties of the film. Second, we use single particle microrheology to probe the local properties of the film. Tracking the mean-squared displacement of particles as they undergo Brownian motion probes the local viscous properties of any heterogeneous domains. Coupling this technique with the magnetic needle viscometer provides information on the effect local viscous properties have on the bulk properties.

9:24AM P41.00008 Molecular Modeling of Three Phase Contact for Static and Dynamic Contact Angle Phenomena , ATEEQUE MALANI, Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, MIGUEL AMAT, Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ, ANILKUMAR RAGHAVANPILLAI, E.I. du Pont de Nemours, Wilmington, DE, ERNEST WYSONG, Experimental Section, E.I. du Pont de Nemours, Wilmington, DE, GREGORY RUTLEDGE, Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA — Interfacial phenomena arise in a number of industrially important situations, such as repellency of liquids on surfaces, condensation, etc. In designing materials for such applications, the key component is their wetting behavior, which is characterized by three-phase static and dynamic contact angle phenomena. Molecular modeling has the potential to provide basic insight into the detailed picture of the three-phase contact line resolved on the sub-nanometer scale which is essential for the success of these materials. We have proposed a computational strategy to study three-phase contact phenomena, where buoyancy of a solid rod or particle is studied in a planar liquid film. The contact angle is readily evaluated by measuring the position of solid and liquid interfaces. As proof of concept, the methodology has been validated extensively using a simple Lennard-Jones (LJ) fluid in contact with an LJ surface. In the dynamic contact angle analysis, the evolution of contact angle as a function of force applied to the rod or particle is characterized by the pinning and slipping of the three phase contact line. Ultimately, complete wetting or de-wetting is observed, allowing molecular level characterization of the contact angle hysteresis.

9:36AM P41.00009 Nonlinear electrohydrodynamics of a viscous droplet, PAUL SALIPANTE, PETIA VLAHOVSKA, Brown University — A classic result due to G.I.Taylor is that a drop placed in a uniform electric field adopts a prolate or oblate spheroidal shape, the flow and shape being axisymmetrically aligned with the applied field. We report an instability and transition to a nonaxisymmetric rotational flow in strong fields, similar to the rotation of solid dielectric spheres observed by Quincke in the 19th century. Our experiments reveal novel droplet behaviors such as tumbling, oscillations and chaotic dynamics even under creeping flow conditions. A phase diagram demonstrates the dependence of these behaviors on drop size, viscosity ratio and electric field strength. The theoretical model, which includes anisotropy in the polarization relaxation, elucidates the interplay of interface deformation and charging as the source of the rich nonlinear dynamics.

9:48AM P41.00010 Breakup of Bubbles or Drops by Capillary Waves Induced by Coalescence or Other Excitations, FENG HUA ZHANG, Singapore-MIT Alliance, National University of Singapore, Singapore, PETER TABOREK, Department of Physics and Astronomy, University of California, Irvine, USA, JUSTIN BURTON, James Franck Institute, University of Chicago, Chicago, USA, BOO CHEONG KHOO, Singapore-MIT Alliance, National University of Singapore, Singapore, SIGGI THORODDSEN, King Abdullah University of Science and Technology, Saudi Arabia — Capillary breakup of a bubble or drop by various excitations is ubiquitous in both nature and technology. Examples include coalescence with another bubble or drop, wetting on a solid surface, impact on a solid surface, detachment from a nozzle, or vibrations driven by acoustic, electrical, or magnetic fields. When the excitation ceases, capillary forces on the surface naturally drive the deformed bubble or drop to recover its spherical shape. However, when the viscosity is small, this recovery can lead to nonlinear oscillations of the interface and a singularity in the flow. Here we use high-speed imaging to investigate the coalescence of bubbles and drops of various sizes. In many cases, coalescence leads to pinch-off events and the formation of the satellite and sub-satellite. Our experiments use pressured xenon gas in glycerol/water mixtures so that the density ratio and viscosity ratio can be varied over many orders of magnitude. We characterize the generation, propagation, and convergence of capillary waves, the formation time and sizes of satellites, and the dynamics of two-fluid pinch-off as a function of the density ratio and viscosity ratio. The work shall benefit the wide-spread applications and fulfill the scientific and public curiosities.

10:00AM P41.00011 Thermo-actuated migration in a micro-system, MARIE-CAROLINE JULLIEN, UMR 7083 CNRS ESPCI, BERTRAND SELVA, Unité Mixte Rhodia CNRS 5258, ISABELLE CANTAT, Université de Rennes 1, MMN, LABORATOIRE GULLIVER TEAM, LOF TEAM, INSTITUT DE PHYSIQUE DE RENNES TEAM — Digital microfluidics require element displacement by simple means featuring high integration rates. Within this context, the transport and handling of elements constitutes a problem [Squires and Quake, 2005]. This context has rekindled interest in the Marangoni surface effect, which refers to tangential stresses along an interface. Producing a surface tension gradient by imposing a temperature gradient is especially efficient and easy to control. In a recent paper, we have shown [Selva et al., Phys. Fluids (2011)] that a bubble undergoing a constant temperature gradient is indeed set into motion. However, the direction of motion (toward the cooler side) is in contradiction with experiments performed at the millimetre scale in which bubble migration is driven towards hotter regions. We believe this observation is due to the PDMS deformability. Indeed, PDMS expands when the temperature increases. A temperature gradient inside a microsystem results in a cavity thickness gradient, and thus leads to the bubble travelling towards the thicker part of the cavity. The physical phenomena involved in such a system are multifaceted (PDMS dilation, thermocapillarity, solutocapillarity) and may have either complementary or opposite effects depending on the experimental conditions.

10:12AM P41.00012 Towards an effective surface tension at a foam/water interface¹, HERVE CAPS, ARIANE BRONFORT, CHARLES DUBOIS, GILES DELON, GRASP - University of Liege — Foams are defined as assemblies of gas bubbles immersed into a continuous liquid phase. Depending on the ration between the total volume occupied by the foam and the amount of liquid inside the foam, different rheological behaviors are observed. Beside the numerous studies on the foam's bulk behavior, poor is known concerning the interface between a foam and the liquid bath it has been generated from. This interface is however separating two identical liquids where, one of these, also contained a dispersed phase. Our studies aim in describing this interface in terms of an effective surface tension, while considering the foam as a continuous medium. Monodisperse foams are produced in Hele-Shaw cells and the features of the boundary between the foam and the baliquid pool is studied by means of hydrodynamical instabilities. Namely, Faraday waves, Rayleigh-Taylor instability and Saffmann-Taylor fingering are considered. Among these instabilities, the shearing of the interface is studied within a rotating drum experiment, similarly to the granular case.

¹ESA MAP - FNRS-FRS - Belspo Prodex

10:24AM P41.00013 Continuous dielectrophoretic centering of compound droplets, GREG RANDALL, BRENT BLUE, General Atomics — Compound droplets, or droplets-within-droplets, are traditionally key components in applications ranging from drug delivery to the food industry. Presently, millimeter-sized compound droplets are precursors for foam shell targets in inertial fusion energy work. A key constraint is a uniform foam shell thickness, which in turn requires a centered core in the compound droplet precursor. Previously, Bei et al. (2009, 2010) have shown that compound droplets could be centered in a static fluid using an electric field of 0.7 kV/cm at 20 MHz. To apply centering to existing or future applications, it is imperative to develop a continuous droplet centering process by overcoming the additional complications from motion. Here, we present analysis and experimental data of a continuous droplet centering device that uses an electric field to force a core droplet to the center of a moving compound drop. Our analysis focuses on how interfacial rheology and electrohydrodynamic flows affect the centering dynamics and droplet deformation. Proof-of-principle experiments are performed in a vertical channel using buoyancy to drive a solution of compound droplets stabilized with phospholipid and protein emulsifiers through a kV/cm electric field.

10:36AM P41.00014 The Dynamics of Coupled Droplets Under Gravity Condition, HAIDER HEKIRI, TAKUMI HAWA, School of Aerospace and Mechanical Engineering, The University of Oklahoma — The dynamics of a two-dimensional, incompressible, and two coupled spherical-cap water droplets pinned in a straight channel is investigated under gravity condition through the use of CFD. Since the capillary length is three times as large as the channel width, the effect of gravity is small but not negligible. In this simulations FLUENT with a 2-D pressure based solver is utilized. The suspended droplet states are measured by the location of the center of mass of the droplet. Under no gravity condition we find that there is a critical volume, V_c , where a bifurcation of asymmetric states occurs. However, gravity changes the pitchfork bifurcation diagram of coupled droplets systems into two separate branches of equilibrium states. The primary branch describes a gradual and stable change of the droplet states from symmetric to non-symmetric as V is increased across V_c . The secondary branch appears at a certain modified critical volume, V_{mc} , and describes two additional non-symmetric states for $V > V_{mc}$. CFD demonstrated that the large-amplitude state along the secondary branch is stable whereas the small-amplitude states are unstable.

Wednesday, February 29, 2012 8:00AM - 11:00AM –
Session P42 DBIO GSNP: Focus Session: Evolutionary Systems Biology II - From molecules to cells 156C

8:00AM P42.00001 Statistical Physics Approaches to RNA Editing¹ , RALF BUNDSCHUH, Ohio State University — The central dogma of molecular Biology states that DNA is transcribed base by base into RNA which is in turn translated into proteins. However, some organisms edit their RNA before translation by inserting, deleting, or substituting individual or short stretches of bases. In many instances the mechanisms by which an organism recognizes the positions at which to edit or by which it performs the actual editing are unknown. One model system that stands out by its very high rate of on average one out of 25 bases being edited are the *Myxomycetes*, a class of slime molds. In this talk we will show how the computational methods and concepts from statistical Physics can be used to analyze DNA and protein sequence data to predict editing sites in these slime molds and to guide experiments that identified previously unknown types of editing as well as the complete set of editing events in the slime mold *Physarum polycephalum*.

¹This presentation is based on work supported by the National Science Foundation under grant number DMR-0706002.

8:36AM P42.00002 Biophysical Models of Evolution: Application to Transcription Factor Binding Sites in Yeast , MICHAEL MANHART, ALLAN HALDANE, ALEXANDRE MOROZOV, Rutgers University — There has been growing interest in understanding the physical driving forces of evolution at the molecular scale, in particular how biophysics determines the fitness landscapes that shape the evolution of DNA and proteins. To that end we study a model of molecular evolution that explicitly incorporates the underlying biophysics. Using population genetics, we derive a steady-state distribution of monomorphic populations evolving on an arbitrary fitness landscape. Compared to previous studies, we find this result is universal for a large class of population models and fully incorporates both stochastic effects and strong natural selection. This distribution can then be used to infer the underlying fitness landscape from genomic data. This model can be applied to a variety of systems, but we focus on transcription factor binding sites, which play a crucial role in gene regulatory networks. Since these sites must be bound for successful gene regulation, we consider a simple thermodynamic model of fitness as a function of the free energy for binding a transcription factor at the site. Using empirical energy matrices and genome-wide sets of binding sites from the yeast *Saccharomyces cerevisiae*, we use this model to infer the role of DNA-protein interaction physics in evolution.

8:48AM P42.00003 The Fitness of Genomic Order¹ , QIUCEN ZHANG, SAURABH VYAWAHARE, ROBERT AUSTIN, Department of Physics, Princeton University — Most bacteria have a single circular chromosome that can range in size from 160,000 to 12,200,000 base pairs. Considering the typical gene density, i.e. 1 gene per 1,000 base pairs, both the number of genes and the ways to arrange are huge. Intuitively, the arrangement of genes on the circle is not important if all of them can be replicated. However, there is typically one origin of replication, and when bacteria is attacked by genotoxic stress during replication, the whole replication process can not be finished. As a result, which gene is replicated first, which is second, ..., becomes very important. Experimentally, we found a broad increase of DNA copy number near the origin of replication (OriC) of bacteria *E.coli* (~3200 genes) under genotoxic stress. Since the genes near OriC are mostly efflux pump genes, we propose that there is fitness advantage for those rapid stress response genes got replicated first, because they can facilitate the replication of the rest of genome. Similar to bacterial evolution to present genomic order, in the somatic evolution of cancer, genomic shuffling was also frequently observed, especially under genotoxic chemotherapy. Such re-arrangement of genome can be viewed as a journey to optimal point in the rugged fitness landscape of genomic order.

¹The research described was supported by Award Number U54CA143803 from the National Cancer Institute.

9:00AM P42.00004 Plasticity of metabolic networks and the evolution of C4 photosynthesis , ELI BOGART, CHRIS MYERS, Cornell University — Over 50 groups of plants have independently developed a common mechanism (C4 photosynthesis) for increasing the efficiency of photosynthetic carbon dioxide assimilation. Understanding the high degree of evolvability of the C4 system could offer useful guidance for attempts to introduce it artificially to other plants. Previously, the nonlinear relationship between carbon dioxide levels and rates of carbon assimilation and photorespiration has prevented the application of genome-scale metabolic models to the problem of the evolution of the pathway. We apply a nonlinear optimization method to find feasible flux distributions in a plant metabolic model, allowing us to explore the plasticity of the metabolic network and characterize the fitness landscape of the transition from C3 to C4 photosynthesis.

9:12AM P42.00005 Uncovering principles of cellular decision-making , GUROL SUEL, UT Southwestern — Cells can cope with unpredictable environmental conditions by differentiating into appropriate states. In this talk, I will present our recent attempts to understand the role of genetic circuits in regulating the underlying process of cellular decision-making. Specifically, we are interested in how interactions within and across genetic circuits enable cells to choose among alternative fates. To address this question my laboratory is employing systems and synthetic biology approaches. Our ultimate goal is to uncover possible evolutionary pressures that may have selected for specific gene circuit architectures, dynamics and noise properties.

9:48AM P42.00006 Role of Multisite Phosphorylation in Timing of a Yeast Cell Cycle Event¹ , VOLKAN SEVIM, University of California, San Francisco, XIAOJING YANG, University of California, San Francisco; Peking University, KAI-YEUNG LAU, University of California, San Francisco, CHAO TANG, University of California, San Francisco; Peking University — We study the biochemical network that triggers the S phase in yeast cell cycle. Key components of this network are three proteins: two kinases and an inhibitor. First kinase, Cln1/2-Cdk, acts as an input signal, phosphorylating the inhibitor, Sic1. The second kinase, Clb5/6-Cdk, is sequestered into an inactive complex by Sic1. Clb5/6-Cdk is the output signal of the circuit. Sic1 has nine phosphorylation sites, and phosphorylation of six or more of them causes it to degrade rapidly, leading to a sharp rise of free Clb5/6-Cdk. Our experiments indicate that multisite phosphorylation (MSP) is responsible for the timing robustness of this sharp transition. We study the role of MSP in timing using computer simulations. Preliminary results indicate that, MSP does not bring timing robustness when each kinase can phosphorylate each site with identical specificity. We employ in silico evolution to find the specificity configuration for the phosphorylation sites that leads to most robust timing under extrinsic noise.

¹ This research was supported in part by Lui Fellowship, Li Foundation, Sandler Family Supporting Foundation, NSF, NIH (P50 GM081879), Ministry of Sci. and Tech. of China (2009CB918500) and Natl. Natural Sci. Foundation of China

10:00AM P42.00007 Precision of sensing, memory and fluctuating environments , GERARDO AQUINO, ROBERT ENDRES, Division of Molecular Biosciences & Centre for Integrated Systems Biology at Imperial College, Imperial College London — Multiple cell types were recently shown to sense their chemical environment with astonishing accuracy, crucial for nutrient scavenging, mating, immune response, and development. It is currently unknown if this sensing near the single-molecule detection limit is due to highly precise single measurements, or due to learning over time. In this work, we analyze if cell memory can allow cells to sense beyond the current estimates of the fundamental physical limit. By merging Bayesian inference with information theoretic concepts, we derive analytical formulas which show that memory improves sensing in correlated fluctuating environments, but not in strongly uncorrelated environments. Despite many analogies with problem solving strategies in engineering, our theory shows fundamental differences in interpreting noisy stimuli in the microscopic and macroscopic world.

10:12AM P42.00008 Rapidly evolving microorganisms with high biofuel tolerance¹, SAURABH VYAWAHARE, QIUCEN ZHANG, WENDY LANG, ROBERT AUSTIN, Department of Physics, Princeton University, Princeton NJ 08544 — Replacing non-renewable energy sources is one of the biggest and most exciting challenges of our generation. Algae and bacteria are poised to become major renewable biofuels if strains can be developed that provide a high, consistent and robust yield of oil. One major stumbling block towards this goal is the lack of tolerance to high concentrations of biofuels like isobutanol. Using traditional bioengineering techniques to remedy this face the hurdle of identifying the correct pathway or gene to modify. But the multiplicity of interactions inside a cell makes it very hard to determine what to modify a priori. Instead, we propose a technology that does not require prior knowledge of the genes or pathways to modify. In our approach that marries microfabrication and ecology, spatial heterogeneity is used as a knob to speed up evolution in the desired direction. Recently, we have successfully used this approach to demonstrate the rapid emergence of bacterial antibiotic resistance in as little as ten hours. Here, we describe our experimental results in developing new strains of micro-organisms with high oil tolerance. Besides biofuel production, our work is also relevant to oil spill clean-ups.

¹Supported by Award Number U54CA143803 from the National Cancer Institute is gratefully acknowledged

10:24AM P42.00009 A Cahn-Hilliard model of vascularized tumor growth in a complex evolving confinement using a diffuse domain approach¹, YAO-LI CHUANG, University of New Mexico, Dept. Pathology, VITTORIO CRISTINI, University of New Mexico, Dept. Pathology and Dept. Chemical Engineering, YING CHEN, XIANGRONG LI, University of California, Irvine, Dept. Math, HERMANN FRIEBOES, University of Louisville, Dept. Bioengineering, JOHN LOWENGRUB, University of California, Irvine, Dept. Math — Understanding the spatiotemporal evolution of tumor growth is essential for developing effective strategies to treat cancers. Various studies have suggested that spatial heterogeneity during tumors growth is a key factor associated with subsequent tumor invasion and the effectiveness of chemotherapy. Spatial heterogeneity may arise due to morphological instability of the tumors and the complex tissue structure surrounding the tumors. In previous works, we have used a Cahn-Hilliard tumor growth model to study the morphological instability for tumors in non-resisting tissues. However, most tumors are surrounded by complex tissue structures and confined in the capsules of some organs or between certain basement membranes. The capsules and basement membranes may be distorted by interacting with the evolving tumors, affecting the morphological instability. Here we adopt a novel diffuse domain approach to adapt our previous Cahn-Hilliard model for tumor growth in such complex evolving environments. As an example, we apply the model to simulate the evolution of lymphoma in a lymph node, incorporating also the tumor-induced angiogenesis.

¹supported by NIH-PSOC grant 1U54CA143907-01

10:36AM P42.00010 Emergence of Information Transmission in a prebiotic RNA Reactor, BENEDIKT OBERMAYER, Harvard University, HUBERT KRAMMER, DIETER BRAUN, ULRICH GERLAND, LMU Muenchen — A poorly understood step in the transition from a chemical to a biological world is the emergence of self-replicating molecular systems. We study how a precursor for such a replicator might arise in a hydrothermal RNA reactor, which accumulates longer sequences from unbiased monomer influx and random ligation. In the reactor, intra- and intermolecular base pairing locally protects from random cleavage. Analyzing stochastic simulations, we observe a strong bias towards long sequences with complex secondary structures, which would facilitate the emergence of ribozymes. Further, we find temporal sequence correlations that constitute a signature of information transmission, weaker but of the same form as in a true replicator.

10:48AM P42.00011 Towards molecular evolution with thermal traps, CHRISTOF MAST, Systems Biophysics, SEVERIN SCHINK, Arnold-Sommerfeld-Center, HUBERT KRAMMER, Systems Biophysics, BENEDIKT OBERMAYER, Arnold-Sommerfeld-Center, ULRICH GERLAND, Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, LMU Munich, DIETER BRAUN, Systems Biophysics and Center for Nanoscience, LMU Munich — Live evolves by replication and selection of nucleotide polymers. Our experiments aim to drive molecular replication and selection with physical nonequilibrium boundary conditions. We discuss three approaches. Replication Trap. Molecules are exponentially accumulated by a combination of thermophoresis and convection, driven both by the same thermal gradient [1]. We have shown last year that with the help of a polymerase protein, concurrent replication and accumulation is possible [2]. Convection is melting and annealing the DNA in an oscillatory pattern, doubling the DNA in each cycle. Trapped polymerization. The chemical equilibrium of polymerization is expected to shift in the thermal trap. As the trap accumulates the monomers, polymerization yields longer polymers. However, since the trap is exponentially length selective, distributions beyond exponential tails are predicted. Replication by selective degradation. Replication typically is discussed as template directed polymerization. We showed that selective degradation and a thermal trap leads to replication-like behavior using only non templated polymerization [3]. The progression of information is given by the faster degradation of single stranded over double stranded RNA. [1] PNAS 104, 9346 (2007) [2] PRL 104, 188102 (2010) [3] PRL 107, 018101 (2011)

Wednesday, February 29, 2012 8:00AM - 11:00AM –
Session P43 DBIO: Invited Session: High Content Biophysical Data for Dynamic Studies in Cancer 157AB

8:00AM P43.00001 Tissue Refractive Index Fluctuations Report on Cancer Development, GABRIEL POPESCU, University of Illinois at Urbana-Champaign — The gold standard in histopathology relies on manual investigation of stained tissue biopsies. A sensitive and quantitative method for *in situ* tissue specimen inspection is highly desirable, as it will allow early disease diagnosis and automatic screening. Here we demonstrate that *quantitative phase imaging* of entire unstained biopsies has the potential to fulfill this requirement. Our data indicates that the refractive index distribution of histopathology slides, which contains information about the molecular scale organization of tissue, reveals prostate tumors. These optical maps report on subtle, *nanoscale morphological properties* of tissues and cells that cannot be recovered by common stains, including hematoxylin and eosin (H&E). We found that cancer progression significantly alters the tissue organization, as exhibited in our refractive index maps. Furthermore, using the quantitative phase information, we obtained the spatially resolved scattering mean free path and anisotropy factor *g* for entire biopsies and demonstrated their direct correlation with tumor presence. We found that these scattering parameters are able to distinguish between two adjacent grades, which is a difficult task and relevant for determining patient treatment. In essence, our results show that the tissue refractive index reports on the nanoscale tissue architecture and, in principle, can be used as an intrinsic marker for cancer diagnosis.

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8:36AM P43.00002 TBA, NONGJIAN TAO, —

9:12AM P43.00003 Time-lapse Microscopy of Colorectal Tumorigenesis In Vivo, SEOK-HYUN (ANDY) YUN, Harvard Medical School — No abstract available.

9:48AM P43.00004 High Content Bio-Chemo-Mechanical Screening and Modeling to Study Heterogeneity and Metastasis of Cancer for Drug Target Discovery, STEPHEN WONG, The Methodist Hospital Research Institute — No abstract available.

10:24AM P43.00005 The Fluid Phase of Solid Tumors: Real-time Access to Cancer in Individual Patients, PETER KUHN, The Scripps Research Institute — No abstract available.

Wednesday, February 29, 2012 8:00AM - 10:48AM —

Session P44 DPOLY: Focus Session: Block Copolymer Micelles and Polymersomes 157C

8:00AM P44.00001 Modeling of Interactions Between Spherical Micelles for Diblock Copolymers in Selective Solvents, RAGHURAM THIAGARAJAN, DAVID MORSE, Department of Chemical Engineering and Materials Science, University of Minnesota — The self-assembly of spherical micelles formed in systems with a diblock copolymer AB, consisting of a solvent-philic block (B) and a solvent-phobic block (A), in selective solvents (S) is studied here. Effective interactions between spherical micelles for a model system are quantified using self-consistent field modeling in real space, for the dilute regime $\phi_{AB} < 0.2$, as well as using a pseudo-spectral implementation of SCFT, for the concentrated regime $\phi_{AB} > 0.2$. We show that the free energy of BCC, and FCC phases can be described in terms of a single effective pair potential that depends on micelle aggregation number, but the aggregation number changes significantly with concentration as well as temperature.

8:12AM P44.00002 Dissipative particle dynamics study of relationship between wall thickness and size in polymer vesicles¹, MENGYING XIAO, Nanjing University, Institute of Theoretical and Computational Chemistry, Key Laboratory of Mesoscopic Chemistry, RONG WANG, Nanjing University, Department of Polymer Science and Engineering, State Key Laboratory of Coordination Chemistry, DAIQIAN XIE, Nanjing University, Institute of Theoretical and Computational Chemistry, Key Laboratory of Mesoscopic Chemistry — Vesicles and membrane properties have long been thought to be essential for reproducing the natural environment of living cells. By using dissipative particle dynamics method, we have studied the relationship between wall thickness and size of vesicles obtained from A1BnA1 block copolymers, where block A is hydrophilic and block B is hydrophobic. Our findings suggest that, the wall thickness is sensitive to the size of vesicles at a low block length ratio of B/A, but insensitive to the size at a large ratio. It shows both weak and strong effects with a crossover point in between. These behaviors are consistent with the experimental results of Eisenberg and co-workers. Besides, an additional crossover point also has been observed. With the B/A ratio increases, the relationship goes from strong to weak behavior, and this transformation first appears to affect the outer area for large sized vesicles, and then to the inner area for small sized vesicles. These results may also be useful in delivery applications through controlling the hydrophobic membrane and the hydrophilic coronas.

¹This work has been supported by NNSFC (Nos. 20874046, 21074053 and 21133006) and NBRPC (No. 2010CB923303).

8:24AM P44.00003 Effect of Hydrophobic Block Length on Vesicle Formation of Block Copolymers¹, RONG WANG, Nanjing University, Department of Polymer Science and Engineering, State Key Laboratory of Coordination Chemistry, MENGYING XIAO, DAIQIAN XIE, Nanjing University, Institute of Theoretical and Computational Chemistry, Key Laboratory of Mesoscopic Chemistry — Self-assembly of amphiphilic block copolymers result in a wide range of aggregates in aqueous solution, including spheres, rods, lamellae, vesicles, and large compound vesicles with an inverted core-shell structure surrounded by hydrophilic surface. In the work, we carried out a systematic investigation of A1BnA1 triblock copolymers with different hydrophobic block length by using the dissipative particle dynamics (DPD). As the B/A ratio increase further, no well-defined disk-like micelles (bilayer structures) are seen. Spherical micelles rearrange internally and swell the hydrophilic group in the center until vesicles are formed. Because the longer chains appear to drift slowly, it is clear that the rearrangement process becomes slower in the system with longer hydrophobic block, which needs more time to form vesicles. The segregation of A segments (hydrophilic group) leaves in the internal layer when the two small spherical micelles merge into a larger one. We observe that the existence of the two pathways of vesicles formation based on the hydrophobic block length using DPD particle models.

¹This work has been supported by NNSFC (Nos. 20874046, 21074053 and 21133006) and NBRPC (No. 2010CB923303).

8:36AM P44.00004 Nanostructured assemblies from amphiphilic ABC multiblock polymers¹, MARC A. HILLMYER, University of Minnesota — Amphiphilic AB diblock copolymers containing a water compatible segment can self-assemble in aqueous media to give supramolecular structures that include simple spherical micelles and macromolecular vesicles termed polymersomes. Amphiphilic ABA triblocks with hydrophobic end blocks can adopt analogous structures but can also form gels at high polymer concentrations. The structural and chemical diversity demonstrated in block copolymer micelles and gels makes them attractive for applications ranging from drug delivery to personal care products to nanoreactors. The inclusion of a third block in amphiphilic ABC triblock systems can lead to a much wider array of self-assembled structures that depend not only on composition but also on block sequence, architecture and incompatibility considerations. I will present our recent efforts on tuning micelle and gel structure and behavior using controlled architecture ABC triblocks. The combination of diverse polymer segments into a single macromolecule is a powerful method for development of self-assembled structures with both new form and new function.

¹This work was supported primarily by the MRSEC Program of the National Science Foundation under Award Number DMR-0819885.

9:12AM P44.00005 The Morphology of Lipid Aggregates based on the Interplay among Molecular Architectures, Hydrophobic-Hydrophilic and Coulombic Interactions and their Kinetics, MU-PING NIEH, Institute of Materials Science, Department of Chemical, Materials and Biomolecular Engineering, University of Connecticut, Storrs, CT 06269 — Lipids resemble amphiphilic diblock copolymers in the many ways in terms of rich resultant structures, which are controlled by spontaneous curvature and molecular interaction, except that the molecular length scale of interest is smaller. One of the most commonly studied systems is so-called "bicelle" ("bilayered micelle"), which is composed of a long- and a short- chain lipid, spontaneously forming discoidal micelles in aqueous solutions under certain conditions. The lamellae of "bicellar mixtures" have been used as magnetically alignable templates for structural study of membrane-associated proteins since they provide a native bilayered environment for the proteins in study. In this talk, I will summarize how and why a variety of morphology can be obtained from the "bicellar" system based on the molecular architectures (spontaneous curvatures) of the lipids, inter-particle Coulombic interaction and hydrophobic-hydrophilic interaction. Most interestingly, many of these structures are kinetically controlled but have robust formation mechanisms and high stability. Currently, we are particularly interested in how the exchange rate of the lipid molecules affects the kinetics.

9:48AM P44.00006 Phase Behavior and Kinetics of Diblock Copolymer in Selective Solvent¹, JULIAN SPRING, RAMA BANSIL, Boston University — Synchrotron based time-resolved small angle x-ray scattering (SAXS) was used to study the kinetics of the formation of a gyroid phase in solutions of a poly (styrene -isoprene) (SI) diblock copolymer in dimethyl phthalate, a selective solvent for the polystyrene block. Temperature ramp measurements over the range of 70-130C show the transition from hexagonally-packed cylinders (HEX) to Gyroid phase for 75% and 80% (w/v) samples to be 117C and 96C, respectively. Results of temperature jump experiments to different jump depths to examine the kinetics of this transition will be presented. In addition to the Bragg scattering from the ordered phases, we were able to observe the temperature dependence of the diffuse scattering near $q=0$. The temperature dependence of the correlation length shows a crossover from $\sqrt{T}$ near the glass transition for polystyrene to linear in T near the HEX to Gyroid transition. The effect of adding low molecular weight linear homopolymer PS to the samples on the phase behavior will be discussed.

¹This research was supported by NSF-DMR grant no. 0804784.

10:00AM P44.00007 Phase Behavior of Gradient Copolymer Solution, GUNJA PANDAV, University of Texas at Austin, KEITH GALLOW, YUEH-LIN LOO, Princeton University, VENKAT GANESAN, University of Texas at Austin — We study the behavior of amphiphilic linear gradient copolymer chains under poor solvent conditions. Using Bond Fluctuation model and parallel tempering algorithm, we explore qualitative behavior of this class of polymers with varying gradient strength; which is the largest difference in the instantaneous composition along the polymer chain. Under poor solvent conditions, the chains collapse to form micelles. We find a linear dependence of hydrophilic to hydrophobic transition temperature on gradient strength. Systematic analysis of these clusters reveals a strong dependence of micelle properties on gradient strength. Also, we discuss our results with reference to recent experiments on synthesis and cloud point depression in gradient copolymers confirming gradient strength as key parameter in tuning micelle properties.

10:12AM P44.00008 Self-Assembly of Novel Amphiphilic 21-Arm, Star-Like Coil-Rod Diblock Copolymers at Interfaces, ZHIQUN LIN, LEI ZHAO, XINCHANG PANG, CHAOWEI FENG, Georgia Institute of Technology — A series of novel amphiphilic 21-arm, star-like diblock copolymers, poly(acrylic acid)-*b*-poly(3-hexylthiophene) (PAA-*b*-P3HT) based on β -cyclodextrin (β -CD) with well defined molecular architectures and ratio of two chemically distinct blocks were prepared, for the first time, via a combination of quasi-living Grignard metathesis method (GRIM), click reaction, and atom transfer radical polymerization (ATRP). The star-like PAA-*b*-P3HT diblock copolymers consist of hydrophilic coil-like PAA cores and hydrophobic rod-like P3HT shells with narrow molecular weight distribution and controllable molecular weight of each block. Owing to the compact structure, the amphiphilic star-like PAA-*b*-P3HT formed a unimolecular micelle. Vesicles based on these novel amphiphilic star-like, coil-rod diblock copolymers were readily produced at the oil/water interface by crosslinking hydrophilic coil-like PAA cores with a bifunctional crosslinker, ethylenediamine. They also self-assembled into a nanotubular structure at the air/water interface.

10:24AM P44.00009 Formation and Characterization of Anisotropic Block Copolymer Gels, CHYA YAN LIAW, DERK JOESTER, WESLEY BURGHARDT, KENNETH SHULL, Northwestern University — Cylindrical micelles formed from block copolymer solutions closely mimic biological fibers that are presumed to guide mineral formation during biosynthesis of hard tissues like bone. The goal of our work is to use acrylic block copolymers as oriented templates for studying mineral formation reactions in model systems where the structure of the underlying template is well characterized and reproducible. Self-consistent mean field theory is first applied to investigate the thermodynamically stable micellar morphologies as a function of temperature and block copolymer composition. Small-angle x-ray scattering, optical birefringence and shear rheometry are used to study the morphology development during thermal processing. Initial experiments are based on a thermally-reversible alcohol-soluble system that can be converted to an aqueous gel by hydrolysis of a poly(*t*-butyl methacrylate) block to a poly(methacrylic acid) block. Aligned cylindrical domains are formed in the alcohol-based system when shear is applied in an appropriate temperature regime, which is below the critical micelle temperature but above the temperature at which the relaxation time of the gels becomes too large. Processing strategies for producing the desired cylindrical morphologies are being developed that account for both thermodynamic and kinetic effects.

10:36AM P44.00010 Stimuli-responsive block copolypeptides, VENKATA KRISHNA KOTHARANGANNAGARI, University of Fribourg, ANTONI SANCHEZ-FERRER, ETH Zurich, JANNE RUOKOLAINEN, Aalto University, RAFFAELE MEZZENGA, ETH Zurich — Stimuli-responsive polypeptide block copolymers are appealing systems due to the morphological polymorphic states they can exhibit in selective solvents, including micelles, vesicles, fibrils, and more complex supramolecular aggregates. Their morphologies can be engineered a-priori by the relative block lengths, the solvent composition, and their concentration. However controlling the morphology upon external stimuli offers clear benefits, since changes in structure and morphology can be induced on demand. In this talk, we present two examples of stimuli-responsive block copolypeptides: in a first case, a photoresponsive PLGA-PEO diblock is discussed capable to reversibly undergo micellization-dissolution-micellization upon visible or UV light exposure, due to spiropyran units decorating the PLGA block; in the second case a PBLG-PDMS-PBLG triblock copolymer undergoing reversible thermal-induced organogelation is also presented. The changes in morphology are correlated, in both cases to the variations in molecular conformations of the polypeptide blocks.

Wednesday, February 29, 2012 8:00AM - 11:00AM – Session P45 DPOLY: Surfaces, Interfaces, and Polymeric Thin Films - Surface Instabilities 159

8:00AM P45.00001 Buckling in a particle film, ANDREW CROLL, Department of Physics, North Dakota State University — When a thin rigid plate is adhered to a soft substrate and compressed, the plate will buckle out of plane to accommodate the applied stress. The out of plane bending is resisted by the substrate and the result is a sinusoidal topography (wrinkles). When the plate is replaced by a collection of closely packed particles similar phenomena results – the positions of the particles move out of plane and follow a roughly sinusoidal curve. Due to the similarity of the end state of each system, the same continuum theory is often applied to model the behaviour. Here, we use a carefully constructed experimental system consisting of micron-scale polymer and silica spheres on a PDMS elastomer substrate to demonstrate the physical differences between a continuum plate and a discrete set of particles. In particular, because we can easily track the position of each particle in three dimensions with confocal microscopy, we have access to all of the particle motion. We note that the wrinkling is independent of particle modulus, and highly dependent on particle packing. This leads us to suggest that the underlying physics is granular (and not continuum) in nature. This result may have implications in biology, where elastic continua are often made of discrete building blocks (e.g. cells).

8:12AM P45.00002 Defect induced shape instabilities in textured Membranes, DANIEL A. VEGA, Dep. of Physics, IFISUR, Univ. Nac. del Sur. Conicet, Argentina, MARCÉLO A. VILLAR, Dep. of Chem. Eng. PLAPIQUI, Univ. Nac. del Sur. Conicet, Argentina, ALDO D. PEZZUTTI, Dep. of Physics, IFISUR, Univ. Nac. del Sur. Conicet, Argentina — We study the dynamics of defect annihilation and quasi-equilibrium configurations in flexible textured membranes suffering a symmetry breaking phase transition. The phase separation process and relaxational properties are described through a Brazovskii-Helfrich-Canham Hamiltonian. Topological defects favor the development of local curvature to geometrically screen out the intrinsic stress field generated by the perturbations to the low symmetry phase. While in hexagonal systems the unbinding of dislocations and Carraro-Nelson interactions between disclinations slow down the dynamics, in smectic systems we found a wrinkled state where the bending forces are balanced by the out-of-plane hoop stretching generated by positive disclinations. The wrinkled configuration found in the smectic systems show features that resemble those found in flexible thin films under small external loads.

8:24AM P45.00003 Dewetting Dynamics from Polymer Interfaces, ANDREI FLUERASU¹, Brookhaven National Laboratory, LAURENCE LURIO², Department of Physics, Northern Illinois University, JYOTSANA LAL³, Argonne National Laboratory — The dewetting dynamics from metastable polymer/polymer interfaces is studied using X-ray Photon Correlation Spectroscopy (XPCS). In addition to more “usual” situations where XPCS correlation functions are used to measure out-of-plane height fluctuations (e.g. capillary waves), we show how this novel method can be used to measure in-situ in-plane motion of the dewetting film. The experimental correlation functions associated with this motion are fitted remarkably well by a simple model considering the growth of dewetting rims in the beam footprint.

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8:36AM P45.00004 Nanoscale Confinement Induced Control of Polymer Thin Film Instabilities, DIYA BANDYOPADHYAY, ARVIND MODI, ALAMGIR KARIM, Department of Polymer Engineering, The University of Akron, Akron, OH 44325 — Control of stability and wettability of polymer thin films is invaluable to a range of functional coatings with applications from electronics to biomedical coatings, yet simple non-chemical modification strategies to accomplish this are generally lacking. We demonstrate a novel route to effectively control instabilities in model polystyrene films on partially wetting and non-wetting solid substrates that would otherwise lead to film dewetting. The method involves top down confining capillary force lithography at various length scales. Systematic experimental studies on silicon and silicon oxide substrates supported by analytical theory shows that for confining pattern wavelengths less than ~ 10 times film thickness, stabilizing surface tension forces dominate the overall energy balance of the system giving rise to stable films under confinement. Interestingly, thermal annealing at elevated temperatures after removal of confinement does not revert to growth of longer instability modes and stability of PS films is retained. These results pave the way for important new technological applications of otherwise unstable polymer films.

8:48AM P45.00005 The influence of the solid/liquid interface on the dewetting of ultra thin polymer films, MATTHIAS LESSEL, MISCHA KLOS, Experimental Physics, Saarland University, OLIVER BAEUMCHEN, Dept. of Physics & Astronomy, McMaster University, KARIN JACOBS, Experimental Physics, Saarland University — In recent years, many studies showed that a thin liquid film on a solid surface in air bears more complexity than expected from a simple three-layer-system: e.g. a highly mobile surface layer in case the liquid is an unentangled polystyrene (PS) melt (Yang et al., *Science* 2010; Seemann et al., *J. of Polym. Sci.* 2006) or the PS melt can slip over the solid substrate (Baumchen et al., *PRL* 2009). Our study focuses on such phenomena and explores their influence on dewetting (speed, morphology, etc.). We use hydrophilic and -phobic Si wafer (either covered by a highly ordered silane layer or by a thin layer of an amorphous fluoropolymer, AF 1600). On each of the substrates, one expects for a certain set of parameters spinodal dewetting for the PS melt. Yet experimentally, a much higher hole density is observed for both types of hydrophobic wafers than is theoretically expected. Moreover, the two hydrophobic coatings induce different dewetting speeds: the PS melt dewets faster on the silane covered Si wafer. The difference is attributed to slip (silane) or to no slip (AF 1600) conditions at the PS/substrate interface, which is also observable in the type of liquid front profile, which in turn changes the dewetting morphology.

9:00AM P45.00006 Viscoelastic properties of ultrathin polystyrene films by dewetting from liquid glycerol¹, JINHUA WANG, GREGORY MCKENNA, Department of Chemical Engineering, Texas Tech University, Lubbock, Texas, 79409 — There is considerable interest in studying the behaviors of polymers at the nanoscale. A liquid dewetting device originally proposed by Bodiguel and Fretigny^[1] was built in our lab to study the size effect on the viscoelastic behaviors of ultrathin polystyrene (PS) films. PS with molecular weight of 278 kg/mol and 984 kg/mol and various thermal treatments were examined. The glass transition temperature (T_g) reduction and film stiffening were observed in films less than 20 nm in thickness and the properties of ultrathin PS films are different from the bulk PS. The value of the plateau compliance changes linearly with film thickness. No molecular weight effect was found on the liquid dewetting behaviors of these PS films. Interestingly, even though the dewetting occurs on liquid glycerol, the apparent T_g reductions are less than observed in SiO₂ substrate supported films.

[1] H. Bodiguel and C. Fretigny, “Viscoelastic dewetting of a polymer film on a liquid substrate,” *Eur.Phys. J. E.*, 19, 185-193 (2006).

¹The authors thank the National Science Foundation under grant DMR-0804438 for support of this work.

9:12AM P45.00007 Evolution of non-equilibrium entanglement networks in spincoat thin polymer films, KARI DALNOKI-VERESS, JOSHUA MCGRAW, PAUL FOWLER, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1 — Measuring the rheology of non-equilibrium thin polymer films has received significant attention recently. Experiments are typically performed on thin polymer films that inherit their structure from spin coating. While the results of several rheological experiments paint a clear picture, details of molecular configurations in spincoat polymer films are still unknown. Here we present the results of crazing measurements which demonstrate that the effective entanglement density of thin polymer films changes as a function of annealing toward a stable equilibrium value. The effective entanglement density plateaus with a time scale on the same order as the bulk reptation time.

9:24AM P45.00008 Evolution of Chitosan Film Thickness Profiles During Spincoating, CHRISTOPHER MURRAY, Lakehead University Orillia, MAXIMILIANO GIULIANI, JOHN DUTCHER, University of Guelph — Many hygroscopic biopolymers can be processed using aqueous solutions. For example, biopolymer films can be prepared by spincoating from dilute biopolymer solutions. We have spincoated ultrathin films of chitosan onto silicon substrates under controlled relative humidity (RH) using acetic acid solutions. Since the solvent is much less volatile than organic solvents that are typically used to spincoat thin films of synthetic polymers, the dynamics associated with the spincoating process can be several orders of magnitude slower. Because of the slow evaporation of the solvent, it is possible to control the thickness by controlling the RH value in the spincoating chamber. To gain insight into the spincoating process, we have collected images of the film during spincoating using a high-speed camera. This has allowed us to determine the evolution of the radial profile of the chitosan film thickness, which can be correlated with the final film thickness values measured using ellipsometry. We compare the measured film thickness profiles with those predicted by theoretical models of spincoating.

9:36AM P45.00009 Spreading of polymer droplets on thin polymer films, SARA L. CORMIER, JOSHUA D. MCGRAW, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1 — We present experimental results of small ($r \sim 10 \mu\text{m}$) polystyrene droplets spreading on thin polystyrene films. Previous experimental work has extensively explored droplets spreading on various types of solid substrates. However, to our knowledge, micron-sized liquid droplets spreading on the same liquid substrate have not been previously studied due to the difficulty of preparing such a geometry. Initially a glassy droplet is placed atop a glassy thin film and a distinct interface exists, upon heating the interface heals quickly. During spreading we must thus consider not only the flow of the polymer droplet but also that of the supporting film. This droplet-on-liquid geometry is fundamentally different from previous studies and allows us to probe the nanorheology of thin polymer films. We observe a characteristic power law spreading that is dependent on the size of the droplet as well as the height of the substrate film. The preparation and study of such samples provides many opportunities because the droplet and supporting film may be of the same polymer, the same polymer but differing molecular weight, or two different polymers.

9:48AM P45.00010 Experimental Study of Particle Behavior on a Curved Polymer Interface¹

KATHLEEN MCENNIS, CHUAN ZENG, BENNY DAVIDOVITCH, ANTHONY D. DINSMORE, THOMAS P. RUSSELL, University of Massachusetts Amherst — A spherical particle bound to an anisotropically curved liquid interface, such as a cylinder or catenoid, cannot maintain a constant contact angle without deforming the interface. Theory predicts that because of this deformation, individual particles will experience a capillary force toward lower negative Gaussian curvature. To test this prediction, particles are deposited from suspension onto interfaces of non-uniform shape. Melted polystyrene (PS) confined on chemically patterned surfaces creates semi-cylinders a few hundred microns in diameter. Microscopic catenoids are created by placing a melted PS film in an electric field. After cooling, PS vitrifies and the particles are frozen in place. The location of particles is observed by optical, scanning electron, and scanning force microscopy (SFM). Particles are observed to migrate to the rims of the catenoids while particles on semi-cylinders cluster, but show no preference for location. At these size scales and particle concentrations, the predicted single-particle behavior is not observed. SFM is used to determine the validity of the assumed constant contact angle boundary condition at the particle's surface. The implication of these results on curvature induced particle assembly will be discussed.

¹We acknowledge support from NSF-supported MRSEC on Polymers at UMass (DMR- 0820506), NSF CBET-0967620, and the U.S. DOE Office of Basic Energy Sciences (DE-FG02-96ER45612).

10:00AM P45.00011 Tension amplification in branched macromolecules

ALEXANDRU BACANU, JAMES BROCK, University of North Carolina at Chapel Hill, SERGEY PANYUKOV, P. N. Lebedev Physics Institute, MICHAEL RUBINSTEIN, University of North Carolina at Chapel Hill — A molecule's topology can greatly affect the distribution of tension within its bonds. Pom-pom molecules consist of a short linear spacer linking two star polymers, each containing z long arms. The striking ability of this molecular architecture to magnify spacer tension in solution by several orders of magnitude, from the pN to the nN level is due to the steric repulsion between densely packed side chains. In fact, the tension can increase to values that significantly alter the molecule's chemical properties, or even initiate the scission of a carbon-carbon covalent bond in the spacer chain. We study the tension distribution in the spacer and in side branches using molecular dynamics simulations and scaling theory. The dependences of observables such as spacer tension and root-mean-square spacer length on the number of side chains, chemical spacer length, and length of side branches have been quantified. Scaling models are used to explain the interrelated phenomena of tension amplification and spacer elongation and to interpret the results of molecular dynamics simulations.

10:12AM P45.00012 Viscous memory effects on the generation of hierarchical morphologies at an emulsified oil/water interface

MELANIE L. MORRIS, MICHAEL C. GROSS, ASMI PANIGRAHI, RYAN M. DEACON, PATRICK CHAN, JASON J. BENKOSKI, Johns Hopkins University Applied Physics Laboratory — A defining feature of biological materials is their fractal morphology. Cancellous bone, pulmonary alveoli, small intestine villi, neural networks, and bladder epithelium are just a few examples of biological structures with hierarchically organized topographies spanning multiple length scales. Herein we present a self-assembly method that faithfully reproduces the topographic features of these biomaterials. The system consists of a photocurable monomer and water. To this quasi-two-component system we add surfactants that sculpt the interface into the desired shape. The resulting structures are then solidified by crosslinking with UV light. Drawing from the rich phase behavior of oil/water/surfactant systems, we demonstrate complex fractal morphologies over many length scales ranging from several mm down to 100 nm. Quantitative image analysis reveals fractal morphologies with at least four distinct levels of hierarchy. Increasing viscosity, in particular, shows a strong correlation with the number of hierarchical levels.

10:24AM P45.00013 Effect of Molecular Architecture on the Wetting Properties of Polymers¹

EMMANOUIL GLYNOS, BRADLEY FRIEBERG, PETER GREEN, University of Michigan, Ann Arbor — We show that the wetting properties of star-shaped polystyrene (PS) macromolecules possessing sufficiently high functionality, f higher than 4, differ significantly from their linear analogues of otherwise identical chemical structure. The equilibrium contact angles of macroscopic droplets composed of star-shaped macromolecules on silicon oxide substrate, are as much as one order of magnitude smaller than their linear analogues, provided that f is equal to or greater than 8 and the degree of polymerization per arm length, N_{arm} , is sufficiently small. The corresponding line tensions of the star polymers are as much as two orders of magnitude smaller. The dewetting characteristics of the linear and star polymers also differ. Linear PS chains dewet leaving an adsorbed layer of nanoscopic dimensions; this layer is also structurally unstable and breaks up into nano-droplets, leaving a precursor layer at the boundary of the macroscopic droplets. The thickness of this layer is consistent with expectations based on the shape of the effective interface potential. The corresponding nanoscopic layer of star-shaped polymers, of sufficiently large f and sufficiently small N_{arm} , remains structurally stable. These effects are discussed in terms of the role of molecular architecture and entropic effects on the structure and dynamics of macromolecules at interfaces.

¹This work was supported by the National Science Foundation, Division of Materials Research, Polymers Program 0906425

10:36AM P45.00014 Surface Segregation of Well-Defined Comb Polymers¹

BOXI LIU, RODERIC QUIRK, MARK FOSTER, The University of Akron, DAVID WU, Colorado School of Mines — Blending polymers with different chain architectures may prove useful in controlling interfacial properties by controlling interfacial segregation. A linear response theory by Wu *et al.* predicts that a long-chain branched polymer blended with its linear analog will be preferentially segregated to the surface and interface of the blend film. The comb architecture is particularly promising for achieving substantial surface segregation. In particular, its high degree of branching provides a substantial driving force for surface segregation when chain ends prefer the surface. Comb polystyrenes with well-defined architectural details were prepared by living anionic polymerization via the "grafting-through" approach. Neutron reflectivity (NR) and secondary ion mass spectrometry (SIMS) analyses reveal that the comb polymers that are still miscible with linear analogs in the bulk segregate so strongly to the surface that the surface concentration is nearly 100 vol%. The effect on the surface segregation of bulk concentration and chain end chemistry will be discussed.

¹NSF support (CBET 0730692 & 0731319) is gratefully acknowledged.

10:48AM P45.00015 Size Dependent Nucleation of Confined 2-Decanol

SAMUEL AMANUEL, HILLARY BAUER, ALEXANDREA SAFIQ, JARGALSAIKHAN DULMAA, AMER KHRAISAT, Department of Physics and Astronomy, Union College, Schenectady, NY 12308, DEPARTMENT OF PHYSICS AND ASTRONOMY, UNION COLLEGE, SCHENECTADY, NY 12308 TEAM — We have studied freezing and melting of physically confined 2-decanol in nano porous silica using a Differential Scanning Calorimeter (DSC). Both melting and freezing temperatures are suppressed for physically confined 2-decanol. In the presence of bulk, freezing of the confined system is triggered by freezing of the bulk where nucleation is heterogeneous. There is, however, a cutoff size between 100 nm and 300 nm where phase transition is no longer initiated through heterogeneous nucleation. Below the cutoff size, nucleation is homogeneous where the confined system has to be supercooled further before any phase transition can occur. Melting of the confined system, on the other hand, is not influenced by the presence or absence of the bulk.

Wednesday, February 29, 2012 8:00AM - 11:00AM –
Session P46 DPOLY: Invited Session: DNA-Programmable Particle Assembly 160AB

8:00AM P46.00001 Self-Replication of Nanoscale tiles and patterns , PAUL CHAIKIN, New York University —

We want to make a “non-biological” system which can self-replicate. The idea is to design particles with specific and reversible and irreversible interactions, introduce seed motifs, and cycle the system in such a way that a copy is made. Repeating the cycle would double the number of offspring in each generation leading to exponential growth. Using the chemistry of DNA either on colloids or on DNA tiles makes the specific recognition part easy. In the case of DNA tiles we have in fact replicated the seed at least to the third generation. The DNA linkers can also be self-protected so that particles don't interact unless they are held together for sufficient time – a nano-contact glue. Chemical modification of the DNA allows us to permanently crosslink hybridized strands for irreversible bonds and a new type of photolithography. We have also designed and produced colloidal particles that use novel “lock and key” geometries to get specific and reversible physical interactions.

With Tong Wang, Ruojie Sha, Remi Dreyfus, Mirjam E. Leunissen, Corinna Maass, David J. Pine, and Nadrian C. Seeman.

8:36AM P46.00002 Inverse Problem in Self-assembly¹ , ALEXEI TKACHENKO, Brookhaven National Laboratory —

By decorating colloids and nanoparticles with DNA, one can introduce highly selective key-lock interactions between them. This leads to a new class of systems and problems in soft condensed matter physics. In particular, this opens a possibility to solve inverse problem in self-assembly: how to build an arbitrary desired structure with the bottom-up approach? I will present a theoretical and computational analysis of the hierarchical strategy in attacking this problem. It involves self-assembly of particular building blocks (“octopus particles”), that in turn would assemble into the target structure. On a conceptual level, our approach combines elements of three different brands of programmable self assembly: DNA nanotechnology, nanoparticle-DNA assemblies and patchy colloids. I will discuss the general design principles, theoretical and practical limitations of this approach, and illustrate them with our simulation results. Our crucial result is that not only it is possible to design a system that has a given nanostructure as a ground state, but one can also program and optimize the kinetic pathway for its self-assembly.

¹Acknowledgement: This research carried out at the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the US DOE, Office of BES, under Contract No. DE-AC02-98CH10886.

9:12AM P46.00003 Structural flexibility of DNA-Nanoparticle Assemblies¹ , DMYTRO NYKYPANCHUK, Brookhaven National Laboratory —

Encoding interactions between nanoparticles using DNA allows for creation of new classes of materials in which particles arrange in superlattices with the structure mainly defined by particle geometry and interactions between DNA shells. The phase behavior in these systems quite often can be rationalized using the interaction energy maximization argument for DNA provided key-lock recognition. However, a polymeric nature of DNA connections can bring about an unexpected phase behavior with structures typically not observed for non-directional interactions. In addition, DNA sensitivity to various specific and non-specific stimuli provides for precise lattice tunability within a given phase. We will provide several examples of phase change in systems of DNA interacting nanoparticles, where unusual, low dimensional structures form due to collective behavior of DNA chains. We will also discuss various ways to dynamically change superlattice parameters using physical variables such as electrostatic interactions or external osmotic pressure for continuous lattice tunability or using DNA machinery to program a step-wise change in the lattice parameter of the assemblies.

¹Research was supported by the U.S. DOE Office of Science and Office of Basic Energy Sciences under contract No. DE-AC-02-98CH10886.

9:48AM P46.00004 Nanoparticle Superlattice Engineering with DNA , CHAD MIRKIN, Northwestern University —

Recent developments in strategies for assembling nanomaterials have allowed us to draw a direct analogy between the assembly of solid state atomic lattices and the construction of nanoparticle superlattices. Herein, we present a set of six design rules for using DNA as a programmable linker to deliberately stabilize nine distinct colloidal crystal structures, with lattice parameters that are tailorable over the 25-150 nm size regime. These rules are analogous to those put forth by Pauling decades ago to explain the relative stability of lattices composed of atoms and small molecules. It is ideal to use DNA as a nanoscale bond to connect nanoparticles to achieve colloidal superlattice structures in this system, since its programmable nature allows for facile control over nanoparticle bond length and strength, and nanoparticle bond selectivity. This assembly method affords simultaneous and independent control over nanoparticle structure, crystallographic symmetry, and lattice parameters with nanometer scale precision. Further, we have developed a phase diagram that predicts the design parameters necessary to achieve a lattice with a given symmetry and lattice parameters a priori. The rules developed in this work present a major advance towards true materials by design, as they effectively separate the identity of a particle core (and thereby its physical properties) from the variables that control its assembly.

10:24AM P46.00005 Real-space crystallography and transformations of DNA-directed particle superlattices , JOHN CROCKER, University of Pennsylvania —

DNA is a versatile tool for directing the controlled self-assembly of nanoscopic and microscopic objects. The interactions between microspheres due to the hybridization of DNA strands grafted to their surface have been measured and can be modeled in detail, using well-known polymer physics and DNA thermodynamics. Knowledge of the potential, in turn, enables the exploration of the complex phase diagram and self-assembly kinetics in simulation. In experiment, at high densities of long grafted DNA strands, and temperatures where the binding is reversible, these system readily form colloidal crystals having a diverse range of symmetries. For interactions that favor alloying between two same-sized colloidal species, our experimental observations compare favorably to a simulation framework that predicts the equilibrium phase behavior, crystal growth kinetics and solid-solid transitions. We will discuss the crystallography of the novel alloy structures formed and address how particle size and heterogeneity affect nucleation and growth rates.

Wednesday, February 29, 2012 8:00AM - 11:00AM —

Session P47 DPOLY: Biopolymers: Molecules, Solutions, Networks, and Gels 160C

8:00AM P47.00001 Sub-nm porous membrane based on cyclic peptide nanotubes¹ , CHEN ZHANG, RAMI HOURANI, CHANGYI LI, University of California at Berkeley, BRETT HELMS, The Molecular Foundry, Lawrence Berkeley National Laboratory, TING XU, University of California at Berkeley —

Porous thin films containing subnanometer channels oriented normal to surface exhibit unique transport and separation properties and can serve as selective membranes for different applications. Generating flexible nanoporous films with densely packed vertical channels over large areas remains a significant challenge. We developed a new approach where the growth of cyclic peptide nanotubes can be directed in a structural framework set by the self-assembly of block copolymers. Conjugating polymers to cyclic peptides enables the nanotube subunits be selectively solubilized in one copolymer microdomain. Conjugated polymers mediate nanotube-polymer interaction to guide nanotube growth. This led to subnanometer porous membranes containing high-density arrays of through channels. In parallel, we also studied how to modify the interior of nanotubes with controlled geometry. Artificial amino acid is introduced in the primary sequence of cyclic peptide with a functional group presented in the nanotube interior without disrupting the high aspect ratio nanotubes. The new design of such a cyclic peptide enables one to modulate the nanotube growth process to be compatible with the polymer processing window, hence opening a viable way of fabricating polymeric membranes for different application

¹DOE-BES, DOE-EFRC-Gas Separation, ARO, Janes Lewis Fellowship

8:12AM P47.00002 Gel-on-Brush Model of Airway Surface of the Lung: its Predictive Role in Chronic Pulmonary Disease¹, LIHENG CAI, BRIAN BUTTON, CAMILLE EHRE, RICHARD BOUCHER, MICHAEL RUBINSTEIN, University of North Carolina at Chapel Hill — Clearance of mucus is the primary defense mechanism that protects airways from inhaled infectious and toxic agents. The current two-layer Gel-on-Liquid model in which a gel-like mucus is propelled on top of a “watery” periciliary layer (PCL) surrounding the cilia does not adequately describe efficient mucociliary clearance in health nor properly predict failure of mucus clearance in disease. We propose and provide evidence for a qualitatively different Gel-on-Brush model with a gel-like mucus layer in contact with a “brush-like” periciliary layer, composed of macromolecules tethered to the airway surface. The relative osmotic moduli of the mucus layer to the “brush-like” PCL layer explain both the stability of mucus clearance in health and its failure in airway disease. Our Gel-on-Brush model of airway surface layer opens important new directions for treatments of airway disease.

¹This work was supported by Cystic Fibrosis Foundation (RUBINSTEIN07XX0, BUTTON07XX0, and BUTTON11G0); NSF CHE-0911588, DMR-0907515, DMR-1121107, DMR-1122483, and CBET-0609087; and NIH K01DK080847, P50HL107168, R01HL077546, and P01HL34322.

8:24AM P47.00003 Experimental and Computational Analysis of Structural and Mechanical Properties of Fibrin Gels, OLEG KIM, ZHILIANG XU, Department of Applied and Computational Mathematics and Statistics, University of Notre Dame, IN, ALISA WOLBERG, Department of Pathology and Laboratory Medicine, University of North Carolina, USA, ELLIOT ROSEN, Department of Medical and Molecular Genetics, Indiana University School of Medicine, Indianapolis, USA, MARK ALBER, Department of Applied and Computational Mathematics and Statistics, University of Notre Dame, IN. — An important area in coagulation research is the study of the structural stability of a blood clot, which has important medical consequences. The stability of clots is closely related to the fibrin networks, which provides the structural support for a blood clot. We synthesized, studied, and compared fibrin networks, with and without cells, formed under wild type and hemophilic conditions. The 3D structure of each fibrin network was reconstructed from z-stacks of 2D confocal microscopy sections by implementing novel image analysis algorithms. These 3D images were utilized to establish microstructure-based models for studying the relationship between the structural features and the mechanical properties of the fibrin networks. The mechanical properties were assessed by analyzing the networks' responses to uniaxial tensile and shear stresses, simulating the impact of blood flow on the fibrin network. We will show in this talk that the elasticity of the fiber network predicted by the model agrees well with prior experimental data for small networks. We will also show that a nonlinear worm-like chain model correctly predicts both the alignment of the fibers and the elastic properties of the networks as the clot sample is stretched.

8:36AM P47.00004 Block copolymer self-assembly for the responsive reinforcement of injectable protein hydrogels, M.J. GLASSMAN, Massachusetts Institute of Technology, S. LI, J. CHAN, California Institute of Technology, B.D. OLSEN, Massachusetts Institute of Technology — Shear-thinning injectable protein hydrogels are emerging as important biomaterials for the minimally-invasive implantation of scaffolds for tissue engineering and drug delivery. In this work, responsive block copolymer self-assembly is employed to trigger nanostructure formation in hydrogels made from artificial associative proteins, producing hydrogels with resistance to shear-thinning post injection, reduced erosion rate, higher toughness, and dramatically reduced creep compliance. Polymer-protein-polymer triblock copolymers have been synthesized by conjugating poly(N-isopropylacrylamide) to either end of a protein midblock decorated with self-associating pentavalent sticker domains. Self-assembly at elevated temperatures introduces a second physical network into the protein hydrogel with an independent and tunable relaxation time. The phase behavior of these dual-network hydrogels has been explored, revealing the ability to access nanostructured morphologies, and the effect of self-assembled polymer domains on the linear mechanics and toughness of injectable hydrogels has been investigated.

8:48AM P47.00005 Electrophoresis of DNA-protein conjugates: hydrodynamic end effects and electrostatic interactions, MYKYTA V. CHUBYNSKY, GARY W. SLATER, Department of Physics, University of Ottawa, Canada — DNA fragments can be separated by length in free solution by attaching them to neutral or positively charged “drag-tags” (e.g., proteins), a technique known as end-labeled free-solution electrophoresis (ELFSE). We first extend a previous theory of ELFSE for neutral drag-tags to the case of weakly charged drag-tags. The simplest variant of the theory assumes that all parts contribute equally to the mobility (no end effects) and that both the DNA and the drag-tag are fully flexible and do not interact. We analyze the influence of these assumptions. We obtain the exact (within the Kirkwood-Riseman approximation) form of the function describing the end effects for flexible polymers. The main significance of the end effects is the $N^{-3/4}$ (instead of N^{-1}) form of the correction to the mobility for large DNA lengths N . We also show that the end effects are weaker for semiflexible and stiff polymers. Using a simple model, we study how the conformation of the drag-tag changes due to the electrostatic interaction with the DNA and how this influences the mobility.

9:00AM P47.00006 The local dynamics of unfolded versus folded tRNA in comparison to synthetic polyelectrolytes and the role of electrostatic interactions, JOON HO ROH, University of Maryland and Johns Hopkins University, MADHU TYAGI, NIST Center for Neutron Research and University of Maryland, ROBERT M. BRIBER, University of Maryland, SARAH A. WOODSON, Johns Hopkins University, ALEXEI SOKOLOV, University of Tennessee — The local dynamics of RNA is strongly coupled to biological functions such as ligand recognition and catalysis. We have used quasielastic neutron scattering spectroscopy to follow the local motion of RNA and a synthetic polyelectrolyte as a function of Mg^{2+} concentration. We have observed that increasing Mg^{2+} concentration increases the picosecond to nanosecond dynamics of hydrated tRNA while stabilizing the tRNA folded structure. Analyses of the atomic mean-squared displacement, relaxation time, persistence length, and fraction of mobile atoms showed that unfolded tRNA is more rigid than in the folded state. This same behavior was observed for sulfonated polystyrene indicating that the increased dynamics in arises from charge screening of the polyelectrolyte rather than specific interactions. These results are opposite to what is observed for proteins for the relationship between the unfolded/folded states and the internal dynamics where the folded state is observed to be more rigid than the unfolded state. We conclude that the local dynamics for both bio- and synthetic polymers are strongly influenced by the electrostatic environment.

9:12AM P47.00007 Physical Structure of Methylcellulose Hydrogels, JOSEPH LOTT, JOHN MCALLISTER, SARA ARVIDSON, FRANK BATES, TIMOTHY LODGE, University of Minnesota — Methylcellulose (MC) is a chemically modified polysaccharide in which there is a partial substitution of hydroxyl groups with methoxy moieties. This results in a polymer that is water soluble at low temperatures and displays lower critical solution temperature (LCST) phase behavior at elevated temperatures. As such, aqueous solutions of MC have long been employed and studied due to their ability to form gels as temperature is increased. Currently, there is no consensus on the detailed mechanism of the gelation process, so a precise determination of the physical structure present in these materials may lead the way to new mechanistic understanding. Transmission electron microscopy (TEM) performed under cryogenic conditions is a powerful tool for the study of hydrogels as it allows direct imaging of the network while preserving the structure in the gel. Cryo-TEM investigations suggest that the hydrogel is composed of fibril-like aggregates comprising multiple polymer chains. Small-angle neutron scattering (SANS) provides a complimentary method to establish the detailed structure of the hydrogel network. We will report the effects of molecular weight, concentration, and temperature on the resultant physical structures within the gel.

9:24AM P47.00008 Mesoscopic Simulations of Free Solution Electrophoresis of Polyelectrolytes with Finite Debye Length, GARY SLATER, OWEN HICKEY, TYLER SHENDRUK, University of Ottawa — The mobility of charged oligomers results from a complex interplay between electrostatic and hydrodynamic interactions leading to a competition between counter-ion condensation and cooperative shearing within the diffuse layer. Simulations of polyelectrolytes that include explicit ions are computationally expensive, while algorithms that couple infinitely thin Debye layers to mesoscopic fluid models are only useful in the long chain limit because they fail to predict the rise and non-monotonicity of the mobility. We present a hybrid mesoscale simulation technique that utilizes multi-particle collision dynamics (MPCD) to simulate surrounding solvent molecules and the Debye-Hückel approximation to assign effective charge to the MPCD particles. This hybrid scheme can capture the electro-hydrodynamics without having to explicitly include counter-ions or make costly electrostatic calculations. This MPCD-MD Debye-Hückel method shows great potential for simulating electrophoretic behavior of polyelectrolytes in novel microfluidic devices.

9:36AM P47.00009 Interfacial adsorption and aggregation of amphiphilic proteins, DAVID CHEUNG, University of Warwick — The adsorption and aggregation on liquid interfaces of proteins is important in many biological contexts, such as the formation of aerial structures, immune response, and catalysis. Likewise the adsorption of proteins onto interfaces has applications in food technology, drug delivery, and in personal care products. As such there has been much interest in the study of a wide range of biomolecules at liquid interfaces. One class of proteins that has attracted particular attention are hydrophobins, small, fungal proteins with a distinct, amphiphilic surface structure. This makes these proteins highly surface active and they recently attracted much interest. In order to understand their potential applications a microscopic description of their interfacial and self-assembly is necessary and molecular simulation provides a powerful tool for providing this. In this presentation I will describe some recent work using coarse-grained molecular dynamics simulations to study the interfacial and aggregation behaviour of hydrophobins. Specifically this will present the calculation of their adsorption strength at oil-water and air-water interfaces, investigate the stability of hydrophobin aggregates in solution and their interaction with surfactants.

9:48AM P47.00010 Viscoelastic and poroelastic relaxations of polymer-loaded gels, EDWIN CHAN, National Institute of Standards and Technology, BLESSING DEEYAA, University of Maryland, PETER JOHNSON, CHRISTOPHER STAFFORD, National Institute of Standards and Technology — Gel layers are prevalent in many applications including water purification, fuel cells, tissue engineering and drug delivery. In these materials, their performance is closely linked to controlling transport of solutes such as solvent or polymer. Thus, understanding the critical time- and length-scale that regulate solute transport will enable development of membrane materials with the desired performance. In this contribution, we present the Poroelastic Indentation Relaxation (PRI) approach in quantifying the viscoelastic and poroelastic relaxations of geometrically-confined hydrogel layers. We demonstrate this indentation-based measurement approach in characterizing several materials properties including diffusion coefficient, shear modulus, and average pore dimensions of the hydrogel independent of the extent of geometric confinement. Additionally, we present a relaxation model that accounts for the viscoelastic and poroelastic contributions to the total relaxation process. Finally, we show that the PRI approach can quantify diffusion of solvent and polymer solution in a single test simply by changing the extent of deformation.

10:00AM P47.00011 Mechanical Characterization of Photo-crosslinkable Hydrogels with AFM¹, ALYSSA MCKENNA, Mount Holyoke College, MYUNGHWAN BYUN, RYAN HAYWARD, University of Massachusetts Amherst, KATHERINE AIDALA, Mount Holyoke College — Stimuli-responsive hydrogel films formed from photo-crosslinkable polymers are versatile materials for controlled drug delivery devices, three-dimensional micro-assemblies, and components in microfluidic systems. For such applications, it is important to understand both the mechanical properties and the dynamics responses of these materials. We describe the use of atomic force microscope (AFM) based indentation experiments to characterize the properties of poly(*N*-isopropylacrylamide) copolymer films, crosslinked by activation of pendent benzophenone units using ultraviolet light. In particular, we study how the elastic modulus of the material, determined using the Johnson, Kendall, and Roberts model, depends on UV dose, and simultaneously investigate stress relaxation in these materials in the context of viscoelastic and poroelastic relaxation models.

¹Support was provided by UMass Center on Polymers, DMR-0820506.

10:12AM P47.00012 Tough hydrogels from hydrophobically associating polymers¹, ROBERT WEISS, JINKUN HAO, University of Akron — Physical gels can be formed by interchain associations involving hydrophobic interactions. The viscoelastic and mechanical behavior of physically crosslinked copolymer hydrogels synthesized from *N*, *N*-dimethylacrylamide (DMA) and 2-(*N*-ethylperfluorooctane sulfonamido) ethyl acrylate (FOSA), with varying FOSA content, were studied by rheology and static tensile testing. The strong hydrophobic association of the FOSA moieties in an aqueous environment produced core-shell nanodomains (6 nm diameter) that provided the physical crosslinks. The PDMA-FOSA hydrogels exhibited excellent mechanical properties: modulus of 80 – 130 kPa, elongation at break of 1000 – 1600 %, tensile strength of 500 kPa, and toughness of 4 –6 MPa, depending on the FOSA concentration. The physical hydrogels were much more efficient at dissipating stress than the chemical hydrogels. Dynamic viscoelastic and stress relaxation experiments of the physical hydrogels and a chemically crosslinked PDMA hydrogel showed that the physical gel was more viscous than chemical gel and displayed much greater stress relaxation. That result was attributed to the extra energy dissipation mechanism provided by the reversible, hydrophobic crosslinks.

¹This research was partially supported by a grant from the Polymer Program of the National Science Foundation (Grant DMR- 0960461)

10:24AM P47.00013 Characterization of the Interfacial Adhesion for Responsive Hydrogels on Substrates, CHANDLER BENJAMIN, JOHN SPRINGMANN, SHAHZAD CHINDHY, WENDY CRONE, University of Wisconsin-Madison, CRONE LAB TEAM — In recent years a growing collection of responsive hydrogels have been developed which are capable of reversibly responding to a range of stimuli. These hydrogels operate in a hydrated environment and respond with significant volumetric reversible transformation through absorption or release of water within the polymeric network. Polymeric hydrogels in this class of shape memory materials have been successfully implemented in microfluidic and biomedical devices as components such as microchannels, micro-orifices, microvalves, micropumps and microcompressors. In practice, the hydrogel component is often polymerized on a substrate or within the confines of a channel in order to create responsive components. It is well known that the adhesion of a swelling hydrogel with its substrate varies with substrate properties. We show an experimental method to quantify the interfacial adhesion of responsive hydrogels with a substrate. This work provides a valuable method and theoretical basis for characterizing and optimizing the adhesion of responsive hydrogels.

10:36AM P47.00014 Resilient Synthetic PEG/PDMS Hydrogels Inspired by Natural Resilin¹, JUN CUI, MELISSA LACKEY, GREGORY TEW, ALFRED CROSBY, University of Massachusetts Amherst — Novel synthetic hydrogels are developed by incorporating hydrophobic polydimethylsiloxane (PDMS) into hydrophilic poly(ethylene glycol) (PEG)-based network using thiol-norbornene chemistry. The properties of these hydrogel are comparable to natural resilin, which is an elastic protein, existing in many insects, such as the tendons of flea and the wings of dragonfly, with extraordinary ability of mechanical energy storage. The energy storage efficiency (resilience) of the hydrogels is more than 97% even at tensile strains up to 170%. In addition, the Young's modulus of the hydrogels ranges from 3 kPa to 300 kPa by increasing the volume fraction of the PDMS in the network. These unique properties are attributed to the well-defined network and negligible secondary structure, provided by the versatile and efficient chemistry.

¹NSF PIRE (NSF-0730243), ARO W911NF-09-1-0373 and ONR N00014-10-1-0348

10:48AM P47.00015 pH-dependent and pH-independent self-assembling behavior of surfactant-like peptides, LEONID GUREVICH, PETER FOJAN, Aalborg University, BIOPHYSICS GROUP TEAM — Self-assembly of amphiphilic peptides designed during the last years by several research groups leads to a large variety of 3D-structures that already found applications in stabilization of large protein complexes, cell culturing systems etc. In this report, we present synthesis and characterization of two novel families of amphiphilic peptides KA_n and KA_nW ($n=6,5,4$) that exhibits clear charge separation controllable by pH of the environment. As the pH changes from acidic to basic, the charge on the ends of the peptide molecule varies eventually leading to reorganization of KA_n micelles and even micellar inversion. On contrary, the bulky geometry of the tryptophan residue in KA_nW limits the variation of the surfactant parameter and hence largely prevents assembly into spherical or cylindrical micelles while favouring flatter geometries. The studied short peptide families demonstrate formation of ordered aggregates with well-defined secondary structure from short unstructured peptides and provide a simple system where factors responsible for self-assembly can be singled out and studied one by one. The ability to control the shape and structure of peptide aggregates can provide basis for novel designer pH sensitive materials including drug delivery and controlled release systems.

Wednesday, February 29, 2012 8:00AM - 11:00AM –
Session P48 DPOLY: Focus Session: Crystallization in Single-, Multicomponent, and Hybrid Systems II 161

8:00AM P48.00001 Shear-induced homogeneous crystallisation in confined columns of polymer, JESSICA L. CARVALHO, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1 — In previous work, we have studied the crystallisation of a system of dewetted poly(ethylene oxide) (PEO) droplets. We have shown that this defect-free system nucleates homogeneously within the droplet volume. By capping this droplet system, a parallel plate geometry is obtained with the droplets forming isolated PEO columns (a capillary bridge) between the substrate and the cap. With this geometry we are able to investigate how the application of an oscillatory shear mediates the crystal nucleation step in small, defect-free volumes of material. These studies are typically carried out in bulk systems which are dominated by heterogeneous defects, here we will present our first results on the effect of shear on homogeneous nucleation.

8:12AM P48.00002 Chain Folding in Polymer Crystals Detected by Solid-state NMR¹, TOSHIKAZU MIYOSHI, The University of Akron — Polymer crystallization induces transitions from random coils in the melt states to bilayer structures consisting of chain-folded crystals and disordered amorphous regions. Although the concept of chain folding is well recognized, there have been continuous debates about adjacent re-entry fractions of polymer chains crystallized at different physical conditions. To understand chain-folding structures in complex systems, spatial selectivity to access short-range polymer-polymer interactions is necessary. In this talk, we will propose a novel approach using solid-state NMR and selective isotope labeling for characterizing chain-folding of polymer chains. Spatial selectivity in double quantum NMR reveals adjacent re-entry fractions in the bulk crystals at different conditions.

¹NSF-DMR1105829

8:24AM P48.00003 Forming hierarchically ordered hybrid materials using polymer crystallization, CHRISTOPHER LI, BIN DONG, TIAN ZHOU, WENDA WANG, Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104 — Hierarchically ordered hybrid materials are of great interest for next generation advanced materials research. In this presentation, we will present our recent results on employing polymer single crystals (PSC) to template nanoparticle assembly, leading to hierarchically ordered hybrid materials. Tailor-made, free-standing NP frames and wires containing single or multiple types of NPs have been obtained by using an in-situ polymer crystallization method. End functionalized poly(ethylene oxide) and polycaprolactone single crystals were used as the templates. Gold and magnetite NPs were successfully patterned as evidenced by transmission electron microscopy experiments. Interaction between NPs, free polymer chain as well as PSC has been systematically monitored using Surface Plasmon Resonance. It has been found that NP-free polymer chain interaction holds the key to forming ordered NP patterns in solution.

8:36AM P48.00004 Understanding Molecular Epitaxial Mechanism of the γ -form Crystal and Chain Tilt in the α -form Single Crystal of Isotactic Polypropylene, YAN CAO, RYAN VAN HORN, GUOLIANG ZHANG, HAO-JAN SUN, The University of Akron, KWANG-UN JEONG, Chonbuk National University Jeonju, FINIZIA AURIEMMA, CLAUDIO DE ROSA, Università di Napoli "Federico II", BERNARD LOTZ, Institut Charles Sadron (CNRS-Université de Strasbourg), STEPHEN CHENG, The University of Akron — We attempt to investigate how the epitaxial domination of the crystal morphologies takes place in the γ -form of the chain-folded crystals using high molecular weight isotactic polypropylene (i-PP) samples with a controlled number of stereodefects. Two different morphologies were identified *via* transmission electron and atomic force microscopies (TEM and AFM). One is needle-like and the other is "flat". Based on the tilted selected area electron diffraction (SAED) results from TEM, the microscopic formation mechanism of the "needle" and "flat" morphology was discussed and it revealed that in the "flat" γ -form crystal, the initial α -form single crystal had to have a stem orientation tilted away from the thin film normal within the ac-plane around the b-axis. Elongated α_2 -form lath-like single crystals were grown from thin film melt at $T_x = 145^\circ\text{C} - 155^\circ\text{C}$ using commercial sample. SAED experimental results show that the stems in these lath-like single crystals were tilted at an unusual 17° angle around the b-axis. This 17° -stem tilt in the α_2 -form single crystals favors the $(10\bar{2})$ fold surface and appears to depend upon both conformational and chain folding constraints.

8:48AM P48.00005 Kinetic Control of the Halogen Distribution in Crystals of Precisely Substituted Polyethylenes, RUFINA ALAMO, PAPATYA KANER, CAROLINA RUIZ-ORTA, FAMU-FSU College of Engineering, Tallahassee, Florida 32312, EMINE BOZ, KENNETH B. WAGENER, University of Florida, Department of Chemistry, Gainesville, FL 32611 — Isothermally crystallized polyethylenes with precise chlorine substitution on each and every 21, 19, 15 or 9 backbone carbon display a drastic change in crystalline structure in a narrow interval of crystallization temperatures. The structural change occurs within one degree of undercooling and is accompanied by a change in WAXD patterns, a sharp increase in melting temperature, an increase in TG conformers and a decrease in SAXS periodicity. These changes correlate with a different distribution of Cl atoms in the crystallites. Under fast crystallization kinetics, the Cl distribution in the crystallites is disordered, while slower crystallization rates favor intermolecular staggering of chlorines and a herringbone structure. The drastic change in morphology is enabled by the precise halogen placement in the chain and driven by the selection of the nucleus stem in the initial stages of the crystallization. Exquisite kinetic control of the crystallization in novel polyolefins of this nature allows strategies for generating nanostructures at the lamellar and sub-lamellar level not feasible in classical branched polyethylenes.

9:00AM P48.00006 On the Width of the Crystallization Process, ANDREW OCHOA, MIRCEA CHIPARA, The University of Texas Pan American — Differential Scanning Calorimetry (DSC) is the most frequently used experimental techniques for the study of crystallization process in polymers and polymer-based nanocomposites. The experimental data are discussed within various theoretical approaches. Isothermal crystallization studies are typically discussed within the Avrami theory of phase change. However, the as recorded experimental data represent the time dependence of the derivative of the crystallinity degree (versus time) rather than the crystallinity degree. From the experimental point of view, the DSC parameters that are considered are the DSC peak position, the area under the DSC curve, and an empirical not very well defined onset temperature. However, all experimental data points are involved in the Avrami analysis after integration (in the Avrami analysis of the dependence representing the degree of crystallinity versus time). However, no effort has been done to understand the significance of the width of the as recorded DSC spectrum. A detailed analysis of the significance of the width of the DSC spectrum is presented. The connection between the width of the DSC spectrum and the exponent of the Avrami equation is analyzed in detail for the case in which nucleation is negligible. Tentatively, the as obtained results are extended to non-isothermal crystallization kinetics, recorded for various heating rates and to the Ozawa treatment of crystallization of polymers in non isothermal conditions.

9:12AM P48.00007 Crystallization and Ordering of Giant Molecules based on Nano-atoms, STEPHEN Z.D. CHENG, Department of Polymer Science, College of Polymer Science and Polymer Engineering, The University of Akron — To create new functional materials for advanced technologies, control over their hierarchical structures and orders is vital for obtaining the desired properties. We utilized and functionalized fullerene (C60) and polyhedral oligomeric silsesquioxane (POSS), and assembled these particles with polymers to form those hierarchical structures. The structures of these assemblies along with the resulting ordered structures were analyzed to determine their structure-property relationships. One of the most illustrating examples is a series of novel giant surfactants and lipids possessing a well-defined amphiphilic head and polymeric tails. Various architectures of this class of materials have been constructed and their self-assembly processes in solution, in the condensed bulk and thin films have been investigated. Another set of examples are “nano-atoms.” These classes of molecules are designed to possess features of molecular Janus particles with various symmetry breakings. When specific interactions are introduced, these “nano-atoms”: are functioned as building blocks to construct different amplified molecules and further to self-assemble into hierarchical ordered structures. Their thermodynamic phase diagrams and kinetic pathways are explored to understand this new class of materials and their potential applications in modern technologies.

9:48AM P48.00008 Morphologies in Semi-Crystalline Precise Acid- and Ion-Containing Polymers, KAREN WINEY, University of Pennsylvania — For over a decade we have endeavored to quantify the morphologies in ion-containing polymers using a combination of X-ray scattering and electron microscopy methods. We are motivated by the promise that when we know the polymer physics connecting chemical structure, nanoscale morphology, and physical properties, new strategies for improving polymer properties will be evident. This is particularly challenging in semi-crystalline polymers. Recently, we have been exploring the morphologies in precise acid copolymers and in the ionomers made neutralizing these precise copolymers. The precise copolymers are synthesized by Prof. K. Wagener's group at the University of Florida using acyclic diene metathesis and have functional groups attached to every 9th, 15th or 21st carbon along a linear polyethylene molecule. The precision of these molecules gives rise to well-defined hierarchical structures including acid-decorated polyethylene lamellae and acid or ionic aggregates arranged on cubic lattices. The temperature dependence of these polyethylene-based copolymers is dominated by the crystallization of the polymer. Stretching these materials can induce anisotropy that has facilitated our determination of these hierarchical morphologies and plans are underway to initiate in situ tensile deformation and X-ray scattering to probe the dynamic morphology.

10:24AM P48.00009 Nanohybrid shish kebab paper: Crystal growth and film properties¹, ERIC D. LAIRD, BING LI, SHAN CHENG, BIN DONG, RANJITA K. BOSE, KENNETH K.S. LAU, CHRISTOPHER Y. LI, Drexel University — Polyethylene single crystals were uniformly grown heterogeneously from carbon nanotubes (CNTs) in solution, forming the nanohybrid shish kebab (NHSK) structure. We demonstrate that highly uniform, free-standing nanohybrid buckypaper with high CNT contents (13-70%) could be produced from vacuum-filtrated polymer single crystal-decorated CNTs. In this way, polymer crystals served as unique spacers for CNTs so that uniform hybrid buckypaper films could be obtained without CNT agglomeration. Wetting techniques, thermal analysis, and scanning electron microscopy were used to elucidate the effect of polymer single crystals on the resultant structure. Surface roughness of NHSK paper could be controlled by tuning the polymer single crystal size (CNT separation distance). Superhydrophobic NHSK papers were obtained with high surface adhesion, which mimics the rose petal effect. Conductivity of the NHSK papers also varied with polymer crystal size. Great enhancement of important properties could be achieved through the formation of ternary hybrids. To that end, initiated- and oxidative chemical vapor deposition methods extend NHSK buckypaper applicability by providing functional polymer surfaces. NHSK papers may find applications in sensors, electrochemical devices and coatings.

¹NSF-IGERT DGE-0221664, NSF DMR-0804838

10:36AM P48.00010 Role of lamellar thickness in the kinetics of polymer crystal growth¹, WENBING HU, State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University — The lamellar thickness of polymer crystals reflects their thermodynamic metastability and meanwhile decides the linear crystal growth rates on their lateral sides. The traditional theories about the growth kinetics of polymer crystals, like Lauritzen-Hoffman theory and Sadler-Gilmer theory, attributed the effect of lamellar thickness to the free energy barrier at the lateral growth front, in order to explain the slower growth of thicker crystals observed at higher temperatures. We studied the linear growth rates of flat-on-oriented polymer crystals in ultra-thin films, by means of dynamic Monte Carlo simulations of lattice polymers. We found that at the same temperatures, the thicker crystals are actually growing faster. The effect of lamellar thickness has no relation with the free energy barrier; rather, it is only related with the driving force for crystal growth. On the basis of the intramolecular crystal nucleation model, we discussed a reasonable microscopic image on the growth kinetics of polymer crystals.

¹The financial support of NNSFC (Grant No. 20825415) and the National Basic Research Program of China (Grant No. 2011CB606100) is appreciated.

10:48AM P48.00011 Isothermal crystallization kinetics of Poly (lactic acid) studied by ultrafast chip calorimeter¹, JING JIANG, WEI JIANG, ZIJIE HUANG, DONGSHAN ZHOU, GI XUE, Nanjing University, DONGSHAN ZHOU TEAM — Poly (lactic acid) (PLA) is a biocompatible, biodegradable polymer which has attracted much attention. The crystallization ability, as one of the most factors influencing the physical properties of the biomaterials such as thermal, mechanical, and biodegradable properties, has been widely studied mainly by differential scanning calorimeters. However, although the crystallization of PLA is relatively slow, it's difficult to avoid the crystallization from the nuclei or the structure reorganization of the metastable crystalline formed during the annealing process when we use the normal DSC with the heating rate on the level of tens of K/min. With the chip calorimeter whose scanning rate can go up to 1000 K/s, we can avoid the structure reorganization of metastable crystalline during the heating. In this case we annealed the PLA sample in the 80-120°C temperature range and found the relationship between the onset the melting temperature T_m and crystallization temperature T_c is $T_m = 0.53T_c + 213.5$ and the equilibrium melting temperature is $T_{m,f} = 179.6^\circ\text{C}$.

¹This work is financially supported by the National Basic Research Program of China (973 Program, 2012CB821500) and National Natural Science Foundation of China (No: 20874045, 21027006)

Wednesday, February 29, 2012 8:00AM - 10:48AM –

Session P49 DMP DPOLY: Focus Session: Organic Electronics and Photonics - Interfaces and Contacts 162A

8:00AM P49.00001 Charge transfer and polarization at interfaces with conjugated molecules, NORBERT KOCH, HU-Berlin & HZB — The function and efficiency of organic electronic devices is determined to a significant extent by the electronic properties of organic/organic heterojunctions and interfaces between electrodes and organic semiconductors. The energy level alignment between metal electrodes and active organic layers can be adjusted over wide ranges by employing interlayers of strong molecular acceptors and donors that undergo charge transfer reactions with the metal. It will be shown that such interlayers lead to lower charge injection barriers than pristine metals, even when the work function is the same. It is argued that the molecularly modified electrodes are electronically more rigid than their pristine metal counterparts, i.e., the electron spill-out at the organic-terminated surface is less pronounced compared to metal surfaces. The energy levels at organic/organic heterojunctions comprising donors and acceptors as used in organic photovoltaic cells are essentially independent of deposition sequence, as long as supporting electrodes do not induce energy level pinning. When a high work function electrode is used, the energy levels may become Fermi-level pinned and an electric field drops right at the heterojunction. This effect is exemplified for the donor diindenoperylene and the acceptor C60. The electric field distribution within an organic opto-electronic device may thus be adjusted locally by employing interfacial energy level pinning, even at weakly interacting organic/organic interfaces.

8:36AM P49.00002 Tuning Contact Recombination and Open-Circuit Voltage in Polymer Solar Cells via Self-Assembled Monolayer Adsorption, HE WANG, ENRIQUE GOMEZ, Department of Chemical and Biological Engineering, Princeton University, ZELEI GUAN, Department of Electrical Engineering, Princeton University, CHERNO JAYE, DANIEL FISCHER, National Institute of Standards and Technology, ANTOINE KAHN, Department of Electrical Engineering, Princeton University, YUEH-LIN LOO, Department of Chemical and Biological Engineering, Princeton University — We adsorbed fluoro-alkyl and hydrogenated-alkyl phosphonic acid derivatives onto indium tin oxide (ITO) for forming self-assembled monolayers (FSAMs and HSAMs, respectively) to tune the open-circuit voltage (V_{oc}) of polymer solar cells. The adsorption of FSAM and HSAM alters the work function of ITO from 4.3 eV to 5.5 eV and 4.0 eV, respectively, as verified by ultraviolet photoemission spectroscopy. Polymer solar cells having FSAM-, HSAM-treated ITO, and bare ITO as anodes display V_{oc} of 0.58V, 0.48V, and 0.31V, respectively. Yet, the hole injection barrier from the anode to the active layer is the same for all three devices. Inverse photoemission spectroscopy measurements indicate that the energy barrier for minority carrier transport to the anode is largest for solar cells comprising FSAM-treated ITO and lowest for devices with bare ITO as anode. Since a high energy barrier for minority carrier transport results in lower contact recombination at the anode, it is this energy barrier that is responsible for differences in the V_{oc} s observed in polymer solar cells having anodes that have been pre-treated with SAMs.

8:48AM P49.00003 Electronic Structure of Organic-Metal Interfaces¹, SUNG-YOUNG HONG, PO-CHUN YEH, JERRY DADAP, RICHARD M. OSGOOD, Columbia University — Organic self-assembled monolayers (SAMs) are important to the understanding of molecular electronics as well as the study of charge transfer in photovoltaic applications. We use two-photon photoemission (2PPE) to investigate the interfacial electronic structure of SAMs on metals. In particular we study the unoccupied states of thiolates and fluorinated thiolates on Cu(111) as a function of molecular coverage using both monochromatic and time-resolved bichromatic 2PPE. While accurate measurements have been made on mostly full monolayer systems, similar effort on detailed coverage-dependence has not yet been reported. We track the formation of the interfacial dipole layer as well as the emergence of intermediate and final states vs. coverage.

¹Work is supported by DOE EFRC grant CU08-9796

9:00AM P49.00004 Fermi level pinning by integer charge transfer at electrode-organic semiconductor interfaces, DENIZ CAKIR, MENNO BOKDAM, GEERT BROCKS, University of Twente — The atomic structure of interfaces between conducting electrodes and molecular organic materials varies considerably. Yet experiments show that pinning of the Fermi level, which is observed at such interfaces, does not depend upon the structural details. In this work [1], we develop a general model to explain Fermi level pinning, and formulate simple expressions for the pinning levels, based upon integer charge transfer between the conductor and the molecular layer. In particular, we show that DFT calculations give good values for the pinning levels.

[1] Appl. Phys. Lett 98, 113303 (2011).

9:12AM P49.00005 Analysis of interface states in blend of polythiophene and polyselenophene: experiments and theory, HELENE ANTAYA, MACIEJ SAKOWICZ, CARLOS SILVA, MICHEL COTE, University of Montreal — Organic photovoltaic devices are presently the subject of intense research since they could eventually propose solar energy solutions at a much reduced cost compared to inorganic devices. Presently, electron transport in organic photovoltaic devices is achieved with a fullerene derivative (PCBM) but this solution has some disadvantages. First, the ratio of PCBM to polymer has to be quite high to assume good electronic transport, and second, the relatively high cost of PCBM is not ideal with the goal to reduce the cost of the device. For these reasons, a replacement for PCBM is desirable and an all polymer device solution is viewed as the best avenue. Since polythiophene (P3HT) is ideal for hole transport, its isovalent polyselenophene (P3HS) where sulfur atoms are replaced with selenium atoms might offer an interesting alternative to PCBM. The physical processes in organic devices are quite different from those of inorganic devices. Charge separation in organic devices is achieved by forming an interface between two organic materials with type 2 level alignment. However, because of the large binding energies observed in organic compounds, there is often the presence of H-aggregate states at the junction between the two organic materials. In this presentation, we will report the results of interface states in a blend of polythiophene and polyselenophene. Photoluminescence spectra will be presented along with calculations of these states with the help of the time-dependent density-functional theory.

9:24AM P49.00006 Controlling Side Chain Density of Electron Donating Polymers for Improving V_{OC} in Polymer Solar Cells, B.J. KIM, K.H. KIM, C.H. CHO, H. KANG, KAIST, S.C. YOON, KRIST — The ability to tune the LUMO/HOMO levels of electroactive materials in active layer of polymer solar cells is critical in controlling their optical and electrochemical properties because the HOMO and LUMO offsets between the polymer donor and the electron acceptor strongly affect charge separation and the open circuit voltage (V_{OC}) of a solar cell. Here, we developed two series of electroactive materials for improving V_{OC} in polymer solar cells. First, we enable facile control over the number of solubilizing groups ultimately tethered to the fullerene by tuning the molar ratio between reactants from 1:1 to 1:3, thus producing *o*-xylenyl C₆₀ mono-, bis-, and tris-adducts (OXCMA, OXCBA, and OXCTA) as electron acceptors with different LUMO levels. As the number of solubilizing groups increased, V_{OC} values of the P3HT-based BHJ solar cells increased from 0.63, 0.83, to 0.98 V. Second, we present a series of novel poly[3-(4-*n*-octyl)phenylthiophene] (POPT) derivatives (POPT, POPTT, and POTQT) as electron donors with different side-chain density. As a result of lower HOMO levels by decrease in the side-chain density of the polymers, the devices consisting of POPT, POPTT, and POTQT with PCBM showed increased V_{OC} values of 0.58, 0.63, and 0.75 V, respectively.

9:36AM P49.00007 Charge Injection Mechanism at Carbon Nanotube-Organic Semiconductor Interface¹, BIDDUT K. SARKER, Nanoscience Technology Center and Department of Physics, University of Central Florida, SAIFUL I. KHONDAKER, Nanoscience Technology Center, Department of Physics, and School of Electrical Engineering and Computer Science, University of Central Florida — One of the major challenges in the fabrication of high performance organic electronic devices is to overcome the inefficient charge injection from metal electrodes into organic semiconductors caused by large interfacial contact barrier. One potential key step of improving the charge injection is to employ single-walled carbon nanotubes as electrodes. Towards this end, we fabricated pentacene field effect transistor using densely aligned carbon nanotube array electrodes with open-ended and parallel tips. The room temperature electronic transport measurements of the devices show excellent transistor properties with field effect mobility of up to 0.65 cm²/Vs and current on-off ratio of up to 1.7×10⁶, which are higher than that of the control devices fabricated with gold electrodes. The high-performance of the devices is attributed to lower charge injection barrier at carbon nanotubes and pentacene interface. In order to find the direct evidence of the low injection barrier, we carry out low temperature electron transport measurement of our devices. We will present the detailed analysis of the low temperature data.

¹This work is partially supported by U.S. National Science Foundation under Grant ECCS 1102228

9:48AM P49.00008 Does Organic Field Effect Transistors (OFETs) Device Performance using Single-walled Carbon Nanotubes (SWNTs) Depend on the Density of SWNT in the Electrode?¹, NARAE KANG, BIDDUT K. SARKER, Nanoscience Technology Center, and Department of Physics, University of Central Florida, SAIFUL I. KHONDAKER, Nanoscience Technology Center, and Department of Physics, and School of Electrical Engineering and Computer Science, University of Central Florida, — Carbon nanotubes as an electrode material for organic field effect transistors (OFETs) have attracted significant attention. One open question is that whether the density of the Single-walled carbon nanotubes (SWNTs) in the electrode has any influence in the device performance of OFETs. In order to address this issue, we fabricated OFETs using SWNT aligned array electrode, where we varied the linear density of the nanotubes in the array of the electrodes during dielectrophoretic assembly of high quality surfactant free and stable aqueous SWNT solution. The source and drain of SWNT electrodes have been formed by electron beam lithography (EBL) and oxygen plasma etching. The OFETs were fabricated by depositing a thin film of poly (3-hexylthiophene) on the SWNT electrodes. We will present detailed result of our study.

¹This work is partially supported by U.S. National Science Foundation under Grant ECCS 1102228

10:00AM P49.00009 Work function recovery of air exposed molybdenum oxide thin films with vacuum annealing, IRFAN IRFAN, University of Rochester, ALEXANDER TURNISKE, University of Wisconsin, ZHENAN BAO, Stanford University, YONGLI GAO, University of Rochester — We report substantial work function (WF) recovery of air exposed molybdenum oxide thin films with vacuum annealing. The high WF (~6.8 eV) of thermally evaporated MoO_x thin film was observed to decrease sharply to ~5.6 eV with an air exposure of one hour. The drop in the WF was accompanied with a very thin layer of oxygen rich adsorbate on the MoO_x film. The WF of the exposed MoO_x film started to gradually recover with increasing annealing temperature in a vacuum chamber having base pressure of 8 × 10⁻¹¹ torr. The saturation in the WF recovery was observed around 460 °C, with WF ~6.4 eV. The adsorb layer was found to be removed after the vacuum annealing. We further studied the interface formation between the annealed MoO_x and copper phthalocyanine (CuPc). The highest occupied molecular orbital (HOMO) level of CuPc was observed to be almost pinned to the Fermi level, strongly suggesting an efficient hole injection through the vacuum annealed MoO_x film.

10:12AM P49.00010 Ab-initio calculation of energy level alignment and vacuum level shift at CuPc/C60 interfaces¹, NA SAI, XIAOYANG ZHU, JAMES CHELIKOWSKY, University of Texas at Austin, KEVIN LEUNG, Sandia National Laboratory — The alignment of the donor and acceptor energy levels is of crucial importance for organic photovoltaic performance. We investigate the interfacial electronic structure and energy level alignment of copper phthalocyanine (CuPc)/fullerene (C60) using ab-initio density functional theory calculations including van der Waals interactions and hybrid density functionals. We show that energy level alignment critically depends on the standing-up and lying-down orientation of the CuPc molecules relative to C60 at the interface. We calculate the magnitude of the interface dipole at different molecular orientations and compare them to the vacuum level shift observed in photoemission spectroscopy. The validity of existing theoretical models which invoke charge transfer on this organic interface will be discussed in light of our predictions. Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

¹This work is supported as part of the program “Understanding charge separation and transfer at interfaces in energy materials”, an Energy Frontier Research Center funded by the U.S. DOE Office of Basic Energy Sciences under Award number DE-SC0001091.

10:24AM P49.00011 Solution based cathode deposition for polymer light emitting devices, MARIAN TZOLOV, STEPHEN SWIONTEK, Department of Physics, Lock Haven University of PA — We report on a method for deposition of cathodes for polymer light-emitting devices (PLEDs), which is fundamentally different than the widely used thermal evaporation of metals. The thermal evaporation is well established in the industry but is very different than the solution processing of the rest of the PLEDs. It requires much more sophisticated equipment and much longer processing time than the solution processing. The metal evaporation requires temperatures around 1000°C with all following requirements for materials handling. Proposing a method alternative to the already well-established thermal evaporation technique is a challenging task, and we are demonstrating only the principal feasibility of a solution based deposition of the cathodes. It is based on electroless deposition of silver. The process is compatible with the solution processing of the rest of the device and allows to finalize the entire device using solution based processes. We demonstrate the most representative current-voltage characteristics, emission spectra, stability tests, and microstructure of the newly developed electrode. These initial experiments demonstrate the feasibility of the proposed method and point avenues for further improvement.

10:36AM P49.00012 Organic solar cells: How can the theory guide the experience?, NICOLAS BERUBE, VINCENT GOSSELIN, HUGO LEPAGE, MICHEL COTE, Universite de Montreal — Research in organic photovoltaic applications are receiving a great interest in the last few years as they offer an environmentally clean and low-cost solution to the world's rising energy needs. One of the main problems limiting the efficiency of an organic solar cell device is the strong binding energy of the excitons, typically of a few hundreds of meV, which is ten to one hundred times more than in inorganic devices. Another limiting factor, persistent in P3HT:PCBM devices, can be the misalignment of the the HOMO (Highest Occupied Molecular Orbital) and the LUMO (Lowest Unoccupied Molecular Orbital) energy levels of the different components of the solar cell. Scharber's model (Scharber, M.C., Adv. Mater. 18, 789) is a simple yet interesting approach for predicting the efficiency of those devices, mainly based on the values of the HOMO and the LUMO and reasonable assumptions for the exciton binding energy. In this presentation, we will discuss how theoretical calculations based on density-functional theory can provide a guide to find promising polymers for photovoltaic cells. The accuracy, limits and possible expansions of Scharber's model will be examined, and a number of interesting polymer candidates to reach and perhaps break the well-known 10 % efficiency will be presented.

Wednesday, February 29, 2012 8:00AM - 11:00AM –

Session P50 DPOLY: Focus Session: Dynamics of Polymers: Phenomena due to Confinement; Glass Transition 162B

8:00AM P50.00001 Theoretical prospects for understanding the glass transition in polymer thin films, SCOTT MILNER, Penn State University — Observations of confinement effects on the glass transition in thin polymer films remain vexing to theorists. Many experiments at sufficiently low frequencies consistently find that the free surfaces of many polymer films, whether freely suspended or supported, have anomalously low glass transition temperatures. This surface effect appears to be independent of molecular weight, and persists 10-20nm into the film. In contrast, freely suspended films have been observed by ellipsometry and other bulk-sensitive techniques to have anomalously low film-averaged T_g values, depending strongly on both film thickness and molecular weight for Mw above about 4×10^5 g/mol. The dependence on Mw persists to astonishingly large values ($\sim 10^7$ g/mol). Recent work of Pye and Roth strongly suggests the presence of two distinct mechanisms in these films, one operative at the free surface and Mw-independent, one depending on Mw and giving a weak second glass transition at considerably lower temperatures. In this talk, I will review the status of various theoretical proposals we have explored for explaining some of these disparate phenomena, including the effects of interrupted percolation at the free surface and the “sliding mechanism” originally suggested by de Gennes for Mw-dependent lowering of T_g . I will describe the present prospects for a successful theory, as well as suggest some potentially helpful experiments and analysis.

8:36AM P50.00002 Cooperative Length Scale and Fragility of Polystyrene under Confinement, CHUAN ZHANG, YUNLONG GUO, RODNEY PRIESTLEY, Princeton University — While thin films are an attractive model system to investigate the impact of confinement on glassy behavior, extending studies beyond thin films to geometries of higher dimensionalities is vital from both scientific and technological viewpoints. In this talk, we present the impact of confinement on the characteristic length at the glass transition as well as the fragility for confined polystyrene (PS) nanoparticles under isochoric conditions. We measure the glass transition temperature (T_g), fictive temperature (T_f) and isochoric heat capacity of silica-capped PS nanoparticles as a function of diameter via differential scanning calorimetry. From the measurement of T_f , we obtain the isochoric fragility, and via the fluctuation formula, the characteristic length at the glass transition. We illustrate that confinement under isochoric conditions for PS nanoparticles leads to a significant increase in the isochoric fragility while the characteristic length is reduced with size. At the minimum the results demonstrate a relationship between fragility and the characteristic length of isochorically-confined polymer that is not intuitive from the Adam-Gibbs theory.

8:48AM P50.00003 Impact of systematic chain architecture changes on the glass transition and modulus of thin polymer films, BRYAN VOGT, University of Akron, JESSICA TORRES, Intel, CHRISTOPHER STAFFORD, NIST, RICHARD REGISTER, Princeton University, DAVID UHRIG, Oak Ridge National Laboratory — We will discuss two systems that significantly impact the thin film behavior with minor changes in chemistry and chain architecture. First, two polymers based on 5-(2-phenylethyl)norbornene are examined. Depending on the polymerization route chosen, the resulting polymer backbone is comprised of either bicyclic (norbornyl) units, which leads to a relatively rigid polymer with a high bulk T_g , or monocyclic (cyclopentyl) units, which leads to a more flexible structure with a lower bulk T_g . The modulus and T_g of the rigid bicyclic polymer is thickness independent down to <10 nm, whereas the modulus of the more flexible monocyclic polymer decreases with decreasing thickness. By hydrogenation of the pendant phenyl ring to the cyclohexyl counterpart, we illustrate that minor changes in the relative flexibility of the side chain do not impact the observed thin film behavior. Second, a series of polystyrene with controlled branching including linear, comb, 6-arm star and centipede. Based upon the molecular mass of the arms, the comb polymer has a significantly larger persistence length and interestingly exhibits only a modest decrease in T_g (9 K) at 5 nm, while the moduli is thickness independent.

9:00AM P50.00004 A Direct Relationship between Enhanced Surface Mobility and Tg Reduction in Thin Polymer Films, ZAHRA FAKHRAAI, Department of Chemistry, University of Pennsylvania, JAMES A. FORREST, DONGPING QI, Department of Physics and Astronomy, University of Waterloo — Cooling rate dependent Tg measurements of thin polymer films show a strong correlation between the cooling rate and the confinement effects. It is observed that the Tg is more strongly dependent on the cooling rate as the film thickness is decreased. The confinement effects also become weaker at higher cooling rates and it appears that both for thick films and high cooling rates the confinement effect vanishes. The results can be plotted on an Arrhenius plot by assuming that the cooling rate is inversely related to the relaxation time as the temperature that the system falls out of equilibrium (Tg). The surface relaxation times can be independently measured using nano-hole relaxation and nanoparticle embedding techniques and the results can be plotted on the same Arrhenius plot. It is observed that the surface relaxation has much weaker temperature dependence, with an activation energy that matches the limit of zero film thickness for the rate-dependent Tg measurements. The strong correlation between surface properties obtained by direct mechanical measurements with the Tg measurements obtained by ellipsometry suggest that these two phenomena are from the same origin and one cannot be explained without the other.

9:12AM P50.00005 Reduced Glass Transition Temperatures of Thin Polymer Films - Confinement Effect or Artifact?, OLIVER BAEUMCHEN, JOSHUA D. MCGRAW, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1, JAMES A. FORREST, Department of Physics and Astronomy and Guelph-Waterloo Physics Institute, University of Waterloo, Waterloo, ON, Canada, N2L 3G1, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1 — For two decades there have been reports of measurements of reduced glass transition temperatures (T_g) in polymer, and in particular poly-styrene, films. These results have motivated theoretical models and a variety of sophisticated experiments probing interfacial polymer properties. While the much larger reductions in T_g for free standing films have suggested the importance of the free surface, a significant concern has been raised about a possible correlation between anomalous dynamics and incomplete equilibration of the sample. Here, we present new ellipsometry measurements which unambiguously address this concern. The glass transition in free standing and supported films can be changed by many 10's of degrees by manipulating the interfacial properties. Taken together with previous work the results clearly reveal the importance of free interfaces as we transition from two, to one, to zero free interfaces.

9:24AM P50.00006 Confinement in thin polymer films near Tg leads to factors of 10 to 1000 reductions in dye translational diffusion, JOHN TORKELOSON, HUI DENG, MANISH MUNDRA, Northwestern University — A breakthrough time/fluorescence resonance energy transfer method is used to measure out-of-plane translational diffusion coefficients of small-molecule dyes in thin polymer films near the glass transition temperature, Tg. The bulk translational diffusion coefficient is a strong function of dye size, increasing by a factor of 100 in polystyrene when dye molecular volume decreases by 25%. Reduction in PS film thickness below 500 nm leads to a factor of 1000 decrease in Disperse Red 1 diffusion coefficient while reduction below 140 nm leads to slightly more than a factor of 10 decrease in decacyclene diffusion coefficient. At a thickness less than 100 nm, the diffusion coefficients for the two dyes are identical within error. Similar effects have been observed in poly(methyl methacrylate) and polysulfone films at $T_g + 3$ K. These effects are not directly correlated with the Tg-confinement effect in these polymers as the length scales for confinement effects are much smaller in the case of Tg and in some of the polymers both diffusivity and Tg decrease with confinement.

9:36AM P50.00007 Measuring the glass transition of polymer nanodroplets, CHAD DALEY, JAMES FORREST, University of Waterloo — Despite almost 2 decades of measuring the glass transition temperature (T_g) in thin polymer films, there is no consensus on the magnitude (or even the existence) of observed T_g reductions. Recent suggestions that reduced T_g values in thin polystyrene films may be nothing more than a complicated artifact of sample preparation must be taken very seriously. Reduced T_g values are reported only for polymer films prepared on a non-wetting substrate where the film is unstable with respect to dewetting. In all cases only kinetic metastability allows one to measure a T_g value. The fundamental problem is that an unambiguous measure of T_g can only be obtained as the sample is cooled from the equilibrium liquid. No experiments involving thin polymer films have yet satisfied this condition. Our approach is to use samples prepared in the equilibrium state atop a non-wetting substrate (a collection of spherical caps). Since the droplets are already in the equilibrium state, they can be annealed for arbitrarily large times without evolution of the structure. We describe dilatometric measurements of T_g for nanometer sized spherical caps of polystyrene. This technique can be used to investigate the effect of annealing history and to extend the studies of T_g in high surface area to volume systems beyond polymers and into other molecular glass forming materials.

9:48AM P50.00008 Molecular motion in polymer thin films exhibits fast and slow subpopulations., KEEWOOK PAENG, MARK EDIGER, University of Wisconsin-Madison — The reorientation of dilute fluorescent probes in thin polymer films was studied using a photobleaching technique. The existence of two subsets of probe molecules with different dynamics was revealed by temperature-ramping and isothermal anisotropy measurements. For freestanding polystyrene films, the slow subset shows bulk-like dynamics while the more mobile subset reorients 4 orders of magnitude faster at $T_g - 5$ K. The difference in dynamics becomes larger as temperature decreases and disappears as temperature approaches T_g . We interpret the fraction of the sample with fast dynamics as a high mobility layer at the film surfaces. The thickness of this mobile surface layer increases with temperature and does not depend on the molecular weight of the polymer and total film thickness. The mobile surface layer exists in various freestanding polymer thin films including polystyrene and poly(methyl methacrylate) and is also present in supported films of these polymers.

10:00AM P50.00009 Confinement Effects of Neighboring Polymer Domains on the T_g s of Infinitely Dilute Blend Components and Ultrathin Film Layers, CHRISTOPHER EVANS, ROBERT SANDOVAL, JOHN TORKELSON, Northwestern University — Using fluorescence, we study the glass transition temperature (T_g) of a polymer species near the limit of infinite dilution. In blends with very dilute polystyrene (PS), intrinsic (unlabeled) and extrinsic dye-labeled fluorescence exhibit quantitative agreement for PS component T_g s. Dilute (0.1 wt%) PS T_g is strongly perturbed towards the matrix T_g ; e.g., 38 C in PnBMA and 119 C in PMMA. These dilute component T_g s yield a range of self-concentrations (0.18-0.47) in the framework of the Lodge-McLeish model. We also study multilayer, nanoconfined films with neighboring polymer domains by fluorescence. For PS supported on a bulk underlayer, the T_g of sub-100 nm PS is perturbed towards the underlayer T_g . For example, the 45 C T_g of a 14-nm PS layer on bulk PnBMA approaches the T_g for 0.1 wt% PS in PnBMA. These results underscore the role of neighboring polymer domains on the dynamics of an infinitely dilute species or an ultrathin polymer film layer and indicate that T_g -confinement effects in blends and thin films can be viewed as variations of the same physical phenomenon.

10:12AM P50.00010 Molecular Weight Dependent and Independent Glass Transition Temperature Reductions Coexisting in High MW Free-Standing Polystyrene Films, JUSTIN PYE, CONNIE ROTH, Dept of Physics, Emory University — Using transmission ellipsometry, we have measured the thermal expansion of ultrathin, high molecular weight (MW), free-standing polystyrene films over an extended temperature range. For two different MWs, we observed two distinct reduced glass transition temperatures (T_g s), separated by up to 60 K, within single films with thicknesses h less than 70 nm. The lower transition follows the previously seen MW dependent, linear $T_g(h)$ behavior, while we also observe the presence of a much stronger upper transition that is MW independent and exhibits the same $T_g(h)$ dependence as supported and low MW free-standing films. This represents the first experimental evidence indicating that two separate mechanisms can act simultaneously on thin free-standing polymer films to propagate enhanced mobility from the free surface into the material. The change in thermal expansion through the transitions indicate that $\sim 90\%$ of the film (matrix) solidifies at the upper transition with only $\sim 10\%$ of the material remaining mobile, freezing in at the lower transition. Surprisingly, when we compare our results to the existing literature, and especially the low MW free-standing film data, we conclude that the upper transition encompasses the free surface region and associated gradient in dynamics. This leaves open the question about where the small ($\sim 10\%$) fraction of material that has ultrafast, MW dependent dynamics resides within the film.

10:24AM P50.00011 Glass Transition and Physical Aging in Thin Polymer Films: A Unified Picture of Confinement, CONNIE ROTH, Dept. of Physics, Emory University — The effect of confinement on the glass transition, structural relaxation, and other material properties has garnered a great deal of attention during the past two decades. Despite the common misperception, there is considerably more agreement than disagreement (or "controversy") of the phenomena in the existing literature. This talk will summarize current experimental findings in the field, focusing on the author's recent work that links physical aging in thin polymer films to T_g changes near a free surface. We also demonstrate that the intricate molecular weight dependence of the film thickness dependent T_g reductions in free-standing films result from two separate mechanisms acting simultaneously on the films. From these results a universal picture is starting to emerge with some effects common to colloidal and small molecule glasses as well.

Wednesday, February 29, 2012 8:00AM - 11:00AM —

Session P51 DCMP DFD: Colloids III: Shear and Hydrodynamics Boston Convention Center 154

8:00AM P51.00001 Confined colloidal suspensions under simple shear, XINLIANG XU, STUART RICE, AARON DINNER, James Franck Institute, University of Chicago — Here we report a study of a simple model system, a colloidal suspension of near hard spheres in an otherwise Newtonian fluid using Stokesian Dynamics (SD) simulations in combination with Non-Equilibrium Umbrella Sampling (NEUS) techniques. The suspension is confined by an external potential in the y direction and is driven far out of equilibrium with a simple shear flow. At moderate shear rate, the suspension forms layers normal to the flow gradient direction, in contrast to equilibrium. In addition to that, novel anisotropic structures (strings in vorticity direction at low density for example) are observed within each layer. We use Non-Equilibrium Umbrella Sampling to explore the relationship between this string structure and the strength of the layer formation. Furthermore we have also studied the relationship between the non-Newtonian behavior of the suspension and the strength of the layer structure.

8:12AM P51.00002 The nonlinear structural response of colloidal suspensions under large amplitude oscillatory shear, NEIL Y.C. LIN, XIANG CHENG, ITAI COHEN, Physics Department, Cornell University — When a colloidal suspension is under oscillatory shear, the particle configuration has a flow-induced anisotropy. While these structural rearrangements have been intensively studied in the linear regime where the amplitude of the applied shear is small, the nonlinear structural response of suspensions under large amplitude oscillatory shear is poorly understood. Using a shear cell coupled to a fast confocal microscope, we directly measured the microscopic structure of colloidal suspensions under large amplitude oscillatory shear. To quantify the structural response, we integrated the pair correlation function over all contact positions; this quantity is proportional to the entropic stress of the suspension. We investigated the structural/stress response of colloidal suspensions systematically with increasing shear amplitudes. We observed strong nonlinear responses in both dense and dilute suspensions under large amplitude oscillatory shear. At even higher amplitudes, we found an overshoot of the stress response in dense suspensions. Our results provide insight on the microscopic structural origin of the nonlinear response of sheared colloidal suspensions.

8:24AM P51.00003 Imaging the microscopic structure of shear thinning and thickening colloidal suspensions, XIANG CHENG, Cornell University, JONATHAN MCCOY, Colby College, JACOB ISRAELACHVILI, University of California Santa Barbara, ITAI COHEN, Cornell University — The viscosity of colloidal suspensions can vary by orders of magnitude depending on how quickly they are sheared. Although this non-Newtonian behavior is believed to arise from the arrangement of suspended particles and their mutual interactions, microscopic particle dynamics in such suspensions are difficult to measure directly. Here, by combining fast confocal microscopy with simultaneous force measurements, we systematically investigate a suspension's structure as it transitions through regimes of different flow signatures. Our measurements of the microscopic single-particle dynamics unambiguously show that shear thinning results from the decreased relative contribution of entropic forces and that shear thickening arises from particle clustering induced by inter-particle hydrodynamic lubrication forces. Furthermore, we explore out-of-equilibrium structures of sheared colloidal suspensions and report a novel string phase, where particles link into log-rolling strings normal to the plane of shear. Our techniques illustrate an approach that complements current methods for determining the microscopic origins of non-Newtonian flow behavior in complex fluids.

8:36AM P51.00004 Shear induced diffusion in hard sphere glasses, NICK KOUMAKIS, GEORGE PETEKIDIS, FORTH & Univ. of Crete, Greece, JOHN BRADY, Chemical Engineering, Caltech, USA, FORTH TEAM, CALTECH TEAM — The response of dense hard sphere suspensions is examined during the application of steady and non-linear oscillatory shear using Brownian Dynamics (BD) simulations and experimental Light Scattering echo coupled with rheology. At rest, volume fractions around the glass transition exhibit long or infinite relaxation times. However, non-linear shear induces out of cage motions of comparable time scale to the applied rates. We found two distinct regimes in terms of stresses and dynamic response under shear. One regime for lower rates or frequencies of oscillation, governed by Brownian activated diffusion, and a second for higher rates related to shear activated diffusion. A linear dependence with rate was found for the diffusivity in the high rate regime, mirroring the viscous loss due to shear activated particle rearrangements, while diffusivities in the Brownian activated regime showed a power law exponent of less than unity. The exponent was found to increase with volume fraction. For applied rates inducing diffusivities above the in-cage diffusivity at rest, we find a time window of super-diffusive behavior, between the short time (in-cage) and long time (out-of cage) diffusivities under shear, a signature of a dynamic breaking and reforming of the cage.

8:48AM P51.00005 Diffusion in sheared athermal soft-particle suspensions: the role of inertia and dissipation mechanism, CRAIG MALONEY, KAMRAN KARIMI, Carnegie Mellon — We perform numerical simulations to study diffusion in a model bi-disperse frictionless athermal soft-particle suspension of disks in two dimensions (2D). To model athermal shear, we damp the motion of a particle *either* with respect to the globally imposed flow *or* with respect to its near neighbors. We study shear flows at various rate $\dot{\gamma}$, system size L , and damping strength b at packing fractions well above the random close packing point. At low $\dot{\gamma}$, we find a quasi-static effective transverse diffusion co-efficient, D_{eff} , which has very weak dependence on ϕ , b , or the damping mechanism yet has a pronounced linear dependence on L in agreement with what is observed in conventional models of bulk metallic glasses. Away from the quasi-static regime, D_{eff} no longer depends on L , and b has a profound impact on the scaling behavior of D_{eff} with $\dot{\gamma}$.

9:00AM P51.00006 Shear thinning in soft particle suspensions, PANAYIOTIS VOUDOURIS, Eindhoven University of Technology (a) Department of Mechanical Engineering, Materials Technology (b) Institute for Complex Molecular Systems, BERCO VAN DER ZANDEN, Eindhoven University of Technology - Department of Mechanical Engineering, DANIEL FLOREA, ZAHRA FAHIMI, HANS WYSS, Eindhoven University of Technology (a) Department of Mechanical Engineering, Materials Technology (b) Institute for Complex Molecular Systems — Suspensions of soft deformable particles are encountered in a wide range of food and biological materials. Examples are biological cells, micelles, vesicles or microgel particles. While the behavior of suspensions of hard spheres - the classical model system of colloid science - is reasonably well understood, a full understanding of these soft particle suspensions remains elusive. The relation between single particle properties and macroscopic mechanical behavior still remains poorly understood in these materials. Here we examine the surprising shear thinning behavior that is observed in soft particle suspensions as a function of particle softness. We use poly-N-isopropylacrylamide (p-NIPAM) microgel particles as a model system to study this effect in detail. These soft spheres show significant shear thinning even at very large Peclet numbers, where this would not be observed for hard particles. The degree of shear thinning is directly related to the single particle elastic properties, which we characterize by the recently developed Capillary Micromechanics technique. We present a simple model that qualitatively accounts for the observed behavior.

9:12AM P51.00007 Anisotropic Diffusion of Colloidal Particles in a Shear Flow, BRIAN LEAHY, DESMOND ONG, XIANG CHENG, ITAI COHEN, Cornell University — Asymmetrically-shaped particles show anisotropic diffusive behavior along different particle axes. This anisotropic diffusion, however, is averaged out on long time scales due to the rotational diffusion of the particles. Here we report on an experimental study of anisotropic colloidal dimers suspended in an oscillatory shear flow. A preferred orientation of the dimers arises due to the applied oscillatory shear. This results in anisotropic particle diffusion that is persistent at long time scales. We compare our results to a simple model of diffusing particles in a shear flow, and comment briefly on the possibility of using this result for assembling out-of-equilibrium colloidal structures.

9:24AM P51.00008 Pattern formation in colloidal explosions: Theory and experiment, ARTHUR STRAUBE¹, Humboldt University of Berlin, Germany, ARD LOUIS COLLABORATION², JÖRG BAUMGARTL, CLEMENS BECHINGER COLLABORATION³, ROEL DULLENS COLLABORATION⁴ — We study the nonequilibrium pattern formation that emerges when magnetically repelling colloids, trapped by optical tweezers, are abruptly released, forming colloidal explosions [EPL 94, 48008 (2011)]. For multiple colloids in a single trap, we observe a pattern of expanding concentric rings. For colloids individually trapped in a line, we observe explosions with a zigzag pattern that persists even when magnetic interactions are much weaker than those that break the linear symmetry in equilibrium. Theory and computer simulations quantitatively describe these phenomena both in and out of equilibrium. An analysis of the mode spectrum allows us to accurately quantify the nonharmonic nature of the optical traps. Colloidal explosions provide a new way to generate well-characterized nonequilibrium behavior in colloidal systems.

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9:36AM P51.00009 Universal Scaling Law of Diffusion and Hydrodynamic Corrections in Colloidal Monolayers¹, XIAO-GUANG MA, Hong Kong University of Science and Technology, WEI CHEN, Fudan University, Shanghai, China, ZIREN WANG, YUAN PENG, YILONG HAN, PENG TONG, Hong Kong University of Science and Technology — Using dense monolayers of colloidal particles and the techniques of optical microscopy and particle tracking, we tested the universal scaling law of the diffusion constant of colloidal particles as a function of excess entropy. By varying the area fraction of the colloidal monolayer, we measured the diffusion constant and the corresponding pair correlation function of the colloidal particles, from which the excess entropy can be calculated. It is found that the universal scaling law applies to a monolayer of latex suspensions at an air-water interface when the inter-particle repulsions are dominant over the hydrodynamic interactions. For colloidal monolayers of hard spheres at the air-water interface and near a solid wall, the universal scaling law starts to deviate from its original form as the short-ranged hydrodynamic interactions increase.

¹Work supported in part by the Research Grants Council of Hong Kong SAR.

9:48AM P51.00010 Long Range Hydrodynamic Correlations in Quasi-One-Dimensional Circular and Linear Geometries, EKATERINA KOSHELEVA, Harvard Univ., BRIAN LEAHY, Cornell Univ., HAIM DIAMANT, Tel Aviv Univ., STUART A. RICE, BINHUA LIN, Univ. of Chicago — We report the results of studies of the collective and pair diffusion coefficients of particles in two quasi-one-dimensional geometries: straight 2 mm long channels and rings with radii between 3 and 35 μm . We investigate, for both geometries, the observed density dependence in the collective diffusion coefficient as predicted by Frydel and Diamant (Phys. Rev. Letts. 104, 248302 (2010)). The origin of this density dependence is the nonvanishing $q = 0$ component of the Green's function of the linearized one-dimensional hydrodynamic equation, which is indicative of the hydrodynamic coupling resulting from collective motion of particles in periodic or infinite quasi-one-dimensional geometries.

10:00AM P51.00011 Using artificial microswimmers for particle separation, VYACHESLAV R. MISKO, University of Antwerp, Belgium, WEN YANG, Taiyuan University of Science and Technology, P.R. China, KWINTEN NELISSEN, University of Antwerp, Belgium, MINGHUI KONG, Institute of Plasma Physics, Hefei, P.R. China, FRANCOIS M. PEETERS, University of Antwerp, Belgium — Microscopic self-propelled swimmers capable of autonomous navigation through complex environments provide appealing opportunities for localization, pick-up and delivery of micro- and nanoscopic objects. Inspired by motile cells and bacteria, man-made microswimmers have been created, and their motion was studied experimentally in patterned surroundings [1]. We propose to use artificial microswimmers – Janus spheres [2] illuminated by light – as “driving agents” that move through a binary mixture of colloidal particles. We demonstrated [3] that binary mixtures can be effectively separated in this way. We analyzed the main features of the particle separation and explained mechanisms of different regimes including the one with a velocity inversion. Our finding can be readily verified in experiments with colloidal binary mixtures and could be of use for various biological and medical applications.

[1] G. Volpe et al., Soft Matter **7**, 8810 (2011).

[2] Q. Chen et al., Science **331**, 199 (2011).

[3] W. Yang, V.R. Misko, K. Nelissen, M. Kong, and F.M. Peeters, arXiv:1109.5099 (2011).

10:12AM P51.00012 Diffusion in Dense Inhomogeneous Colloid Suspensions in Narrow Channels, BINHUA LIN, EMILY WONDER, STUART A. RICE, Univ. of Chicago — We report the results of a study of single particle diffusion in dense colloid fluids confined in a ribbon channel geometry that is intermediate between quasi-one-dimensional (q1D) and quasi-two-dimensional (q2D). In all of the systems studied the colloid density distribution transverse to the ribbon channel is stratified with peak amplitudes that depend on the colloid density. Although the virtual walls that confine a stratum are structured with a scale length of the colloid diameter, that structure does not have an apparent influence on the single particle diffusion, which shows the characteristic features of diffusion in a q1D channel with smooth walls. We find that for all channel widths and packing fractions studied the single particle transverse diffusion coefficient in a stratum is smaller than the single particle longitudinal diffusion coefficient in the same stratum, and that the single particle longitudinal diffusion coefficient varies very little from stratum to stratum, being only slightly smaller in the dense strata next to the walls than in central strata. The lack of variation of the longitudinal diffusion coefficient with apparent stratum density is explained by application of the Fischer-Methfessel approximation to the local density in an inhomogeneous liquid. The ratio of the transverse to longitudinal diffusion coefficients varies very slowly with ribbon width, implying a very slow transition from q1D to q2D behavior.

10:24AM P51.00013 Flow of concentrated emulsion in a microchannel: walls effects and roughness impact, VINCENT MANSARD, ANNIE COLIN, LOF, Universite de Bordeaux, LYDÉRIC BOCQUET, LPMC, Université Lyon 1 — Soft glassy materials have ubiquitous rheological properties. At small stress they deform elastically. For stress above a threshold they flow like liquids. At microscale, they are composed of highly disordered particles caged by the neighborhood. Flow happens by successive cage-jumps -or rearrangement. We study concentrated emulsion as a model fluid. When it flows in confined geometry, the viscosity does not correspond to the rheometer measurements but obeys to a non-local relation (Goyon-2008) due to rearrangement's correlation. As they impose viscosity's boundary conditions, walls modify the flow. We study carefully the conditions imposed by the walls and the impact of the roughness. In a microchannel, we create a Poiseuille flow. Using a fast confocal microscope we visualize the droplets and measure the velocity with high spatial resolution. At high stress, we observe one or two discontinuities of the velocity at respectively one and two droplets' diameters. They are due to stratification of the first droplets' layers. Far from them the non-local model remains valid. We create roughness by adding controlled size patterns. The roughness modifies the apparition of the stratifications and the limit conditions on the viscosity. We will compare these results with theory.

10:36AM P51.00014 Non-equilibrium dynamics in particle-interface systems, ANNA WANG, School of Engineering and Applied Sciences, Harvard University, RYAN MCGORTY¹, University of California, San Francisco, DAVID M. KAZ², University of California, Berkeley, VINOTHAN N. MANOHARAN³, School of Engineering and Applied Sciences, Harvard University — When a particle is at equilibrium at a fluid-fluid interface, its position can be calculated with Young's law (which has been used since 1805). The non-equilibrium behavior of particles at fluid-fluid interfaces, however, is only just beginning to be studied. In this talk, we will discuss the behavior of colloidal particles as they approach and meet an oil-water interface. A variety of different systems, such as approach from both the aqueous and oil phases and using aqueous phases of various salt concentrations will be compared. The motion of the polymer microspheres is captured using digital holographic microscopy in real time. As the holograms are simply two-dimensional images, the frame rate is limited only by the CMOS sensor and frame rates of up to 2000fps are used in this study. We then analyze the high frame rate data to recover the three-dimensional trajectory and fluctuations of the particles.

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10:48AM P51.00015 Granular Fluid Kinetics Approach to Modeling Soft Colloid and Polymer Materials¹, DIMITER PETSEV², JHOAN TORO-MENDOZA³, University of New Mexico, FRANK VAN SWOL⁴, University of New Mexico and Sandia National Laboratories — The objective of this study is to understand the fundamental laws governing the Brownian motion of viscoelastic particles suspended in solvent at macroscopic equilibrium. Our hypothesis is that the internal degrees of freedom of the particles couple to their translational Brownian motion and affect their mean square displacement. Our system is similar to granular fluids with the important distinction that the energy absorbed by the particles during a collision is returned back thus maintaining a global thermodynamic equilibrium. We propose a new Molecular Dynamics model system that consists of tracer Brownian particles, solvent, and a virtual third component that serves as a thermal bath. The energy that is lost in an inelastic collision between Brownian and solvent particles is returned to the bath. The bath particles are undergoing elastic collisions among themselves and also with the solvent and Brownian particles. This provides a mechanism to restore and maintain an overall thermal equilibrium in the whole system. We report data on the effect of particle inelasticity on the translational diffusion.

¹This work was supported by NSF Grants 0844645 and 0611616.

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Wednesday, February 29, 2012 8:00AM - 11:00AM –
Session P52 GSNP DFD: Focus Session: Extreme Mechanics - Structures for Form and Function 153C

8:00AM P52.00001 Soft Robots: Manipulation, Mobility, and Fast Actuation, ROBERT SHEPHERD, FILIP ILIEVSKI, WONJAE CHOI, ADAM STOKES, STEPHEN MORIN, AARON MAZZEO, REBECCA KRAMER, Harvard, CARMEL MAJIDI, Carnegie Mellon, ROB WOOD, GEORGE WHITESIDES, Harvard — Material innovation will be a key feature in the next generation of robots. A simple, pneumatically powered actuator composed of only soft-elastomers can perform the function of a complex arrangement of mechanical components and electric motors. This talk will focus on soft-lithography as a simple method to fabricate robots—composed of exclusively soft materials (elastomeric polymers). These robots have sophisticated capabilities: a gripper (with no electrical sensors) can manipulate delicate and irregularly shaped objects and a quadrupedal robot can walk to an obstacle (a gap smaller than its walking height) then shrink its body and squeeze through the gap using an undulatory gait. This talk will also introduce a new method of rapidly actuating soft robots. Using this new method, a robot can be caused to jump more than 30 times its height in under 200 milliseconds.

8:12AM P52.00002 Low-Dimensional Generalized Coordinate Models of Large-Deformation Elastic Joints¹, LAEL ODHNER, AARON DOLLAR, Department of Mechanical Engineering, Yale University — In the field of robotics, it is increasingly common to use elastic elements such as rods, beams or sheets to allow motion between the rigid links of a robot, rather than conventional sliding mechanisms such as pin joints. Although these elastic joints are simpler to manufacture, especially at meso- and micro-scales, representational simplicity is sacrificed. It is far easier to compute the Lagrangian of a robot using joint angles as generalized coordinates, rather than by considering the large-deformation continuum behavior of elastic joints. In this talk, we will discuss our work toward finding accurate, low-dimensional discretizations of elastic joint mechanics, suitable for use in generalized coordinate models of robot kinematics and dynamics. We use modally parameterized backbone curves to describe the kinematic configuration of the elastic joints, and compute the energy associated with deformation using rod and shell theory. In the plane, only three smooth deformation modes are sufficient to describe Euler-Bernoulli bending of 90 degrees to within 1 percent. Parametric models for the three-dimensional motion of sheet hinges are more complex, but can be simplified significantly using boundary conditions and constraints imposed by ruled surface assumptions.

¹This work is supported by National Science Foundation grant IIS-0952856.

8:24AM P52.00003 Liquid-Embedded Elastomer Electronics, REBECCA KRAMER, Harvard University, CARMEL MAJIDI, Carnegie Mellon University, YONG-LAE PARK, JAMIE PAIK, ROBERT WOOD, Harvard University — Hyperelastic sensors are fabricated by embedding a silicone rubber film with microchannels of conductive liquid. In the case of soft tactile sensors, pressing the surface of the elastomer will deform the cross-section of underlying channels and change their electrical resistance. Soft pressure sensors may be employed in a variety of applications. For example, a network of pressure sensors can serve as artificial skin by yielding detailed information about contact pressures. This concept was demonstrated in a hyperelastic keypad, where perpendicular conductive channels form a quasi-planar network within an elastomeric matrix that registers the location, intensity and duration of applied pressure. In a second demonstration, soft curvature sensors were used for joint angle proprioception. Because the sensors are soft and stretchable, they conform to the host without interfering with the natural mechanics of motion. This marked the first use of liquid-embedded elastomer electronics to monitor human or robotic motion. Finally, liquid-embedded elastomers may be implemented as conductors in applications that call for flexible or stretchable circuitry, such as robotic origami.

8:36AM P52.00004 Extreme Mechanics in Soft Pneumatic Robots and Soft Microfluidic Electronics and Sensors, CARMEL MAJIDI, Carnegie Mellon University — In the near future, machines and robots will be completely soft, stretchable, impact resistance, and capable of adapting their shape and functionality to changes in mission and environment. Similar to biological tissue and soft-body organisms, these next-generation technologies will contain no rigid parts and instead be composed entirely of soft elastomers, gels, fluids, and other non-rigid matter. Using a combination of rapid prototyping tools, microfabrication methods, and emerging techniques in so-called “soft lithography,” scientists and engineers are currently introducing exciting new families of soft pneumatic robots, soft microfluidic sensors, and hyperelastic electronics that can be stretched to as much as 10x their natural length. Progress has been guided by an interdisciplinary collection of insights from chemistry, life sciences, robotics, microelectronics, and solid mechanics. In virtually every technology and application domain, mechanics and elasticity have a central role in governing functionality and design. Moreover, in contrast to conventional machines and electronics, soft pneumatic systems and microfluidics typically operate in the finite deformation regime, with materials stretching to several times their natural length. In this talk, I will review emerging paradigms in soft pneumatic robotics and soft microfluidic electronics and highlight modeling and design challenges that arise from the extreme mechanics of inflation, locomotion, sensor operation, and human interaction. I will also discuss perceived challenges and opportunities in a broad range of potential application, from medicine to wearable computing.

9:12AM P52.00005 Macrocomposite mechanical design, modeling, and behavior of physical models of bioinspired fish armor , ASHLEY BROWNING, Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, CHRISTINE ORTIZ, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, MARY C. BOYCE, Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139 — The macrocomposite design of flexible biological exoskeletons, consisting of overlapping mineralized armor units embedded in a compliant tissue, is a key determinant of their mechanical function (e.g penetration resistance and biomechanical flexibility). Here, we investigate the role of macrocomposite structure, composition, geometric orientation, and spatial distribution in a flexible model natural armor system present in the majority of teleost fish species. Physical multi-material composite models are fabricated using a combination of 3-D printing and molding methods. Mechanical experiments using digital image correlation enable measurement of both the macroscopic response and underlying deformation mechanisms during various loading scenarios. Finite element-based mechanical models yield detailed insights into the roles and the tradeoffs of the composite structure providing constraint, shear, and bending mechanisms to impart protection and flexibility.

9:24AM P52.00006 Periodic Structural Solids: Mechanics and Multifunctional Applications , LIFENG WANG, Clarkson University — Triply periodic minimal surfaces have been of great interest to mathematicians, physical scientists, material scientists, and biologists. Close physical approximations to triply periodic minimal surfaces arise in a few material systems, such as block copolymers, nanocomposites, and biological exoskeletons. Here, we demonstrate the potential to design and fabricate two-component periodically ordered structures which correspond to the level set structures associated with triply periodic minimal surfaces. These structures are shown to have a unique combination of stiffness, strength, and energy absorption, as well as damage tolerance. The results provide guidelines for engineering and tailoring the nonlinear mechanical behavior and energy absorption of cocontinuous composites for a wide range of applications and further creating multifunctional materials. For example, polymeric materials which can change shape and material properties in response to external stimuli (temperature or electric field) can provide additional functionality when used as one of the phases, such as 3D shape memory. The periodic and multiphase nature of the structures also enables mechanically tunable band gap (phononic or photonic) materials, and tunable sensors in tissue engineering.

9:36AM P52.00007 Honeycombs with hierarchical organization¹ , AMIN AJDARI, BABAK HAGHPANAH JAHROMI, JIM PAPADOPOULOS, ASHKAN VAZIRI, Northeastern University — We investigated the mechanical behavior of two-dimensional hierarchical honeycomb structures using analytical, numerical and experimental methods. Hierarchical honeycombs were constructed by replacing every three-edge vertex of a regular hexagonal lattice with a smaller hexagon. Repeating this process builds a fractal-appearing structure. The resulting isotropic in-plane elastic properties (effective elastic modulus and Poisson's ratio) of this structure are controlled by the dimension ratios for different hierarchical orders. Hierarchical honeycombs of first and second order can be up to 2.0 and 3.5 times stiffer than regular honeycomb at the same mass (i.e., same overall average density). The Poisson's ratio varies from nearly 1.0 (when planar "bulk" modulus is considerably greater than Young's modulus, so the structure acts "incompressible" for most loadings) to 0.28, depending on the dimension ratios. The work provides insight into the role of structural organization in regulating the mechanical behavior of materials, and new opportunities for developing low-weight cellular structures with tailorable properties.

¹This work was supported in part by the U.S. Air Force Office of Scientific Research under AFOSR YIP grant award, #FA 9550-10-1-0145 and in part by the U.S. Department of Homeland Security under Award Number 2008-ST-061-ED0001.

9:48AM P52.00008 Buckling-induced Tunable Chirality in Rationally-Designed Surface-Attached Cellular Structures¹ , SICONG SHAN, SUNG HOON KANG, WIM NOORDUIN, School of Engineering and Applied Sciences, Harvard University, MUGHEES KHAN, Wyss Institute for Biologically Inspired Engineering, KATIA BERTOLDI, JOANNA AIZENBERG, School of Engineering and Applied Sciences, Harvard University — Chirality is crucial in understanding and controlling the behavior of living and non-living systems since the presence or absence of chirality in the structures plays important roles in their interactions with molecules, enzymes, light, and mechanical stress. Processes that induce chirality have been extensively studied at the molecular and macroscopic scales, but are relatively unexplored at the mesoscale. By rational design based on modeling, we experimentally demonstrate the controlled reversible switching between achiral and chiral configurations using swelling/de-swelling of surface-attached cellular structures. Importantly, the buckling patterns and the associated symmetry reduction of the initially achiral centrosymmetric structures could be tuned, simply by changing their dimensions. This approach opens the way to deterministically select to select the appearance of either mixed (racemic) or chiral phases. In the case of chiral transformations, spontaneous symmetry breaking resulted in the formation of large uniform areas of structures of single handedness. The fundamental understanding of this process provides a general route to designing deterministically deformable structures with dynamically switchable mechanical and/or optical properties.

¹Materials Research Science and Engineering Center under NSF Award No. DMR-0820484

10:00AM P52.00009 Buckling-induced Planar Chirality of Porous Elastic Structure , JONGMIN SHIM, SICONG SHAN, SUNG H. KANG, PAI WANG, Harvard University, BETH R. CHEN, University of Michigan, Ann Arbor, JOANNA AIZENBERG, KATIA BERTOLDI, Harvard University — We present two periodic elastomeric structures which develop planar chirality induced by buckling under uniaxial/biaxial loading. The geometry of the structure comprises a 2-D plate patterned with a regular array of circular voids. Two specific circular void arrangements are obtained by investigating buckling-induced pattern transformations for void closure. Beyond the critical load, the thin ligaments between two adjacent voids buckle leading to a cooperative buckling cascade within the 2-D plate. Both micro-scale swelling experiments and finite element simulations are used to explore the underlying mechanics in detail and to show a proof of concept of the proposed structures. During swelling, the initial non-chiral pattern of the circular voids is transformed to a deformed pattern which exhibits planar chirality through buckling-induced symmetry breaking. In order to explore the effect of planar chirality, we perform an acoustic band structure calculation at different level of deformation. The planar chirality is found to strongly affect the in-plane phononic band gaps, providing opportunities for tunable phononic band structures.

10:12AM P52.00010 Anisotropy-induced wave steering in periodic linear and nonlinear lattices , FILIPPO CASADEI, JULIAN RIMOLI, MASSIMO RUZZENE, Georgia Institute of Technology — Structural lattice configurations can be designed with tailored topologies which provide them with unusual behaviors, such as negative bulk modulus, negative Poisson's ratios, or extreme anisotropy¹. The latter is of particular relevance to explore the inherent anisotropic behavior of periodic lattices as a design paradigm for wave guiding and steering applications. The equivalent material anisotropy of square and skew periodic lattices is investigated through the application of Bloch's theorem² to the finite element discretization of the representative unit cell. The in-plane directions of wave propagation are determined through detailed analysis of the longitudinal and shear wave velocities, and verified through full-field wave propagation simulations. Similar wave behaviors are investigated analytically and experimentally for multilayer composite panels with anisotropic lay-ups in order to demonstrate the feasibility of micro structural design as an effective approach for wave management.

¹M. Ruzzene et al. *Physica Status Solidi B*, **242**, 665 (2005)

²Bloch F., *Z. Physik* **52**, 555 (1928)

10:24AM P52.00011 2-D Phononic Crystals – Unraveling the Effect of Void Distribution in Porous Structures, PAI WANG, JONGMIN SHIM, KATIA BERTOLDI¹, Harvard University, KATIA'S GROUP TEAM² — Phononic crystals are periodic materials consisting of different constituents with the capability to control the propagation of elastic waves. In this study, the dispersion relations of two-dimensional phononic crystals with *circular voids* are investigated using Bloch-wave analysis. Porous patterns are derived from the *Laves tilings*, which are duals of the eleven *convex uniform tilings* of the *Euclidean plane*. Numerical simulations are performed on the microstructures using finite element method. Frequency band-gaps are calculated and compared among different geometric configurations, void-volume fractions, and material properties, providing valuable insight into the behavior of phononic crystals. The predictive technical procedure developed here offers opportunities for the design of mechanical wave filters that have many potential applications such as noise-cancelling devices, acoustic wave guides and vibration isolators.

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10:36AM P52.00012 Guiding of High Amplitude Stress Waves Through Stress-Induced Domain Switching in Multiphase Materials, JULIAN RIMOLI, LUCA GUIDONI, BRETT REICHARD, MASSIMO RUZZENE, Georgia Institute of Technology — Periodic and graded Multiphase Materials (MMs) are of great interest to scientists and engineers because of their unique static and dynamic mechanical properties, and the design flexibility they provide. In the linear range operation, MMs can be designed to attenuate vibrations over wide frequency bands and in specified directions, as defined by topology, geometry and material of the unit cell. Similarly, unit cell design and topology can be selected to obtain a desired anisotropy in the material, which can be exploited to alter the path of propagation of elastic and high amplitude stress waves. Specifically, steering of waves in preferential directions can be achieved through the proper arrangement of periodic hard inclusions within a matrix. Such a capability is extremely important for the design of materials capable of guiding stress waves to propagate along specified paths. In the present work, we explore the use of periodic metamaterials for wave management in force protection applications. We define topologies which adapt to high amplitude mechanical inputs, and study through numerical simulations and experiments local and global instabilities which lead to adaptive mechanical behavior through topological and structural modifications.

10:48AM P52.00013 Soft Modes and Deformations of Three-Dimensional Isostatic Periodic Lattices, ANTON SOUSLOV, Georgia Institute of Technology, T.C. LUBENSKY, University of Pennsylvania — Each particle in a three-dimensional isostatic lattice is connected by springs on average to six nearest neighbors, a condition obtained by J.C. Maxwell for marginal stability. The cubic and pyrochlore lattices satisfy this condition. By calculating the dispersion relations and the density of states for phonons in these lattices, we expand on previous studies of isostatic periodic structures [1], which have largely been focused on the simpler two-dimensional cases. The low energy phonon spectrum of these lattices exhibits features common to isostatic systems in any dimension, such as the presence of floppy modes and the scaling of a divergent length and a vanishing critical frequency. However, the allowed symmetries of an elasticity theory and the number of floppy modes depend on dimension and play a crucial role in the structure of the low-frequency response. We relate these findings to the isostatic transition in systems of close-packed athermal spheres and look at an analogy with three-dimensional crystals with zeolite structure.

[1] A. Souslov, A. J. Liu, and T. C. Lubensky, Phys. Rev. Lett. 103, 205503 (2009)

Wednesday, February 29, 2012 8:00AM - 11:00AM – Session P53 GSNP: Disordered Systems: Packing 153B

8:00AM P53.00001 Analytical Construction of A Dense Packing of Truncated Tetrahedra and Its Melting Properties, YANG JIAO, SALVATORE TORQUATO, Princeton University — Dense polyhedron packings are useful models of a variety of condensed matter and biological systems and have intrigued scientists and mathematicians for centuries. Here, we analytically construct the densest known packing of truncated tetrahedra with a remarkably high packing fraction $207/208=0.995\ 192$, which is amazingly close to unity and strongly implies its optimality. This construction is based on a generalized organizing principle for polyhedra that lack central symmetry that we introduce here. The packing characteristics and equilibrium melting properties of the putative optimal packing as the system undergoes decompression are discussed.

8:12AM P53.00002 Packing fraction of dimers and anisotropic objects, TAISHAN ZHU, YULIANG JIN, HERNAN A MAKSE, Levich Institute and Physics Department, the City College of New York, New York, NY 10031, USA, MAXIMILIEN DANISCH, ENS, Cachan, ADRIAN BAULE, School of Mathematical Sciences Queen Mary, University of London — We present a statistical theory and computer simulations for the calculation of the average volume in jammed assemblies of dimer shaped objects and other anisotropic particles like spherocylinders. The theory predicts the volume fraction as a function of the coordination number of the particles.

8:24AM P53.00003 Statistical Mechanics of Athermal Packings: Incorporating Basin Volumes, ASHWIN S. S., Departments of Mechanical Engineering & Materials Science and Physics, Yale University, JERZY BLAWZDZIEWICZ, Mechanical Engineering, Texas Tech University, COREY S. O'HERN, Departments of Mechanical Engineering & Materials Science and Physics, Yale University, MARK D. SHATTUCK, Benjamin Levich Institute and Physics Department, The City College of the New York — We present a first principles formalism for the statistical mechanics of athermal packings subject to driving beyond the weak limit. Edwards hypothesized a statistical mechanics of flat measure associated with packings explored at fixed density. This ensemble has been found to work well in the limit of very weak (but non-zero) driving. Beyond the weak driving limit, the probability measures associated with jammed states become proportional to the volume of basins of attractions associated with the packings on the density landscape. We propose here, a statistical mechanics which takes into consideration the volume of basins of attraction under certain approximations. Further, the statistical mechanics takes into account the protocol by writing the partition function in terms of an integral over protocol dependent generalized coordinates. This will allow an extremum principle to determine states, in these out of equilibrium systems.

8:36AM P53.00004 Polydisperse sphere packing in high dimensions, a search for an upper critical dimension, PETER MORSE, Department of Physics: University of Oregon, MAXIME CLUSEL, Laboratoire Charles Coulomb UMR 5221, CNRS and Université Montpellier 2, F-34095, Montpellier, France, ERIC CORWIN, Department of Physics: University of Oregon — The recently introduced granocentric model for polydisperse sphere packings has been shown to be in good agreement with experimental and simulational data in two and three dimensions. This model relies on two effective parameters that have to be estimated from experimental/simulational results. The non-trivial values obtained allow the model to take into account the essential effects of correlations in the packing. Once these parameters are set, the model provides a full statistical description of a sphere packing for a given polydispersity. We investigate the evolution of these effective parameters with the spatial dimension to see if, in analogy with the upper critical dimension in critical phenomena, there exists a dimension above which correlations become irrelevant and the model parameters can be fixed *a priori* as a function of polydispersity. This would turn the model into a proper theory of polydisperse sphere packings at that upper critical dimension. We perform infinite temperature quench simulations of frictionless polydisperse sphere packings in dimensions 2-8 using a parallel algorithm implemented on a GPGPU. We analyze the resulting packings by implementing an algorithm to calculate the additively weighted Voronoi diagram in arbitrary dimension.

8:48AM P53.00005 Constraint percolation on hyperbolic lattices , JORGE LOPEZ, J.M. SCHWARZ, Physics Department, Syracuse University — Constraint percolation models include constraints on the occupation of sites to, for example, better understand the onset of glassiness in glass-forming liquids. The dynamical glass transition in the Fredrickson-Andersen model simplifies to the study of the percolation transition in k -core percolation where every occupied site must have at least k occupied neighbors. Other constraint percolation models, such as force-balance percolation, have been introduced to begin to account for mechanical equilibrium on each particle arising during the onset of jamming. To study a mean-field-like version of force-balance percolation in which the directionality of forces becomes important, we consider clusters with occupied particles satisfying the $k = 3$ -core condition and lying inside a triangle determined by three of its occupied neighbors. The model is constructed on a tessellation of the Poincaré disk, thus, bearing a hyperbolic structure. Models on such spaces exhibit mean-field-like behavior and also play an important role in generating geometric frustration in glassy systems. We analytically investigate the conditions under which there exists a transition as well as the underlying nature of the transition. We also present numerical results to compare with our analytical results.

9:00AM P53.00006 Cavity method for Edwards ensemble of jammed matter , HERNAN MAKSE, LIN BO, YULIANG JIN, the City College of New York, CHAOMING SONG, Northeastern University, SOFT MATTER AND COMPLEX SYSTEMS LAB TEAM — Two theoretical frameworks have emerged to investigate the problem of random close packings: the Edwards statistical mechanics and the cavity method for glassy systems. Here we propose a model that combines both approaches into a single Hamiltonian imposing force balance constraints and minimization of the volume of the system. The formalism can be put into the framework of constraint optimization problems as recently proposed. The cavity method then solves the problem of force balance providing a prediction of the coordination number of the jammed packing. The model can be applied to spherical frictionless and frictional particles as well as non-spherical particles providing a prediction of the coordination number as a function of the aspect ratio of the particles.

9:12AM P53.00007 Glass Transition and Random Close Packing above Three Dimensions¹ , PATRICK CHARBONNEAU, Duke University, ATSUSHI IKEDA, Universite Montpellier 2, GIORGIO PARISI, Sapienza Universita di Roma, FRANCESCO ZAMPONI, Ecole Normale Supérieure — Motivated by a recently identified severe discrepancy between a static and a dynamic theory of glasses, we numerically investigate the behavior of dense hard spheres in spatial dimensions 3 to 12. Our results are consistent with the static replica theory, but disagree with the dynamic mode-coupling theory, indicating that key ingredients of high-dimensional physics are missing from the latter. We also obtain numerical estimates of the random close packing density, which provides new insights into the mathematical problem of packing spheres in large dimension.

¹NSF Support No. DMR-1055586

9:24AM P53.00008 Packing Squares in a Torus¹ , DONALD BLAIR, CHRISTIAN SANTANGELO, JON MACHTA, University of Massachusetts Amherst — We study the densest packings of N unit squares in a torus (i.e., using periodic, square boundary conditions in 2D) using both analytical methods and simulated annealing. We find a rich array of dense packing solutions: density-one packings when N is the sum of two square integers, a family of “gapped bricklayer” Bravais lattice solutions with density $N/(N+1)$, and some surprising non-Bravais lattice configurations – including lattices of holes, as well as a configuration for $N=23$ in which not all squares share the same orientation. We assess the entropy of some of these configurations, as well as the frequency and orientation of density-one solutions as N goes to infinity.

¹With support from NSF grants DMR-0907235 and DMR-0846582, as well as the NSF-funded Center for Hierarchical Manufacturing, CMMI-1025020

9:36AM P53.00009 Characterization of Basin Volumes in Mechanically Stable Packings¹ , MARK D. SHATTUCK, Benjamin Levich Institute and Physics Department of The City College of New York, S.S. ASHWIN, Departments of Mechanical Engineering & Material Science and Physics, Yale University, JERZY BLAWZDZIEWICZ, Department of Mechanical Engineering, Texas Tech University, COREY S. O’HERN, Departments of Mechanical Engineering & Material Science and Physics, Yale University — There are a finite number of distinct mechanically stable (MS) packings in granular systems composed of frictionless particles. For typical packing-generation protocols employed in experimental and numerical studies, the probabilities with which the MS packings occur are highly nonuniform and depend strongly on preparation protocol. Despite intense work, it is extremely difficult to predict *a priori* the MS packing probabilities. We describe a novel computational method for calculating the MS packing probabilities by directly measuring the volume of the MS packing ‘basin of attraction’, which we define as the collection of initial points in configuration space at *zero packing fraction* that map to a given MS packing by following a particular dynamics in the density landscape. We show that there is a small core region with size l_c surrounding each MS packing in configuration space in which all initial conditions map to a given MS packing. However, we find that the MS packing probabilities are not strongly correlated with l_c and thus they are determined by complex geometric features of the landscape that are distant from the MS packing.

¹Supported by NSF CBET-0968013, CBET-0967262, NSF PREM DMR-0934206

9:48AM P53.00010 ABSTRACT WITHDRAWN —

10:00AM P53.00011 Hierarchical freezing in a lattice model with a nonperiodic ground state¹ , JOSHUA E.S. SOCOLAR, TRAVIS BYINGTON, Duke University — A recent result in tiling theory provides a two-dimensional lattice model with nearest and next-nearest neighbor interactions that has a limit-periodic ground state. During a slow quench from the high temperature, disordered phase, the ground state emerges through an infinite sequence of phase transitions, all related by renormalizations of the temperature scale with the sequence of critical temperatures approaching zero. As the temperature is decreased, sublattices with increasingly large lattice constants become ordered. Quenching at any finite rate eventually results in glass-like state due to kinetic barriers created by simultaneous freezing on sublattices with different lattice constants.

¹Supported by NSF’s Research Triangle MRSEC (DMR-1121107).

10:12AM P53.00012 Degenerate Quasicrystal of Hard Triangular Bipyramids Stabilized by Entropic Forces , AMIR HAJI-AKBARI, MICHAEL ENGEL, SHARON GLOTZER, University of Michigan — The assembly of hard polyhedra into novel ordered structures has recently received much attention. Here we focus on triangular bipyramids (TBPs)- i.e. dimers of hard tetrahedra- which pack densely in a simple triclinic crystal with two particles per unit cell [1]. This packing is referred to as the TBP crystal. We show that hard TBPs do not form this densest packing in simulation. Instead, they assemble into a different, far more complicated structure, a dodecagonal quasicrystal, which, in the level of monomers, is identical to the quasicrystal recently discovered in the hard tetrahedron system [2], but the way that tetrahedra pair into TBPs in the nearest neighbor network is random, making it the first degenerate quasicrystal reported in the literature [3]. This notion of degeneracy is in the level of decorating individual tiles and is different from the degeneracy of a quasiperiodic random tiling arising from phason flips [4]. The $(3.4.3^2.4)$ approximant of the quasicrystal is shown to be more stable than the TBP crystal at densities below 79.7%.

[1] Chen ER, Engel M, Sharon SC, Disc. Comp. Geom. 44:253 (2010).

[2] Haji-Akbari A, Engel M, et al. Nature 462:773 (2009).

[3] Haji-Akbari A, Engel M, Glotzer SC, arXiv:1106.5561 [PRL, in press].

[4] Elser V, PRL 54: 1730 (1985)

10:24AM P53.00013 A Novel Decomposition of the Structure of Jammed Packings¹, MARK KANNER, MARK SHATTUCK, CUNY Graduate Center and the Benjamin Levich Institute and Physics Department of the City College of New York, CORY O'HERN, Departments of Mechanical Engineering and Physics, Yale University — We use simulations of 2D bidisperse disks to determine the properties of jammed packings and investigate the statistical mechanics of these systems. We have created a novel method for classifying structural subunits of a packing, using the structures to calculate relevant physical quantities. The classification scheme is based on a 20 type decomposition of the Delaunay triangles extracted from the centers of the particles in the packing. We find that the distribution of each type has a universal form, independent of total number of particles N in the packing for $N=8-10,000$, and that the parameters describing this form saturate as N is increased beyond $N=20$. We measure the distribution of the particle connections, the area distributions of the different structures, and nearest neighbor distributions. We explore the extent to which the nearest-neighbor distributions can predict the properties of the entire packing.

¹Supported by NSF (CBET-0968013)

10:36AM P53.00014 8x8 and 10x10 Hyperspace Representations of SU(3) and 10-fold Point-Symmetry Group of Quasicrystals¹, ALEXANDER ANIMALU², Emeritus Professor of Physics — In order to further elucidate the unexpected 10-fold point-symmetry group structure of quasi-crystals for which the 2011 Nobel Prize in chemistry was awarded to Daniel Shechtman, we explore a correspondence principle between the number of (projective) geometric elements (points[vertices] + lines[edges] + planes[faces]) of primitive cells of periodic or quasi-periodic arrangement of hard or deformable spheres in 3-dimensional space of crystallography and elements of quantum field theory of particle physics [points (particles, lines (particles, planes (currents] and hence construct $8 \times 8 = 64 = 28 + 36 = 26 + 38$, and $10 \times 10 = 100 = 64 + 36 = 74 + 26$ hyperspace representations of the SU(3) symmetry of elementary particle physics and quasicrystals of condensed matter (solid state) physics respectively. As a result, we predict the Cabibbo-like angles in leptonic decay of hadrons in elementary-particle physics and the observed 10-fold symmetric diffraction pattern of quasi-crystals.

¹Supported by International Centre for Basic Research, Abuja, Nigeria.

²Dept. of Physics & Astronomy, University of Nigeria, Nsukka, Nigeria

10:48AM P53.00015 Competition of Bergman-type approximants with other packing motifs in the Cu-Zr system, FENG ZHANG, MIN JIN, X.W. WANG, CAI-ZHUANG WANG, M.J. KRAMER, M.I. MENDELEV, KAI-MING HO, Ames Laboratory, US DOE, and Iowa State University — Knowledge about the topological and chemical ordering in metallic liquids and glasses is essential in predicting phase selection and understanding glass formation dynamics. Taking the Cu-Zr system as an example, previous studies have established Bergman-type medium-range ordering (MRO) from a structural analysis with cluster alignment methods [1]. In this study, we examine the thermodynamic stability of a crystalline approximant of Bergman-type quasicrystals [2] against packing geometries existing in other intermetallic compounds for a wide range of Cu compositions. The most stable structures for each structural motif at each Cu composition are obtained using an efficient genetic-algorithm search. Our results show that the Bergman-type approximant structure is thermodynamically favored over other packing geometries at the glass-forming region with Cu compositions around 65%, reaffirming the Bergman-type MRO is the lowest energy in Cu-Zr glasses.

[1] X. W. Fang, C. Z. Wang, Y. X. Yao, Z. J. Ding, and K. M. Ho, Phys. Rev. B 82, 184204 (2010).

[2] G. Bergman J. L. T. Waugh, and L. Pauling, Acta Cryst. 10, 254 (1957).

Wednesday, February 29, 2012 8:00AM - 9:48AM – Session P54 DCMP: Superconductivity: Thermodynamics and Phases 152

8:00AM P54.00001 Magnetic field scaling of the specific heat of $\text{La}_{1.92}\text{Sr}_{0.08}\text{CuO}_4$ up to 30 Teslas¹, JONATHON KEMPER, NHMFL-Florida State University — The catalogue of experimental data on cuprate superconductivity has thoroughly characterized multiple different energy scales. Despite this, the complicated relationships between these energy scales remain poorly understood. New specific heat data on the underdoped cuprate $\text{La}_{1.92}\text{Sr}_{0.08}\text{CuO}_4$, performed in magnetic fields up to 30 Teslas demonstrates how the specific heat scaling behavior evolves as the cyclotron energy approaches the thermal energy at the superconducting transition temperature, T_c , and the mean-field calculated upper critical field, known as H_{c2} . This scaling behavior gives new insight into the complicated relationship of the various energy scales of the cuprate superconductor in the vortex state.

¹Funded by the State of Florida and the NSF

8:12AM P54.00002 High Magnetic Field Specific Heat in Cuprate Superconductors, SCOTT RIGGS, Stanford University, OSKAR VAFEK, JON BETTS, FEDOR BALAKIREV, ALBERT MIGLIORI, National High Magnetic Field Lab, DOUG BONN, WALTER HARDY, RUIXING LIANG, UBC, GREG BOEBINGER, National High Magnetic Field Lab — We present new high magnetic field specific heat results for both underdoped YBCO 6.51 and overdoped LSCO. With these measurements we show that across different families of cuprates and across the superconducting-doping phase diagram, 45T does very little to suppress the d-wave superconducting gap. We discuss possible interpretations of the specific heat data through the use of bandstructure, previous high field magnetization measurements, and proposed Fermi surface reconstruction scenarios.

8:24AM P54.00003 Evolution of the phase diagrams in the pseudoternary system $\text{Pr}_{1-x}\text{Nd}_x\text{Os}_4\text{Sb}_{12}$ ¹, P.-C. HO, Physics/California State University, Fresno, R.B. BAUMBACH, L. SHU, M.B. MAPLE, Physics/University of California, San Diego, S. ZHAO, D.E. MACLAUGHLIN, Physics/University of California, Riverside, T. YANAGISAWA, Hokkaido University, Japan — The pseudo ternary system $\text{Pr}_{1-x}\text{Nd}_x\text{Os}_4\text{Sb}_{12}$ has been used as a model system to investigate the effect of ferromagnetism (FM) on the unconventional superconductivity (SC), the high field ordered phase (HFOP), and quantum critical behavior [1], that was observed in $\text{PrOs}_4\text{Sb}_{12}$. SC in this system disappears near the Nd concentration $x \sim 0.58$. Between $x \sim 0.33$ and ~ 0.58 , weak FM, confirmed by the μSR experiments [2], was found to coexist with SC. In order to further inspect the possible quantum critical behavior, a power-law analysis of the temperature dependence of the electrical resistivity data was performed. Upon suppression of SC, for samples in the range $0.33 < x < 0.58$, the power-law exponent decreases from ~ 1.8 toward 1 in the temperature region below 2.5 K, resembling non-Fermi liquid behavior. Detailed T-x, H-x, and H-T phase diagrams for various x will be discussed.

[1] Ho, et. al., PRB 83, 024511 (2011).

[2] Ho, et. al., 2010 APS March Meeting, A38.00005 (2010).

¹Research at CSU-Fresno is supported by NSF DMR-1104544; at UC San Diego by NSF DMR-0802478 and US DOE DE FG02-04ER46105; at UC Riverside by NSF DMR-0801407; at Hokkaido U by MEXT, Japan.

8:36AM P54.00004 Resonant Ultrasound study of underdoped single crystal YBCO cuprates, ARKADY SHEKHTER, VICTOR FANELLI, NHMFL, Pulsed Field Facility, LANL, Los Alamos, NM, SCOTT RIGGS, Stanford University, Stanford, CA, YOKO SUZUKI, JON B. BETTS, ALBERT MIGLIORI, NHMFL, Pulsed Field Facility, LANL, Los Alamos, NM, GREG BOEBINGER, NHMFL, FSU, Tallahassee, FL, BRAD RAMSHAW, RUIXING LIANG, WALTER HARDY, DOUG BONN, UBC, Vancouver, Canada — We measure elastic constants and ultrasound attenuation in ultra-high quality underdoped YBCO cuprate single crystal samples. We observe a phase transition at the pseudogap temperature and reveal additional phase structure inside the pseudogap phase.

8:48AM P54.00005 A Pre-Formed Pair Approach to the Dynamical (THz) Complex Conductivity in the Cuprates, DAN WULIN, VIVEK MISHRA, KATHRYN LEVIN, University of Chicago — In this talk we present a theory for $\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega)$ in the underdoped cuprates. Our work presumes that the pseudogap is associated with preformed pairs. We demonstrate how the puzzling extended range of finite $\sigma_2(\omega)$ above T_c (implying a “dynamical superfluid density”) arises from a new form of pair breaking contribution to $\sigma_2(\omega)$. This is only present in these moderately clean superconductors because of stronger than BCS attraction (BCS-BEC). Sum rule compatibility and good semiquantitative agreement with experiment is found.

9:00AM P54.00006 Origin of multiple quantum oscillation frequencies from single carrier nodal pocket in the underdoped cuprate superconductor YBCO, SUCHITRA E. SEBASTIAN, G.G. LONZARICH, University of Cambridge, N. HARRISON, M.M. ALTARAWNEH, NHMFL, Los Alamos, R. LIANG, D.A. BONN, W.N. HARDY, University of British Columbia — Quantum oscillations are measured in the underdoped high T_c cuprate superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$, revealing multiple frequencies. An extended study over a broad angular range and magnetic field range up to 95 T accompanied by detailed harmonic analysis is presented, establishing the multiple frequencies to arise from Fermi surface reconstruction yielding a single carrier nodal pocket. Scenarios are presented for the origin of multiple frequencies from this nodal pocket.

9:12AM P54.00007 ABSTRACT MOVED TO L21.00008 —

9:24AM P54.00008 Synthesis, $P - T$ phase diagram, and T_c of $R_2\text{Ba}_4\text{Cu}_7\text{O}_{15}$ ($R = \text{Dy}, \text{Y}, \text{DyY}, \text{GdY}$)¹, SEYED AHMAD SABOK-SAYR, BOGDAN DABROWSKI, STANISLAW KOLESNIK, Department of Physics, Northern Illinois University — The oxygen pressure - temperature phase diagrams of $R_2\text{Ba}_4\text{Cu}_{15}$ ($R = \text{Dy}, \text{Y}, \text{Er}, \text{DyY}, \text{GdY}, \text{and EuY}$) superconductors have been investigated in the temperature range between 850 and 1025°C and the pressure range between 1 and 50 atm. O_2 . The relative fraction of the phases: 123, 124, and 247, was determined by studying the intensity of the x-ray diffraction peaks of each phase. The condition at which the phase pure 247 exists was determined to be $P = 10 \text{ atm}$ and $T = 1025^\circ\text{C}$. Under these conditions samples with larger size $R = \text{LaY}, \text{NdY}, \text{SmY}, \text{and Eu}$ fail to form pure 247 phase. Annealing at $P = 200 \text{ atm. O}_2$ and 400°C was used to increase oxygen content of the as-synthesized materials and to induce superconductivity. The highest transition temperatures of 70K were observed for $R = \text{Y}$ compositions.

¹supported by the Institute for Nano Science, Engineering, and Technology (InSET) at NIU

9:36AM P54.00009 Pseudogap temperature along the Widom line of a first-order transition in doped Mott insulators, GIOVANNI SORDI, Institut Laue-Langevin, Grenoble, France, PATRICK SEMON, Universite de Sherbrooke, K. HAULE, Rutgers University, A.-M. S. TREMBLAY, Universite de Sherbrooke and Canadian Institute for Advanced Research — A state of matter with unusual physical properties, dubbed “the pseudogap”, appears below a characteristic temperature T^* in hole-doped high-temperature superconductors. In many cases, it is not even clear whether T^* is a crossover or a phase transition. We construct the normal-state phase diagram of the two dimensional Hubbard model using cellular dynamical mean-field theory. We find that T^* is a crossover line above the critical endpoint of a first-order phase transition between two metallic phases, one with a pseudogap and one without. Thus T^* appears in a new light: it is an unexpected example of a phenomenon observed in fluids, namely a sharp crossover between different dynamical regimes along a line of thermodynamic anomalies that appears above a first-order phase transition, the Widom line. Our findings thus suggest that the critical point of a first-order transition, and not a quantum critical point, can be the organizing principle for the rich behavior of the normal state of the cuprates. Refs: G. Sordi et al., PRL 104, 226402 (2010); G. Sordi et al., PRB 84, 075161 (2011); G. Sordi et al., arXiv:1110.1392 (2011).

Wednesday, February 29, 2012 11:15AM - 2:15PM — Session Q2 GMAG: Invited Session: Manipulating Spin Waves 204AB

11:15AM Q2.00001 Magnons, Spin Current and Spin Seebeck Effect, SADAMICHI MAEKAWA, Japan Atomic Energy Agency — When metals and semiconductors are placed in a temperature gradient, the electric voltage is generated. This mechanism to convert heat into electricity, the so-called Seebeck effect, has attracted much attention recently as the mechanism for utilizing wasted heat energy. [1]. Ferromagnetic insulators are good conductors of spin current, i.e., the flow of electron spins [2]. When they are placed in a temperature gradient, generated are magnons, spin current and the spin voltage [3], i.e., spin accumulation. Once the spin voltage is converted into the electric voltage by inverse spin Hall effect in attached metal films such as Pt, the electric voltage is obtained from heat energy [4-5]. This is called the spin Seebeck effect. Here, we present the linear-response theory of spin Seebeck effect based on the fluctuation-dissipation theorem [6-8] and discuss a variety of the devices.

[1] S. Maekawa et al, *Physics of Transition Metal Oxides* (Springer, 2004).

[2] S. Maekawa: *Nature Materials* **8**, 777 (2009).

[3] *Concept in Spin Electronics*, eds. S. Maekawa (Oxford University Press, 2006).

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[5] K. Uchida et al., *Nature Materials* **9**, 894 (2010)

[6] H. Adachi et al., *APL* **97**, 252506 (2010) and *Phys. Rev. B* **83**, 094410 (2011).

[7] J. Ohe et al., *Phys. Rev. B* (2011)

[8] K. Uchida et al., *Appl. Phys. Lett.* **97**, 104419 (2010).

11:51AM Q2.00002 Spin Wave Transport in Microscopic Magnetic Structures¹, HELMUT SCHULTHEISS, Materials Science Division, Argonne National Laboratory, and Department of Physics and Research Center OPTIMAS, University of Kaiserslautern — The coherent transport of spin information is one of the great challenges in condensed matter physics and is of fundamental importance for the development of spintronic devices. Spin waves carry angular momentum and can be utilized to transport spin information over distances much larger than the spin diffusion length in metals. Recent experiments showing that spin waves can be manipulated via spin currents and vice versa due to spin torque, spin pumping, spin Hall and spin Seebeck effects have drawn great attention to the transport properties of spin waves. Fundamental topics are spin-wave propagation characteristics in microstructures with reduced dimensionality^{2,3}, realization of spin-wave transport in two-dimensional waveguides, including directional changes along the spin-wave propagation path⁴, and the effect of nonlinear damping mechanisms when spin waves are spatially confined in microstructures. We use phase- and time-resolved Brillouin light scattering microscopy to address these topics in micron-sized spin-wave conduits made from permalloy. These experiments allow us to develop a simple model for calculating dispersion relations in spin-wave conduits. This model can be applied to understand how spin waves are transported in conduits with broken translation symmetry and how nonlinear damping via four-magnon-scattering is enhanced due to spatial confinement.

¹Financial support was through the German Science Foundation DPG and the U.S. Department of Energy, Office of Science under Contract no. DE-AC02-06CH11357

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³K. Vogt, H. Schultheiss, S. J. Hermsdoerfer, P. Pirro, A. A. Serga, and B. Hillebrands, Appl. Phys. Lett. **95** 182508 (2009)

⁴P. Clausen, K. Vogt, H. Schultheiss, S. Schäfer, B. Obry, G. Wolf, P. Pirro, B. Leven, and B. Hillebrands, Appl. Phys. Lett. **99**, 162505 (2011)

12:27PM Q2.00003 Using magnons to probe spintronic materials properties¹, ROBERT MCMICHAEL, Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD — For many spin-based electronic devices, from the read sensors in modern hard disk drives to future spintronic logic concepts, the device physics originates in spin polarized currents in ferromagnetic metals. In this talk, I will describe a novel “Spin Wave Doppler” method that uses the interaction of spin waves with spin-polarized currents to determine the spin drift velocity and the spin current polarization [1]. Owing to differences between the band structures of majority-spin and minority-spin electrons, the electrical current also carries an angular momentum current and magnetic moment current. Passing these coupled currents through a magnetic wire changes the linear excitations of the magnetization, i.e. spin waves. Interestingly, the excitations can be described as drifting “downstream” with the electron flow. We measure this drift velocity by monitoring the spin-wave-mediated transmission between pairs of periodically patterned antennas on magnetic wires as a function of current density in the wire. The transmission frequency resonance shifts by $2\pi\Delta f = \mathbf{v} \cdot \mathbf{k}$ where the drift velocity v is proportional to both the current density and the current polarization P . I will discuss measurements of the spin polarization of the current in $\text{Ni}_{80}\text{Fe}_{20}$ [2], and novel alloys $(\text{CoFe})_{1-x}\text{Ga}_x$ [3] and $(\text{Ni}_{80}\text{Fe}_{20})_{1-x}\text{Gd}_x$ [4].

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¹Collaborators include M. Zhu, C. L. Dennis, B. D. Soe, M. J. Carey, S. Maat, J. R. Childress, R. L. Thomas, V. Misra, K. H. Aschenbach and T. Mewes

1:03PM Q2.00004 Interaction between spin-wave excitations and pure spin currents in magnetic structures¹, ANTONIO AZEVEDO, Departamento de Física, Universidade Federal de Pernambuco, 50670-901, Recife, PE, Brazil — The generation of pure spin current (PSC) in magnetic structures has attracted much attention not only for its fundamental importance in spintronics, but also because it opens up potential applications. One of the most exciting aspects of this area is the interplay between spin-waves (SW) and PSC. Here we report experimental results in which the PSC, generated by both spin pumping (SPE) [1] and spin Seebeck (SSE) [2] effects, can exert a spin-transfer torque sufficient to compensate the SW relaxation in yttrium iron garnet (YIG)/non-magnetic structures. By measuring the propagation of SW packets in single-crystal YIG films we were able to observe the amplification of volume and magnetostatic modes (MSW) by both SSE and SHE [3,4]. The excitation and detection of the SW packets is carried out by using a MSW delay line device. In both cases the amplification is attributed to the spin-transfer torque due to PSC generated by SSE as well as SHE. It will also be presented new results in which PSC are simultaneously excited by SSE and SPE effects in YIG films. While the spin current generated by SPE is obtained by exciting the ferromagnetic resonance (FMR) of the YIG film, the spin current due to SSE is created by applying a temperature gradient along the film plane. The effect of the superposition of both spin currents is characterized by measuring the spin Hall voltage (V_H) along thin strips of Pt deposited on top of the YIG films. Whereas V_H corresponding to the uniform FMR is amplified due to the SSE the voltages corresponding to the other magnetostatic spin-wave modes are attenuated [5].

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1:39PM Q2.00005 Manipulation of Spin Waves in Yttrium Iron Garnet Thin Films through Interfacial Spin Scattering, MINGZHONG WU, Department of Physics, Colorado State University — Spin waves in magnetic films have many properties that can be utilized for microwave signal processing and logic operations. These applications, however, are bottlenecked by the damping of spin waves. This presentation reports on a new method for the amplification of spin waves. Specifically, the presentation reports the electric manipulation of spin waves in yttrium iron garnet (YIG) thin films via interfacial spin scattering (ISS). Experiments used a 4.6 μm -thick YIG film strip with a 20 nm-thick Pt capping layer. A dc pulse was applied to the Pt film that produced a spin current along the Pt thickness direction via the spin-Hall effect. As the spin current scatters off the surface of the YIG film, it exerts a torque on the YIG surface spins. Due to the dipolar and exchange interactions, the effect of this torque is extended to other spins across the YIG thickness and thereby to spin-wave pulses traveling in the YIG film. The net effect of the ISS process depends critically on the relative orientation of (1) the magnetic moments of the electrons in the Pt layer that scatter off the YIG surface and (2) the precession axis of the magnetic moments on the YIG surface. When they are anti-parallel, the spin-wave damping is reduced and the amplitude of a traveling spin-wave pulse is increased. In a parallel configuration, the pulse experiences an enhanced attenuation.

Wednesday, February 29, 2012 11:15AM - 2:15PM –

Session Q3 DCMP: Invited Session: Recent Advances in Pnictide Superconductors 205AB

11:15AM Q3.00001 Study of the Multiorbital Hubbard Model for the Fe-Superconductors Beyond Weak Coupling , ELBIO DAGOTTO, Department of Physics, University of Tennessee and Materials Science and Technology Division, Oak Ridge National Laboratory — A variety of experimental and theoretical investigations indicate that the pnictides and chalcogenides are materials with on-site Hubbard repulsion intermediate between weak coupling, where simple nesting ideas apply, and strong coupling where the spins are localized. For this reason, it is desirable to broaden the range of couplings theoretically studied as well as the many-body models and techniques employed. In this talk, an extensive analysis of model Hamiltonians for the Fe-based superconductors is presented. The multiorbital Hubbard models with two, three, and five orbitals are studied, via the Hartree-Fock approximation and exact diagonalization techniques. The main topics to be discussed are: magnetic ordering tendencies [1], range of realistic Hubbard repulsion and Hund couplings [2], orbital-weight redistribution at the Fermi surface and comparison with photoemission data [3], low-temperature transport properties [4], and competing pairing channels [5]. The possible magnetic states of the $\sqrt{5} \times \sqrt{5}$ Fe-vacancy arrangement will also be presented [6]. The experimental reports of local moments at room temperature leads to our most recent efforts employing a three-orbital spin-fermion model, analyzed via Monte Carlo simulations, to study the temperature dependence of the (anisotropic) conductance [7]. It is concluded that considerable progress has been made in the understanding of these materials in spite of their difficult range of intermediate couplings. However, the existence of several open problems will also be discussed.

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11:51AM Q3.00002 Doping - dependent anisotropy of the superconducting gap in underdoped pnictide superconductors , RUSLAN PROZOROV, The Ames Laboratory — The in-plane London penetration depth, $\Delta\lambda(T)$, was studied in single crystals of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ ("Ba122") and $\text{Ca}_{10}(\text{Pt}_3\text{As}_8)[(\text{Fe}_{1-x}\text{Pt}_x)_2\text{As}_2]_5$ ("10-3-8"). Whereas in Ba122 magnetism and superconductivity coexist in the underdoped regime, the 10-3-8 compound exhibits a clear separation of two order parameters. By comparing the results obtained in these two systems, we could study general features of the superconducting gap structure as function of doping in the underdoped regime. Similar to all other pnictides, the low-temperature variation of London penetration depth exhibits a power-law behavior, $\Delta\lambda(T) = AT^n$, in both systems. Moving towards the underdoped edge of the superconducting dome, the exponent n decreases well below scattering - limited value of $n = 2$ and, at the same time, the pre-factor A increases. Both trends indicate an increasing anisotropy of the superconducting gap in more underdoped compounds. These and previous results suggest that the development of the superconducting gap anisotropy towards the underdoped edge of the superconducting dome is an intrinsic property of iron pnictides, similar to the known tendency on the overdoped side where magnetism and superconductivity do not interfere.

In collaboration with M.A. Tanatar, H. Kim, The Ames Laboratory; Bing Shen, Hai-Hu Wen, Nanjing University; and N. Ni, R.J. Cava, Princeton University.

12:27PM Q3.00003 Nematic susceptibility and quantum criticality in Fe-pnictide superconductors , JAMES ANALYTIS, Stanford Institute for Material and Energy Science — The concept of broken symmetry is ubiquitous in condensed matter physics because it allows us to write the proper Hamiltonian description of an electron in a solid. Determining which symmetry is broken and how it is broken is therefore crucial. I will present results from transport and magnetization experiments on both underdoped and overdoped pnictide superconductors of the "122" structural motif that help reveal the intrinsic symmetry of the electronic ground state. We reveal the nature of the nematic susceptibility as optimal doping is approached on the underdoped side, and the breakdown of Fermi liquid like quasiparticles from the overdoped side. We discuss the universality of these properties to other pnictides.

1:03PM Q3.00004 Controlling vortex pinning and vortex phase diagrams of FeAs-based superconductors through particle irradiation and substitution , ULRICH WELP, Argonne National Laboratory — The prominent vortex pinning features of the Ba-122 and Sm-1111 family of pnictide superconductors are presented. For isovalently doped $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ we observe the systematic evolution of vortex pinning with increasing P-doping from fishtail behavior to a distinct peak effect near the irreversibility field to a reversible magnetization and Bean Livingston surface barriers. The enhancement of vortex pinning resulting from heavy ion and proton irradiation is shown to arise from delta-Tc-type pinning. These results will be compared to those on optimally doped $\text{BaKFe}_2\text{As}_2$ and $\text{SmFeAs}(\text{O}_{1-x}\text{F}_x)$. High-energy heavy-ion irradiation induced defects lead to a decrease in the superconducting anisotropy, an increase in the slope of the temperature dependence of the irreversibility line and only small suppression of Tc. In all cases, we see a large enhancement of the critical current following particle irradiation. In particular, on $\text{BaKFe}_2\text{As}_2$ irradiated to a dose matching field of 21 T with 1.3-GeV Pb-ions, $J_c \sim 4 \text{ MA/cm}^2$ at 5 K and in 7 T || c is achieved, comparable to results for YBCO coated conductors at the same temperature and field.

In collaboration with L. Fang, Y. Jia, J. A. Schlueter, H. Claus, C. Chaparro, G. Sheet, A. E. Koshelev, G. W. Crabtree, W. K. Kwok, Materials Science Division, Argonne National Laboratory, Argonne, Illinois, USA; S. F. Xu, Physics Division, Argonne National Laboratory, Argonne, Illinois, USA; H. F. Hu, J. M. Zuo, Department of Materials Science and Engineering, University of Illinois, Urbana, Illinois, USA; A. Kayani, Physics Department, Western Michigan University, Kalamazoo, Michigan, USA; H.-H. Wen, University of Nanjing, Nanjing, China; and N. D. Zhigadlo, J. Karpinski, Solid State Physics Laboratory, ETH Zurich, Switzerland.

This work was supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the DoE, Office of Basic Energy Sciences (LF, YJ, HC, AEK, CC, GS, GWC, HFH, JMJ), by the DoE, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357 (UW, JAS, WKK) and by the ATLAS accelerator at Argonne (SFZ).

1:39PM Q3.00005 Unusual electronic structure and pairing in the $K_x\text{Fe}_{2-y}\text{Se}_2$ and $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ superconductors, DONGLAI FENG, State Key Laboratory of Surface Physic and Department of Physics, Fudan University, Shanghai, China — In this talk, we present the angle resolved photoemission study of the unusual electronic structure and pairing behavior in two rather unique iron based superconductors: $K_x\text{Fe}_{2-y}\text{Se}_2$ and $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$. For $K_x\text{Fe}_{2-y}\text{Se}_2$, large electron Fermi surfaces are observed around the zone corners with an almost isotropic superconducting gap of 10.3 meV, while there is no hole Fermi surface near the zone center, which demonstrate the inter-band scattering or Fermi surface nesting is not a necessary ingredient for the unconventional superconductivity in iron-based superconductors. Moreover, two insulating and one semiconducting parental phases of $K_x\text{Fe}_{2-y}\text{Se}_2$ were identified. The two insulating phases exhibit Mott-insulator-like signatures, and one of the insulating phases is mesoscopically phase-separated from the superconducting/semiconducting phase in the superconductor/semiconductor [2]. For $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$, which is a prototypical iron-based superconductor with nodal gap behaviors, we have determined the systematic change of its low energy electronic structures as a function of the Phosphor concentration. We found the so-called iso-valent doping actually introduce significant amount of holes into the system. The chemical pressure effect is largely a doping effect in addition to the non-rigid band behavior [3]. Moreover, we report the direct observation of a circular line node on the largest hole Fermi surface around the Z point at the Brillouin zone boundary. We found that the nodes are due to the strong three dimensional character of this Fermi surface (large k_z dispersion, strong mixing of $d_{3z^2-r^2}$ orbitals), instead of d-wave pairing or other scenarios involving the electron pockets [4].

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Wednesday, February 29, 2012 11:15AM - 2:15PM – Session Q4 DAMOP: Focus Session: Many-body Quantum Phases in Cold Atom Systems 205C

11:15AM Q4.00001 Orbital ice: an exact Coulomb phase on the diamond optical lattice¹, GIA-WEI CHERN, University of Wisconsin at Madison and Los Alamos National Lab, CONGJUN WU, University of California, San Diego — The rapid advances in loading and controlling alkali atoms on the excited bands of optical lattices have made it possible to investigate orbital-related many-body physics in new settings. Here we demonstrate the existence of orbital Coulomb phase as the exact ground state of p -orbital exchange Hamiltonian on the diamond lattice. The Coulomb phase is an emergent state characterized by algebraic dipolar correlations and a gauge structure resulting from local constraints (ice rules) of the underlying lattice models. For most ice models on the pyrochlore lattice, these local constraints are a direct consequence of minimizing the energy of each individual tetrahedron. On the contrary, the orbital ice rules are emergent phenomena resulting from the quantum orbital dynamics. We show that the orbital ice model exhibits an emergent geometrical frustration by mapping the degenerate quantum orbital ground states to the spin-ice states obeying the 2-in-2-out constraints on the pyrochlore lattice. We also discuss possible realization of the orbital ice model in optical lattices with p -band fermionic cold atoms. [1] Gia-Wei Chern and Congjun Wu, arXiv:1104.1614 (2011).

¹GWC thanks the supported of ICAM and NSF Grant DMR-0844115. CW acknowledges the support of NSF under DMR-1105945 and AFOSR-YIP program.

11:27AM Q4.00002 Time reversal symmetry breaking of p -orbital bosons in a one-dimensional optical lattice¹, XIAOPENG LI, ZIXU ZHANG, W. VINCENT LIU, University of Pittsburgh — We study bosons loaded in a one-dimensional optical lattice of two-fold p -orbital degeneracy at each site. Our numerical simulations find an anti-ferro-orbital $p_x + ip_y$, a homogeneous p_x Mott insulator phase and two kinds of superfluid phases distinguished by the orbital order (anti-ferro-orbital and para-orbital). The anti-ferro-orbital order breaks time reversal symmetry. Experimentally observable evidence is predicted for the phase transition between the two different superfluid phases. We also discover that the quantum noise measurement is able to provide a concrete evidence of time reversal symmetry breaking in the first Mott phase.

¹A. W. Mellon Fellowship

11:39AM Q4.00003 Correlated phases of bosons in tilted, frustrated lattices¹, SUBIR SACHDEV, Harvard University, SUSANNE PIELAWA, WIEZMANN INSTITUTE OF SCIENCE, TAKUAYA KITAGAWA, EREZ BERG, Harvard University — We study the “tilting” of Mott insulators of bosons into metastable states. These are described by Hamiltonians acting on resonant subspaces, and have rich possibilities for correlated phases with non-trivial entanglement of pseudospin degrees of freedom measuring the boson density. We extend a previous study (Phys. Rev. B 66, 075128 (2002)) of cubic lattices to a variety of lattices and tilt directions in 2 dimensions: square, triangular, decorated square, and kagome, while noting the significance of three-body interactions. We find quantum phases with Ising density wave order, with superfluidity transverse to the tilt direction, a sliding Luttinger liquid phase, and quantum liquid states with no broken symmetry. Some cases map onto effective quantum dimer models.

¹Supported by DMR-1103860 and by a MURI grant from AFOSR.

11:51AM Q4.00004 Quantum simulations with ultracold atoms¹, NIKOLAY PROKOFIEV, University of Massachusetts, Amherst — Precise understanding of strongly interacting systems, from electrons in materials and frustrated magnets to nuclear matter, is a major challenge for modern physics. Often, theoretical description of key models is severely plagued by the intricate quantum mechanics at play. This prompted a challenging effort of using ultra-cold atoms to realize Feynman’s emulators of fundamental microscopic models. I will discuss some of the current efforts in realizing quantum simulators for cold bosonic and fermionic systems and how the theory tries to caught up with the experiment in making reliable predictions for strongly interacting quantum matter.

¹NSF, grant PHY-1005543, ARO DARPA OLE

12:27PM Q4.00005 A Mott Glass to Superfluid Transition for Random Bosons in Two Dimensions, DAVID PEKKER, SHANKAR IYER, GIL REFAEL, Caltech — We study the zero temperature superfluid-insulator transition for a two-dimensional model of interacting, lattice bosons in the presence of quenched disorder and particle-hole symmetry. We follow the approach of a recent series of papers by Altman, Kafri, Polkovnikov, and Refael, in which the strong disorder renormalization group is used to study disordered bosons in one dimension. Adapting this method to two dimensions, we study several different species of disorder and uncover universal features of the superfluid-insulator transition. In particular, we locate an unstable finite disorder fixed point that governs the transition between the superfluid and a gapless, glassy insulator. We present numerical evidence that this glassy phase is the incompressible Mott glass and that the transition from this phase to the superfluid is driven by percolation-type process. Finally, we provide estimates of the critical exponents governing this transition.

12:39PM Q4.00006 Disordered Supersolids in the Extended Bose-Hubbard Model¹, VITO SCAROLA, BHARGAV KEMBURI, Virginia Tech — Studies of the extended Bose-Hubbard model seek to capture the essential properties of a wide variety of physical systems including helium, Josephson junction arrays, certain narrow-band superconductors, and bosons in optical lattices. We theoretically study the stability of lattice supersolid states in the extended Bose-Hubbard model with bounded spatial disorder. We construct a disorder mean field theory and compare with quantum Monte Carlo calculations. We find that the supersolid survives weak disorder on the simple cubic lattice. We also find that increasing disorder strength can transform a lattice solid into a supersolid as it tends to percolate through the disorder landscape.

¹This work is supported by AFOSR (FA9550-11-1-0313) and DARPA-YFA (N66001-1-1-4122).

12:51PM Q4.00007 Density instabilities in a two-dimensional dipolar Fermi gas, MEERA PARISH, University College London, FRANCESCA MARCHETTI, Universidad Autonoma de Madrid — We investigate the inhomogeneous phases of fermionic polar molecules confined in a single two-dimensional (2D) layer, where the molecule dipole moments are all aligned by an external electric field. We show that the Random Phase Approximation (RPA) for the density-density response function is never accurate for the 2D dipolar Fermi gas. To incorporate correlations beyond RPA, we use an improved version of the Singwi-Tosi-Land-Sjolander scheme, which has been successful for electron systems. In addition to density-wave instabilities, our formalism captures the collapse instability that is expected from Hartree-Fock calculations but is absent from RPA. Crucially, we find that when the dipoles are oriented perpendicular to the layer, the system spontaneously breaks rotational symmetry and forms a stripe phase, in defiance of conventional wisdom.

1:03PM Q4.00008 Scaling of noise correlations of hard-core bosons in incommensurate lattices, KAI HE, Georgetown University, INDUBALA I. SATIJA, George Mason University; Joint Quantum Institute, NIST, CHARLES W. CLARK, Joint Quantum Institute, NIST, ANA MARIA REY, JILA, NIST, MARCOS RIGOL, Georgetown University — We study the scaling of the momentum distribution function and the noise correlations in the Mott insulator, Bose glass, and superfluid quantum phases of hard-core bosons subjected to quasi-periodic disorder. The exponents of the correlation functions at the superfluid to Bose-glass transition are found to be approximately one half of the ones that characterize the superfluid phase. We also find a divergence in the derivative of the noise correlation peaks with respect to the strength of disorder at the superfluid to Bose-glass critical point. This behavior is found not to occur in the corresponding free fermion system, where an Anderson-like transition takes place at the same critical point.

1:15PM Q4.00009 Quantum Orders and Space-Time Vortices for Spin 2 Atomic Chains, ARI TURNER, University of Amsterdam, FRANK POLLMANN, Max-Planck-Institute for the Physics of Complex Systems, ASHVIN VISHWANATH, University of California, Berkeley — Laser cooled atoms with spin can become magnetically ordered, like electrons in solids, but a greater variety of orders is possible in this setting. Spin one atoms can form nematic states with the symmetry of an undirected line segment while spin two atoms can form states with the symmetry of a tetrahedron. Such atoms could be confined to a one-dimensional optical lattice. In one dimension, quantum fluctuations become much more significant, and lead to a few interesting phases. In particular, the nematic state spontaneously breaks translational symmetry. If a state has a Berry's phase of a certain order under rotations, the fluctuations will often be modulated with a period of the same order. I will argue that this connection can be broken for a non-abelian symmetry group—both uniform and periodic phases can be stabilized. As an example, computer calculations (with DMRG) on a tetrahedral state find both a uniform and a period 3 phase.

1:27PM Q4.00010 Thermal versus quantum fluctuations of optical lattice fermions, CHRIS HOOLEY, SUPA, University of St Andrews, UK, VIVALDO CAMPO, Universidade Federal de Sao Carlos, Brazil, KLAUS CAPELLE, Universidade Federal do ABC, Brazil, JORGE QUINTANILLA, SEPnet, University of Kent and STFC Rutherford Appleton Laboratory, UK, VITO SCAROLA, Virginia Tech, USA — We show that, for fermionic atoms in a one-dimensional optical lattice, the fraction of atoms in doubly occupied sites is a highly non-monotonic function of temperature. We demonstrate that this property persists even in the presence of realistic harmonic confinement, and that it leads to a suppression of entropy at intermediate temperatures that offers a clear route to adiabatic cooling. Our interpretation of the suppression is that such intermediate temperatures are simultaneously too high for quantum coherence and too low for significant thermal excitation of double occupancy thus offering a clear indicator of the onset of quantum fluctuations.

1:39PM Q4.00011 Tunable quantum glasses and phase transitions of atoms and photons: first-predictions for glassy physics with many-body cavity QED¹, PHILIPP STRACK, SUBIR SACHDEV, Harvard University — Recent studies of strongly interacting atoms and photons in opticalcavity have rekindled interest in the Dicke model of atomic qubitsto discrete photon cavity modes. In this talk, we argue thatof the Dicke model with variable atom-photon couplings canrise to a ground state phase diagram exhibiting quantum phasebetween paramagnetic, ferromagnetic, and a spin glass phase. These quantum optics realizations of quantum glasses are distinctive to condensed matter systems and provide new opportunities for glassy physics with many-bodyQED. The photon-mediated random couplings between the atomic qubitssing spins) are truly long-ranged and the theory for these systemsanalytically tractable. We compute atomic and photon spectrafunctions across this phase diagram, and outline how ourcan be observed in experiments.

¹Supported by DFG grant Str 1176/1-1, by NSF grant DMR-1103860, and by a MURI grant from AFOSR.

1:51PM Q4.00012 ABSTRACT WITHDRAWN —

2:03PM Q4.00013 The boson-Hubbard model on a kagome lattice with a sextic ring-exchange term¹, VALERY ROUSSEAU, KA-MING TAM, JUANA MORENO, MARK JARRELL, Louisiana State University (LSU) — We present exact quantum Monte Carlo simulations of hard-core bosons in a two-dimensional Kagome lattice with a sextic ring-exchange term. We study how the superfluid density evolves as the ring-exchange interactions are increased. We show that the system becomes unstable in the limit of large interactions at all fillings and undergoes a phase separation, except at $\frac{1}{3}$ and $\frac{2}{3}$ fillings for which the superfluid density vanishes and a solid state forms.

¹This work was supported by the National Science Foundation through OISE-0952300, the TeraGrid re- sources provided by NICS under grant number TG- DMR100007, the high performance computational re- sources provided by the Louisiana Optical Network

Wednesday, February 29, 2012 11:15AM - 2:15PM —
Session Q5 DCMP: Nonequilibrium and Gauge/Gravity Duality 206A

11:15AM Q5.00001 Solution to the d=2 Hertz-Millis problem from a hairy electron star¹, KA WAI LO, University of Illinois at Urbana Champaign, MOHAMMAD EDALATI, University of Texas at Austin, PHILIP PHILLIPS, University of Illinois at Urbana Champaign — We use holography to study the spontaneous condensation of a neutral order parameter in a (2+1)-dimensional field theory at zero-temperature and finite density, dual to the electron star background of Hartnoll and Tavanfar. An appealing feature of this field theory is the emergence of an IR Lifshitz fixed-point with a finite dynamical critical exponent z , which is due to the strong interaction between critical bosonic degrees of freedom and a finite density of fermions (metallic quantum criticality). We show that under some circumstances the electron star background develops a neutral scalar hair whose holographic interpretation is that the boundary field theory undergoes a quantum phase transition, with a Berezinski-Kosterlitz-Thouless character, to a phase with a neutral order parameter. Including the backreaction of the bulk neutral scalar on the background, we argue that the two phases across the quantum critical point have different z , a novelty that exists in certain quantum phase transitions in condensed matter systems. We also analyze the system at finite temperature and find that the phase transition becomes, as expected, second-order. Embedding the neutral scalar into a higher form, a variety of interesting phases could potentially be realized for the boundary field

¹National Science Foundation Division of Material Research 0940992

11:27AM Q5.00002 Non-Relativistic Holographic Quantum Liquids¹, JUVEN WANG, ALLAN ADAMS, Massachusetts Institute of Technology — We explore the phase structure of a holographic toy model of superfluid states in non-relativistic conformal field theories. At low background mass density, we find a familiar second-order transition to a superfluid phase at finite temperature. Increasing the chemical potential for the probe charge density drives this transition strongly first order as the low-temperature superfluid phase merges with a thermodynamically disfavored high-temperature condensed phase. At high background mass density, the system reenters the normal phase as the temperature is lowered further, hinting at a zero-temperature quantum phase transition as the background density is varied. Given the unusual thermodynamics of the background black hole, however, it seems likely that the true ground state is another configuration altogether.

¹The work based on: <http://arxiv.org/abs/1103.3472> and works to appear on arXiv.org.

11:39AM Q5.00003 Striped Superconductor and Holography, GEORGE SIOPSIS, University of Tennessee at Knoxville, JIMMY HUTASOIT, West Virginia University, JASON THERRIEN, SUMAN GANGULI, University of Tennessee at Knoxville — Using gauge/gravity duality, we analytically study the properties of a strongly coupled striped superconductor, with the charge density wave sourced by a modulated chemical potential. The calculation is done in the large modulation wavenumber Q regime and comparing the results with numerical calculations, we find good agreement for $Q \geq 3T_c$. In the absence of a homogeneous term in the chemical potential, we show that the critical temperature scales as a negative power of Q for scaling dimensions $\Delta < \frac{3}{2}$, whereas for $\Delta > \frac{3}{2}$, there is no phase transition above a certain critical value of Q . The order parameter or the condensate is found to scale as a positive power of Q such that the gap is proportional to Q . We discuss how these results change if a homogeneous term is added to the chemical potential. We also calculate the conductivity with its spatial dependence.

11:51AM Q5.00004 Holographic noise near quantum critical points¹, ANDREW GREEN, London Centre of Nanotechnology, JULIAN SONNER, DAMTP, University of Cambridge — The dynamical scaling present in equilibrium correlations near to a quantum critical point suggests the possibility of universal, out-of-equilibrium steady states. This has been demonstrated in analyses of the response of the bosonic Hubbard model to a strong electric field. The universal out-of-equilibrium behaviour is particularly apparent in the current noise; at high field, a current noise power $S_j \propto \sqrt{E}$ was found which was interpreted as Johnson-like with an effective temperature $\propto \sqrt{E}$ [Phys. Rev. Lett. 97, 227003 (2006)]. We revisit this problem using the holographic mapping to a classical gravitational system. We recover a current noise that extends the previously known equilibrium and strongly out-of-equilibrium results with a full interpolation between the two: $S_j \propto T_{eff}$ with $T_{eff} = (T^4 + E^2/\pi^4)^{1/4}$.

¹We acknowledge financial support from Trinity College Cambridge, the EPSRC and KITP Santa Barbara

12:03PM Q5.00005 Out-of-equilibrium conductivity and current noise at quantum critical points, ANDREW BERRIDGE, London Centre for Nanotechnology, M.J. BHASEEN, Cavendish Laboratory, Cambridge, A.G. GREEN, London Centre for Nanotechnology — Quantum critical points display universal behaviour across a wide range of physical systems. These effects appear in both thermodynamics and transport. Such behaviour should also be present out-of-equilibrium where, for example, the current and current noise should follow scaling laws as a function of applied field. These expectations have been borne out in calculations for out-of-equilibrium transport at the Superfluid-Mott Insulator quantum critical point of the Bose-Hubbard model [?, ?]. These analyses extend the quantum Boltzmann description [?] of equilibrium transport using a trick of the $1/N$ expansion. Here we use an epsilon expansion to obtain similar results. This approach has the advantage of making the physical constraints of the results more transparent. We also present preliminary analysis of the evolution to the non-equilibrium steady state after the electric field is applied.

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12:15PM Q5.00006 Wigner-Mott scaling of transport near the two-dimensional metal-insulator transition, MILOS RADONJIC, DARKO TANASKOVIC, Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia, VLADIMIR DOBROSavlJEVIC, Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854 — Thermal destructions of heavy quasiparticles often dominates the transport behavior of many strongly correlated materials. It typically leads to pronounced resistivity maxima in the incoherent regime around the coherence temperature T^* , reflecting the tendency of carriers to undergo Mott localization following the demise of the Fermi liquid. This behavior is best pronounced in the vicinity of interaction-driven (Mott-like) metal-insulator transitions, where the T^* decreases, while the resistivity maximum ρ_{max} increases. Here we show that, in this regime, the entire family of resistivity curves display a characteristic scaling behavior $\rho(T)/\rho_{max} \approx F(T/T_{max})$, while the ρ_{max} and $T_{max} \sim T^*$ assume a powerlaw dependence on the quasi-particle effective mass m^* . Remarkably, precisely such trends are found from an appropriate scaling analysis of experimental data obtained from diluted two-dimensional electron gases in zero magnetic fields. Our analysis provides strong evidence that inelastic electron-electron scattering – and not disorder effects – dominates finite temperature transport in these systems, validating the Wigner-Mott picture of the two-dimensional metal-insulator transition.

12:27PM Q5.00007 Finite-size effects in transport data from Quantum Monte Carlo simulations, RAIMUNDO ROCHA DOS SANTOS, RUBEM MONDANI, Universidade Federal do Rio de Janeiro, KARIM BOUADIM, Ohio State University, THEREZA PAIVA, Universidade Federal do Rio de Janeiro — We have examined the behavior of the compressibility, of the dc-conductivity, and of the Drude weight as probes of the density-driven metal-insulator transition in the Hubbard model on a square lattice. These quantities have been obtained through determinantal quantum Monte Carlo simulations at finite temperatures on lattices up to 16×16 sites. While the compressibility and the dc-conductivity are known to suffer from ‘closed-shell’ effects due to the presence of artificial gaps in the spectrum (caused by the finiteness of the lattices), we have established that the former tracks the average sign of the fermionic determinant, and that a shortcut often used to calculate the conductivity may neglect important corrections. We have also performed systematic studies of the dependence of our data with the imaginary-time interval. Our analyses also show that, by contrast, the Drude weight is not too sensitive to finite-size effects, being much more reliable as a probe to the insulating state.

12:39PM Q5.00008 Universal transport near a continuous Mott transition in two dimensions, WILLIAM WITCZAK-KREMPA, University of Toronto, POUYAN GHAEMI, University of Illinois at Urbana-Champaign, TODADRI SENTHIL, MIT, YONG BAEK KIM, University of Toronto — We discuss the universal transport signatures near a zero-temperature continuous Mott transition between a Fermi liquid and a spin liquid in 2 spatial dimensions. This transition can be described using a slave-rotor field theory, where the electron is decomposed into a fermionic spinon and charge-carrying rotor, both interacting with an emergent $U(1)$ gauge field. The universal part of the non-zero temperature charge transport is determined by the dynamics of the charged rotors and is affected by the gauge fluctuations. Explicit predictions for the behavior of the electrical conductivity are made via the solution of a quantum kinetic equation using controlled approximations.

12:51PM Q5.00009 Dissipation-Induced Quantum Phase Transition in a Resonant Level¹, HENOK MEBRAHTU, IVAN BORZENETS, DONG E. LIU, HUAIXIU ZHENG, YURI BOMZE, Duke University, ALEX SMIRNOV, North Carolina State University, HAROLD BARANGER, GLEB FINKELSTEIN, Duke University — We measure conductance through a resonant level coupled to a dissipative environment, which suppresses tunneling rate at low energies. Our sample consists of a single-walled carbon nanotube quantum dot contacted by resistive metal leads that serve as the dissipative environment. We study the shape of the resonant conductance peak, with the expectation that its width and height, both dependent on the tunneling rate, will be suppressed at low temperatures. However, we observe distinct regimes, including a case where the resonant tunneling conductance reaches the unitary limit, despite the presence of dissipation. We discuss the implication of these findings for a dissipation-induced quantum phase transition and extract the scaling exponents.

¹Work supported by U.S. DOE

1:03PM Q5.00010 Collective excitations and low temperature transport properties of bismuth¹, PIOTR CHUDZINSKI, THIERRY GIAMARCHI, DPMC, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Geneva 4, Switzerland — We examine the influence of collective excitations on the transport properties (resistivity and magneto-optical conductivity) for semimetals, focusing on the case of bismuth. We show, using a random-phase approximation (RPA), that the properties of the system are drastically affected by the presence of an acoustic-plasmon mode, which is a consequence of the presence of two types of carriers (electrons and holes) in this system. We find a crossover temperature T^* separating two different regimes of transport. At high temperatures where $T > T^*$, the Baber scattering explains quantitatively the dc resistivity experiments, while at low temperatures where $T < T^*$, the interactions of the carriers with this collective mode lead to a T^{-5} behavior of the resistivity. We examine other consequences of the presence of this mode. In particular a two-plasmon edge feature in the magneto-optical conductivity is predicted. We compare our results with the experimental findings on bismuth. We discuss the limitations and extensions of our results beyond the RPA, and examine the case of other semimetals such as $1T - TiSe_2$.

¹supported by MaNEP

1:15PM Q5.00011 Photo-excitation and relaxation dynamics in junction of double-exchange systems, WATARU KOSHIBAE, CMRG, RIKEN, Japan, NAOTO NAGAOSA, Dept. of Appl. Phys., Univ. of Tokyo, CMRG, CERG, RIKEN, Japan, NOBUO FURUKAWA, ERATO-MF, Aoyama-Gakuin Univ., Japan — The photo-induced insulator-metal (I-M) transition is studied by the numerical simulation of real-time quantum dynamics of a double-exchange model. We find a characteristic multiplication of particle-hole (p-h) pairs by a p-h pair of high energy during the I-M transition. To examine the conversion from the p-h pairs into electric energy, we perform the numerical study on the junction systems combined by the double exchange models. The numerical results have been revealed including (i) the threshold behavior with respect to the intensity and energy of light, (ii) p-h pairs are well separated and pair annihilation is suppressed, (iii) enhancement of collected carrier by meta-stability of I-M transition.

1:27PM Q5.00012 Photo excited state in spin-charge coupled correlated electron system, SUMIO ISHIHARA, YU KANAMORI, Department of Physics, Tohoku University, HIROAKI MATSUEDA, Sendai National College of Technology, JUN OHARA, Department of Physics, Tohoku University — Recent ultrafast optical techniques open up a new frontier for research of the phase transition. Photo-induced phase is transient and highly nonequilibrium. photo-induced phenomena in correlated electron systems offer large possibility of new hidden phases which do not realize in the thermal equilibrium state, and prompt several theoretical challenges. In this talk, I will talk about recent our theoretical results for the photo-induced phase transition in correlated electron systems. We study the photo-induced spin state change in itinerant correlated electron system, motivated from the experiments in perovskite cobaltites [1]. The effective models before and after photon-pumping are derived from the two-orbital Hubbard model and are analyzed by the exact diagonalization method. When a photon is introduced in the low-spin band insulator, we found a spin-polarized bound state of photo-excited hole and the high-spin state. This bound state directly reflects the optical pump-probe spectra. These results well explain the recent femtosecond spectroscopy experiments in perovskite cobaltites We also show the unusual double-exchange interaction in photo excited state.

[1] Y. Kanamori, H. Matsueda and S. Ishihara, Phys. Rev. Lett. 107, 167403-1-5 (2011)

1:39PM Q5.00013 Non-equilibrium steady state of field-driven strongly correlated electrons¹, WOO-RAM LEE, School of Physics, Korea Institute for Advanced Study, Seoul 130-722, Korea, JONG EUN HAN, Department of Physics, State University of New York at Buffalo, Buffalo, New York 14260, USA, KWON PARK, School of Physics, Korea Institute for Advanced Study, Seoul 130-722, Korea — We theoretically study the nature of non-equilibrium steady state of strongly correlated electrons on lattices under the influence of a static electric field. We describe the dynamics of steady state by the Floquet theory, and the electron correlation by the dynamical mean-field theory, respectively. We find that the steady-state current in a closed system is characterized by the Bloch oscillation in the metallic regime, while it vanishes in the Mott-insulating regime. Importantly, the coherent contribution to the current can be captured by measuring the quasiparticle weight in the local spectral density as in equilibrium. Based on these criteria, we draw the non-equilibrium phase diagram as a function of the strength of electric field and the on-site interaction at zero temperature. *References: [1] A. V. Jura, J. K. Freericks, and Th. Pruschke, Phys. Rev. Lett. 101, 196401 (2008); [2] N. Tsuji, T. Oka, and H. Aoki, Phys. Rev. B 78, 235124 (2008).

¹We thank Korea Institute for Advanced Study for providing computing resources (KIAS Linux Cluster System) for this work.

1:51PM Q5.00014 Dynamical DMRG study of non-linear optical response in one-dimensional dimerized Hubbard model with nearest neighbor Coulomb interaction and alternating on-site potential, SHIGETOSHI SOTA, TAKAMI TOHYAMA, Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto, Japan, SERGUEI BRAZOVSKII, LPTMS-CNRS, University Paris-Sud, Orsay, France — The optical response of organic compounds has been attracting much attention. The one of the reasons is the huge non-linear and ultrafast optical response [K. Yamamoto *et. al.*, J. Phys. Soc. Jpn. **77**, 074709(2008)]. In order to investigate such optical properties, we carry out dynamical DMRG calculations to obtain optical responses in the 1/4-filled one-dimensional Hubbard model including the nearest neighbor Coulomb interaction and the alternating electron hopping. The charge gap [S. Nishimoto, M. Takahashi, and Y. Ohta, J. Phys. Soc. Jpn. **69**, 1594(2000)] and the bound state [H. Benthien and E. Jeckelmann, Eur. Phys. J. B **44**, 287(2005)] in this model have been discussed based on DMRG calculations. In the present study, we introduce an alternating on-site potential giving the polarization in the system into the dimerized Hubbard model, which breaks the reflection symmetry of the system. In this talk, we discuss the obtained linear and the 2nd order non-linear optical susceptibility in order to make a prediction for non-linear optical experiments in the future.

2:03PM Q5.00015 Non-Kondo mechanism of resistivity upturn in a spin-ice Kondo lattice model, YUKITOSHI MOTOME, Dept. Appl. Phys., Univ. of Tokyo, MASAFUMI UDAGAWA, Dept. Appl. Phys., Univ. of Tokyo, MPI-PKS, Dresden, HIROAKI ISHIZUKA, Dept. Appl. Phys., Univ. of Tokyo — Ice rule is a configurational constraint observed in a broad range of systems in which two-state variables are defined at the vertices of a pyrochlore lattice. The constraint enforces the so-called 'two-in two-out' configuration; two out of four neighboring sites within each tetrahedron are in the opposite state to the other two. Under this peculiar local constraint, the system remains disordered, whereas the ground state is characterized by macroscopic degeneracy with a hidden gauge structure. Recent experiments on pyrochlore metallic oxides have promoted interest in itinerant electrons coupled with such ice-rule type localized moments. Here we investigate how electronic and transport properties are affected by the coupling to the spin ice by applying a cellular dynamical mean-field theory to a spin-ice type Kondo lattice model. We found that a spin-ice liquid state emerges in a wide temperature range at low electron density, in which two-in two-out local correlation well develops in the absence of long-range ordering. In this spin liquid state, the resistivity shows an upturn because of an anomalous scattering of electrons by the local spin-ice type correlation. The details of this non-Kondo resistivity upturn will be discussed in relation with experiments in pyrochlore oxides.

Wednesday, February 29, 2012 11:15AM - 2:15PM – Session Q6 DMP: Carbon Nanotubes: Electronic and Thermal Properties 206B

11:15AM Q6.00001 Ultra-short single-wall carbon nanotube NEMS transistors, ANDREW C. MCRAE, JOSHUA O. ISLAND, VAHID TAYARI, SERAP YİĞEN, A.R. CHAMPAGNE, Department of Physics, Concordia University, Montreal, Canada — We study electron transport in clean suspended single-wall carbon nanotube (SWCNT) transistors hosting a single quantum dot (QD) ranging in length from a few tens of nm down to ≈ 3 nm. To fabricate these ultra-short QD transistors, we align narrow gold bow-tie junctions on top of individual SWCNTs and suspend the devices. We then use a feedback-controlled electromigration to break the gold junctions and expose nm-sized sections of the SWCNTs. We measure electron transport in these devices at low temperature and show that they form clean and tunable quantum dot transistors. We observe QD excited states which correspond to both the stretching and flexural vibronic modes. The out-of-plane vibron resonances approach the THz range, and show that these ultra-short suspended transistors are promising candidates to develop highly sensitive NEMS and explore the strong electron-vibron coupling regime.

11:27AM Q6.00002 Measurement of intrinsic resistivity of individual single walled carbon nanotubes with known-chirality, MITSUhide TAKEKOSHI, VIKRAM DESHPANDE, ZHENGYI ZHANG, Columbia University, YUHEI MIYAUCHI, Kyoto University, TONY HEINZ, JAMES HONE, PHILIP KIM, Columbia University — We report the electrical resistivity measured on individual single walled nanotubes (SWNTs) whose atomic structures are characterized by Rayleigh and Raman spectroscopy. Since electrical transport of SWNTs on substrates is predominantly limited by surface polar phonon from substrate at elevated temperatures, intrinsic transport properties of SWNTs limited by nanotube phonons remained to be probed experimentally. Here we present electrical transport measurement of long suspended individual SWNTs with exactly assigned atomic structures. SWNTs are grown by the chemical vapor deposition method on pre-patterned electrodes and their exact chiral indices are obtained using Rayleigh and Raman spectroscopy. We investigate temperature dependent resistivity of metallic SWNTs in the diffusive regime. We will discuss the chirality dependence of the electron-acoustic phonon interaction inferred from the temperature dependent intrinsic resistivity of SWNTs.

11:39AM Q6.00003 Probing Magnetic Susceptibility Anisotropy of Large-Diameter Armchair Carbon Nanotubes via Magnetic Linear Dichroism Spectroscopy, ERIK HAROZ, JUNICHIRO KONO, Rice University, Dept. of ECE, THOMAS SEARLES, Morehouse Univ., Dept. of Physics, XIAOMIN TU, MING ZHENG, JEFFREY FAGAN, National Institute of Standards & Technology, Polymer Division, STEPHEN MCGILL, DMITRY SMIRNOV, National High Magnetic Field Laboratory — We studied magnetic susceptibility anisotropy, via magnetic linear dichroism spectroscopy, of aqueous suspensions of single-walled carbon nanotubes in high magnetic fields up to 22T using a unique magnet system (Split-Florida Helix magnet). Specifically, we measured magnetic susceptibility anisotropies, $\Delta\chi$, of several armchair species ranging from (5,5)-(13,13) at room temperature over an excitation wavelength range of 400-900 nm. For large diameter armchairs such as (12,12) and (13,13), we have observed some of the strongest alignment in a static magnetic field due to their large diameters. Results will be discussed in comparison with detailed calculations involving the Aharonov-Bohm effect.

11:51AM Q6.00004 Helical modes and Majorana fermions in carbon nanotubes, JELENA KLINOVAJA, MANUEL SCHMIDT, BERND BRAUNECKER, DANIEL LOSS, Department of Physics, University of Basel — We derive an effective low-energy theory for metallic (armchair and nonarmchair) single-wall nanotubes in the presence of an electric field perpendicular to the nanotube axis, and in the presence of magnetic fields, taking into account spin-orbit interactions and screening effects on the basis of a microscopic tight-binding model [1,2]. The interplay between electric field and spin-orbit interaction allows us to tune armchair nanotubes into a helical conductor in both Dirac valleys. Metallic nonarmchair nanotubes are gapped by the surface curvature, yet helical conduction modes can be restored in one of the valleys by a magnetic field along the nanotube axis. If in proximity with a superconductor, helical modes give rise to Majorana bound states. Furthermore, we discuss electric dipole spin resonance in carbon nanotubes, and find that the Rabi frequency shows a pronounced dependence on the momentum along the nanotube.

[1] J. Klinovaja, M. Schmidt, B. Braunecker, and D. Loss, Phys. Rev. Lett. **106**, 156809 (2011).

[2] J. Klinovaja, M. Schmidt, B. Braunecker, and D. Loss, Phys. Rev. B **84**, 085452 (2011).

12:03PM Q6.00005 Extracting Diameter and Chirality Dependences of Optical and Electronic Properties of Semiconducting Single-Wall Carbon Nanotubes from First-Principles Calculations

, RODRIGO B. CAPAZ, Universidade Federal do Rio de Janeiro, Brazil, JACK DESLIPPE, Lawrence Berkeley National Laboratory, STEVEN G. LOUIE, U. C. Berkeley and Lawrence Berkeley National Laboratory — First-principles methods based on the combination of density-functional theory (DFT) for ground-state properties, GW approximation for quasiparticle properties and Bethe-Salpeter equation (BSE) for optical properties represent the state-of-art for accurate and reliable calculations of optical and electronic properties of solids and molecules. For semiconducting carbon nanotubes (CNTs), they have been applied successfully to selected small-diameter tubes. In this work, we systematically calculate such properties for all zig-zag semiconducting single-wall carbon nanotubes with diameters ranging from (10,0) to (20,0) CNTs, allowing us to extract in a reliable way the diameter and chirality dependence of many properties, such as: (i) optical transition energies; (ii) quasiparticle band gaps; (iii) exciton binding energies; (iv) bright-dark exciton splittings; (v) excited exciton states properties; (vi) transverse-polarized exciton states properties; (vii) electron and hole effective masses (and therefore excitonic reduced masses). All properties are described with good accuracy by diameter- and chirality-dependent analytical formulas, with parameters extracted from the first-principles calculations.

12:15PM Q6.00006 Modeling the Thermal Conductivity of Nanocomposites Using Monte-Carlo Methods and Realistic Nanotube Configurations¹

, KHOA BUI, DIMITRIOS PAPAVALASSILOU, The University of Oklahoma — The effective thermal conductivity (K_{eff}) of carbon nanotube (CNT) composites is affected by the thermal boundary resistance (TBR) and by the dispersion pattern and geometry of the CNTs. We have previously modeled CNTs as straight cylinders and found that the TBR between CNTs ($TBR_{CNT-CNT}$) can suppress K_{eff} at high volume fractions of CNTs [1]. Effective medium theory results assume that the CNTs are in a perfect dispersion state and exclude the $TBR_{CNT-CNT}$ [2]. In this work, we report on the development of an algorithm for generating CNTs with worm-like geometry in 3D, and with different persistence lengths. These worm-like CNTs are then randomly placed in a periodic box representing a realistic state, since the persistence length of a CNT can be obtained from microscopic images. The use of these CNT geometries in conjunction with off-lattice Monte Carlo simulations [1] in order to study the effective thermal properties of nanocomposites will be discussed, as well as the effects of the persistence length on K_{eff} and comparisons to straight cylinder models. **References** [1] K. Bui, B.P. Grady, D.V. Papavassiliou, Chem. Phys. Lett., 508(4-6), 248-251, 2011 [2] C.W. Nan, G. Liu, Y. Lin, M. Li, App. Phys. Lett., 85(16), 3549-3551, 2006

¹Department of Energy, DE-FG02-06ER64239; AFOSR, FA9550-10-1-0031

12:27PM Q6.00007 Computational study of the thermal conductivity of defective carbon nanostructures¹

, ZACHARIAS FTHENAKIS, DAVID TOMANEK, Michigan State University — We use molecular dynamics simulations to study the role of defects on the thermal conductivity in low-dimensional graphitic nanostructures such as schwarzites (3D), graphene (2D), carbon nanotubes and graphene nanoribbons (1D). Since the simulations are very demanding due to the very long phonon mean free path, we describe forces acting on carbon atoms by a parameterized valence force field. Our calculations make use of the non-equilibrium molecular dynamics technique, which incorporates the constant-temperature Nose-Hoover thermostat and non-equilibrium driving forces, which mimic the effect of the heat flow. We study different types of defects, including vacancies and isotope impurities, and show that their importance changes with changing dimension of the system.

¹Supported by the National Science Foundation Cooperative Agreement #EEC-0832785, titled “NSEC: Center for High-rate Nanomanufacturing”.

12:39PM Q6.00008 Near-field heat transfer between an array of SWNTs and a quartz substrate¹

, ANDREI NEMILENTSAU, SLAVA ROTKIN, Department of Physics, Lehigh University — The near-field heat transfer between a quartz substrate and a sparse array of SWNTs oriented normal to the substrate was studied theoretically. The heat power transferred from the hot quartz substrate to the cold SWNTs was expressed through the electric field Green tensor of the system using the fluctuation-dissipation theorem. The integral equation for the Green tensor was obtained and solved numerically. The spectra of the transferred power were calculated and the pronounced resonance lines in the spectra were demonstrated at the frequencies of the polariton resonances in the quartz and antenna resonances of the surface plasmons in the SWNTs. The dependence of the transferred power on separation between the SWNTs and the substrate and on the SWNTs lengths in the array was also studied.

¹Supported by DoD (AFOSR # FA9550-11-1-0185).

12:51PM Q6.00009 Ab initio studies of mechanical, electric, and magnetic properties of functionalized carbon nanotubes¹

, KAROLINA MILOWSKA, MAGDALENA BIROWSKA, JACEK A. MAJEWSKI, University of Warsaw — We present results of extensive theoretical studies of mechanical, electric, and magnetic properties of functionalized carbon nanotubes (CNTs). Our studies are based on the ab initio calculations in the framework of the density functional theory. We have performed calculations for various metallic and semiconductor single wall CNTs, functionalized with simple organic molecules such as OH, COOH, NH_n, CH_n and metals, Al, Fe, Ni, Cu, Zn, and Pd. We have determined the stability of the functionalized CNTs, their elastic moduli, conductance, and magnetic moments (in the case of CNTs decorated with magnetic ions). These studies shed light on physical mechanisms governing the binding of the adsorbed molecules and also provide valuable quantitative predictions that are of importance for design of novel composite materials and functional devices. In particular, we find out that the Young's modulus of functionalized CNTs is smaller than in the case of bare CNTs, however it is large enough to provide a strong enforcement of composites. The functionalization with molecules leads also to the metallization of semiconducting CNTs, being relevant in the context of CNT interconnects, whereas the functionalization with metals might be used to cut CNTs into ribbons.

¹The studies were carried out within the SiCMAT Project financed under the European Funds for Regional Development (Contract No. UDA-POIG.01.03.01-14-155/09).

1:03PM Q6.00010 Nanotube based engine

, OLEG SHKLYAEV, ERIC MOCKENSTURM, Department of Mechanical and Nuclear Engineering, The Pennsylvania State University, University Park, PA, 16802-6300, USA, VIN CRESPI, Department of Physics and Materials Research Institute, The Pennsylvania State University, University Park, PA, 16802-6300, USA — We discuss a mechanism for converting electrical energy into translational motion using a variable-shape bistable carbon nanotube. Clamping one tube end open and the other one closed, we use an applied voltage to switch the tube between mostly collapsed and mostly inflated shapes. Devices based on such a double-pinned tube geometry can operate as a voltage-controlled constant-force spring, a charge-controlled harmonic spring, or an electromechanical engine performing work by coupling to a propagating collapsed/inflected transition region. Making an analogy to ideal-gas thermodynamics, constant-voltage, constant-charge, and constant-geometry operational regimes correspond to isothermal, adiabatic and isochoric processes. Constant-voltage, constant-charge, and constant-geometry processes coupled can be combined into cycles analogous to those of a heat engine. Unlike a heat engine, the tube bistability enables it to collect useful work on both inflation and collapse motions, thus eliminating the need for external forces to restore the system to its initial state during the operational cycle.

1:15PM Q6.00011 Influence of temperature and adsorbates on a carbon nanotube resonator by molecular dynamics simulations, HEEYUEN KOH, JAMES CANNON, SHIGEO MARUYAMA, JUNICHIRO SHIOMI, the University of Tokyo — The bending modes of carbon nanotube have been studied for ultralow mass and force sensing and its tunable resonance frequency. On the other hand, the nonlinear damping of flexural mode has been shown to be vulnerable to temperature and adsorbates. For this reason, we have studied the interaction between mechanical and thermal characteristics in a carbon nanotube cantilever resonator observing the phase space trajectories, strain-stress distributions, and lattice vibrational spectra for various temperatures and adsorbate conditions. The calculation was based on molecular dynamics simulations using the REBO potential, where a carbon nanotube was excited by sinusoidal mechanical forcing at a tube end with constant-temperature boundary condition. The result confirms that the localized strain distribution is in agreement with previous high-resolution transmission electron microscopy result. Based on the simulations, the dynamic Young's modulus and the damping coefficient will be extracted in the frequency domain for different nanotube length and chirality, and will be compared with the continuum theories. In addition, the interaction between the first resonance mode and the background phonons will be discussed based on the obtained dissipated thermal energy and the phonon energy spectra.

1:27PM Q6.00012 Electron Spin Resonance as a route to Spin-Gap detection in Carbon Nanotubes, DARRYL H. NGAI, ANDRE' LECLAIR, EUN-AH KIM, Cornell University — The recent observation of a charge-neutral excitation gap in ultraclean carbon nanotubes¹ raises the intriguing possibility of a phase with gapless charge spectrum and gapped spin spectrum: the Luther-Emery liquid. We note that ESR would be an ideal probe to directly test whether the observed gap is a spin-gap, as it probes the non-local correlations of conduction electron spins. We focus on the Luther-Emery point ($K_s = 1/2$, also known as free fermion point) where an explicit calculation of relevant spin-spin correlation function is possible, to calculate the ESR signal in a Luther-Emery liquid. At high frequencies of $\omega > 2\Delta_s$ where Δ_s is the spin-gap, the ESR signal of the Luther-Emery liquid will exhibit a second peak at magnetic fields away from the resonance condition of $B = \omega/\mu_B g K_s$. We discuss how to measure the spin-gap from the location of this additional peak as a function of applied field strength.

¹V. V. Deshpande *et al.*, Science **323**, 106 (2009)

1:39PM Q6.00013 Coherent non-local transport in quantum wires with strongly coupled electrodes¹, YANFEI YANG, GEORGY FEDOROV², PAOLA BARBARA, Department of Physics, Georgetown University, Washington, DC, SERHII SHAFRANIUK, Department of Physics and Astronomy, Northwestern University, Evanston, IL, BENJAMIN COOPER, RUPERT LEWIS, CHRISTOPHER LOBB, Department of Physics, CNAM and JQI, University of Maryland, College Park, MD — We report a one-dimensional non-local experiment, where the conductance of a section of carbon nanotube shows regular oscillations due to coherent and ballistic transport in an adjacent section. This occurs in spite of wide strongly coupled contact electrodes, which are expected to divide the nanotube into independent sections. Our simulations show that the electrodes form shallow and wide barriers, which maintain quantum coherence between the adjacent sections.

¹This work was supported by the NSF (DMR-0907220). G.F. acknowledges financial support from the Russian Ministry of Science and Education (grant no. 16.513.12.3004) and the RFBR (grant no. 10-02-92671-NNF-a)

²Current affiliation: Russian Research Centre "Kurchatov Institute", Moscow, 123182, Russia

1:51PM Q6.00014 Nanofissure formation during selective breakdown of m-SWNT in an aligned array, UDAI BHANU, SHASHANK SHEKHAR, Nanoscience Technology Center, and Department of Physics, University of Central Florida, SAIFUL I. KHONDAKER, Nanoscience Technology Center, and Department of Physics, and School of Electrical Engineering and Computer Science University of Central Florida — Selective removal of metallic single walled carbon nanotubes (m-SWNT) in an aligned array is needed for restoring semiconducting properties and better device performance. The selective removal is done via electrical breakdown of m-SWNT while applying a large gate voltage to preserve semiconducting SWNT. In this work, we show using electrical measurements and scanning electron microscopy imaging that in a sufficiently dense array, not only the m-SWNT breaks down but also s-SWNT breaks down in a correlated fashion giving rise to a nano fissure pattern. This is in contrast to the established understanding that SWNTs are broken in a random fashion. The origin of the correlated breakdown is due to the electrostatic field of the broken nanotubes that produces locally inhomogeneous current and Joule heating distributions in the neighboring intact nanotubes triggering their breakdowns in the vicinity of the broken nanotubes

2:03PM Q6.00015 An optically pumped InGaAsP/InP quantum dot rolled-up microtube laser, PABLO BIANUCCI, Department of Engineering Physics, École Polytechnique de Montréal, Montreal QC, H3C 3A7, M. HADI TAVAKOLI DASTJERDI, SHOUVIK MUKHERJEE, MEHRDAD DJAVID, Department of Electrical Engineering, McGill University, Montreal QC, H3A 2A7, PHILIP POOLE, Institute for Microstructural Sciences, National Research Council, Ottawa, Ontario K1A 0R6, Canada, ZETIAN MI, Department of Electrical Engineering, McGill University, Montreal QC, H3A 2A7 — Rolled-up quantum dot microtubes are a promising candidate for light sources in integrated photonics. We have fabricated InGaAsP/InAs quantum dot rolled-up microtubes from InGaAsP strained bilayers with embedded InAs quantum dots (grown by chemical beam epitaxy). In room-temperature photoluminescence experiments we have observed resonant-mode emission with wavelengths in the telecom range. This resonant emission is consistent with whispering gallery modes. At a temperature of 82 K, we have demonstrated multi-mode lasing under continuous wave optical pumping. We estimate an ultra-low lasing threshold near 1.25 μ Ws of absorbed optical power.

Wednesday, February 29, 2012 11:15AM - 2:15PM –
Session Q7 DMP DCOMP: Focus Session: Computational Design of Materials: Graphene - Strain, defect and interface engineering 207

11:15AM Q7.00001 Formation of hydrogenated graphene nanoripples by strain engineering and directed surface self-assembly¹, ZHENGFEI WANG, YU ZHANG, FENG LIU, University of Utah, Department of Materials Science and Engineering, FENG LIU'S GROUP TEAM — We propose a class of semiconducting graphene-based nanostructures: hydrogenated graphene nanoripples (HGNRs), based on continuum-mechanics analysis and first-principles calculations. They are formed via a two-step combinatorial approach: first by strain-engineered pattern formation of graphene nanoripples, followed by a curvature-directed self-assembly of H adsorption. It offers a high level of control of the structure and morphology of the HGNRs, and hence of their band gaps, which share common features with graphene nanoribbons. A cycle of H adsorption (desorption) at (from) the same surface locations completes a reversible metal-semiconductor-metal transition with the same band gap.

¹This work was supported by DOE-BES program.

11:27AM Q7.00002 Engineering electronic properties of armchair graphene nanoribbons using strain and functional species, XIHONG PENG, FU TANG, SELINA VELASQUEZ, ANDREW COPPLE, Arizona State University — First principles density-functional theory calculations were performed to study effects of strain, edge passivation, and surface functional species on structural and electronic properties. Particularly band gap and work function, of armchair graphene nanoribbons (AGNRs), are addressed. It was found that the band gap of the O-passivated AGNRs experiences a direct-to-indirect transition with sufficient tensile strain. The indirect band gap reduces to zero with further increased strain. The work function was found to increase with uniaxial tensile strain while decreasing with compression. The variation of the work function under strain is primarily due to the shift of the Fermi energy with strain. For AGNRs with edge carbon atoms passivated by oxygen, the work function is higher than that of nanoribbons with edge passivated by hydrogen under a moderate strain. The difference between work functions in these two edge passivations is enlarged (reduced) under a sufficient tensile (compressive) strain. Furthermore, the effect of surface species decoration, such as H, F, or OH with different covering density, was investigated. It was found the work function varies with the type and coverage of surface functional species. F and OH decoration increase the work function while H decreases it. The surface functional species were decorated on either one side or both sides of AGNRs. The difference in the work functions between one-side and two-side decorations was found to be relatively small, which may suggest the introduced surface dipole plays a minor role.

11:39AM Q7.00003 Electronic Band Engineering of Epitaxial Graphene by Atomic Intercalation, THUSHARI JAYASEKERA, Department of Physics, Southern Illinois University, Carbondale, IL, 62901, ANDREAS SANDIN, SHU XU, Department of Physics, North Carolina State University, Raleigh, NC 27695, VIRGINIA WHEELER, D.K. GASKILL, U.S. Naval Research Laboratory, Washington, DC 20375, J.E. ROWE, Department of Physics, North Carolina State University, Raleigh, NC 27695, K.W. KIM, Department of Electrical and Computer Engineering, North Carolina State University, Raleigh, NC 27695, DANIEL B. DOUGHERTY, M. BUONGIORNO NARDELLI, Department of Physics, North Carolina State University, Raleigh, NC 27695 — Using calculations from first principles, we have investigated possible ways of engineering the electronic band structure of epitaxial graphene on SiC. In particular, intercalation of different atomic species, such as Hydrogen, Fluorine, Sodium, Germanium, Carbon and Silicon is shown to modify and tune the interface electronic properties and band alignments. Our results suggest that intercalation in graphene is quite different from that in graphite, and could provide a fundamentally new way to achieve electronic control in graphene electronics.

11:51AM Q7.00004 Interplay of Defects, Magnetism, Ripples and Strain in Graphene¹, ELTON J.G. SANTOS, Department of Physics and School of Engineering and Applied Sciences, Harvard University, 17 Oxford Street, Cambridge 02138, MA, ANDRES AYUELA, DANIEL SANCHEZ-PORTAL, Centro de Fisica de Materiales MFC, CSIC-UPV/EHU and Donostia International Physics Center, Paseo Manuel de Lardizabal 4/5, San Sebastian, 20018, Spain — We present a comprehensive study based on first-principles calculations about the interplay of four important ingredients on the electronic structure of graphene: defects + magnetism + ripples + strain. So far they have not been taken into account simultaneously in a set of ab initio calculations. Furthermore, we focus on the strain dependence of the properties of carbon monovacancies, with special attention to magnetic spin moments. We demonstrated that such defects show a very rich structural and spin phase-diagram with many spin solutions as function of strain. At zero strain the vacancy shows a spin moment of 1.5 Bohrs that increases up to 2 Bohrs with stretching. Changes are more dramatic under compression: the vacancy becomes non-magnetic under a compression larger than 2%. This transition is linked to the structural modifications associated with the formation of ripples in the graphene layer. Our results suggest that such interplay could have important implications for the design of future spintronics devices based on graphene derivatives, as for example a spin-strain switch based on vacancies.

¹We acknowledge support from Basque Departamento de Educacion and the UPV/EHU (Grant No. IT-366-07), the Spanish Ministerio de Educacion y Ciencia (Grant No. FIS2010-19609-CO2-02) and the ETORTEK program.

12:03PM Q7.00005 Spin switching in organic molecules by strain engineering in graphene¹, BIPLAB SANYAL, SUMANTA BHANDARY, Department of Physics and Astronomy, Uppsala University, SAURABH GHOSH, Cornell University, USA, HEIKE HERPER, HEIKO WENDE, University of Duisburg-Essen, Germany, OLLE ERIKSSON, Department of Physics and Astronomy, Uppsala University — One of the primary objectives in molecular nano-spintronics is to manipulate the spin states of organic molecules with a d-electron center, by suitable external means. Here, we demonstrate by first principles density functional calculations, as well as second order perturbation theory, that a strain induced change of the spin state, from $S=1 \rightarrow S=2$, takes place for an iron porphyrin (FeP) molecule deposited at a divacancy site in a graphene lattice. The process is reversible in a sense that the application of tensile or compressive strains in the graphene lattice can stabilize FeP in different spin states, each with a unique saturation moment and easy axis orientation. The effect is brought about by a change in Fe-N bond length in FeP, which influences the molecular level diagram as well as the interaction between the C atoms of the graphene layer and the molecular orbitals of FeP. We propose that the spin switching should be detected by x-ray magnetic circular dichroism experiments through the contributions from spin dipole and magnetic anisotropy.

¹We gratefully acknowledge financial support from STINT Institutional Grant for Young Researchers, Swedish Research Council (VR) and a KOF grant from Uppsala University and SNIC for supercomputing allocations.

12:15PM Q7.00006 The magnetism in graphene under strain, YI CHEN CHANG, STEPHAN HAAS, University of Southern California, COMPUTATIONAL CONDENSED MATTER THEORY GROUP TEAM — We theoretically study the magnetic features in graphene dot under mechanical deformation using the mean field Hubbard model. The edge local magnetic moment (ELMM) is considerably modified in accordance with an effective quantum well originating from a strain-induced gauge field. Applying a uniaxial strain along the zigzag or armchair directions enhances or dampens the ELMM due to the development of the edge quantum wells. Whereas a circular arc bending deformation is applied, the inner and outer edge display ELMM caused by nonuniform gauge field, a direct consequence of the presence of the bulk localized states. These states suggest that an effective single well potential is introduced by a nonuniform pseudo-magnetic field.

12:27PM Q7.00007 Vacancy-induced order-to-disorder transition in single-layer graphene, CORINNE CARPENTER, ASHWIN RAMASUBRAMANIAM, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — Defect engineering provides a potential route for tuning the mechanical, electronic, and chemical properties of graphene. While individual defects in single-layer graphene have been investigated in much detail, the outcomes of collective interactions of multiple defects remain elusive. In this work, we address the collective interaction of populations of vacancies in single-layer graphene using classical molecular-dynamics simulations based on reliable bond-order potentials; we examine random vacancy distributions with the vacancy concentration and temperature being the key parameters in the analysis. We demonstrate that a crystalline-to-amorphous structural transition occurs as the vacancy concentration in single-layer graphene increases beyond a critical level; the transition leads to complete loss of long-range order in the graphene layer. The onset of this order-to-disorder transition typically occurs over the vacancy concentration range from 10 to 20% and is independent of the details of the interatomic interactions in the classical potentials employed. We present a systematic parametric study of the phenomenon and discuss the implications of our findings for the mechanical and electronic properties of single-layer graphene.

12:39PM Q7.00008 Two magnetic impurities in graphene¹, FEI-MING HU, Aalto University, School of Science, Finland, JAME GUBERNATIS, Los Alamos National Laboratory, Los Alamos, New Mexico, USA, HAI-QING LIN, Beijing Computational Science Research Center, Beijing, China and The Chinese University of Hong Kong, Hong Kong, China, RISTO NIEMINEN, Aalto University, School of Science, Finland — We theoretically investigate two magnetic impurities in graphene. We mainly study the indirect interaction between the two magnetic impurities mediated by conducting electrons, which is so called RKKY interaction. The spin-spin and charge-charge correlation functions are calculated by quantum Monte Carlo simulations when the Fermi energy of the system is changed by gate voltage. The spectral density of the two impurities is also studied by maximum entropy methods.

¹We thank the CSC in Finland for computer resources.

12:51PM Q7.00009 Power-Law Correlated Disorder in Graphene and Square Nanoribbons¹, NANCY SANDLER, GREG PETERSEN, Ohio University — Two dimensional metal-insulator transitions have remained an active topic in condensed matter physics do to the lack of a general model that can predict when an MIT occurs. With the creation of truly 2D crystals and nanostructures, the question has become increasingly relevant. Though initially predicted to not contain a MIT transition, the inclusion of electron-electron interactions and/or spatial disorder can drive a MIT in some 2D systems. In the case of graphene, correlated ripples are present even when the nanoribbons are freestanding and can have an effect on the transport properties while electron-electron interactions are normally considered negligible. To explore the effect of ripples, we model graphene with a long-range power-law spatial correlation of the form $\langle \epsilon_i^2 \rangle = 1/(1 + |\vec{r}_i/a|)^\alpha$ where ϵ_i , $\vec{r}$, a , and α are the on-site energy, position, lattice constant, and strength of the correlation respectively. It should be noted that much work has been completed on short-range correlations but little on truly long-range correlations. We also present our finding for the square lattice for comparison.

[1] Abrahams E. Phys. Rev. Lett. 42, 673-676 (1979)

[2] Abrahams E. Ann. Phys. 8 (1999) 7-9, 539-548

¹This work has been supported by the NSF-PIRE mwn/ciam and NSF Grant DMR-0710581.

1:03PM Q7.00010 Thermally-driven Isotope Separation Across Nanoporous Graphene¹, JOSHUA SCHRIER, Haverford College — Experiment and theory indicate that a single graphene sheet is impermeable to gases even as small as helium; pores are required for transmission of atoms and molecules. Nanoporous forms of graphene, such as two-dimensional polyphenylene (2D-PP), consist of a regular array of sub-nanometer pores which can be used for separating atoms and molecules by size. Because the nanoporous graphene barrier is only an atom-thick, quantum tunneling plays a role in the transmission of atoms through the nanoporous barrier, even at room temperature. This talk describes how the mass-dependence of the tunneling, combined with a temperature gradient, can be used to separate isotope mixtures under conditions where classical transmission cannot. Using transition state theory, we show that the zero-point and tunneling contributions lead to isotopic separations in opposite directions with respect to the temperature gradient. We examine the separation of ³He/⁴He across a 2D-PP membrane under modest temperature and pressure conditions. We will also describe 2D-PP bilayer structures that yield resonant tunneling of helium atoms, and new nanoporous graphene structures suitable for separating heavier noble-gas isotopes.

¹Partially supported by the Donors of the American Chemical Society Petroleum Research Fund and Research Corporation for Science Advancement's Cottrell Scholar grant, and used resources of the National Energy Research Scientific Computing Center.

1:15PM Q7.00011 Phonon instabilities in graphene¹, KLAUS ZIEGLER, Universitaet Augsburg, Germany, EUGENE KOGAN, Bar-Ilan University, Israel — We study the thermal distribution of phonons in graphene and compare in-plane and out-of-plane contributions with a focus on two in-plane modes that represent intervalley scattering. Due to the two electronic bands there are also two out-of-plane phonon modes with respect to the two sublattices. The electron-phonon interaction softens the phonon modes with a tendency to create instabilities for a sufficiently large electron-phonon coupling. The instabilities are characterized by phase transitions, where one of the out-of-plane mode undergoes an Ising transition by spontaneously breaking the sublattice symmetry. The in-plane modes undergo a Berezinskii-Kosterlitz-Thouless transition. We calculate the critical points of the instabilities, the renormalization of the phonon frequencies and the phonon frequency splitting for in-plane modes. The possibility to observe these instabilities in doped graphene and their consequences for transport are discussed.

¹Deutsche Forschungsgemeinschaft

1:27PM Q7.00012 Electronic Properties of Epitaxial Graphene on Si(111)-7×7 and 3CS-SiC(100) Substrates, SHU XU, North Carolina State University, THUSHARI JAYASEKERA, Southern Illinois University, MARCO BUONGIORNO NARDELLI, North Carolina State University — The synthesis of epitaxial graphene is an attractive method for industrial-scale fabrication and mass production of graphene-based electronic devices. Recently, efforts of epitaxial growth of graphitic carbon films on Si(111)-7×7 and 3CS-SiC(100) substrates have been undertaken in order to explore new potential substrates compatible with conventional Si technology. In this talk, we will discuss the electronic properties of epitaxial graphene on Si (111)-7×7 and 3CS-SiC(100) substrates using calculations from first principles based on Density Functional Theory. In particular, we found that a single graphene layer on Si(111)-7×7 displays ripples of about 0.5 Å and shows an n type electronic behavior. We also calculated the band structures for a graphene bilayer on 3CS-SiC(100) surface with different stacking sequences. While AA stacking on Si face and turbostratic stacking on C face show n type behavior, turbostratic stacking on Si face and AA stacking on C face show p type behavior. On both faces, the first carbon plane is covalently bonded to the substrate and serves as a buffer layer similarly to the graphene/6H-SiC(0001) system previously studied.

1:39PM Q7.00013 Graphene-nickel interface: hybridization and magnetization, TESFAYE ABTEW, BI-CHING SHIH, PEIHONG ZHANG, University at Buffalo, The State University of New York — The unique properties of graphene have opened up a new avenue for fundamental research as well as technological applications. Whereas the in-plane sp^2 bonding is primarily responsible for the overall structural stability and mechanical strength of graphene, the out-of-plane $pp-\pi$ states control its transport and interfacing properties. In this talk, we present a first principles study of the single layer graphene/Ni(111) interface. We discuss how hybridization between the carbon $pp-\pi$ and nickel d orbitals modifies the electronic and magnetic properties of the interface.

We acknowledge the computational support provided by the Center for Computational Research at the University at Buffalo, SUNY. This work is supported by the Department of Energy under Grant No. DE-SC0002623 and by the National Science Foundation under Grant No. DMR-0946404.

1:51PM Q7.00014 Correlated magnetic states in domain and grain boundaries in graphene¹

, RICARDO W. NUNES, SIMONE S. ALEXANDRE, U. F. Minas Gerais - Brazil, ALINE D. LUCIO, U. F. Lavras - Brazil, ANTONIO H. CASTRO NETO, Graphene Research Centre and Physics Dept. National Univ. Singapore and Physics Dept. Boston Univ. — Ab initio calculations indicate that while the electronic states introduced by grain boundaries in graphene are only partially confined to the defect core, a domain boundary introduces states near the Fermi level that are very strongly confined to the core of the defect, and that display a ferromagnetic ground state. The domain boundary is fully immersed within the graphene matrix, hence this magnetic state is protected from reconstruction effects that have hampered experimental detection in the case of ribbon edge states. Furthermore, our calculations suggest that charge transfer between one-dimensional extended defects and the bulk in graphene is short ranged for both grain and domain boundaries. <http://arxiv.org/abs/1109.6923>

¹SSA, RWN, and ALD acknowledge support from Brazilian Agencies Capes, CNPq, Fapemig e ICNT Carbon Materials. AHCN acknowledges support from NRF-CRP award Novel 2D Materials (R-144-000-295-282), US/DOE grant DE-FG02-08ER46512, and

2:03PM Q7.00015 A Nanocluster Based Study of Silicon Carbide Nanocones: Existence and Stability¹

, KAPIL ADHIKARI, ASOK RAY, Department of Physics, University of Texas at Arlington — A systematic study of silicon carbide nanocones of different disclination angles and different tip geometries using the finite cluster approximation is presented. The geometries of the nanocones have been spin optimized using the hybrid functional B3LYP (Becke's three-parameter exchange functional and the Lee-Yang-Parr correlation functional) and the all electron 3-21G* basis set. The study indicates that the binding energy per atom or the cohesive energy of the nanocones depends not only on the size of the nanocones but also on the disclination angle of the nanocones. The electronic properties of nanocones depend on disclination angles, size of the nanocone clusters and the edge structure of the nanocones. Given similar cluster size, silicon carbide appears to favor tubular structures over two dimensional graphene-like structures. For relatively smaller clusters the B.E./atom oscillates in all cases except in nanocones of disclination angle 300°. This indicates the greater stability of nanocones of some particular size as compared with its neighboring sizes. A study of binding energies, NBO charge, density of states and HOMO-LUMO gaps has been performed for all nanocones from disclination angles of 60° to 300°.

¹This work is supported by the Welch Foundation, Houston, TX (Grant No. Y-1525)

Wednesday, February 29, 2012 11:15AM - 2:15PM – Session Q8 DMP GMAG: Focus Session: Spin Liquids II 208

11:15AM Q8.00001 Absence of magnetic order and unusual spin dynamics in the spin liquid candidate Na₄Ir₃O₈

, PETER BAKER, FRANCIS PRATT, ISIS Facility, STFC Rutherford Appleton Laboratory, DHARMALINGHAM PRABHAKARAN, ANDREW STEELE, TOM LANCASTER, BILL HAYES, STEPHEN BLUNDELL, Oxford University Department of Physics — Na₄Ir₃O₈ has spin-1/2 iridium ions on a hyperkagome lattice of corner sharing triangles and is a candidate three-dimensional spin liquid [1], which has led to active theoretical study [2,3,4]. Previously reported measurements have shown no evidence for magnetic ordering down to temperatures around three orders of magnitude below the Curie-Weiss constant of ~ 650K [1]. We have carried out muon-spin relaxation measurements which exclude magnetic ordering above 55mK. The field dependence of the muon spin relaxation rate provides further information on the spin dynamics with a temperature-dependent crossover between power laws at intermediate fields suggesting that more than one energy scale is relevant to the fluctuations in this system. [1] Y. Okamoto *et al.*, Phys. Rev. Lett. **99**, 137207 (2007). [2] M. J. Lawler *et al.*, Phys. Rev. Lett. **100**, 227201 (2008). [3] Yi Zhou *et al.*, Phys. Rev. Lett. **101**, 197201 (2008). [4] E. J. Bergholtz *et al.*, Phys. Rev. Lett. **105**, 237202 (2010).

11:27AM Q8.00002 Short range magnetic correlations and the possible role of frustration in the heavy-fermion CeCu₄Ga

, B.G. UELAND, C.F. MICLEA, K. GOFRYK, Los Alamos National Laboratory, J.S. GARDNER, Indiana University / NIST Center for Neutron Research, F. RONNING, R. MOVSHOVICH, E.D. BAUER, J.D. THOMPSON, Los Alamos National Laboratory — Neutron scattering, longitudinal and transverse resistivity, heat capacity, ac susceptibility, and magnetization measurements on single and polycrystalline samples of the heavy-fermion compound CeCu₄Ga suggest that its hexagonal lattice and disorder due to Ga substitution may frustrate formation of the long-range magnetic order found in its parent CeCu₅. The absence of magnetic Bragg peaks in neutron diffraction data, field-dependent specific heat data, a Weiss temperature of ~ 10 K, and diffuse scattering below ~1 K which can be fit to an isotropic model describing spin-spin correlations between third through fifth nearest neighbors support this suggestion. Kondo behavior also plays a role in determining the physical properties of CeCu₄Ga.

11:39AM Q8.00003 Mean field phase diagram of the layered perovskite (Li, Na)₂IrO₃ in the strong interaction limit: possible realization of spin liquid phases¹

, MEHDI KARGARIAN, JUN WEN, GREGORY A. FIETE, The University of Texas at Austin — We study the phase diagram of layered perovskite (Li, Na)₂IrO₃ with an underlying honeycomb lattice structure in the strongly interacting limit. Because of the strong spin-orbit coupling of iridium, the effective spin exchange model is highly anisotropic and frustrated. We use the Schwinger fermion approach to map out the phase diagram of the model. At the mean field level several spin liquid phases are found: a gapless spin liquid, a chiral spin liquid, and a helical spin liquid phase. Moreover, in the strong exchange coupling limit we obtain a dimerized phase. The gapless spin liquid phase is characterized by Dirac nodes. In the chiral phase the Dirac nodes are gapped in the bulk, and the system possess a nonzero Chern number signifying existence of chiral modes along the boundary of the system. The helical phase preserves time reversal symmetry, has a bulk gap, and features helical gapless edge modes along boundary analogous to those in topological insulators with a nontrivial invariant. We further investigate the nature of the spin liquid phase by considering the gauge fluctuations above the mean field solution. The chiral spin liquid phase is stable as it breaks time reversal symmetry and acquires a nonzero Chern-Simons term in the effective low energy theory.

¹We gratefully acknowledge funding from ARO grant W911NF-09-1-0527 and NSF grant DMR- 0955778.

11:51AM Q8.00004 Magnetic torque measurement in a gapless spin-liquid state of EtMe₃Sb[Pd(dmit)₂]₂

, DAIKI WATANABE, YOSHINORI SENSU, MINORU YAMASHITA, SHO TONEGAWA, TAKASADA SHIBAUCHI, YUJI MATSUDA, Department of Physics, Kyoto University, YUGO OSHIMA, REIZO KATO, Riken, TAICHI TERASHIMA, SHINYA UJI, NIMS, ILYA SHEIKIN, LNCMI — The organic Mott insulator EtMe₃Sb[Pd(dmit)₂]₂ with nearly identical 2D triangular lattice of $S = 1/2$ is the most promising candidate material of a quantum spin liquid, in which gapless spin excitations have been reported by the thermal transport measurements [1]. However, it remains unsettled whether the observed gapless excitations are magnetic ($S \geq 1/2$) or nonmagnetic ($S = 0$). The magnetic torque measurement is a powerful tool to probe the magnetic properties down to very low temperature, because it is not affected by isotropic impurities. We report the magnetic torque measurements of EtMe₃Sb[Pd(dmit)₂]₂ down to 30 mK up to 32 T. A finite magnetic susceptibility is observed at the lowest temperature. Magnetization increases linearly with the magnetic field up to 32 T without exhibiting any anomaly. These results indicate that the gapless excitations reported by the thermal conductivity measurements are magnetic and that the present system is in an algebraic spin liquid phase.

[1] M. Yamashita *et al.*, Science **328**, 1246 (2010).

12:03PM Q8.00005 Field-Dependent Instability of the Candidate Quantum Spin Liquid in $\text{EtMe}_3\text{Sb}[\text{Pd}(\text{dmit})_2]_2$ as Revealed by NMR, GEORGIOS KOUTROULAKIS, Los Alamos National Laboratory, TONG ZHOU, STUART E. BROWN, UCLA, JOE D. THOMPSON, Los Alamos National Laboratory, REIZO KATO, RIKEN — In recent years, the two-dimensional spin-1/2 triangular lattice of the organic salt $\text{EtMe}_3\text{Sb}[\text{Pd}(\text{dmit})_2]_2$ has emerged as a candidate for the realization of a quantum spin liquid. Furthermore, thermal conductivity and nuclear magnetic resonance (NMR) experiments unveiled the presence of a low-temperature instability in the spin liquid state, the opening of a spin gap. We performed a detailed ^{13}C NMR study on this material at low temperatures ($30\text{mK} \leq T \leq 1.5\text{ K}$) and for a wide range of external magnetic field values ($B_0 = 0.6 - 9\text{ T}$). In finite fields, a clear break in the temperature derivative of the spin-lattice relaxation is observed at a temperature $T_m(B_0)$, with T_m following the empirical form $T_m(B_0) \sim |B_0 - B_c|^{1/2}$. Moreover, a uniform broadening of the NMR line for finite fields suggests the presence of a small field-induced staggered magnetization. We discuss these results in the context of possible instabilities, and existing thermodynamic data.

12:15PM Q8.00006 Low temperature magnetodielectric coupling in the spin-liquid candidate $\kappa\text{-(BEDT-TTF)}_2\text{Cu}_2(\text{CN})_3$, MARIO POIRIER, SAMUEL PARENT, ALEX COTE, Universite de Sherbrooke, KAZUYA MIYAGAWA, Tokyo University, YASUHIRO SHIMIZU, Nagoya University, KAZUSHI KANODA, Tokyo University — In the context of geometrical frustration of exchange coupling between spins on dimer orbitals, the possibility of a quantum spin-liquid state has been inferred for the quasi-2D organic Mott insulator $\kappa\text{-(BEDT-TTF)}_2\text{Cu}_2(\text{CN})_3$. However, because the geometrical frustration effect is not strong, it has been proposed that the suppression of magnetic order could result from fluctuating quantum electric dipoles. Indeed, non-trivial charge degrees of freedom survive in this dimer Mott insulator as observed in dielectric measurements. Here, we report in-plane microwave dielectric measurements that reveal a coupling of the electric dipoles to the spins at low temperatures. Anomalies in the complex dielectric permittivity are observed at 6 K and around 3–4 K. The one at 6 K is in clear correlation with the thermal expansion measurements for which a second-order phase transition was inferred. The second dielectric anomaly is frequency dependent and cannot be associated to a phase transition; however, it is rapidly modified and ultimately suppressed by a magnetic field which effects are highly anisotropic. These results could be consistent with the scenario of a dipolar-spin liquid phase where spins couple to the dipoles through the interdimer charge fluctuation. Such a phase appears inhomogeneous since the dielectric anomalies are sensitive to thermal cycling and small pressures.

12:27PM Q8.00007 Coulombic Quantum Liquids in Spin-1/2 Pyrochlores, LUCILE SAVARY, University of California, Santa Barbara, LEON BALENTS, Kavli Institute for Theoretical Physics, University of California, Santa Barbara — We develop a non-perturbative “gauge Mean Field Theory” (gMFT) method to study a general effective spin-1/2 model for magnetism in rare earth pyrochlores. gMFT is based on a novel exact slave-particle formulation, and matches both the perturbative regime near the classical spin ice limit and the semiclassical approximation far from it. We show that the full phase diagram contains two exotic phases: a quantum spin liquid and a coulombic ferromagnet, both of which support deconfined spinon excitations and emergent quantum electrodynamics. Phenomenological properties of these phases are discussed.

12:39PM Q8.00008 Spin Liquid Ground State of Spin-1/2 Square $J_1\text{-}J_2$ Heisenberg Model, HONG-CHEN JIANG, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106, HONG YAO, Department of Physics, Stanford University, Stanford, CA 94305, LEON BALENTS, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106 — We perform highly accurate density matrix renormalization group (DMRG) simulations to investigate the ground state properties of the spin-1/2 antiferromagnetic (AFM) square lattice Heisenberg $J_1\text{-}J_2$ model on numerous long cylinders with circumference up to 10 lattice spacings. Besides finding the conventional Neel AFM phase at small $J_2/J_1 < 0.41$ and the stripe AFM phase at large $J_2/J_1 > 0.62$, we establish an intriguing gapped quantum spin liquid phase within the parameter space $0.41 < J_2/J_1 < 0.62$ by showing the absence of various conventional broken symmetries as well as by identifying topological features such as finite topological entanglement entropy and topological “even-odd” effect.

12:51PM Q8.00009 Projected wave function study of Z_2 spin liquids on the kagome lattice for the spin-1/2 quantum Heisenberg antiferromagnet, FEDERICO BECCA, CNR Istituto Officina dei Materiali and SISSA, YASIR IQBAL, DIDIER POILBLANC, Laboratoire de Physique Theorique UMR-5152, CNRS and Universite' de Toulouse — Within the class of Gutzwiller projected fermionic wave functions, by using quantum variational Monte Carlo simulations, we investigated the energetics of all possible Z_2 spin liquids that can potentially occur as ground states of the nearest-neighbor $S=1/2$ quantum Heisenberg model on the Kagome lattice [1]. We conclusively show that all gapped and gapless Z_2 spin liquids are higher in energy compared to the $U(1)$ gapless states in whose neighborhoods they lie. In particular, the most promising gapped Z_2 spin liquid (the so-called $Z_2[0, \pi|\beta]$ state), conjectured to describe the ground state [2], is always higher in energy compared to the $U(1)$ Dirac spin liquid. We also extended the $U(1)$ Dirac state and the uniform RVB spin liquid to include next-nearest-neighbor hopping terms, and studied its local and global stability towards various valence bond crystal patterns. We found that a non-trivial 36-site VBC is stabilized upon addition of a small ferromagnetic exchange coupling [3].

[1] Y. Iqbal, F. Becca, and D. Poilblanc, Phys. Rev. B 84, 020407(R) (2011)

[2] Y.-M. Lu, Y. Ran, and P.A. Lee, Phys. Rev. B 83, 224413 (2011)

[3] Y. Iqbal, F. Becca, and D. Poilblanc, Phys. Rev. B 83, 100404(R) (2011)

1:03PM Q8.00010 Edge states of $(2+1)D$ BF theory as the effective field theory of translational invariant Z_2 spin liquids¹, GIL YOUNG CHO, JOEL MOORE, Physics Department, University of California, Berkeley — We classify $(2+1)$ -dimensional BF field theory as the effective field theory for the achiral and translation invariant Z_2 spin liquids on the square lattice. We use the pattern of the crystal momenta of BF field theory to find the corresponding Z_2 spin liquid. Then, we show that some classes of Z_2 spin liquids can support gapless helical edge states depending on the projective symmetry group of the effective BF theory. We supplement this effective theory by studying possible projective symmetry group of Z_2 spin liquids.

¹Funding support for this work was provided by FENA (G.Y.C) and NSF DMR-0804413 (J.E.M.).

1:15PM Q8.00011 ESR lineshape for a two-dimensional spin liquid state with spinon Fermi surface¹, OLEG STARYKH, RACHEL GLENN, MIKHAIL RAIKH, University of Utah — We propose that ESR experiment can be an informative probe of a putative spin-liquid ground state with a spinon Fermi surface. Our proposal is based on the assumption that in addition to strong and frustrated Heisenberg exchange interactions, the spins also interact via an asymmetric Dzyaloshinskii-Moriya interaction (DMI). We argue that in a spin-liquid state the DMI plays the role of a spin-orbit interaction well-known in low-dimensional conductors. Assuming further spin-orbit interaction to be of Rashba type, we calculate the ESR absorption spectrum of a two-dimensional fermion gas subject to Zeeman and spin-orbit fields. Finite spin-orbit coupling translates into a finite absorption spectrum width. Remarkably, the ESR signal diverges as an inverse square-root at the edges of the spectrum.

¹Supported by NSF DMR-0808842 and MRSEC DMR-1121252

1:27PM Q8.00012 Loop condensation in quantum dimer models , C.M. HERDMAN, K.B. WHALEY, UC Berkeley

— The formation of topological order is well understood in terms of the mechanism of loop condensation in systems with loop-like degrees of freedom. Various quantum dimer models possess exotic liquid states, including topologically ordered phases. Dimer models can be mapped to loop models and these dimer liquid phases may be described as loop condensates. We present a numerical study of the geometric properties of the loop condensates in quantum dimer models and related models using classical Monte Carlo as well as ground state quantum Monte Carlo calculations.

1:39PM Q8.00013 Gapless fractionalized vortex liquids in frustrated quantum antiferromagnets , CHONG WANG, SENTHIL TODADRI, MIT

— The standard theoretical approach to gapless spin liquid phases of two-dimensional frustrated quantum antiferromagnets invokes the concept of fermionic slave particles into which the spin fractionalizes. As an alternate we explore new kinds of gapless spin liquid phases in frustrated quantum magnets with XY anisotropy where the vortex of the spin fractionalizes into gapless itinerant fermions. The resulting gapless fractionalized vortex liquid phases are studied within a slave particle framework that is dual to the usual one. We demonstrate the stability of some such phases and describe their properties.

1:51PM Q8.00014 Properties of the short ranged RVB wavefunction on non-bipartite lattices via Pfaffian Monte Carlo¹ , JULIA WILDEBOER, ALEXANDER SEIDEL, Washington University in Saint Louis

— We introduce a Monte Carlo scheme to investigate the nearest neighbor version of Anderson's resonating-valence-bond (RVB) spin-1/2 wave function on the kagome and on the triangular lattice. For the kagome lattice there exists a parent Hamiltonian for this state, but even in the absence of a known Hamiltonian, wave functions of RVB type are interesting as such. The corresponding RVB wave function on the square lattice has recently enjoyed much attention, and it was shown that earlier findings about the criticality of the *dimer*-liquid wave function on the square lattice qualitatively carry over to the analogous *spin*-liquid wave function on this lattice. On bipartite lattices, the spin-1/2 RVB wave functions are amenable to MC methods based on a loop gas picture. For other lattices, this method has a sign problem. We present a method that is free of this sign problem, making use of a Pfaffian presentation of the wave function in the orthogonal Ising basis. Our results for both open and periodic boundary conditions show that spin-spin and "dimer-dimer" type correlation function are exponentially decaying. Time and/or results permitting, we also comment on the behavior of the monomer correlations, and mention possible applications of our method to other problems.

¹This research was supported by the National Science Foundation under Grant No. DMR-0907793.

2:03PM Q8.00015 Exact Chiral Spin Liquid on the Ruby Lattice and Mean-Field Perturbations of Gamma Matrix Models¹ , SETH WHITSITT, VICTOR CHUA, GREGORY A. FIETE, Department of Physics, University of Texas at Austin

— We report recent results on the study of an exactly solvable spin-3/2 model of the Kitaev type [A. Kitaev, Ann. Phys. 321, 2 (2006)] and related mean-field studies. The model is a Yao-Zhang-Kivelson Gamma Matrix (GM) extension [H. Yao, S.C. Zhang, and S.A. Kivelson, Phys. Rev. Lett. 102, 217202 (2009)] on the ruby or rhombihexadeltile lattice. We show that the model admits an exact chiral spin liquid ground state solution with emergent free spinon excitations and interesting bandstructure. Specifically, we find gapped phases with chiral edge modes resulting from topologically non-trivial Chern numbers and gapless phases with interesting spinon Fermi surfaces. We have also studied the addition of perturbations to this and other GM Kitaev systems (kagome, square) which leads to weakly interacting spinons. We have applied a mean-field analysis to explore the interplay between these interactions and the gapless spin liquid phases.

¹NSF grant DMR-0955778

Wednesday, February 29, 2012 11:15AM - 2:03PM –

Session Q9 DMP GMAG: Focus Session: Complex Bulk Oxide: Doped and Undoped Manganites 209

11:15AM Q9.00001 Weak ferromagnetism in lightly electron-doped CaMnO_3 , HIROMASA OHNISHI,

TAICHI KOSUGI, SHOJI ISHIBASHI, Nanosystem Research Institute (NRI), National Institute of Advanced Industrial Science and Technology (AIST), KIY-OYUKI TERAOKA, Research Center for Integrated Science (RCIS), Japan Advanced Institute of Science and Technology (JAIST) — The origin of the weak ferromagnetism, that is observed in lightly electron-doped CaMnO_3 , is studied by means of the non-collinear spin density functional theory, including the spin-orbit interaction. We show that the spin-canting in the G-type antiferromagnetic structure is realized by the electron-doping, and the canting angle becomes larger with increase of the doping amount. The estimated canting angle is in a good agreement with the experimental value of the Ce-doped CaMnO_3 [1] The spin-canted state is stabilized by the double-exchange interaction, and the spin-orbit interaction does not play a crucial role in this phenomenon. In addition, the spin-canted state shows metallic behavior by the double-exchange transfer that gives a reasonable interpretation for the experimental electronic transport property [2] We also clarify a possibility of the antiferromagnetic-ferromagnetic phase separation [3] that will be realized when doped-electrons are strongly localized.

[1] E.N. Caspi et al., Phys. Rev. B 69, 104402 (2004).

[2] P.-H. Xiang et al., Appl. Phys. Lett. 94, 062109 (2009).

[3] E. Dagotto et al., Phys.Rep. 344, 1 (2001).

11:27AM Q9.00002 Synthesis, Structural and Magnetic Characterization of Rare Earth Doped SrMnO_3 Compounds , M.A. JUAREZ-ROSETE, E. CHAVIRA, J.I. BETANCOURT, Instituto de Investigaciones en Materiales, UNAM, Mexico

DF 04510, E.E. MARINERO, Hitachi San Jose Research Center, 3403 Yerba Buena Road, San Jose, CA 95135, L. BUCIO, X. BOKHIMI, Instituto de Fisica, UNAM, Mexico DF 04510 — We report on our ongoing work on the synthesis, characterization and magnetic studies of Rare Earth (RE) containing RE- SrMnO_3 compounds. The aim of the study is to determine how different RE elements influence the magnetic properties of said materials. We have so far investigated the incorporation of Dy and Yb into the SrMnO_3 unit cell. To this effect we have employed solid state reaction synthesis methods to fabricate said compounds. The reaction products evolution were monitored as a function of time by XRD, TGA and SEM. Measurements of lattice parameters and Rietveld refinement of the XRD spectra, indicate that Dy and Yb are incorporated substitutionally in SrMnO_3 . Temperature dependent magnetic measurements, on the other hand, reveal a common transition temperature around 41 K for both Dy and Yb doped SrMnO_3 . We are in the process of synthesizing additional materials containing additional RE elements to investigate how the electronic properties of said RE may influence the magnetic properties of these compounds.

11:39AM Q9.00003 Far-IR spectra of magnons, crystal field transitions, and phonons in hexagonal $RE\text{MnO}_3$ ($RE=\text{Er, Tm, Yb, Lu}$) single crystals¹, E.C. STANDARD, T.N. STANISLAVCHUK, R. BASISTYY, A.A. SIRENKO, Dept of Phys, NJIT, Newark NJ, USA, T.D. KANG, ReCFI, Dept of Phys and Astronomy, Seoul National U., Seoul, Korea, N. LEE, S-W. CHEONG, Rutgers Center for Emergent Materials and Dept of Phys and Astronomy, Rutgers U., NJ, USA — Far-IR spectra of hexagonal $RE\text{MnO}_3$ ($RE=\text{Er, Tm, Yb, Lu}$) single crystals have been studied between $T=1.6$ K and 300 K using transmission in high magnetic field and rotating analyzer ellipsometry. The symmetry of the IR optical phonons and their oscillator strengths were determined for compounds with different RE ions. The temperature dependence of the phonon frequencies revealed a strong spin-phonon interaction in the temperature range below $T_N \sim 70$ K. The effective g-factors have been determined for the AFM resonances and crystal field transitions using external magnetic fields up to 10 T. The frequency of the AFM resonances around 50 cm^{-1} increases systematically with a decrease of the RE ion radius. The observed effects are analyzed taking into account main magnetic interactions in the system including exchange of the Mn^{3+} spins with RE^{3+} paramagnetic moments. The magnetic ordering of RE ions was observed at low temperatures $T < 3.5$ K and in strong magnetic fields.

¹Work at NJIT and Rutgers was supported by DOE DE-FG02-07ER46382. Use of NSLS-BNL was supported by DOE DE-AC02-98CH10886.

11:51AM Q9.00004 Direct observation of collective magnetism at ferroelectric domain walls in multiferroic ErMnO_3 , YANAN GENG, NARA LEE, YOUNGJAI CHOI, SANG-WOOK CHEONG, WEIDA WU, Rutgers Center for Emergent Materials & Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, 08854 — Multiferroic hexagonal manganites $RE\text{MnO}_3$ ($RE = \text{Ho, Er, Lu, etc.}$) have been of great interest because of the coexistence of ferroelectric and magnetic orders. Herein we report cryogenic magnetic force microscopy (MFM) studies of flux-grown ErMnO_3 single crystals with vortex ferroelectric domain pattern. By uniquely correlating ambient piezo-response force microscopy and low temperature MFM images at the same location, we identified alternating uncompensated magnetic moments at ferroelectric domain walls that correlate over entire vortex network, suggesting collective magnetism at ferroelectric vortex domain walls.

12:03PM Q9.00005 Maximally localized Wannier functions in LaMnO_3 within PBE+ U , hybrid functionals, and GW: an efficient route to construct ab-initio tight-binding parameters for e_g perovskites, ROMAN KOVACIK, School of Physics, Trinity College Dublin, Dublin 2, Ireland, CESARE FRANCHINI, MARTIJN MARSMAN, Faculty of Physics, University of Vienna and Center for Computational Materials Science, A-1090 Wien, Austria, CLAUDE EDERER, School of Physics, Trinity College Dublin, Dublin 2, Ireland — Using the newly developed VASP2WANNIER90 interface we have constructed maximally localized Wannier functions [1] (MLWFs) for the e_g states of the prototypical Jahn-Teller magnetic perovskite LaMnO_3 at different levels of approximation for the exchange-correlation kernel. These include conventional density functional theory (DFT) with and without additional on-site Hubbard U term, hybrid-DFT, and single shot GW. By suitably mapping the MLWFs onto an effective e_g tight-binding (TB) Hamiltonian [2,3] we have computed a complete set of TB parameters providing the band dispersion in excellent agreement with the underlying *ab initio* and MLWF bands. The method-dependent changes of the TB parameters and their interplay with the electron-electron interaction term are discussed and interpreted, outlining a guidance for more elaborate treatments of correlation effects in effective Hamiltonian-based approaches.

[1] I. Souza, N. Marzari, and D. Vanderbilt, Phys.Rev.B 65, 035109 (2001).

[2] R. Kováčik and C. Ederer, Phys.Rev.B 81, 245108 (2010).

[3] R. Kováčik and C. Ederer, Phys.Rev.B 84, 075118 (2011).

12:15PM Q9.00006 Reverse Monte Carlo Modeling of Pair Distribution Function Data as a Tool for Separating the Coordination Environments of Multiple Atoms Disordered Over a Single Site, GRAHAM KING, ANNA LLOBET, Lujan Neutron Scattering Center, Los Alamos National Laboratory, REBECCA RICCIARDO, JENNIFER SOLIZ, PATRICK WOODWARD, Department of Chemistry, Ohio State University, FARSHID RAMEZANIPOUR, JOHN GREEDAN, Department of Chemistry, McMaster University — The local structures of 8 perovskite compounds which contain equal concentrations of 2 transition metal cations disordered over the B -sites have been investigated using reverse Monte Carlo (RMC) modeling of neutron pair distribution function (PDF) data. Such compounds are known to display a number of interesting magnetic and electronic properties which, due to the cation disorder, cannot be correlated with the average long range structure and so remain poorly understood. In compounds with $B=\text{Mn/Ru}$ there exists a valence degeneracy between $\text{Mn}^{3+}/\text{Ru}^{5+}$ and $\text{Mn}^{4+}/\text{Ru}^{4+}$. We demonstrate that the RMC method can be used as an effective tool to separate out the individual coordination environments of these cations and also to monitor the relative concentrations of the different oxidation states. We find that the valency ratio is governed by the size of the A -site cations. In a different series of $\text{Sr}_2\text{FeMnO}_{6-x}$ perovskites we find that locally the structures are quite different from the average cubic structures, with the local coordination environments more closely resembling those of the brownmillerite structure. In all compounds the octahedra containing Mn^{3+} are Jahn-Teller distorted, even if this distortion is not evident in the average structure.

12:27PM Q9.00007 Direct Visualization of Electric-Field-Driven Migration and Decay of Oxygen Vacancy-induced Stripes in $\text{Pr}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ ¹, DONGMIN CHEN, Institute Of Physics, Chinese Academy of Sciences, ZHAOLIANG LIAO, Institute Of Physics, Chinese Academy of Sciences & Department of Physics and Astronomy, Louisiana State University, XUEDONG BAI, PENG GAO, Institute Of Physics, Chinese Academy of Sciences, JIANDI ZHANG, Department of Physics and Astronomy, Louisiana State University — We report on the microscopic evidence of electric-field driven migration and decay of oxygen vacancy stripes in $\text{Pr}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ (PCMO30). A local lattice stripe phase associated with oxygen vacancy migrating along the applied electric field was imaged in real time by using *in-situ* imaging with high-resolution transmission electron microscopy (TEM). Such a field-driven dynamic oxygen migration process should be responsible to the transport for the resistance switching effects observed in many metal-oxide-metal structures, thus providing a direct microscopic evidence for the oxygen migration model. A decay of oxygen vacancy stripes with a characteristic decay time has been observed, consistent with measurement of resistance relaxation in the materials.

¹Supported by the Chinese Academy of Sciences (NO. KJCX2-SW-W26) and the National Natural Science Foundation of China under Grant No. 90406017. ZL and JZ were partially supported by U.S. DOE under Grant No. DOE DE-SC0002136.

12:39PM Q9.00008 Ultrafast pump-probe reflectance study of multiferroic $\text{Eu}_{0.75}\text{Y}_{0.25}\text{MnO}_3$, D. TALBAYEV, Tulane University, J. LEE, S.A. TRUGMAN, R.P. PRASANKUMAR, A.J. TAYLOR, Los Alamos National Laboratory, R.D. AVERITT, Boston University, C.L. ZHANG, S.-W. CHEONG, Rutgers University — Time resolved dynamical studies of multiferroic materials help unravel the fundamental interactions between various degrees of freedom. We report an ultrafast pump-probe reflectance study of multiferroic $\text{Eu}_{0.75}\text{Y}_{0.25}\text{MnO}_3$. The material undergoes antiferromagnetic ordering and, upon further cooling, ferroelectric ordering that strongly couples to the material's magnetic state. We measured the pump-probe reflectance in this compound using 400- and 800-nm pump and probe pulses. We found that the amplitude of the photoinduced reflectance increases dramatically with the development of local and long-range spin-spin correlations as the temperature is lowered toward the magnetic ordering transition. We also observe a dramatic increase in the rise time, up to 10s of picoseconds, of the photoinduced reflectance. This time scale is consistent with the long response times of the spin system in manganites. We suggest that the modification of the local exchange coupling around the photoinduced electrons and holes is responsible for the observed reflectance behavior, as the optical properties of manganites are known to couple strongly to the local and long-range spin correlations [1].

[1] N.N. Kovaleva et al., Phys. Rev. Lett. **93**, 147204 (2004)

12:51PM Q9.00009 Multiple Magnetic Transitions and Magnetocaloric Effect in (La,Pr,M)MnO₃ (M = Ca, Sr, Ba) Mixed Phase Manganites¹, P.J. LAMPEN, N.S. BINGHAM, M.H. PHAN, H.S. SRIKANTH, University of South Florida, T.L. PHAN, S.C. YU, Chungbuk National University, S.W. CHEONG, Rutgers University — The manganite compound (La,Pr,Ca)MnO₃ is a well-studied system that is known to exhibit a complex phase diagram featuring “strain liquid” and “strain glass” regions in combination with competing ferromagnetic (FM) and charge-ordered antiferromagnetic (CO/AFM) phases. The balance of these phases is sensitive to various perturbations including magnetic and electric field, strain, bandwidth, and A-site cation disorder. The A-site disorder and bandwidth of this compound can be tuned through the replacement of Ca with larger Sr and Ba ions. We report here a systematic study of the influence of cation substitution on the magnetic and magnetocaloric properties of La_{0.35}Pr_{0.275}Mn_{0.375}O₃ (M = Ca, Sr, Ba). Structural properties, including lattice parameters and Mn–O–Mn bond angles, were determined from X-ray diffraction patterns. DC magnetometry studies reveal multiple magnetic transitions in each sample which are probed by magnetocaloric effect (MCE) and transverse susceptibility (TS) experiments. Increasing the average A-site cationic radius is found to strongly impact the magnetic properties and phase behavior of the system.

¹Support provided by DOE-BES Grant No. DEFG02-07ER46438 and FCASST

1:03PM Q9.00010 Evolution of antiferromagnetic order during the colossal magnetoresistive transition, M.A. HOSSAIN, MARK H. BURKHARDT, SLAC, Stanford University, E. WESCHKE, E. SCHIERLE, Helmholtz-Zentrum Berlin, Y. TOMIOKA, National Institute of Advanced Industrial Science and Technology (AIST), Japan, Y. TOKURA, University of Tokyo, J. STÖHR, H.A. DÜRR, SLAC, Stanford University — Pr_{0.7}Ca_{0.3}MnO₃ (PCMO) displays one of the largest colossal magneto-resistances (CMR) among manganites. Magneto-transport data suggest that an insulating antiferromagnetic to metallic ferromagnetic transition occurs as the system goes through a CMR transition with the application of a high magnetic field (3–6T). However, the nature of this transition is a mystery. We report the first high magnetic field resonant soft x-ray scattering (RSXS) experiments on PCMO which follow the evolution of the antiferromagnetic superlattice order through the CMR transition. We find that the antiferromagnetic order is first enhanced by several orders of magnitude before melting away into the metallic ferromagnetic phase. Additional high field x-ray magnetic circular dichroism (XMCD) measurements allow us to track the spin and orbital moments and construct a microscopic picture of the competing forces at the heart of CMR.

1:15PM Q9.00011 Low energy magnetic excitations in phase-separated La_{5/8} – yPryCa_{3/8}MnO₃, JAIME FERNANDEZ-BACA, FENG YE, SONGXUE CHI, WEI TIAN, ORNL, S-W CHEONG, Rutgers University — La_{5/8} – yPryCa_{3/8}MnO₃ (LPCMO) ($y = 0.4$) is one of the prototype materials for the study of phase separation. The end members of the series, La_{5/8}Ca_{3/8}MnO₃ and Pr_{5/8}Ca_{3/8}MnO₃, have a robust low temperature FM metallic and charge ordered insulating states, respectively. Various experimental techniques have shown evidence of two-phase coexistence for intermediate Pr contents. However, a clear understanding of some basic macroscopic signature of phase separation is still lacking. The states of the coexistence phases are different when the system goes through different thermodynamic paths with the application of magnetic field. The zero-field-cooled (ZFC) procedure results in a dominant CO-OO state with little FM clusters at low temperature. Such insulating state is robust against external magnetic field. On the other hand, a zero-field cooled, field warming (ZFC-FW) procedure causes a sudden increase in FM intensity near the glassy transition temperature (TG ~ 25K). In this talk we will present the results of recent elastic and inelastic neutron scattering experiments on a single crystal specimen of LPCMO, which reveal the nature of the complex phase coexistence at low temperatures.

1:27PM Q9.00012 Anisotropic field-induced melting of orbital ordering phase in Pr_{0.6}Ca_{0.4}MnO₃¹, RUN-WEI LI, HUALI LI, YIWEI LIU, Ningbo Institute of Material Technology and Engineering, CAS, Ningbo 315201, P. R. China, JIANDI ZHANG, Louisiana State University, WEI KU, Brookhaven National Laboratory, QINGFENG ZHAN, Ningbo Institute of Material Technology and Engineering, CAS, Ningbo 315201, P. R. China, ZHAOHUA CHENG, BAO-GEN SHEN, Beijing National Laboratory for Condensed Matter Physics & Institute of Physics, CAS, Beijing — The orbital degree of freedom in correlated electron systems plays an essential role in creating versatile phenomena via its coupling with charge, spin, and lattice. One extraordinary phase in doped oxide compounds is the charge/orbital-ordered (OO) antiferromagnetic (AF) insulating state, which, interestingly, can be melted to an orbital-liquid metallic state by external magnetic field. By measuring the field-dependent transport behavior of Pr_{0.6}Ca_{0.4}MnO₃ single crystal at different temperatures, we have found a field-orientation dependent melting of the charge-orbital ordered state, regardless whether or not the system is in AF phase. The field-induced melting is found stronger when the applied field is in the ab (basal)-plane. This can be understood as suppression of the CE-type OO state via spin-orbit coupling induced preference of in-plane orbital direction.

¹Supported by Chinese Academy of Science and National Natural Science Foundation of China. J.Z. is supported by US NSF NSF DMR1005562.

1:39PM Q9.00013 Paramagnetic Spin Correlations in Colossal Magnetoresistive La_{0.7}Ca_{0.3}MnO₃, JEFFREY LYNN, JOEL HELTON, NCRN, National Institute of Standards and Technology, MATTHEW STONE, Oak Ridge National Laboratory, DMITRY SHULYATEV, YAKOV MUKOVSKII, Moscow State Steel and Alloys Institute — Inelastic neutron scattering measurements, taken on the ARCS time-of-flight spectrometer, reveal dynamic spin correlations throughout the Brillouin zone in the colossal magnetoresistive system La_{0.7}Ca_{0.3}MnO₃ at 265 K ($\approx 1.03 T_C$). Well defined correlations are observed in constant- E scans. The long-wavelength behavior can be attributed to spin diffusion, qualitatively consistent with dynamical scaling theory, with a correlation length of ≈ 10 Å. Dynamic correlations are observed at energies up to at least 28 meV, suggesting persistent short range spin correlations in the paramagnetic phase. An additional and unexpected component of the scattering is observed at lower energies which takes the form of ridges of strong scattering running along (H 0 0) and equivalent directions.

1:51PM Q9.00014 Existence of a New Phase in the Intermediate J_{AF} -coupling Regime of the Two-Orbital Model for Manganites¹, CENGIZ SEN, SHUHUA LIANG, ELBIO DAGOTTO, University of Tennessee, Knoxville, TN, and Oak Ridge National Lab, Oak Ridge, TN — We report the existence of a new exotic state in the two-orbital model for manganites in the intermediate J_{AF} coupling regime, analyzed using the standard Monte Carlo technique based on the exact diagonalization of the electronic sector. At density $x = 1/4$, this state shows diagonal ferromagnetic (FM) chains with uniform charge order (CO), stacked in between CE-like zig-zag patterns of spin with less populated staggered CO. The new state exists in a narrow range between the well-known FM metallic and C_xE_{1-x} insulating states, and provide a realization in the clean limit of the nanoscale phase separation scenario of CMR manganites. The existence of many other competing exotic states in this range of couplings will also be discussed.

¹This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division. We acknowledge the computational support through Teragrid resources under grant number TG-DMR110033.

Wednesday, February 29, 2012 11:15AM - 2:15PM –
Session Q10 DCMP DCOMP: Invited Session: Rare Fluctuation Effects in Strongly Disordered Systems 210A

11:15AM Q10.00001 Rare Fluctuation Effects in the Anderson Model of Localization¹, RAVINDRA BHATT, Department of Electrical Engineering and Princeton Center for Theoretical Science, Princeton University, Princeton, NJ 08544 — Two significant advances in the theory of disordered systems in the past three decades have been (i) the development of large disorder Renormalization Group methods, and (ii) a more concerted effort to study of the effects of rare fluctuations or configurations, such as Griffiths' phenomena. A major problem facing the latter in many-body systems has been the enormous numerical resources needed to see these rare phenomena. In this talk, we examine the issue of rare configuration effects in Anderson's original model of localization (1958). In this talk, we examine the issue of rare configuration effects in Anderson's original model of localization. We show that effects due to resonant tunneling among neighboring sites leads not only to anomalous behavior of electronic eigenstates far in the Lifshitz tail, where the density of states is exponentially suppressed, but also leads to singularities in average properties (i.e. the inverse participation ratio) as a function of energy, where the density of states is large. The singular behavior, which separates resonant, Lifshitz-like states from typical, Anderson-localized states, occurs *in the insulating phase*, and thus is present in *all* dimensions [1]. Using the analytic solution of a toy model, as well as numerical results of the Anderson model for several different disorder distributions in dimensions $d = 1, 2$ and 3 , we show that this separation of eigenstates due to rare fluctuations is a ubiquitous property of the Anderson model with *bounded* disorder. This suggests that the half-century-old model, being solvable in polynomial time, is a prime candidate for detailed numerical studies of rare fluctuation effects in disordered systems.

[1] Sonika Johri and R. N. Bhatt, arXiv1106.1131; and in preparation.

¹This research was supported by Department of Energy Grant No. DE-SC0002140.

11:51AM Q10.00002 Electronic Griffiths Phases and Quantum Criticality at Disordered Mott Transitions, VLADIMIR DOBROSAVLJEVIC, Director, Condensed Matter Science - Theory, NHMFL Florida State University — The effects of disorder are investigated in strongly correlated electronic systems near the Mott metal-insulator transition. Correlation effects are found¹ to lead to strong disorder screening, a mechanism restricted to low-lying electronic states, very similar to what is observed in underdoped cuprates. These results suggest, however, that this effect is not specific to disordered d-wave superconductors, but is a generic feature of all disordered Mott systems. In addition, the resulting spatial inhomogeneity rapidly increases² as the Mott insulator is approached at fixed disorder strength. This behavior, which can be described as an Electronic Griffiths Phase, displays all the features expected for disorder-dominated Infinite-Randomness Fixed Point scenario of quantum criticality.

¹E. C. Andrade, E. Miranda, and V. Dobrosavljevic, Phys. Rev. Lett., **102**, 206403 (2009).

²E. C. Andrade, E. Miranda, and V. Dobrosavljevic, Phys. Rev. Lett., **104** (23), 236401 (2010).

12:27PM Q10.00003 Bosons in disordered one-dimensional traps: a new paradigm for the superfluid-insulator transition, GIL REFAEL, California Institute of Technology — No abstract available.

1:03PM Q10.00004 Gaps and Pseudogaps across the inhomogeneous superconductor to paired insulator transition¹, MOHIT RANDERIA, Ohio State University — The mechanism for the disorder-tuned superconductor to insulator transition (SIT) in thin films and the nature of the resulting insulator are still debated, despite decades of research. We use quantum Monte Carlo simulations [1] that treat, on an equal footing, inhomogeneous amplitude variations and phase fluctuations, and go beyond our earlier Bogoliubov-deGennes analysis [2]. We gain new microscopic insights into the SIT, compare our theory with experiments [3] and make testable predictions for local spectroscopic probes. The energy gap in the single-particle density of states survives across the transition, but coherence peaks exist only in the superconducting state. A characteristic pseudogap persists above the critical disorder and critical temperature, in contrast to conventional theories. Surprisingly, the insulator has signatures of pairing with a two-particle gap scale that vanishes at the superconductor-insulator transition, despite a robust single-particle gap. The impact of rare regions on the gaps will also be discussed. In collaboration with K. Bouadim, Y.L.Loh and N. Trivedi.

[1] K. Bouadim, Y.L.Loh, M. Randeria and N. Trivedi, Nature Phys. **7**, 884 (2011).

[2] A. Ghosal, M. Randeria, and N. Trivedi, Phys. Rev. B **65**, 014501 (2001).

[3] B. Sacepe et al., Nature Comm. **1**, 140 (2010); Nature Phys. **7**, 239 (2011); M. Mondal et al., Phys. Rev. Lett. **106**, 047001 (2011).

¹Supported by NSF DMR-0907275 (K.B.), DOE BES DE-FG02-07ER46423 (N.T., Y.L.L.), and NSF DMR-1006532 (M.R.).

1:39PM Q10.00005 Infinite-randomness criticality in disordered metals and superconductors¹, THOMAS VOJTA, Missouri University of Science and Technology — Quantum phase transitions in disordered systems often display unconventional behavior which is dominated by rare strongly coupled spatial regions. In this talk, we investigate magnetic and superconducting quantum phase transitions in disordered metallic systems. We develop a strong-disorder renormalization group method that accounts for both quenched disorder and the dissipation of the critical modes due to the Fermi sea. We find that the quantum phase transition in Heisenberg anti-ferromagnets and the pair-breaking superconductor-metal transition are both governed by non-perturbative infinite-randomness critical points. Even stronger disorder effects arise for metallic magnets with Ising spin symmetry in which the quantum phase transition is completely destroyed by smearing. We determine thermodynamic and transport properties at these transitions and in the associated quantum Griffiths phases. We also discuss the current status of experimental observations of these exotic disorder phenomena in a variety of systems including transition metal compounds, heavy-fermion systems, and superconducting nanowires.

¹Supported by the NSF under grant No. DMR-0906566.

Wednesday, February 29, 2012 11:15AM - 1:51PM –
Session Q11 DMP: Focus Session: Graphene Structure, Stacking, Interactions: Infrared and Terahertz Spectroscopy 210B

11:15AM Q11.00001 Collective modes in gapped bilayer graphene¹, CHRISTOPHER TRIOLA, ENRICO ROSSI, Department of Physics, College of William and Mary, Williamsburg, VA 23188, USA — We calculate the polarizability of gapped bilayer graphene using the four-band continuum model. In the presence of a gap the four-band model and the simplified two-band model return bands that are qualitatively different especially at low energies. We find that because of these differences the static polarizability obtained using the four-band model is qualitatively different from the one obtained using the two-band model. We also find that the differences between the two-band model and the four-band model profoundly affect the dynamical dielectric function, and therefore the properties of the plasmon modes. In addition, we study the effect of trigonal warping and find that it qualitatively modifies the density response function.

¹Work supported in part by the Jeffress Memorial Trust, Grant No. J-1033

11:27AM Q11.00002 Sum-Frequency Vibrational Spectroscopic Studies of Polymer/Graphene Interface, HUI-LING HAN, Department of Physics, University of California, Berkeley, CHUANSHAN TIAN, Department of Physics, Fudan University, China, FENG WANG, YUEN-RON SHEN, Department of Physics, University of California, Berkeley — The interest in alignment of polymer on graphene surfaces has been motivated by a desire to gain a fundamental understanding the interaction between molecule and graphene, and for possible application of graphene for surface chemistry. Graphene-polymer interactions also play an important role in graphene-polymer composites, which exhibit greatly improved electrical conductivity, strength, and thermal stability compared with pure polymer material. Theoretical investigation of graphene-polymer interface has been performed previously using molecular dynamics simulations [1]. However, experimental studies of the interfacial characteristics of graphene-polymer composite has been challenging. Here we investigate the molecular orientation at polymer/graphene interface using phase-sensitive-sum-frequency generation spectroscopy. The sum-frequency spectrum shows clear vibration signatures of CH₂ groups. In particular, it suggests that CH₂ groups pointing toward the graphene surface interact with graphene strongly, which leads to a red shift of vibration frequency as large as 15 cm⁻¹. In this talk I will discuss the implications of our experimental findings.

[1] C. Lv, Q. Xue, D. Xia, M. Ma, J. Xie, and H. Chen, *J. Phys. Chem. C*, **2010**, 114 (14), 6588–6594.

11:39AM Q11.00003 Tunable Quantum-Enhanced Second-Order Optical Nonlinearity From Bilayer Graphene, SANFENG WU, Department of Physics, University of Washington, Seattle, 98195, United States, LI MAO, Department of Physics and Astronomy, Washington State University, Pullman, WA, 99164 USA, WANG YAO, Department of Physics and Center of Theoretical and Computational Physics, The University of Hong Kong, Hong Kong, China, CHUANWEI ZHANG, Department of Physics and Astronomy, Washington State University, Pullman, WA, 99164 USA, XIAODONG XU, Department of Physics and Department of Material Science and Engineering, University of Washington, Seattle, 98195, United States — Bilayer graphene exhibits a tunable band gap when the inversion symmetry is broken. It therefore stimulates much interest on its physical characterization and practical application for mid-infrared (MIR) optoelectronics. Here we focus on its second order nonlinear optical response to the MIR laser excitation under device condition, following a quantum description of nonlinear optical conductivity. Our theoretical study shows that, for a certain laser-frequency range determined by the band-gap, giant second harmonic generation can be excited due to the intrinsic electronic spectrum of bilayer graphene. Electrically tunable $\chi^{(2)}$ on the order of $10^5 pm/V$ can be achieved, 3 orders of magnitude larger than the widely-used nonlinear crystal AgGaSe₂.

11:51AM Q11.00004 Infrared magneto-spectroscopy of graphene-based systems, MILAN ORLITA, Laboratoire National des Champs Magnétiques Intenses, CNRS, Grenoble — The results of infrared magneto-spectroscopy of different graphene-based materials will be presented. These systems involve multi- and mono-layers of epitaxial graphene, decoupled graphene flakes on the surface of graphite as well as bulk graphite. The magneto-optical methods serve us mostly as a tool of Landau level spectroscopy. It is used to study the characteristic response due to massless or massive Dirac-type particles and, e.g., to distinguish materials with graphene layers exhibiting rotational or Bernal stacking. Broadening of inter-Landau level transitions has been traced as a function of magnetic field and energy to evaluate the quality of multi-layer epitaxial graphene in terms of scattering time and carrier mobility. From broadening of overlapping Landau levels we find that the scattering rate increases linearly with energy. Complementary to these experiments, inelastic relaxation processes have been studied in pump-and-probe measurements in THz range. The obtained data indicate that the inelastic processes are significantly slower than the elastic ones, and also that the inelastic relaxation is slowed down when the photon energy is tuned to values below the optical phonon frequency. References: M. Orlita et al., PRL, to be published (2011); S. Winnerl et al., PRL, to be published (2011).

12:27PM Q11.00005 Far-infrared Kerr rotation spectroscopy of graphite and multilayer graphene, JULIEN LEVALLOIS, MICHAËL TRAN, ALEXEY KUZMENKO, University of Geneva — Graphite attracts much attention nowadays as a reference 3D material for graphene. Since the early measurements of the cyclotron effect in graphite over fifty years ago [1], a satisfactory quantitative description of this spectacular phenomenon is missing. The analysis of magneto-optical data was hindered either by a limited set of the used photon energies or by the lack of the optical selectivity between electrons and holes. We overcome this issue by measuring the far-infrared magneto-optical Kerr rotation spectra [2] and achieve a highly accurate unified microscopic description of all spectra in a broad range of magnetic fields (0.5 – 7 T) by taking rigorously the c-axis band dispersion and the trigonal warping into account. We find that the second- and the forth-order cyclotron harmonics are optically almost as strong as the fundamental cyclotron resonance even at high fields. The same effects are expected to strongly influence the magneto-optical spectra of Bernal stacked multilayer graphene and therefore play a major role in the respective applications.

[1] J. K. Galt, W.A. Yager and H.W. Dail Jr., *Phys. Rev.* **103**, 1586 (1956)

[2] J. Levallois, M.K. Tran and A. B. Kuzmenko, arXiv:1110.2754v2; submitted.

12:39PM Q11.00006 “Intrinsic” terahertz plasmons and magnetoplasmons in single layer graphene on SiC, IRIS CRASSEE, DPMC, Université de Genève, Suisse, MILAN ORLITA, LNCMI, CNRS-UJF-UPS-INSA, Grenoble, France, Charles University, Praha, Czech Republic, MAREK POTEMSKI, LNCMI, CNRS-UJF-UPS-INSA, Grenoble, France, DIRK VAN DER MAREL, DPMC, Université de Genève, Suisse, MARKUS OSTLER, THOMAS SEYLLER, University of Erlangen-Nurnberg, Erlangen, Germany, ALEXEY KUZMENKO, DPMC, Université de Genève, Suisse — Plasmons in graphene have lately attracted much attention, to great extent, due to promises for novel technologies. Recently, plasmon absorption in graphene was attained in deliberately patterned structures [1]. We measured the magneto-optical absorption and Faraday rotation response of highly doped single layer graphene, epitaxially grown on Si-terminated SiC substrate. The zero-field spectra show a clear plasmon peak at about 2 THz. In magnetic fields, the plasmon peak splits into two branches, thus showing a characteristic magneto-plasmon behavior which was previously observed in periodic dot structures in GaAs two dimensional electron gases [2]. Hence, in large-scale epitaxial graphene on SiC, light can couple to plasmons in the absence of the intentional patterning of graphene. We suggest that optically-active plasmon absorption in this kind of two-dimensional system arises from laterally confined plasmon modes due to “intrinsic” imperfections of graphene on Si-face of SiC, such as, grain boundaries which we clearly identify with AFM methods.

[1] L. Ju et al., *Nature Nanotechnology* **6**, 630 (2011).

[2] A. J. Allen et al., *Phys Rev B* **28**, 4875 (1983).

12:51PM Q11.00007 Enhanced Optical Dichroism of Graphene Nanoribbons¹, VITOR M. PEREIRA, F. HIPOLITO, Graphene Research Centre and Department of Physics, National University of Singapore, A.J. CHAVES, R.M. RIBEIRO, M.I. VASILEVSKIY, N.M.R. PERES, Department of Physics and Centre of Physics, University of Minho, Portugal. — The optical conductivity of graphene nanoribbons is analytical and exactly derived. It is shown that the absence of translational invariance along the transverse direction allows considerable intra-band absorption in a narrow frequency window that varies with the ribbon width, and lies in the THz band for ribbons 10-100nm wide. In this region the anisotropy in the optical conductivity can be as high as two orders of magnitude, which renders the medium dichroic, and allows near 100% polarizability with just a single layer of graphene. The interplay between the geometrically induced anisotropy with the anisotropy induced by plasmon absorption is also considered and discussed.

¹arXiv:1107.1509

1:03PM Q11.00008 Quasiparticle properties in graphene¹, EUYHEON HWANG, CMTc, University of Maryland at College Park — The quasiparticle properties in both single layer and bilayer graphene are presented. We study the electron self-energy as well as the quasiparticle spectral function in graphene, taking into account electron-electron interaction in the leading order dynamically screened Coulomb coupling and electron-impurity interaction associated with quenched disorder. Our calculation of the self-energy provides the basis for calculating all one-electron properties of graphene. We provide analytical and numerical results for quasiparticle renormalization in graphene. Comparison with existing angle-resolved photoemission spectroscopy measurements shows broad qualitative and semiquantitative agreement between theory and experiment, for both the momentum-distribution and energy-distribution curves in the measured spectra. We also present the inelastic quasiparticle scattering rate and the carrier mean free path for energetic hot electrons as a function of carrier energy, density, and temperature, including both electron-electron and electron-phonon interactions. Our results are directly applicable to device structures where ballistic transport is relevant with inelastic scattering dominating over elastic scattering.

S. Das Sarma, S. Adam, E. H. Hwang, and E. Rossi, Rev. Mod. Phys. 83, 407 (2011).

E. H. Hwang, Ben Yu-Kuang Hu, and S. Das Sarma Phys. Rev. B 76, 115434 (2007).

E. H. Hwang and S. Das Sarma Phys. Rev. B 77, 081412 (2008).

Rajdeep Sensarma, E. H. Hwang, and S. Das Sarma, Phys. Rev. B 84, 041408(R) (2011).

¹This work is done in collaboration with R. Sensarma, B. Hu, and S. Das Sarma, and supported by CNAM, US-ONR and NSF-NRI.

1:39PM Q11.00009 Anisotropy of π -plasmon Dispersion Relation of AA-stacked Graphite, C.W. CHIU, Department of Physics, National Cheng Kung University, Tainan 710, Taiwan, F.L. SHYU, Department of Physics, R.O.C. Military Academy, Kaohsiung 830, Taiwan, M.F. LIN, Department of Physics, National Cheng Kung University, Tainan 710, Taiwan, GODFREY GUMBS, OLEKSIY ROSLYAK, Department of Physics and Astronomy, Hunter College at the City University of New York, 695 Park Avenue New York, NY 10065 USA — The dispersion relation of optical π -plasmons of simple hexagonal intrinsic graphite was calculated within the self-consistent-field approximation. The plasmon frequency ω_p is determined as functions of the wave vector $q_{\parallel}$ along the hexagonal plane in the Brillouin zone and its perpendicular component q_z . These plasmons are isotropic within the plane in the long wavelength limit. As the in-plane wave vector is increased, the plasmon frequency strongly depends on its magnitude and direction (ϕ). Our results reveal that interlayer interaction could enhance anisotropy of in-plane π -plasmons. The group velocity for plasmon propagation along the perpendicular direction may be positive or negative depending on the choice of in-plane wave vector.

Wednesday, February 29, 2012 11:15AM - 2:15PM –
Session Q12 DMP: Focus Session: Graphene: Growth, Mechanical Exfoliation, and Properties
- SiC and Growth Kinetics 210C

11:15AM Q12.00001 From above or from below? Determining how graphene layers form on SiC(0001), JAMES HANNON, IBM Research Division — SiC decomposes when heated above 1200 C in vacuum. Silicon desorbs, while the carbon left behind can coalesce to form graphene. Growth of graphene on the SiC(0001) surface (“Si face”) and the SiC(000-1) (“C face”) is very different. On the Si face, graphene growth is epitaxial, while on the C face the growth is generally much less ordered. On the Si face, the observed epitaxy suggests that new graphene layers form under existing one, that is, at the SiC/graphene interface. The lack of epitaxy on the C face suggests that the growth mode on this surface might be different. To test this, we grew ultra-thin epitaxial SiC films (1 nm) on both SiC(0001) and SiC(000-1) via CVD using isotopically pure carbon-13. We then formed graphene via high-temperature thermal decomposition. We used medium energy ion scattering to determine where the carbon-13 was located within the graphene film. For both the Si face and C-face, we find that the carbon-13 is located predominantly in the outmost graphene layer, confirming that graphene grows “from the inside out” on both surfaces [1]. This work was performed in collaboration with Matt Copel and Ruud Tromp.

[1] Phys. Rev. Lett. 107, 166101 (2011)

11:51AM Q12.00002 STM/STS study of ridges on epitaxial graphene/SiC¹, Y.Y. LI, Y. LIU, M. WEINERT, L. LI, Department of Physics, University of Wisconsin, Milwaukee, WI 53211 — The graphitization of hexagonal SiC surfaces provides a viable alternative for the synthesis of wafer-sized graphene for mass device production. During later stages of growth, ridges are often observed on the graphene layers as a result of bending and buckling to relieve the strain between the graphene and SiC substrate. In this work, we show, by atomic resolution STM/STS, that these ridges are in fact bulged regions of the graphene layer, forming one-dimensional (nanowire) and zero-dimensional (quantum dot) nanostructures. We further show that their structures can be manipulated by the pressure exerted by the STM tip during imaging. These results and their impact on the electronic properties of epitaxial graphene on SiC(0001) will be presented at the meeting.

¹Supported by DOE (DE-FG02-05ER46228)

12:03PM Q12.00003 Scalable templated growth of graphene patterns on SiC and their electronic properties, MING RUAN, JAMES PALMER, JOHN HANKINSON, YIKE HU, BAIQIAN ZHANG, ZELEI GUO, RUI DONG, ANTON SIDOROV, ZHIGANG JIANG, School of Physics, Georgia Institute of Technology, CLAIRE BERGER, CNRS- Institut Néel, Grenoble, France & School of Physics, Georgia Institute of Technology, WALT DE HEER, School of Physics, Georgia Institute of Technology — Conventional graphene growth research focuses on SiC on-axis surfaces: SiC (0001) and (000-1). In our previous work, we showed that graphene can be selectively grown on off-axis SiC crystal facets, demonstrated the possibility for templated graphene growth. Here we show scalable production of various devices made with this technique, such as graphene nanoribbons, Hall bars and Aharonov–Bohm rings. Graphene and SiC crystal facets are characterized with SEM and SPM tools. Shubnikov-de Haas oscillations and other phase coherent transport phenomena are observed at low temperature. These observations indicate that the structured epitaxial graphene growth can be a viable method for graphene electronics.

12:15PM Q12.00004 A study of epitaxial graphene/SiC(0001) functionalized by nitrogen doping¹, S. RAJPUT, Y. LIU, Department of Physics, University of Wisconsin, Milwaukee, WI 53211, H. YU, R. F. HICKS, Department of Chemical and Biomolecular Engineering, University of California, Los Angeles, CA 90095, L. LI, Department of Physics, University of Wisconsin, Milwaukee, WI 53211 — In this work, we have carried out nitridation of epitaxial graphene/SiC(0001) using N₂ plasma. The effects of processing conditions on the structure of graphene have been investigated by x-ray photoemission spectroscopy and Raman spectroscopy, and changes in the electronic structures of the nitrogen-doped graphene have been studied using scanning tunneling microscopy. We find that the exposure of epitaxial graphene to nitrogen plasma not only leads to N incorporation, but also creates carbon vacancies, resulting in the formation of N-vacancy complexes.

¹Supported by DOE (DE-FG02-05ER46228)

12:27PM Q12.00005 Creation and sculpting of graphene with ion and electron beams, CHRISTOPHER RUSSO, Harvard University Department of Physics — This talk will cover our recent work on the creation of graphene by ion implantation of carbon into copper substrates followed by a prescribed annealing procedure. We also discuss nanopore nucleation with ion beams and the direct observation of nanopore growth in an aberration corrected TEM. We discuss the cross-sections and knock-on energy transfers required for edge atom removal and demonstrate the controlled growth of monodisperse nanopores in graphene with atomic precision.

1:03PM Q12.00006 Spatially Selective Graphene Formation on Si Substrate¹, NAILI YUE, YONG ZHANG², RAPHAEL TSU, UNC-Charlotte — A uniform large area graphene is useful for applications such as electrode in a touch screen or substrate for growing another material. For applications where graphene is used either as active material (FET for instance) or electrode in a 2-D device array, to form a 2D (electronic) superlattice or photonic crystal, it is critically important to be able to form graphene at selective locations, in desirable size and shape on a substrate, without relying on mechanical cutting. It would be even more significant if the substrate is a Si wafer for coupling with the mature microelectronic technology. We have developed a technique that can achieve these goals. A thin SiC film is first deposited on a Si substrate using MBE. Then, at ambient condition, a focused laser beam is used to convert SiC to graphene at the selected location with the shape and size that can be defined by either a lithographic method or simply by a focused laser beam. The graphene conversion has been verified by structural characterization (TEM, SEM/EDS, etc.) and Raman spectroscopy.

¹Work supported by ARO and CRI.

²yong.zhang@uncc.edu

1:15PM Q12.00007 Surface reconstruction and graphene formation on face-to-face 6H-SiC at 2000 °C, RANDOLPH E. ELMQUIST, MARIANO REAL¹, BRIAN G. BUSH, TIAN SHEN, MARK D. STILES, ERIC A. LASS, National Institute of Standards and Technology — Improved epitaxial graphene films have been widely reported when the sublimation rate of Si is reduced by ambient Ar gas, vapor phase silane, or confined Si vapor. We describe graphene growth on (0001) 6H-SiC samples annealed “face-to-face” [1]; in our modified method the separation is limited only by the flatness of the surfaces. After annealing in 100 kPa Ar gas at 2000 °C for 300 s, atomic force microscopy (AFM) and electrostatic force microscopy (EFM) show graphene coverage is typically between one and a few layers. Samples without prior hydrogen etching undergo surface reconstruction in the graphitization process, resulting in atomically flat terraces with step bunching. Estimates of the sequestered carbon in the form of graphene are compared to calculated levels due to sublimation and diffusion rates where the sublimated gas is dominated by Si atoms below 2100 °C. The 2000 °C samples are contrasted against samples processed between 1700 °C and 1900 °C and transport results on large-scale graphene devices are presented.

[1] X.Z Yu, C.G. Hwang, C.M. Jozwiak, A. Kohl, A.K. Schmid and A. Lanzara, New synthesis method for the growth of epitaxial graphene, Journal of Electron Spectroscopy and Related Phenomena 184 (2011) 100-106.

¹Permanent affiliation: Instituto Nacional de Tecnologia Industrial, Argentina

1:27PM Q12.00008 Imaging grain boundary scattering of graphene in real space, SHUAI-HUA JI¹, JAMES B. HANNON, RUUD M. TROMP, IBM T. J. Watson Research Center, Yorktown Heights, NY, CHOCKALINGAM SUBBIAH, ABHAY PASUPATHY, TONY F. HEINZ, Department of Physics, Columbia University, NY, FRANCES M. ROSS, IBM T. J. Watson Research Center, Yorktown Heights, NY — Graphene grain boundaries are unavoidable defects in most growth methods, in particular chemical vapor deposition and thermal decomposition on the SiC(0001) surface. How electrons are scattered by those grain boundaries has not been experimentally demonstrated at the nanoscale. Here we report atomic-scale images of grain boundary scattering measured by scanning tunneling potentiometry (STP). Monolayer graphene sheets were synthesized on the SiC(0001) surface by thermal decomposition in a background of disilane, using low energy electron microscopy to monitor the graphene thickness during its formation. High resolution scanning tunneling microscopy (STM) reveals graphene grain boundaries and various grain orientations, and STP shows variations in voltage across grains and terraces as current flows across the graphene layer. We have identified two types of grain boundary. One shows a trench structure in STM images; potential mapping shows prominent potential drops. These boundaries between grains appear to be weak links and the dominant scattering locations. The other type of boundary shows a continuous lattice between the grains, with periodic dislocations accommodating the grain misorientation. Potential mapping indicates much weaker scattering despite the grain misorientation. We will discuss transport in polycrystalline graphene based on these measurements.

¹My second affiliation: Department of Physics, Columbia University, NY

1:39PM Q12.00009 Imaging of Electron Beam Induced Current in Epitaxial graphene¹, SHIN MOU, JOHN BOECKL, WEIJIE LU, J.H. PARK, W.C. MITCHEL, Air Force Research Laboratory, STEPHEN TETLAK, Wyle Laboratories — It has been observed that there forms a Schottky junction between graphene and SiC in epitaxial graphene due to the work function difference. As a result, it is viable to apply the electron beam induced current (EBIC) technique on epitaxial graphene due to the fact that it needs a built-in field and ample electron generation volume to generate EBIC. EBIC is an important characterization technique, which identifies electrically active impurities/defects, detects local built-in field, and measures minority carrier diffusion length. In this paper, we use a FEI SEM equipped with a current amplifier to investigate the spatial mapping of EBIC. The incident electron beam generates excited electron-hole pairs in SiC and the minority carriers are collected through the Schottky junction before flowing into graphene. EBIC imaging reveals mesoscopic domains of bright and dark contrast areas due to local EBIC polarity and magnitude, which is believed to be the result of spatial fluctuation in the carrier density in graphene. We also investigate the electron energy dependence, which modulates the EBIC magnitude. With an analytical drift-diffusion current model, we are able to extract the minority carrier diffusion length in the SiC, which is on the order of micro meter.

¹Thanks for the financial support from AFOSR and AFRL.

1:51PM Q12.00010 Writing Graphene Nanoribbons on SiC by Selective Graphitization¹, SEFAAT-TIN TONGAY, MAX LEMAITRE, Department of Material Science and Engineering, University of Florida, JOEL FRIDMANN, Raith USA Inc., Ronkonkoma, New York, ARTHUR F. HEBARD, Department of Physics, University of Florida, BRENT GILA, BILL R. APPLETON, Department of Material Science and Engineering, University of Florida — We describe a new technique for selective graphene growth onto 4H- and 6H-SiC by ion implantation. The presented technique is as easy as patterning (ion implanting) regions where graphene layers are desired followed by annealing to 100 C below the graphitization temperature (T_G) of SiC. We find that ion implantation of SiC lowers the T_G of SiC, allowing selective graphene growth at temperatures below the T_G of pristine SiC and above T_G of implanted SiC. Presented results provide a new technique to pattern device structures ranging from nanometers to microns in size without using conventional lithography and chemical processing.

¹National Science Foundation and Office of Naval Research

2:03PM Q12.00011 Nucleation of uniform mono- and bilayer epitaxial graphene on SiC(000 $\bar{1}$)¹, XIAOSONG WU, RUI ZHANG, Department of Physics, Peking University, YUNLIANG DONG, Department of Physics, Guangxi Normal University, SHUAI GUO, Department of Physics, Peking University, WENJIE KONG, Department of Physics, Guangxi Normal University, ZHIMIN LIAO, DAPENG YU, Department of Physics, Peking University — Early stage of epitaxial graphene growth on SiC(000 $\bar{1}$) has been investigated. Using the confinement controlled sublimation (CCS) method, we have achieved well controlled growth and been able to see the formation of mono- and bilayer graphene islands. The growth features reveal the intriguing growth mechanism. In particular, a new “stepdown” growth mode has been identified. Graphene can propagate tens of micrometers across many SiC steps, while, most importantly, step bunching is avoided and the initial regular stepped SiC surface morphology is preserved. The stepdown growth demonstrates a route towards uniform epitaxial graphene in wafer size without sacrificing the initial substrate surface morphology.

¹This work was supported by NSFC (project 11074007). We also acknowledge the International Science & Technology Cooperation Program of China Sino Swiss Science and Technology Cooperation Program(SSSTC, 2010DFA01810)

Wednesday, February 29, 2012 11:15AM - 2:15PM –
Session Q13 DMP GMAG: Focus Session: Magnetic Nanostructures-Nanoparticle Synthesis and Magnetism 211

11:15AM Q13.00001 Synthesis and properties of magnetic ceramic nanoparticles¹, MONICA SORESCU, Duquesne University — Magnetic ceramic nanoparticles of the type $x\text{In}_2\text{O}_3-(1-x)\alpha\text{-Fe}_2\text{O}_3$, $x\text{V}_2\text{O}_5-(1-x)\alpha\text{-Fe}_2\text{O}_3$ and $x\text{ZnO}-(1-x)\alpha\text{-Fe}_2\text{O}_3$ ($x=0.1-0.7$) were synthesized from the mixed oxides using mechanochemical activation for 0-12 hours. X-ray diffraction was used to derive the phase content, lattice constants and particle size information as function of ball milling time. Mossbauer spectroscopy results correlated with In^{3+} , V^{5+} and Zn^{2+} substitution of Fe^{3+} in the hematite lattice. SEM/EDS measurements revealed that the mechanochemical activation by ball milling produced systems with a wide range of particle size distribution, from nanometer particles to micrometer agglomerates, but with a uniform distribution of the elements. Simultaneous DSC-TGA investigations up to 800 degrees C provided information on the heat flow, weight loss and the enthalpy of transformation in the systems under investigation. This study demonstrates the formation of a nanostructured solid solution for the indium oxide, an iron vanadate (FeVO_4) for the vanadium oxide, and of the zinc ferrite (ZnFe_2O_4) for the zinc oxide. The transformation pathway for each case can be related to the oxidation state of the metallic specie of the oxide used in connection with hematite.

¹National Science Foundation DMR-0854794

11:27AM Q13.00002 Magnetic Interactions in Binary Nanocrystal Superlattices¹, JING CAI, JUN CHEN, ANGANG DONG, XINGCHEN YE, YIJIN KANG, CHRISTOPHER B. MURRAY, JAMES M. KIKKAWA, University of Pennsylvania — The recent development² of highly ordered three-dimensional assemblies of magnetic nanocrystals (NCs) poses new questions for the study of collective magnetic dipolar interactions. Prior literature has focused on changes in blocking temperature in infinite, random assemblies. Here, we study ordered assemblies with two different magnetic NCs and complex superlattice unit cells. Monte Carlo simulations are compared with data to clarify magnetic behaviors in AB_{13} superlattices consisting of two different-sized (14.3 nm and 7.2 nm) Fe_3O_4 NCs, which are superparamagnetic in isolation. This strategy illuminates the individual sublattice properties and their interaction. We show that under certain circumstances, the magnetic response of smaller magnetic NCs may be quenched by the random magnetic field of larger magnetic NCs,³ and that trends in blocking temperature with interaction strength depend strongly on both unit cell geometry and boundary conditions.

¹We are grateful for support from U.S. Army Research Office MURIW911NF-08-1-0364, NSF MRSEC program DMR-0520020, and Department of Energy Office of Basic Energy Sciences DE-SC0002158.

²A. Dong, J. Chen, P. M. Vora, J. M. Kikkawa, and C. B. Murray, Nature 466, 474 (2010).

³J. Chen, A. Dong, J. Cai, X. Ye, Y. Kang, J. M. Kikkawa, and C. B. Murray, Nano. Lett. 10, 5103 (2010).

11:39AM Q13.00003 Fabrication of Iron Oxide Nanoparticle Monolayers by Electrophoretic Deposition¹, ALEX KREJCI, ISABEL GONZALO-JUAN, JAMES DICKERSON, Department of Physics and Astronomy, Vanderbilt University — Magnetic nanoparticle (NP) films are potentially useful in a variety of applications, such as magnetic storage media and ultra-strong permanent magnets. Monolayers of magnetic NPs are specifically interesting as the monolayer geometry maximizes film interactions with dissimilar materials below and above the monolayer. However, many potential commercial and industrial applications of NP films rely on fabrication techniques that are facile, rapid, and site-selective which create homogenous, densely packed, defect-free thin films. Electrophoretic deposition (EPD) is a technique for forming thin films that meets all of these criteria. This work shows, for the first time, EPD's utility in forming monolayers of magnetic NPs. Iron oxide NPs (~14nm) have been synthesized using a solution phase synthesis technique. Repeated centrifugation of the particles prepares the NPs for EPD. The particles are then deposited onto silicon substrates with EPD using dc electric fields. Analysis of the films using scanning electron microscopy and atomic force microscopy shows the particles deposit as NP monolayers. The monolayer density and deposition rate are controlled by varying the suspension concentration and the deposition time. Future research will focus on creating long-range order within the monolayers.

¹This research is partially supported by the United States Office of Naval Research, Award N000140910523, and the National Science Foundation Award DMR-1054161.

11:51AM Q13.00004 Curie temperature reduction in SiO₂-coated ultrafine Fe₃O₄ nanoparticles: Quantitative agreement with a finite-size scaling law, WEI WU, JUN WANG, FAN ZHAO, Ningbo University, GUO-MENG ZHAO, California State University, Los Angeles — We report high-temperature magnetic measurements for SiO₂-coated ultrafine Fe₃O₄ nanoparticles. The Curie temperatures of the ultrafine Fe₃O₄ nanoparticles are significantly reduced and follow a finite-size scaling law predicted from Monte Carlo simulations. Our current result provides the first quantitative confirmation of the finite-size scaling law for quasi-zero-dimensional magnetic systems.

12:03PM Q13.00005 Magnetic properties of Fe nanoparticles: application of the DFT-Inhomogeneous-DMFT approach¹, ALAMGIR KABIR, Department of Physics, University of Central Florida, Orlando, FL 32816, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics and NSTC, University of Central Florida, Orlando, FL 32816 — Dynamical Mean-Field Theory (DMFT) in combination with Density Functional Theory (DFT) has been successfully applied to examine the properties of transition metal elements in which correlation plays an important role. It was recently shown that this approach can also be applied to study correlation effects in nanostructures [1]. Here we present results of a combined DFT-inhomogeneous-DMFT approach used to investigate the size dependent magnetic properties of small iron clusters containing 15 to 19 atoms. For the DMFT impurity solver we use the iterated-perturbation theory approximation. The numerical analysis with the code developed in our group allows one to study systems consisting up to several hundred atoms. The optimized structure of the Fe clusters is obtained from spin polarized DFT calculations. We find our approach to yield better agreement with experimental data [2] than that obtained using DFT and DFT+U, which generally overestimates the magnetization.

[1] V. Turkowski, et al, J. Phys.: Condens. Matt. 22, 462202 (2010).

[2] M. B. Knickelbein, Chem. Phys. Lett. 353, 221(2002).

¹Work supported in part by DOE Grant No. DOE-DE-FG02-07ER46354

12:15PM Q13.00006 Finite-size scaling behavior and intrinsic critical exponents of nickel: Consistent with the three-dimensional Heisenberg model, JUN WANG, WEI WU, FAN ZHAO, Ningbo University, GUO-MENG ZHAO, California State University, Los Angeles — We report high-temperature magnetic measurements of silica-coated nickel nanoparticles. The Curie temperature is found to decrease with decreasing particle size and follow a finite-size scaling relation with the correlation length exponent $\nu = 1.06 \pm 0.07$. The measured exponent is in excellent agreement with the reported values for nickel nanowires and some nickel thin films. By carefully analyzing the reported thickness dependencies of the Curie temperatures for some nickel films, we show that the intrinsic ν value for nickel is 0.73 ± 0.03 while the much larger ν values (about 1.0) found for some other samples might arise from the presence of long-range correlated disorder near the surface. The intrinsic ν value together with the experimental values of other critical exponents consistently shows that the three-dimensional Heisenberg model is sufficient to describe the ferromagnetism of nickel. Our current work thus resolves a long standing controversy in this field.

12:27PM Q13.00007 Self-assembly of Superparamagnetic Nanoparticles with Permanent Magnetization¹, SUVOJIT GHOSH, ISHWAR PURI, Virginia Tech — Magnetic nanoparticles (MNPs) exhibit superparamagnetism when thermal fluctuations overcome the potential barrier for spin reversal set by magnetocrystalline anisotropy. The magnetic moment in such a material oscillates between the easy axes leading to zero net magnetization. Stable colloidal dispersions of MNPs exploit this state to prevent agglomeration. Self-assembly of MNPs presents an excellent bottom up nanofabrication technique due to the wide range of structures that can be formed. A stable dispersion of MNPs is an essential starting point for good control of the process. In this study we explore the theoretical basis for a self-assembled MNP structure with permanent magnetization starting from a dispersion of superparamagnetic MNPs. Magnetostatic coupling of dipole moments enhance the potential barrier for magnetization reversals. We use X-Ray microCT and TEM to visualize the self-assembled structures. We use a stochastic form of the Landau-Lifshitz-Gilbert equation to simulate the magnetization dynamics in each MNP. Permanent magnetization in self-assembled structures generated *in situ* promise several significant applications such as targeted drug delivery, tissue engineering and novel soft composites.

¹The X-Ray microCT scans were supported by NSF Major Research Instrumentation grant (CMMI0923297).

12:39PM Q13.00008 Rate-dependent hysteresis losses in ensembles of magnetic nanoparticle clusters¹, ONDREJ HOVORKA, RICHARD EVANS, The University of York, UK, GARY FRIEDMAN, Drexel University, Philadelphia, USA, ROY CHANTRELL, The University of York, UK, DREXEL UNIVERSITY COLLABORATION — Hysteresis is ubiquitous in magnetic nanoparticle systems and understanding how it emerges from complex interactions and for different time scales is a long-standing issue in magnetism research. Understanding the phenomenon is most important for engineering magnetic nanoparticle structures of well-controlled properties in magnetic recording, hysteresis loss optimization in hyperthermia cancer treatment in biomedicine, or biological and chemical sensing, to name a few examples. In this work we address one of the general questions related to the influence of thermal activation processes on hysteresis loss. Employing large-scale computational modeling based on the master-equation framework we investigate the influence of dipolar interactions on thermal hysteresis loops in ensembles of magnetic nanoparticle chains and clusters. We show that the directional dependence of dipolar interactions results in enhanced or reduced hysteresis loss, depending on the distribution of particles' anisotropy axes and particle chain orientations with respect to the external field. Additional hysteresis loss reduction occurs in case of particle clusters due to possibility of the frustration phenomenon not present for topologically simpler chains.

¹This research was supported by a Marie Curie Intra European Fellowship within the 7th European Community Framework Programme

12:51PM Q13.00009 Size dependence and thermal stability of chiral states in ferromagnetic nanoparticles deposited on a ferromagnetic substrate¹, NAOISE GRISEWOOD, JOHN EVES, HANS-BENJAMIN BRAUN, University College Dublin — Chiral magnetization profiles are observed in many low dimensional systems such as nanoscale particles, thin films, or bulk systems such as multiferroic samples, that are characterized by a lack of inversion symmetry. These spiraling spin structures are often size-dependent and can be attributed to the competition between exchange and anisotropic, or parity breaking Dzyaloshinskii-Moriya (DM) terms. To utilize such spiraling magnetization profiles in novel spintronic devices, it is necessary to understand the mechanisms under which these spiral spin configurations form and how they can be harnessed via an external field. Here we present exact analytic solutions for the magnetization profiles and the associated energies and energy barriers for ferromagnetic nanoparticles deposited on a ferromagnetic substrate. Our method allows us to determine the critical length at which spiral solutions are supported in such samples, which we find to be $l_c = (\pi/2) \sqrt{A/K_e}$ for vanishing applied field and a misfit angle of $\pi/2$ between substrate and nanoparticle anisotropy axis. We also demonstrate that in absence of further pinning effects, the nanoparticles are exclusively in a uniform state for $l < l_c$. We show that our theory is in good agreement with recent experiments.

¹Supported by IRCSET Embark fellowships and grants SFI 08/RFP/PHY1532 and SFI 05/IN1/1853

1:03PM Q13.00010 Magnetic and magnetocaloric properties of NdMnO₃ nanoparticles¹, SAYAN CHANDRA, ANIS BISWAS, M.H. PHAN, H. SRIKANTH, University of South Florida, FUNCTIONAL MATERIALS LABORATORY TEAM — Recently nanosized manganites have attracted considerable attention as the reduction of particle size has exotic effect on their properties. We have studied the magnetic properties and magnetocaloric effect (MCE) of NdMnO₃ nanoparticles with particle size ~20 and 30nm (denoted as S20 and 30 respectively). In temperature dependence of magnetization, M(T), a paramagnetic to ferromagnetic transition is observed at $T_C \sim 70\text{K}$ for S20, which is 5K higher than that for S30 indicating enhancement of ferromagnetic interaction with particle size reduction. In addition to this, an anomaly in M(T) is observed at 20K (T_{CA}) for both S20 and S30, which is attributed to the stabilization of a canted magnetic state (CMS) due to the ordering of Nd^{3+} . The magnetic entropy change [$-\Delta S_M(T)$] is calculated from isothermal magnetization curves using Maxwell relation. There are two maximas in $-\Delta S_M(T)$ at T_C and T_{CA} indicating large MCE over both temperature regions. Interestingly, the relative cooling power is enhanced in case of smaller particle size in which the influence of stabilization of CMS on MCE is less pronounced.

¹DOE-BES Grant No. DEFG02-07ER46438 and FCASST

1:15PM Q13.00011 Effect of the size distributions of magnetic nanoparticles on metastability using phonon-assisted transition rates, YOH YAMAMOTO, KYUNGWHA PARK, Virginia Tech — Experiments show that magnetic nanoparticles have distributions of sizes and shapes, and that the distributions greatly influence static and dynamic properties of the nanoparticles. Therefore, it is critical to understand their properties as a function of the distributions. Previously, we studied an effect of particle size distributions on metastability in magnetization relaxation, using spin $S = 1$ Blume-Capel model with Glauber transition rates. The size distributions were simulated using distributions of magnetic anisotropy parameter D with spins fixed. We found that the lifetime of the metastable state is governed by the smallest particle in a given system. In this talk, we present the effect of size distributions on metastability in magnetization relaxation with phonon-assisted transition rates. These transition rates differ from Glauber dynamics and are derived from weak spin-phonon coupling. In the phonon-assisted transition rates, spin-flips occur via emission or absorption of phonons, and so transitions are forbidden between degenerate states. We investigate magnetization relaxation with distributions of D using kinetic Monte Carlo simulations, when the distributions include values with which such forbidden transitions are expected.

1:27PM Q13.00012 Magnetoelastic coupling in magnetic oxide nanoparticles¹, QI SUN, University of Tennessee, SHEILA BAKER, University of Missouri-Columbia, CHRISTINA BIRKEL, RAM SESHADRI, University of California at Santa Barbara, WOLFGANG TREMEL, Johannes Gutenberg-Universitat, ANDREW CHRISTIANSON, Oak Ridge National Laboratory, JANICE MUSFELDT, University of Tennessee — Phonons are exquisitely sensitive to finite length scale effects in a wide variety of materials. To investigate confinement in combination with strong magnetoelastic interactions, we measured the infrared vibrational properties of MnO and CoFe₂O₄ nanoparticles and their parent compounds. For MnO, a charge and bonding analysis reveals that Born effective charge, local effective charge, total polarizability, and the force constant are overall lower in the nanoparticles compared to the bulk. We find that the spin-lattice coupling drops from $\sim 7 \text{ cm}^{-1}$ in the single crystal to $< 1 \text{ cm}^{-1}$ in the nanoparticles. For CoFe₂O₄, the spectroscopic response is sensitive to the size-induced crossover to the superparamagnetic state, which occurs between 7 and 10 nm, and a spin-phonon coupling analysis supports the core-shell model. Moreover, it provides an estimate of the thickness of the magnetically disordered shell, increasing from 0.4 nm in the 14 nm particles to 0.8 nm in the 5 nm particles, demonstrating that the associated local lattice distortions take place on the length scale of the unit cell. These findings are important for understanding finite length scale effects in magnetic oxides and other more complex functional oxides.

¹This work is supported by the MSD, BES, U.S. DOE and the JDRD and JIAM SEED Programs at UT.

1:39PM Q13.00013 The specific edge effects of 2D core/shell model for spin-crossover nanoparticles¹, AZUSA MURAOKA, Meiji University, KAMEL BOUKHEDDADEN, JORGE LINARÈS, FRANCOIS VARRET, Université de Versailles Saint-Quentin-en-Yvelines — We analyzed the size effect of spin-crossover nanoparticles at the edges of the 2D square lattices core/shell model, where the edge atoms are constrained to the high spin (HS) state. We performed MC simulations using the Ising-like Hamiltonian,

$$H = -J \sum_{\langle i,j \rangle} \sum_{\substack{i' = \pm 1; \\ j' = \pm 1}} S(i,j) S(i+i', j+j') + \left(\frac{\Delta}{2} - \frac{k_B T}{2} \ln g \right) \sum_{\langle i,j \rangle} S(i,j)$$

The molar entropy change is $\Delta S \approx 50 \text{ J/K/mol}$, $\ln g = \Delta S/R \approx 6$ (R is the perfect gas constant), energy gap is $\Delta = 1300 \text{ K}$. The HS fixed edges were based on the observation of an increasing residual HS fraction at low temperature upon particle size reduction. This specific boundary condition acts as a negative pressure which shifts downwards the equilibrium temperature. The interplay between the equilibrium temperature ($= \Delta/k_B \ln g$) variation and the expected variation of the effective interactions in the system leads to a non-monotonous dependence of the hysteresis loop width upon the particle size. We described how the occurrence condition of the first-order transition has to be adapted to the nanoscale.

¹The present work has been supported by the Univ. Versailles, CNRS, GDRI France-Japan, and PRES-UniverSUD (COPECS project).

1:51PM Q13.00014 Magnetic Properties of Single Co Nanoparticles Probed by Tunneling and Microwaves, WENCHAO JIANG, FELIPE TIJIWA BIRK, DRAGOMIR DAVIDOVIC, Georgia Institute of Technology — We present tunneling studies of magnetic hysteresis loops of single Co nanoparticles. The magnetic switching field at mK-temperature is strongly reduced as a function of bias voltage. At 10mV bias voltage, the switching field is reduced by 15%, while the magnetization can be switched by applying a voltage pulse of 10mV. The strong reduction of the switching field is not an artifact due to charge noise or Joule heating, nor it is a result of the electric field dependence of the surface anisotropy. Instead, the reduction represents the case of magnetic excitation driven by the tunnel current. The strength of the effect indicates strongly enhanced coupling between magnetic excitations and the tunnel current in ferromagnets with strongly reduced dimensions. We also present the first measurement of the magnetic relaxation time in a single Co nanoparticle ($\sim$ microsecond), obtained by combining tunneling spectroscopy and microwave pumping.

2:03PM Q13.00015 Exchange Bias Studies in Core/Shell Structures Nanoparticles, HAFSA KHURSHID, SAYAN CHANDRA, University of South Florida, WANFENG LI, University of Delaware, MAN-HUONG PHAN, University of South Florida, GEORGE HADJIPANAYIS, HARIHARAN SRIKANTH, University of Delaware, UNIVERSITY OF DELAWARE COLLABORATION, UNIVERSITY OF SOUTH FLORIDA COLLABORATION — This study is focused on a comparison of magnetic properties of chemically synthesized core/shell structured iron/iron-oxide nanoparticles with different core sizes and comparable shell thickness. Particles were synthesized by high temperature decomposition of iron organometallic compounds. Thermomagnetic data revealed that particles are superparamagnetic at room temperature. The field cooled hysteresis loops showed interesting features of enhanced coercivity and horizontal and vertical shifts along directions of the cooling field, all strongly depend on temperature, indicative of an exchange-bias-like phenomenon. These effects were more pronounced in smaller core size nanoparticles with an exchange bias field of 4098 Oe. The spin-glass-like phase with high-field irreversibility in the iron oxide shells played the role of the fixed phase in the core/shell system and provided the pinning force to the reversible spins. The magnetic domains and higher contributions from the surface anisotropy in the hollow nanoparticles caused enormous magnetic frustration that is the origin of high field irreversibility and vertical shift of hysteresis loop in these particles.

Wednesday, February 29, 2012 11:15AM - 2:15PM –

Session Q14 GMAG DMP FIAP: Focus Session: Spins in Semiconductors - Spin Dependent Transport 212

11:15AM Q14.00001 Determination of Rashba and Dresselhaus coefficient in InGaAs quantum wells¹, SÉBASTIEN FANIEL, Université catholique de Louvain, TORU MATSUURA, Hokkaido University, SHUNSUKE MINESHIGE, GSIST, Hokkaido University, YOSHIKI SEKINE, NTT BRL, NTT Corp, TAKAAKI KOGA, GSIST, Hokkaido University — We report the determination of the intrinsic spin-orbit interaction (SOI) parameters for $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{In}_{0.52}\text{Al}_{0.48}\text{As}$ quantum wells (QWs) from the analysis of the weak antilocalization effect measured at dilution temperature [1]. We found that the Dresselhaus SOI is mostly negligible relative to the Rashba SOI in this system. The intrinsic parameter for the Rashba effect, $a_{\text{SO}} \equiv \alpha/\langle E_z \rangle$, is determined to be $a_{\text{SO}} m^*/m_e = (1.46 - 1.51 \times 10^{-17} N_S [\text{m}^{-2}]) e\text{\AA}^2$, where α is the Rashba SOI coefficient, $\langle E_z \rangle$ is the expected electric field within the QW, m^*/m_e is the electron effective mass ratio, and N_S is the sheet carrier density. The N_S dependence of a_{SO} corresponds to the non-parabolic correction in the effective mass or electron g-factor. These values for $a_{\text{SO}} m^*$, which are in good agreement with the theoretical prediction by Kane's $\mathbf{k} \cdot \mathbf{p}$ theory, were also confirmed by the observation of beatings in the Shubnikov-de Haas oscillations in our most asymmetric QW sample.

[1] S. Faniel *et. al.*, PHYSICAL REVIEW B **83**, 115309 (2011).

¹This work was supported by KAKENHI, Grant-in-Aid for Young Scientists (A), No. 19684009 and Grant-in-Aid for Scientific Research (B), No. 23360001.

11:27AM Q14.00002 Spin-dependent scattering in the presence of polarized nuclei in n-GaAs¹, KEVIN CHRISTIE, CHAD GEPPERT, MUN CHAN, University of Minnesota, QI HU, CHRIS PALMSTRØM, University of California, Santa Barbara, PAUL CROWELL, University of Minnesota — We report on all-electrical measurements of the inverse spin Hall effect (ISHE) in epitaxial (100) Fe/GaAs heterostructures with a channel doping (Si) of $n = 5 \times 10^{16} \text{ cm}^{-3}$ and highly doped Schottky tunnel barriers. Under measurement conditions of large (10-20%) spin accumulation at the injection electrode, a significant dynamic nuclear polarization (DNP) enhances the size of the ISHE. The electron spin dynamics are shown to match the predictions of the usual drift-diffusion model, including the applied, hyperfine, and Knight fields. The DNP, however, also enhances the scattering of spin-polarized carriers, which is not understood. To separate the roles of the electronic and nuclear spin systems, we have employed a pump-probe method to vary the nuclear spin polarization $\langle I \rangle$ and electron spin polarization S independently. The size of the ISHE is proportional to $\langle I \rangle$ when the DNP is small, but it eventually saturates. When the nuclear polarization is fixed, the ISHE is linear in S , as expected. We conclude therefore that the measured signal scales linearly with the spin current multiplied by a transport skewness parameter that depends strongly on $\langle I \rangle$.

¹Supported by the ONR MURI program and the NSF.

11:39AM Q14.00003 Nuclear enhancement of the spin Hall angle in $n\text{-In}_x\text{Ga}_{1-x}\text{As}$ ¹, CHAD GEPPERT, KEVIN CHRISTIE, MUN CHAN, University of Minnesota, QI HU, CHRIS PALMSTRØM, University of California at Santa Barbara, PAUL CROWELL, University of Minnesota — We present measurements of the inverse spin Hall effect in vertical $\text{Fe}/\text{In}_x\text{Ga}_{1-x}\text{As}$ heterostructures as identified via a Hanle effect in the local Hall voltage. The spin Hall angle is greatly enhanced in the presence of polarized nuclei, achieving typical values of $\gamma \simeq 5 \times 10^{-2}$. Phenomenological modeling of the observed line-shapes shows that the nuclear polarization acts as a linear prefactor to the standard spin Hall conductivity. This enhancement far exceeds expectations based on the energy splitting of the electron or nuclear spin systems. Our samples are doped just above the Mott transition ($n \simeq 3n_c$) where metallic impurity band conduction is dominant. A strong coupling between localized moments and delocalized states is evidenced by the temperature dependence and sensitivity to disorder at higher In concentrations. This leads us to interpret our results using an Anderson-like model of polarized impurities whereby both dynamic nuclear polarization and resonant skew scattering arise as a result of a spin polarized doubly occupied (D^-) impurity band.

¹Supported by the ONR MURI program and the NSF.

11:51AM Q14.00004 Spin Hall effect for detection of spin-currents – Realization of a Spin transistor, JOERG WUNDERLICH, Hitachi Cambridge Laboratory, Cambridge CB3 0HE, UK; Institute of Physics ASCR, v.v.i., Cukrovarnická 10, 162 53 Praha 6, Czech Republic — The realization of a viable semiconductor transistor and information processing devices based on the electron spin has fueled intense basic research of three key elements: injection, detection, and manipulation of spins in the semiconductor microchannel. The inverse spin Hall effect (iSHE) detection of spins manipulated by a gate electrode [1] has recently led to the experimental demonstration of a spin transistor device. [2] Here, the spin injection into a 2-dimensional electron gas (2DEG) was done optically in the depletion layer of a reverse biased pn-junction. [3] The iSHE detection is also used for electrical spin injection from a Fe electrode into a lateral GaAs channel combined with a simultaneous non-local spin valve measurement [4-10]. The spins in the channel are manipulated via the Hanle spin precession induced by an applied magnetic field and via a drift of electrons induced by an applied electric field. The output spin signal is suppressed or enhanced depending on the applied electrical bias rendering the device to a spin transistor different from the Datta Das concept. [11]

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12:27PM Q14.00005 Measurement by antilocalization of interactions between InAs surface electrons and magnetic surface species¹, YAO ZHANG, R.L. KALLAHER, V. SOGHOMONIAN, J.J. HEREMANS, Virginia Tech — Weak-antilocalization (WAL) low-temperature magnetotransport measurements are sensitive to electron quantum coherence, and can be used as a sensitive probe of surface quantum states. We experimentally study interactions between surface electrons and local magnetic moments on InAs by comparing WAL on patterned InAs accumulation layers where rare earth ions or Co^{2+} , Co-phthalocyanine, Fe^{3+} , and Fe-phthalocyanine were deposited, with those where no magnetic species were deposited. The magnetic species modify the magnetic spin-flip scattering, which carries information about magnetic interactions, and modify the spin-orbit (SO) scattering, identified via the WAL signal and characterized over temperature. Experiments indicate a mostly temperature-independent magnetic spin-flip scattering, except for Ho^{3+} . The SO scattering also displays a weak temperature dependence, and is increased by the heavy ions, Co^{2+} and Co-phthalocyanine, while suppressed by ferromagnetic Fe^{3+} and Fe-phthalocyanine, in agreement with the expected absence of the WAL in ferromagnets.

¹partial support from DOE DE-FG02-08ER46532

12:39PM Q14.00006 A Quantitative Analysis of the Electrical Detection of Spins Via the Spin Hall Effect and the Non-Local Spin Valve Effect Within a Semiconductor Microchannel, VIVEK AMIN, JAIRO SINOVA, Department of Physics, Texas A&M University, JOERG WUNDERLICH, Hitachi Cambridge Laboratory, ANDY IRVINE, Microelectronics Research Centre, Cavendish Laboratory, RICHARD CAMPION, School of Physics and Astronomy, University of Nottingham, KAMIL OLEJNIK, TOMAS JUNGWIRTH, Institute Of Physics ASCR — Recently, the manipulation of spins via a gate electrode, and their subsequent detection through the Spin Hall Effect, has led to the experimental realization of a spin-based semiconductor transistor. While in this experiment, spin injection was achieved optically via circularly-polarized light, we consider a similar experiment using electrical injection by means of a ferromagnetic contact into a GaAs microchannel instead. The spin current in a lateral semiconductor channel is then detected through the Spin Hall Effect, while the spin accumulation nearby is simultaneously measured through the Non-Local Spin Valve Effect (using another Fe electrode). The spins within the channel are manipulated through the Hanle Effect via an external magnetic field, and through a drift induced by an applied electrical bias. To analyze these results, we use analytical and numerical solutions to the steady-state drift-diffusion equations with a constant magnetic field and a drift velocity modeled by a Heaviside Theta function. Combining these results with the anomalous Hall response function, which takes into account the geometry of the Hall probe in order to obtain the correct Hall angle, we obtain results that are in quantitative agreement with experiments.

12:51PM Q14.00007 Spin-gating of a conventional aluminum single electron transistor, LIVIU P. ZÂRBO, Institute of Physics ASCR, v.v.i., CZ, CHIARA CICCARELLI, ANDY IRVINE, Microelectronics Group, Cavendish Laboratory, University of Cambridge, UK, JÖRG WUNDERLICH, Hitachi Cambridge Laboratory, Cambridge, UK, RICHARD CHAMPION, BRIAN GALLAGHER, School of Physics and Astronomy, University of Nottingham, UK, TOMÁŠ JUNGWIRTH, Institute of Physics ASCR, v.v.i., CZ, ANDREW FERGUSON, Microelectronics Group, Cavendish Laboratory, University of Cambridge, UK — We report the realization of a single electron transistor in which electron transport from an aluminum source electrode to an aluminum drain electrode via an aluminum island is controlled by spins in a capacitively coupled magnetic gate electrode. The origin of the effect is in the change of the chemical potential on the gate, formed by the ferromagnetic semiconductor GaMnAs, with changing the direction of the magnetization. In agreement with experimental observations, microscopically calculated anisotropies of the chemical potential with respect to the magnetization orientation are of the order of $10\mu\text{V}$ which is comparable to the electrical gate voltages required to control the on and off state of the single electron transistor. Our phenomenon belongs to the family of anisotropic magnetoresistance effects which can be observed in ohmic, tunneling or other device geometries. In our case, the entire phenomenon is coded in the dependence of the chemical potential on the spin orientation which allowed us to remove the spin functionality from all current contacts and channels and place it in the capacitively coupled gate electrode. Our spintronic device therefore operates without spin current.

1:03PM Q14.00008 Spin injection from into InSb from CoFe, YONG-JAE KIM, MARTIN RUDOLPH, R.L. KALLAHER, J.J. HEREMANS, Virginia Tech — The strong spin-orbit interaction in InSb is an asset for spin manipulation using electric fields. In order to electrically characterize spin injection and detection in InSb, we experimentally investigate spin injection into InSb from ferromagnetic CoFe electrodes, via non-local spin valve measurements at low temperature. We observe non-local transresistance switching around zero in-plane external magnetic field. We characterize the magnetic properties of the CoFe layer by the Hall signal of the fringing fields and confirm 3-state switching. We verify that the non-local signal is not related to the physical or geometrical magnetoresistance due to the CoFe fringing fields. The non-local spin valve signal is, as typical, dependent on the specific CoFe/InSb interfaces, while the temperature dependence points to a contribution beyond the spin coherence length. We further observe a modification of weak-antilocalization by spin injected carriers and the same phenomenon may contribute to the spin valve transresistance (partial support from DOE DE-FG02-08ER46532).

1:15PM Q14.00009 Top- and Side-Gated InAs Spinfilter Cascades in Magnetic Fields, JAN JACOB, HAUKE LEHMANN, TILL BENTER, ALEXANDER BUHR, JENS KIENITZ, ULRICH MERKT, Universitaet Hamburg, Institut fuer Angewandte Physik — We present results from transport experiments on two-stage Y-shaped spin-filter cascades fabricated from InAs heterostructures. The first Y junction acts as a generator of two oppositely spin-polarized currents by employing the intrinsic spin-Hall effect. When the second filter that is attached to one of the first filter's outputs in a distance corresponding to a multiple of the spin-precession length, the spin polarization is revealed as a conductance imbalance at the outputs. To achieve the required quasi one-dimensional transport modes we reduce either the effective width of the cascade's five wires by side-gate quantum-point contacts or we reduce the carrier concentration by means of a top gate. The latter yields the advantage to keep the width along the cascade's wires constant and thus, by ensuring higher homogeneity of the potential, reduces spurious effects in the measured conductances. The application of a magnetic field perpendicular to the cascade's plane results in a Lorentz force acting on the electrons in the cascade and thereby changing the measured conductance imbalance and the spin polarization. This can be used to quantify the strength of the spin-Hall effect in InAs heterostructures.

1:27PM Q14.00010 Tunable Zeeman-like Spin Splitting with Liquid Gated Field Effect Transistors, HONGTAO YUAN, Department of Applied Physics, University of Tokyo, M.S. BAHRAMY, Correlated Electron Research Group, RIKEN, K. MORIMOTO, H. SHIMOTANI, R. ARITA, University of Tokyo, CH. KLOC, Nanyang Technological University, N. NAGAOSA, Y. IWASA, University of Tokyo — Generation of spin polarized electrons is the most critical step for developing spintronics applications. As an electric and nonmagnetic way to realize spin polarization in energy bands, spin-orbit interaction (SOI) has been widely used for spin manipulation in two-dimensional systems. For example, Rashba-type energy splitting with in-plane-polarized spins near Γ point of Brillouin zone (BZ) is able to be modulated by electric field through tuning spatial inversion asymmetry. However, Zeeman-type energy splitting with out-of-plane spin polarization is known to be sensitive only to magnetic field and supposed never to be affected by external electric field. In this paper, we theoretically uncover and experimental confirm a perpendicular-electric-field induced giant Zeeman spin splitting at low symmetric K and K' points in a layered chalcogenide, 2H-WS_2 . *Ab initio* band calculation and spin texture indicate that an electric field can make low-energy carriers spin-polarized in a out-of-plane Zeeman-type way and a tunable SOI is able to selectively control the size of splitting. A gate-induced crossover from weak localization to weak antilocalization in the magnetotransport serves as an experimental proof for the tunable SOI and spin polarization. The splitting energy deduced from quantum correction of magnetoconductance is as large as 120 meV and satisfied well with the band calculation for Zeeman-type splitting. This finding directly provides us with a new path-way for electrically initializing and manipulating electron spins for spintronics applications.

1:39PM Q14.00011 Anomalous Hall effect in the Presence of Strong Spin-orbit Coupling and Non-trivial Magnetization, JIANPING LIU, HUAWEI GAO, JACOB GAYLES, ARTEM ABANOV, JAIRO SINOVA, Texas A&M University — AHE in ferromagnets with strong spin-orbit coupling (SOC) and homogeneous magnetization has been studied extensively, using both Kubo formalism and semi-classical Boltzmann equation. In the opposite limit of weak SOC in the presence of non-trivial magnetization texture and strong exchange coupling with the carriers (adiabatic limit), the electron spins always align themselves with the direction of the local magnetization and they experience an effective magnetic field arising from this non-trivial magnetization, giving rise to the topological anomalous Hall effect. We study here the transition between the two limits and the joint effect that a strong SOC and non-trivial magnetic textures have on the AHE. We will report on results from both perturbative analytical approaches and bulk numerical simulations. Some of these effects may be present and exploited in current induced manipulation and detection of domain walls.

1:51PM Q14.00012 Spin diffusion and precession at the multiferroic interface and InAs quantum wells, PENG ZHANG, MING-WEI WU, Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, University of Science and Technology of China — We study spin diffusion and precession in a two-dimensional electron gas at the multiferroic interface and InAs quantum wells respectively by means of the kinetic spin Bloch equation approach [Wu *et al.*, Physics reports **493**, 61 (2010)]. At the $\text{AlO}_3/\text{SrTiO}_3/\text{TbMnO}_3$ heterostructure with a temperature being as low as 15 K, the two-dimensional electron gas at the $\text{LaAlO}_3/\text{SrTiO}_3$ interface interacts with the spiral magnetic moments of Mn^{3+} in TbMnO_3 via the Heisenberg exchange interaction. It is demonstrated that the spin diffusion length at the interface is always finite, despite the polarization direction of the injected spins. It is also revealed that the Coulomb scattering plays an important role and effectively suppresses the spin diffusion. The spin precession in InAs quantum wells is investigated with the Rashba spin-orbit coupling being modulated by a gate voltage. The gate-voltage dependence of spin diffusion under different temperatures is studied with all the scattering explicitly included. Our result partially supports the claim of the realization of the Datta-Das spin-injected field effect-transistor by Koo *et al.* [Science **325**, 1515 (2009)]. We also show that the scattering plays an important role in spin diffusion in such a system.

2:03PM Q14.00013 Enhanced photon-assisted spin transport in a quantum dot attached to ferromagnetic leads¹, FABRICIO M. SOUZA, Instituto de Fisica, Universidade Federal de Uberlandia, THIAGO L. CARRARA, Universidade Federal do Triangulo Mineiro, EDSON VERNEK, Instituto de Fisica, Universidade Federal de Uberlandia — Time-dependent transport in quantum dot system (QDs) has received significant attention due to a variety of new quantum physical phenomena emerging in transient time scale.[1] In the present work [2] we investigate real-time dynamics of spin-polarized current in a quantum dot coupled to ferromagnetic leads in both parallel and antiparallel alignments. While an external bias voltage is taken constant in time, a gate terminal, capacitively coupled to the quantum dot, introduces a periodic modulation of the dot level. Using non equilibrium Green's function technique we find that spin polarized electrons can tunnel through the system via additional photon-assisted transmission channels. Owing to a Zeeman splitting of the dot level, it is possible to select a particular spin component to be photon-transferred from the left to the right terminal, with spin dependent current peaks arising at different gate frequencies. The ferromagnetic electrodes enhance or suppress the spin transport depending upon the leads magnetization alignment. The tunnel magnetoresistance also attains negative values due to a photon-assisted inversion of the spin-valve effect. [1] F. M. Souza, Phys. Rev. B **76**, 205315 (2007). [2] F. M. Souza, T. L. Carrara, and E. Vernek, Phys. Rev. B **84**, 115322 (2011).

¹Financial Support: FAPEMIG, CNPq and CAPES.

Wednesday, February 29, 2012 11:15AM - 2:15PM – Session Q16 DCMP: Heavy Fermions - 1-1-5 Systems 251

11:15AM Q16.00001 Strong magnetic fluctuations in superconducting state of CeCoIn_5 ¹, T. HU, H. XIAO², M. DZERO, C.C. ALMASAN, Kent State University, Kent, OH, T.A. SAYLES, M.B. MAPLE, University of California at San Diego, CA — We probe the magnetism inside the superconducting state of CeCoIn_5 by locally suppressing superconductivity and investigating the underlying normal state through current-voltage measurements under applied pressure and external magnetic field in the mixed state. We observe that the vortex core resistivity increases sharply with decreasing temperature (T) for $T < T_c$ and magnetic field. We attribute this result to the presence of critical spin fluctuations near the Neel temperature inside the vortex core. This behavior is greatly suppressed with increasing pressure, due to the suppressed antiferromagnetic order inside the vortex core. Using our experimental results we construct a three-dimensional phase diagram which provides a direct evidence for a quantum critical line inside the superconducting phase. An experimentally obtained explicit equation for the antiferromagnetic boundary inside the superconducting dome shows the close relationship between quantum criticality, antiferromagnetism, and superconductivity.

¹This research was supported by the NSF DMR-1006606 and DMR-0844115, ICAM Branches from Institute for Complex Adaptive Matter, and Ohio Board of Regents Grant OBR-RIP-220573 at KSU and the DOE DE-FG02-04ER46105 at UCSD.

²Permanent address: Institute of Physics, Chinese Academy of Science, Beijing, China

11:27AM Q16.00002 Visualizing the Emergence of Heavy Fermions in a Kondo Lattice (Part I)¹, EDUARDO H. DA SILVA NETO, PEGOR AYNAJIAN, Princeton University, RYAN BAUMBACH, J.D. THOMPSON, Los Alamos National Laboratory, ZACHARY FISK, University of California, Irvine, ERIC BAUER, Los Alamos National Laboratory, ALI YAZDANI, Princeton University — The interaction between magnetic moments and conduction electrons is at the heart of many phenomena in condensed matter physics, from the Kondo effect in magnetic alloys and nanostructures to superconductivity in strongly correlated systems. We use the scanning tunneling microscope (STM) to detect the emergence of these heavy excitations with lowering of temperature in a prototypical 115 family of Ce-based heavy fermion compounds. Experiments on different atomically terminated layers and their modeling are used to demonstrate the sensitivity of the tunneling process to the composite nature of these heavy quasiparticles, which arise from quantum entanglement of itinerant conduction and f -electrons. The momentum space electronic structure of those heavy excitations will be discussed in the next talk by Pegor Aynajian.

¹This work is funded by a DOE-BES grant. Infrastructure at the Princeton Nanoscale Microscopy Laboratory are also supported by grants from NSF-DMR, Keck Foundation, and NSF-MRSEC.

11:39AM Q16.00003 Visualizing the Emergence of Heavy Fermions in a Kondo Lattice (Part II) , PEGOR AYNAJIAN, EDUARDO DA SILVA NETO, Princeton University, RYAN BAUMBACH, JOE THOMPSON, Los Alamos National Laboratory, ZACHARY FISK, University of California Irvine, ERIC BAUER, Los Alamos National Laboratory, ALI YAZDANI, Princeton University — The development of low energy fermionic excitations with heavy mass in compounds with f -orbitals is one of the key concepts in the physics of correlated electronic states and fundamental to the mechanism of unconventional superconductivity in such systems. We use spectroscopic mapping with the scanning tunneling microscope (STM) to detect the emergence of these heavy excitations in the Ce-115 heavy fermion compounds. Scattering and interference of the heavy quasiparticles is used to resolve their energy-momentum structure and to extract their mass enhancement, which develops near the Fermi energy with decreasing temperature. This work is funded by a DOE-BES grant. Infrastructure at the Princeton Nanoscale Microscopy Laboratory are also supported by grants from NSF-DMR, Keck Foundation, and NSF-MRSEC. PA also acknowledges support of a fellowship through the PCCM funded by NSF MERSEC.

11:51AM Q16.00004 Scanning tunneling microscopy studies of heavy fermion compound CeCo(In_{1-x}Cd_x)₅ , ANDRAS GYENIS, PEGOR AYNAJIAN, EDUARDO H. DA SILVA NETO, Princeton University, ZACHARY FISK, University of California, Irvine, ERIC D. BAUER, Los Alamos National Laboratory, ALI YAZDANI, Princeton University — Heavy fermion materials, such as those forming in actinide- or lanthanide-based compounds, have a rich variety of phases from unconventional superconductivity to antiferromagnetism to possibly exotic and non-Fermi liquid states. Central to all these ground states is the interaction between the magnetic impurities and the conduction electrons. In the Ce-based heavy fermions compounds (e.g. CeColn₅), the ground state can be tuned by doping or isovalent substitution, for example, Cd doping tunes the system toward antiferromagnetism. We present scanning tunneling microscopy/spectroscopy measurements on the Cd-doped CeColn₅ heavy fermion compounds as a function of temperature. These results will be analyzed within the context of how tuning the chemical structure impacts the formation of heavy electron band and various ground states of this material system.

12:03PM Q16.00005 Magnetic penetration depth and skin depth study of superconductivity and quantum criticality in Ce_{1-x}R_xCoIn₅ (R=La and Nd) , HYUNSOO KIM, M. A. TANATAR, K. CHO, J. MURPHY, R. PROZOROV, The Ames Laboratory, Ames, IA, R. HU, C. PETROVIC, Brookhaven National Laboratory, Upton, NY — A heavy fermion superconductor CeColn₅ shows different responses to Nd- or La- substitutions for Ce, with the former inducing static magnetic order coexisting with superconductivity for some concentrations. To understand the origin of the differences, we studied the temperature and field dependent in-plane magnetic penetration depth, $\lambda(T)$, in single crystals of (Ce,R)Coln₅ (R=La, Nd). Measurements were performed with a tunnel diode resonator down to 50 mK in a dilution refrigerator, in magnetic field up to 14 T parallel to the c -axis. These low-temperature and high field measurements allowed for the exploration for the full domain of superconductivity and quantum criticality in the $T-H$ phase diagram. Some previously unreported features were observed and will be discussed from the point of view of measured differential magnetic susceptibility. Combined with the contact-less measurements of resistivity via normal-state skin depth, these measurements bring new insight into the interplay between superconductivity and magnetism as well as field-tuned quantum critical behavior of doped 115 systems.

12:15PM Q16.00006 Quantum oscillations study of the Fermi-surface evolution in Yb-substituted CeCoIn₅ , BOBBY PRÉVOST, Département de physique, Université de Montréal, Montréal, QC, Canada, ANDREY POLYAKOV, OLEG IGNATCHIK, Hochschule-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany, SIMON BLACKBURN, ANDREA D. BIANCHI, MICHEL CÔTÉ, GABRIEL SEYFARTH, Département de physique, Université de Montréal, Montréal, QC, Canada, DANIEL HURT, ZACHARY FISK, Department of Physics & Astronomy, University of California Irvine, Irvine, CA, USA, ROY G. GOODRICH, Department of Physics, George Washington University, Washington, DC, USA, JOCHEN WOSNITZA, Hochschule-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — We report results of systematic de Haas-van Alphen (dHvA) studies on Ce_{1-x}Yb_xColn₅ single crystals with varying Yb concentrations x . For a low dilution of $x = 0.1$, the well-documented Fermi surface and the heavy effective masses of CeColn₅ ($x = 0$) remain nearly unchanged. A clear change of the Fermi-surface topology becomes evident for high Yb concentrations of $x = 0.55$, and above. The effective masses are reduced considerably to values between 0.7 and 2.6 free electron masses. Nevertheless, the superconducting transition temperature T_c and upper critical field H_{c2} are only weakly suppressed with x . The angular-resolved dHvA frequencies for YbColn₅ show a good agreement with our density functional theory band-structure calculation with localized 4f electrons and an Yb valence of 2+, which has been used to constructed the Fermi surface.

12:27PM Q16.00007 Field induced QCP in Yb-doped CeCoIn₅¹ , Y.P. SINGH, T. HU, H. XIAO², M. DZERO, C.C. ALMASAN, Kent State University, L. SHU, M.B. MAPLE, University of California San Diego — We performed magnetoresistance and Hall effect measurements on Yb-doped CeColn₅. The longitudinal resistivity data measured in 14 T show that the onset of coherence in the dilute Kondo lattice remains robust with respect to Yb concentration. In addition, we find that the superconducting transition temperature is weakly suppressed with doping ($x \leq 0.2$). Our analysis of the magnetoresistance data allowed us to identify the magnetic field induced quantum critical point and its evolution upon doping. At high Yb concentrations, our Hall effect data point to a possible valence transition of Yb ions. At small doping, our results provide an insight into the nature of the interplay between quantum criticality, magnetism, and unconventional superconductivity, while the behavior of this system at high doping can be characterized by a subtle interplay between Kondo screening on Ce sites and strong valence fluctuations on Yb sites.

¹This research was supported by the NSF DMR-1006606 and DMR-0844115, ICAM Branches Cost Sharing Fund from Institute for Complex Adaptive Matter, and Ohio Board of Regents Grant OBR-RIP-220573 at KSU and the DOE DE-FG02-04ER46105 at UCSD.

²Permanent address: Institute of Physics, Chinese Academy of Science, Beijing, China.

12:39PM Q16.00008 Effect of local electronic tuning in CeCoIn₅ , KRZYSZTOF GOFRYK, FILIP RONNING, M.N. OU, PAUL TOBASH, XIN LU, ERIC BAUER, JOE THOMPSON, Los Alamos National Lab, S. STOYKO, A. MAR, University of Alberta, ZACH FISK, UC Irvine — The relationship between quantum criticality (QC), non-Fermi-liquid (nFL) behavior and the emergence of unconventional superconductivity (SC) in the vicinity of an antiferromagnetic quantum critical point (QCP) is one of the important issues in strongly correlated electron physics. Here we report on the effect of electronic tuning on superconductivity and quantum criticality in CeColn₅ driven by electron (Pt and Sn) and hole doping (Hg). We show that both Pt and Sn doping have similar strong effect on superconductivity and push the system slightly away from the QCP . The sub-linear power law exponent, even at a high doping level (where the superconductivity is suppressed) could point to the formation of electronic inhomogeneity. Moreover, hole doping by Hg can tune the system back to the QCP as demonstrated by an increase of T_c (and subsequently the onset of AFM), a decrease of the coherence temperature T^* and an increase of the power law coefficient n stressing the importance of the interplay of electronic tuning and pair breaking effects.

12:51PM Q16.00009 Doping effects of CeCo_{1-x}Ru_xIn₅ , M.N. OU, Los Alamos National Laboratory; Institute of Physics-Academia Sinica, Y.Y. CHEN, Institute of Physics-Academia Sinica, O. JANKA, S.M. KAUZLARRICH, University of California, K. GOFRYK, R.E. BAUMBACH, E.D. BAUER, J.D. THOMPSON, F. RONNING, Los Alamos National Laboratory — CeColn₅ lies in close proximity to a QCP which can be tuned with chemical doping, pressure or magnetic field. In this work, single crystals of Ruthenium doped CeColn₅ were prepared by means of self-flux in Indium. The lattice structure of CeCo_{1-x}Ru_xIn₅ was identified as tetragonal by powder XRD with slightly increasing lattice constants. The results of electrical resistivity down to 1.8 K reveals that both coherence (T^*) and superconducting transition (T_c) temperatures are decreasing monotonically with increasing Ru doping. Antiferromagnetism is anticipated on the basis of both negative chemical pressure and hole doping. Transport and thermodynamic data will be compared and contrasted with results from Rh and Cd doping.

1:03PM Q16.00010 Effect of Pressure on Superconductivity and the Kondo-Lattice Coherence Temperature in $\text{Ce}_{1-x}\text{R}_x\text{CoIn}_5$ with $\text{R} = \text{Yb}, \text{Y}, \text{Gd}$, BENJAMIN WHITE, JAMES HAMLIN, MARC JANOSCHEK, LEI SHU, RYAN BAUMBACH, KEVIN HUANG, M. BRIAN MAPLE, University of California, San Diego — Generally, rare-earth substitution for Ce in the heavy fermion superconductor CeCoIn_5 suppresses superconductivity rapidly. However, it was recently reported that the correlated electron ground state of $\text{Ce}_{1-x}\text{Yb}_x\text{CoIn}_5$ is stabilized over an anomalously large range in x , perhaps because of cooperative valence fluctuations of the Ce and Yb ions. Motivated by this possibility, we studied the effect of applied pressure on the superconducting critical (T_c) and Kondo-lattice coherence (T^*) temperatures of $\text{Ce}_{1-x}\text{R}_x\text{CoIn}_5$ with $\text{R} = \text{Yb}, \text{Y}$, and Gd in order to compare the effect of Yb substitution with other magnetic and non-magnetic rare-earth ion substitutions. We performed electrical resistivity measurements under pressures up to a maximum of ~ 2.3 GPa in a piston-cylinder clamped high pressure cell using a 50:50 mixture of n -pentane and isoamyl alcohol for the pressure transmitting medium. It was found that the variations of T_c and T^* in $\text{Ce}_{1-x}\text{R}_x\text{CoIn}_5$ under pressure were approximately independent of R . This result implies that the effect of pressure is independent of the magnetic configuration of the rare-earth ion being introduced.

¹Sample synthesis was supported by DOE Grant DE-FG02-04-ER46105. High pressure measurements were supported by DOE grant DE-FG52-06NA26205. Low-temperature measurements were supported by NSF Grant DMR-0802478.

1:15PM Q16.00011 Antiferromagnetic Order in Pauli-Limited Unconventional Superconductors , YASUYUKI KATO, CRISTIAN BATISTA, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, ILYA VEKHTER, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana, 70803, USA — We develop a theory of the coexistence of superconductivity (SC) and antiferromagnetism (AFM) in CeCoIn_5 . We show that in Pauli-limited nodal superconductors the nesting of the quasiparticle pockets induced by Zeeman pair breaking leads to incommensurate AFM with the magnetic moment normal to the field. We compute the phase diagram and find a first order transition to the normal state at low temperatures, the absence of normal state AFM, and the coexistence of SC and AFM at high fields, in agreement with experiments. We also predict the existence of a new double-Q magnetic phase.

1:27PM Q16.00012 Staggered moments in the vortex cores of CeCoIn_5 , L. LU, G. KOUTROULAKIS, M.D. STEWART, V.F. MITROVIĆ, Department of Physics, Brown University, Providence, Rhode Island 02912, M. HORVATIĆ, C. BERTHIER, Grenoble High Magnetic Field Laboratory, CNRS, B.P. 166, 38042 Grenoble Cedex 9, France, G. LAPERTOT, J. FLOUQUET, CEA, INAC, SPSMS, CEA Grenoble, 38054 Grenoble Cedex 9, France — Our previous nuclear magnetic resonance measurements revealed that magnetic field can induce an exotic superconducting phase, characterized by the presence of strong antiferromagnetic fluctuations. In the low field superconducting state, NMR spectra are determined by the inhomogeneous field distribution of a vortex lattice. In the exotic superconducting phase the NMR spectra broaden well beyond what is expected on the basis of the vortex lattice distribution. Here we explore the possibility that this extra broadening of the NMR spectra arises from the staggered magnetization induced locally around the vortex cores.

¹This research is supported by the funds from NSF (DMR-0710551), ANR Grant NO. 06-BLAN-0111, and the LNCMI, under European Community Contract No. RITACT-2003-505474. V.F.M. acknowledges support by the A.P. Sloan Foundation.

1:39PM Q16.00013 Knight Shift anomaly in anti-ferromagnetic Heavy Fermion, CeRhIn_5 , ABIGAIL SHOCKLEY, University of California, Davis — Since their discovery, the CeMIn_5 ($\text{M}=\text{Ir}, \text{Rh}, \text{Co}$) class of heavy fermion superconductors has attracted a lot of attention for their unusual properties. These compounds all have a scaling behavior which Nakatsuji et al (NPF) proposed is best explained by a two-fluid model. Below a characteristic temperature T^* , the f-moments delocalize and form a coherent state with the conduction electrons, similar to super-fluid ^4He . One of the central questions in the field is which energy scale correlates with the onset of coherence, T_{Kondo} or T_{RKKY} . We will present new data on the Knight Shift anomaly in CeRhIn_5 which allows us to learn about the spin correlations as we approach the coherent state. By comparing the Knight shift anomaly in the three cousin compounds, we can explore how the characteristic energy scales of these materials change as we transition from a superconducting to an anti-ferromagnetic ground state.

1:51PM Q16.00014 Strong suppression of superconductivity and Kondo coherence by Yb substitution in CeCoIn_5 epitaxial films , MASAOKI SHIMOZAWA, SATOSHI YASUMOTO, Department of Physics, Kyoto University, MASAYUKI NAKAMURA, RCLTMS, Kyoto University, TATSUYA WATASHIGE, YUTA MIZUKAMI, Department of Physics, Kyoto University, HIROAKI SHISHIDO, Department of Physics and Electronics, Osaka Prefecture University, TAKASADA SHIBAUCHI, Department of Physics, Kyoto University, TAKAHITO TERASHIMA, RCLTMS, Kyoto University, YUJI MATSUDA, Department of Physics, Kyoto University — One of the important issues in strongly correlated electron system is the relationship between unconventional superconductivity and quantum criticality. Among them, the heavy-fermion superconductor CeCoIn_5 is a key material situated near an antiferromagnetic quantum critical point. When rare-earth ions are substituted for Ce, superconductivity and Kondo-lattice coherence are usually suppressed, but it has been recently pointed out from bulk studies that Yb substitution may be distinguished because of its valence instability. Here we report our recent study on $\text{Ce}_{1-x}\text{Yb}_x\text{CoIn}_5$ epitaxial thin films grown by the molecular beam epitaxy, which have high homogeneity. We find that the superconducting transition temperature is suppressed with increasing x much more rapidly than the previous bulk results, and that the coherence temperature is suppressed concurrently. We also observe a systematic reduction of the low-temperature Hall coefficient magnitude with x , establishing that the antiferromagnetic fluctuations fade even by the Yb substitutions.

2:03PM Q16.00015 Extremely strong-coupling superconductivity in artificial two-dimensional Kondo lattices , YUTA MIZUKAMI, Department of Physics, Kyoto University, HIROAKI SHISHIDO, Research Center for Low Temperature and Materials Sciences, Kyoto University, TAKASADA SHIBAUCHI, MASAOKI SHIMOZAWA, SATOSHI YASUMOTO, DAIKI WATANABE, MINORU YAMASHITA, HIROAKI IKEDA, Department of Physics, Kyoto University, TAKAHITO TERASHIMA, Research Center for Low Temperature and Materials Sciences, Kyoto University, HIROSHI KONTANI, Department of Physics, Nagoya University, YUJI MATSUDA, Department of Physics, Kyoto University — Superconductivity with the strongest electron correlations is realized in heavy-fermion system, where almost all of the compounds have three-dimensional nature. It had remained an unanswered question whether superconductivity would persist on reducing the dimensionality of these materials. We succeeded in observing superconductivity in the system of heavy electrons confined within a two dimensional square lattice of Ce atoms, which was realized by fabricating epitaxial superlattices built of alternating layers of heavy-fermion CeCoIn_5 and conventional metal YbCoIn_5 [1]. The field-temperature phase diagram of the superlattices exhibits a striking enhancement of the upper critical field relative to the transition temperature. This implies that the force holding together the superconducting electron pairs takes on an extremely strong-coupled nature as a result of two-dimensionalization. [1]Mizukami et al., Nature Phys. 7, 849 (2011).

Wednesday, February 29, 2012 11:15AM - 2:15PM –
Session Q17 DMP: Focus Session: Nanostructures and Metamaterials, Growth, Structure, and Characterization – Improved Materials and Applications I 252A

11:15AM Q17.00001 Metamaterials and Plasmonics: Improved Material Building Blocks, ALEXANDRA BOLTASSEVA, Purdue University — Optical metamaterials are rationally designed and manufactured materials built of nanostructured unit cells, or “artificial atoms” much smaller than the wavelength of operating light. These materials can be engineered to exhibit optical properties beyond any naturally occurring materials. This field has been gaining momentum over the past several years, as it continues to provide new fascinating ideas promising a variety of exciting applications including for example super-resolution microscopes, extremely efficient light concentrators and invisibility cloaks. In most metamaterial devices, noble metals (primarily gold and silver) have been used as the constituent material to make subwavelength building blocks. But metals suffer from high optical losses that are much too large to create practical and robust metamaterials devices. A recent approach that could unlock the technological potential of plasmonics and optical metamaterials is to look for better plasmonic materials that have a negative real part of dielectric permittivity. Here we provide an overview of two classes of alternative plasmonic materials - doped semiconductors and intermetallics - that could allow realization of novel transformation optics and metamaterial devices with greatly improved performance operating at near infrared and visible frequencies.

11:51AM Q17.00002 Bianisotropy Compensation in Metamaterials, GEORGE KEISER, ANDREW STRIKWERDA, Department of Physics-Boston University, KEBIN FAN, XIN ZHANG, Department of Mechanical Engineering- Boston University, RICHARD AVERITT, Department of Physics- Boston University — The potential scientific and technological applications for metamaterials abound and continue to multiply at an unprecedented rate. However, with applications come non-trivial design challenges. For instance, many metamaterial designs exhibit the phenomenon of bianisotropy, the ability for an incident electric field to excite a magnetic response (and vice versa) in the metamaterial. In many applications, this bianisotropic response is considered a parasitic effect to be avoided whenever possible. Metamaterials can be designed to eliminate bianisotropy at the unit cell level, but the presence of a substrate will inevitably reintroduce bianisotropy into the system. Here, through a judicious choice of unit cell geometry, we have compensated for and removed the effects of substrate-induced bianisotropy in broadside coupled split-ring resonators on a GaAs substrate. We present numerical simulation results, parameter extraction, and experimental measurements at terahertz frequencies to validate this claim.

12:03PM Q17.00003 Indium Tin Oxide Nanorod Building Blocks for Near-Infra-Red Filter Metamaterials¹, SUNG HOON HONG, HUMEYRA CAGLAYAN, NADER ENGHETA, CHERIE KAGAN, University of Pennsylvania — We report arrays of indium tin oxide (ITO) nanorods function as near-infra-red (NIR) filter metamaterials. We fabricated arrays of rectangular cross-section, plasmonic ITO nanorods of varying pitch, width, gap, and height of the nanorods using nanoimprint lithography and chlorine based inductively coupled plasma (ICP) etching processes. The transmission spectrum of the periodic nanorod arrays may be spectrally tuned in the NIR by the geometry of the arrays and the optical response depends on the polarization of the incident light. The nanorod array behaves as an optical nanocircuit. For illumination by an E-field vector parallel to the nanorod array, the array functions as a parallel L-C circuit, acting as a bandpass filter. For illumination by an E-field vector perpendicular to the nanorod array, the array functions as a series L-C circuit, acting as a bandstop filter. We show good agreement between optical measurements of fabricated nanorod arrays and simulations using equivalent circuit theory and finite-difference time-domain (FDTD) methods. The optical properties of the ITO nanorod circuit may be further tuned by filling the gap between the nanorods using various dielectric materials.

¹This work is supported in part by the Office of Naval Research (ONR) Multidisciplinary University Research Initiative (MURI) grant number N00014-10-1-0942.

12:15PM Q17.00004 Measurement of Resonant Frequencies and Modes of Freestanding Nanoparticle Monolayers, PONGSAKORN KANJANABOOS, James Franck Institute and Department of Physics, The University of Chicago, XIAO-MIN LIN, Center for Nanoscale Materials, Argonne National Laboratory, HEINRICH JAEGER, James Franck Institute and Department of Physics, The University of Chicago, JEFFREY GUEST, Center for Nanoscale Materials, Argonne National Laboratory — We recently showed that freestanding membranes of ligated nanoparticles can be assembled in a one-step drying-mediated process [1]. These 10nm thin membranes can stretch over holes up to 100 microns in diameter and are supported by a substrate only along their outer edge, thereby freely suspending of the order of 100 million close-packed particles [2]. Previous work has focused on quasi-static mechanical properties [1-3]. Here we present the first investigation of the full dynamic response of freely suspended nanoparticle membranes, utilizing a high frequency laser interferometer with picometer sensitivity. This instrument allows us to rapidly measure the dynamical properties of freestanding nanoparticle monolayers for the first time including resonant frequencies, quality factors, and images of different modes.

[1] Klara E. Mueggenburg et al., “Elastic membranes of close-packed nanoparticle arrays,” Nature Materials 6, 656-660 (2007).

[2] Jinbo He et al., “Fabrication and Mechanical properties of large-scale freestanding nanoparticle membranes,” Small 6, 1449-1456 (2010).

[3] Pongsakorn Kanjanaboos et al., “Strain Patterning and Direct Measurement of Poisson’s Ratio in Nanoparticle Monolayer Sheets,” Nano Letters 11, 2567-2571 (2011).

12:27PM Q17.00005 Metamaterial Based Terahertz Detector, ANDREW STRIKWERDA, Boston University, HU TAO, Tufts University, EMIL KADLEC, Sandia National Laboratories, KEBIN FAN, Boston University, WILLIE PADILLA, Boston College, RICHARD AVERITT, Boston University, ERIC SHANER, Sandia National Laboratories, XIN ZHANG, Boston University — We have designed, fabricated, and characterized metamaterial enhanced bimaterial cantilever pixels for far-infrared detection. Local heating due to absorption from split ring resonators (SRRs) incorporated directly onto the cantilever pixels leads to mechanical deflection which is readily detected with visible light. Highly responsive pixels have been fabricated for detection at 95 GHz and 693 GHz, demonstrating the frequency agility of our technique, and their subwavelength nature enables their use as a focal plane array (FPA) to image near the diffraction limit. We have obtained single pixel responsivities as high as 16,500 V/W and noise equivalent powers of 10-8 W/Hz^{1/2} with these first-generation devices, which were achieved at room temperature and pressure. Consequently, MMs hold great promise for facilitating the development of a “versatile” THz detector which can a) strongly absorb THz radiation; b) operate at room temperature; c) function as a multi-pixel array for imaging applications; and d) be lightweight and low cost.

12:39PM Q17.00006 Experimental observation of strong microwave-induced force in parallel-plate metallic cavity, Z. MARCET, University of Florida, Hong Kong University of Science and Technology, Z.H. HANG, S.B. WANG, C.T. CHAN, H.B. CHAN, Hong Kong University of Science and Technology — It has long been known that light induced forces have an impact on matter. These forces, albeit small, have found various applications in physics, chemistry and biology. The magnitude of this induced force is directly related to the momentum carried by light. With a much longer wavelength than visible light, microwave radiation is commonly regarded to having negligible mechanical impact on macroscopic objects. Here we present the first experimental demonstration of a strong repulsive force induced by incident microwave radiation in parallel centimeter-sized metallic plates. We found that the microwave radiation induced force can be significantly stronger than the usual photon pressure exerted by the incident beam when the cavity is excited at resonance, as strong electromagnetic energy is trapped inside the cavity walls. There is good agreement between experimental measurement and calculations using a boundary element method and the Maxwell stress tensor formalism. Our effort may bring new applications of microwave manipulations in the microwave and metamaterial communities.

12:51PM Q17.00007 Geometrical structure, multifractal spectra and localized optical modes of aperiodic Vogel spirals. , JACOB TREVINO, Division of Materials Science and Engineering, Boston University, SENG FATT LIEW, HESSO NOH, HUI CAO¹, Department of Applied Physics, Yale University, LUCA DAL NEGRO², Department of Electrical and Computer Engineering, Boston University — We present a numerical study of the structural properties, photonic density of states and bandedge modes of Vogel spiral arrays of dielectric cylinders in air. Specifically, we systematically investigate different types of Vogel spirals obtained by the modulation of the divergence angle parameter above and below the golden angle value (≈ 137.507 degrees). We found that these arrays exhibit large fluctuations in the distribution of neighboring particles characterized by multifractal singularity spectra and pair correlation functions that can be tuned between amorphous and random structures. We also show that the rich structural complexity of Vogel spirals results in a multifractal photonic mode density and isotropic bandedge modes with distinctive spatial localization character. Vogel spiral structures offer the opportunity to create a novel photonic devices that leverage radially localized and isotropic bandedge modes to enhance light-matter coupling, such as optical sensors, light sources, concentrators, and broadband optical couplers.

¹Prof. Cao has a second affiliation: Department of Physics, Yale University

²Prof. Dal Negro has a second affiliation: Division of Materials Science and Engineering, Boston University

1:03PM Q17.00008 Geometrically Structured Dynamic Shadowing Lithography: Structural Growth and Control¹, SHENGRONG YE, AARON ROUTZAHN², R. LLOYD CARROLL³, Department of Chemistry, West Virginia University — Sphere lithography (SL), or nanosphere lithography (NSL), stands out as a versatile technique capable of producing 2D periodic micro- and nanostructures using colloidal crystal as deposition mask. Many of the fundamental aspects of the features produced by SL have been extensively investigated, including the optical, magnetic, electronic, and catalytic behaviors with emphasis toward applications in biosensing, ultrasensitive spectroscopy, and nanodevice fabrication. Previous work has primarily focused on 2D patterning, however, with little attention paid to vertical growth of the SL features. In this work, we will demonstrate the 3D structural evolution of metal dot arrays by SL-based geometrically structured dynamic shadowing lithography (GSDSL). The resulting structure is highly dependent on the nature of the metal that is used as evaporative source. We will specifically focus on the difference in the grain size of several typical metals and illustrate the ability in control of the structural growth through experiment and modeling. We believe that knowledge of the detailed geometry will enable us to understand further information on the physical and chemical properties of the SL substrates.

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1:15PM Q17.00009 Omni-directional active pillar arrays for emission extraction and on-chip generation of optical vortices at $1.55\mu\text{m}$, NATE LAWRENCE, Department Electrical Engineering, Boston University, JACOB TREVINO, Division of Material Science, Boston University, LUCA DAL NEGRO, Department Electrical Engineering, Boston University — We engineer deterministic aperiodic structures (DAS) for omni-directional light extraction, emission profile shaping and direct orbital angular momentum generation from Si-based light emitting devices operating at telecom wavelengths. Omni-directional diffraction is achieved through the use of structures with circularly symmetric Fourier space and is well suited for extracting light from devices, such as LEDs or lasers. To exploit the unique light scattering properties of these structures we have fabricated active pillar arrays of Erbium (Er) doped Silicon-Rich Nitride (SRN) using electron beam lithography (EBL) and reactive ion etching (RIE) while varying geometry to optimize extraction enhancement around $1.55\mu\text{m}$. We find that aperiodic spiral arrays with continuous circular Fourier space give over 10 times extraction enhancement and outperform Archimedean lattices, which are the standard structures commonly utilized for omni-directional extraction. Additionally we directly image the real and reciprocal space of the emitted radiation at $1.55\mu\text{m}$ and demonstrate direct generation of optical vortices with well-defined values of orbital momentum. These results offer the opportunity to engineer novel optical devices that leverage the control of structured light on optical chips, such as novel laser sources, broadband optical couplers and concentrators.

1:27PM Q17.00010 Synthesis and Structural Characterization of Orthorhombic Vanadium Oxide Nanorods, L.M. GARCIA, E. CHAVIRA, Instituto de Investigacion en Materiales, UNAM, Mexico, DF 04510, P. SANTIAGO-JACINTO, L. RENDON, Instituto de Fisica, UNAM, Mexico, DF 04510, E.E. MARINERO, Hitachi San Jose Research Center, 3404 Yerba Buena Road, San Jose, CA 95135, A. TEJADA, E. FREGOSO-ISRAEL, C. FLORES, Instituto de Investigacion en Materiales, UNAM, Mexico, DF 04510 — Nanorod structures for Li storage are of interest for rechargeable battery applications. Vanadium pentoxide is a promising battery cathode material and in this work we report on the synthesis of V_2O_5 orthorhombic single crystal and polycrystalline nanorods by the sol-gel polymerizing acryl amide method via ethylenediamine tetra acetic acid EDTA assisted hydrothermal process. In order to determine the thermodynamic stability of nanostructured polymorphs vanadates, heat treatments were performed from 450°C to 500°C with annealing times ranging from 48 to 72 h. The morphologies and structures of the nanorods were characterized by XRD, SEM and HRTEM. Thermo Gravimetric Analysis (TGA) was employed to monitor reaction mass losses during the course of the synthesis. Nanorod diameters ranging from 50 to 150 nm were observed. The lengths and diameter of the rods depended on the conditions of the preparation, such as concentration, and reaction time.

1:39PM Q17.00011 Nonlinear metamaterials through enhanced impact ionization in GaAs at terahertz frequencies, KEBIN FAN, Boston Univeristy, HAROLD HWANG, Massachusetts Institute of Technology, MENGKUN LIU, ANDREW STRIKWERDA, JINGDI ZHANG, AARON STERNBACH, XIN ZHANG, Boston Univeristy, KEITH NELSON, Massachusetts Institute of Technology, RICHARD AVERITT, Boston Univeristy, BOSTON UNIVERISTY TEAM, MASSACHUSETTS INSTITUTE OF TECHNOLOGY TEAM — We report the experimental observation of a nonlinear response in metamaterial split ring resonators on semi-insulating GaAs at terahertz frequencies. Using metamaterials with narrow gaps (down to $1\mu\text{m}$), a local in-gap THz field of 3.5 MV/cm was achieved with a field enhancement of ~ 20 on resonance. With increasing THz electric field the metamaterial resonance is gradually quenched as the capacitive gap is shorted due to a large change in the local conductivity in the gap. This indicates an increase of the local carrier density by ten orders of magnitude resulting from impact ionization. Hybrid metamaterials with intense local electric fields not only have the potential to serve as a new tool to study nonequilibrium transport phenomena in materials, but also provide a new way to explore nonlinear metamaterials at terahertz frequencies.

1:51PM Q17.00012 Mode nonorthogonality in nonhermitian PT-symmetric optical resonators, GWANGSU YOO, H.-S. SIM, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea, HENNING SCHOMERUS, Department of Physics, Lancaster University, Lancaster LA1 4YB, United Kingdom, QUANTUM ELECTRON TRANSPORT THEORY GROUP TEAM, CENTRE FOR NANOSCALE DYNAMICS AND MATHEMATICAL MODELLING COLLABORATION — PT -symmetric optical resonators combine absorbing regions with active, amplifying regions. The latter are the source of radiation generated via spontaneous and stimulated emission, which embodies quantum noise and can result in lasing. We calculate the frequency-resolved output radiation intensity of such systems and relate it to a suitable measure of excess noise and mode nonorthogonality. The lineshape differs depending on whether the emission lines are isolated (as for weakly amplifying, almost hermitian systems) or overlapping (as for the almost degenerate resonances in the vicinity of exceptional points associated to spontaneous PT -symmetry breaking). The calculations are carried out in the scattering input-output formalism, and are illustrated for a quasi one-dimensional resonator set-up.

2:03PM Q17.00013 Elastic metamaterials and effective medium theory, YING WU, Division of Mathematical and Computer Sciences and Engineering, King Abdullah University of Science and Technology, YUN LAI, Department of Physics, Soochow University, China, PING SHENG, Department of Physics and William Mong Institute of Nano Science and Technology, Hong Kong University of Science and Technology, ZHAO-QING ZHANG, Department of Physics and William Mong Institute of Nano Science and Technology, Hong Kong University of Science and Technology — The unusual properties of a metamaterial are induced by the resonance in its building blocks. We derived an effective medium theory for elastic metamaterials in two dimensions, which is capable of predicting the wave propagation behavior inside the metamaterial near resonances of the building-block. It reveals the connection between resonances and negativities in effective medium parameters. Based on the EMT, we design two types of elastic metamaterials consisting of different resonance structures in their building blocks that can exhibit multiple negative dispersion bands with special characteristics. One is able to produce negative shear modulus and negative mass density simultaneously over a frequency regime, and the other is super-anisotropic. All of these unusual properties are demonstrated by multiple-scattering theory or finite element simulations.

Wednesday, February 29, 2012 11:15AM - 2:15PM –

Session Q18 DMP: Focus Session: Interfaces in Complex Oxides - Electronic, Magnetic and Optical Properties 252B

11:15AM Q18.00001 First principles insights into electronic, magnetic, and dynamic effects at and across oxide interfaces¹, SOHRAB ISMAIL-BEIGI, Yale University — The recent experimental capacity to create high quality epitaxial oxide/oxide interfaces has opened new avenues for research and provides examples of novel materials properties that emerge at the interfaces and in some cases only exist at the interfaces. Furthermore, a coherent, high-quality interface allows degrees of freedom in the two materials to be coupled to each other across the interface thereby creating artificial multi-functional materials systems. Ab initio theoretical approaches can provide key understanding of these complex systems as they can directly describe the interfacial chemical and structural effects on the electronic properties without assumptions or empirical parameters that are derived from bulk properties. Here, we will provide recent examples from our work showing how the presence and structure of the interface can modify the electronic, magnetic, or transport properties. For example, at a ferroelectric/manganite interface we see how the ferroelectric polarization couples to and strongly modifies the magnetism in the manganite. Another example involves dynamic coupling across an insulator/manganite interface where structural fluctuations in the insulator modify the conductivity in the manganite. In part, we will be focusing on the types of structural distortions present at such interfaces, how they are different from or non-existent in the bulk, and which type of distortions create uniquely interfacial phenomena.

¹Primary support from NSF DMR MRSEC 0520495 and partially from NSF CNS 08-21132.

11:51AM Q18.00002 Digital Layered-Manganites: Madelung Energy Effects on Atomic Structure and Properties, B. NELSON-CHEESEMAN, MSD, Argonne Natl Lab, J. RONDINELLI, MSE, Drexell Univ, H. ZHOU, APS, Argonne Natl Lab, M. NIKIFOROV, CNM, Argonne Natl Lab, E. BARNES, MSE, Penn State Univ, A. SHAH, MRL, Univ of IL Urbana-Champaign, S. BADER, MSD/CNM, Argonne Natl Lab, V. GOPALAN, MSE, Penn State Univ, A. BHATTACHARYA, MSD/CNM, Argonne Natl Lab — The atomic monolayer control of molecular beam epitaxy allows one to explore non-equilibrium dopant-cation configurations in correlated oxide thin films, enabling new electronic phases and magnetic properties to emerge. We report the effects of digital A-site cation doping on electronic phase stability and competition in perovskite-derived manganites. In such digitally synthesized films, Madelung energy constraints are expected to play a primary role in minimizing local Coulomb forces. We correlate changes in the electrical and magnetic properties of the ordered manganites and the resulting crystal structures (Mn-O bond lengths and O-Mn-O bond angles) to the compositionally equivalent control films, i.e. those with randomly distributed A-site dopant-cations. DFT calculations predict that these different layering patterns produce different local and extended crystallographic distortions, including a potential multiferroicity induced by a hitherto unknown mechanism. Synchrotron surface X-ray diffraction measurements in combination with COherent Bragg Rod Analysis at the Advanced Photon Source is used to investigate the resulting atomic structure of the different layering variants, while Second Harmonic Generation and Piezoforce Microscopy investigate the ferroelectric properties.

12:03PM Q18.00003 Reduced dimensionality and pseudogap formation in $(\text{LaMnO}_3)_{2n}(\text{SrMnO}_3)_n$ superlattices, ERIC MONKMAN, CAROLINA ADAMO, DANIEL SHAI, JOHN HARTE, DAWEI SHEN, BULAT BURGANOVA, DARRELL SCHLOM, KYLE SHEN, Cornell University — $(\text{LaMnO}_3)_{2n}(\text{SrMnO}_3)_n$ superlattices, composed of the antiferromagnetic insulators LaMnO_3 (LMO) and SrMnO_3 (SMO), are ferromagnetic and metallic for $n < 3$. By increasing the separation between LMO/SMO interfaces for $n \geq 3$, the system goes through a transition from a metallic to insulating ground state whose origin remains unresolved. We present ARPES measurements of $\text{LMO}_{2n}\text{SMO}_n$ superlattices grown by MBE. The electronic structure of states near the Fermi level is similar to the random alloy $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ for small n , but as n is increased we observe the formation of a more 2D state with a preferential occupation of $x^2 - y^2$ orbitals. As the system passes into the insulating state at $n = 3$, a pseudogap forms at the Fermi level: charge carriers are suppressed over a scale of hundreds of meV but without substantial changes to the overall bandstructure. This pseudogap begins to fill as the temperature is increased, but a large suppression in spectral weight at the Fermi level remains at room temperature. Our observations indicate that the insulating state for large- n superlattices is related to strong many-body effects within this system, enhanced by the reduced dimensionality of an interfacial two-dimensional electron liquid.

12:15PM Q18.00004 Cross-sectional Scanning Tunneling Microscopy (XSTM) Investigation on $(\text{SrMnO}_3)_n/(\text{LaMnO}_3)_n$ Heterostructures¹, WEI-CHENG KUO, Department of Electrophysics, National Chiao Tung University, HsinChu 30100, Taiwan, YING-HAO CHU, Department of Materials Science and Engineering, National Chiao Tung University, HsinChu 30100, Taiwan, TZENG-MING UEN, JENH-YIH JUANG, Department of Electrophysics, National Chiao Tung University, HsinChu 30100, Taiwan — Recent advances in obtaining heterostructures between dissimilar transition-metal oxides with atomically sharp interfaces have revealed emerging exotic electronic and magnetic phases in the vicinity of the interface, which are qualitatively different from the parent compounds. In this study, we have grown $(\text{SrMnO}_3)_n/(\text{LaMnO}_3)_n$ heterostructure superlattice, with n being varied from 2 to 8, by laser MBE system with the assistance of the reflection high-energy electron diffraction (RHEED) intensity oscillations on (001) SrTiO_3 single-crystal substrates. The variation of the density of states across the vicinity of the SrMnO_3 - LaMnO_3 interfaces were investigated by scanning tunneling microscopy (STM) to reveal the spatial modulation of the electronic properties arising from formation of the two-dimensional electron system at the interfaces. The effects of the layer number, n , on this electronically-induced contrast, which is generally ascribed to result from the differences in the energy band gaps, carrier concentrations, as well as electron affinities between SrMnO_3 and LaMnO_3 , will be discussed.

¹This work was supported by National Science Council of Taiwan, ROC

12:27PM Q18.00005 Magnetoelectric coupling at the interface of manganite thin films grown on strontium titanate, MATTHEW MARSHALL, FRED WALKER, CHARLES AHN, CRISP, Dept. of Applied Physics, Yale University, New Haven, CT, 06520 — Oxide heterostructures of $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3/\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3/\text{SrTiO}_3$ (PZT/LSMO/STO) have been shown to undergo a large charge-driven magnetoelectric coupling. Switching the polarization state of the ferroelectric PZT layer induces a spin reconstruction in the top atomic layer of the magnetic LSMO layer, changing from ferromagnetic to antiferromagnetic ordering [1]. In this work, the LSMO layer is several unit cells thick. In order to enhance this magnetic switching effect, we have reduced the thickness of the active LSMO layer, replacing part of the LSMO film with LaMnO_3 (LMO), a bulk antiferromagnetic insulator. To carry out this approach, we use oxide molecular beam epitaxy (MBE) to control the composition of thin films of LMO and LSMO/LMO heterostructures on $\text{SrTiO}_3(001)$ with atomic layer precision. Heterostructures grown in this way show a large deviation from the expected behavior for a simple combination of the individual components. We compare measurements of the magnetization for epitaxial LMO on SrTiO_3 and heterostructures of LSMO/LMO grown on SrTiO_3 . Using this approach, one can optimize the properties of the ferromagnetic layer and improve the magnetoelectric switching properties of the PZT/LSMO/STO system. [1] CAF Vaz, et al. Phys. Rev. Lett. 104, 127202 (2010); doi:10.1103/PhysRevLett.104.127202

12:39PM Q18.00006 Density-functional Study of Suppressed Magnetism at $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{SrTiO}_3$ Interfaces¹, JUN HE, Vanderbilt University, ALBINA BORISEVICH, SERGEI KALININ, STEPHEN PENNY-COOK, Oak Ridge National Laboratory, SOKRATES PANTELIDES, Vanderbilt University — The experimentally observed magnetism suppression at interfaces of $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ has attracted increasing attention. Here we report density-functional calculations for the interface systems of $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{SrTiO}_3$. Two interface models are employed to isolate and identify different effects coming from epitaxial strain, symmetry-breaking, charge redistribution, and oxygen vacancy segregation. We found that the strain effect from SrTiO_3 substrate is not significant enough to cause magnetism suppression at the interface. Although the symmetry is broken at interfaces, this effect leads only to a local ground state and does not cause the observed suppression either. The choice of interface termination does have an effect: moderate magnetism suppression is found for SrO/MnO_2 termination. Finally, we considered the effect of oxygen vacancy segregation at the interface. In the scenarios we have tested, oxygen vacancies do not suppress the interfacial magnetism. Thus, a complicated mechanism is needed to explain the suppressed magnetism at $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{SrTiO}_3$ interfaces.

¹Work supported by the Division of Materials Sciences and Engineering, BES, U.S. DoE., Computations were performed at NERSC.

12:51PM Q18.00007 Optical Measurements on Magnetoelectric LSMO/PZT Bilayers, DISHENG CHEN, SRINIVAS POLISETTY, EVAN WOLFE, JINLING ZHOU, MIKEL HOLCOMB, West Virginia University, THANH TRA VU, JAN-CHI YANG, YING-HAO CHU, National Chiao Tung University — Fairly weak magnetoelectric coupling observed in the only single phase material (BeFeO_3) exhibiting magnetism and ferroelectricity at room temperature has pushed scientists to consider alternative systems. Multilayers prove promising theoretically and experimentally, however, most modern techniques are blind to the interfacial mechanisms causing the coupling. Without a full understanding of the physical mechanism for these effects, significant improvements in the design and multiple potential applications of magnetoelectric coupling will be difficult to achieve. Optical measurements including second harmonic generation are crucial tools to solve this problem, as they provide complementary insight into the magnetic/ferroelectric properties and resulting carrier dynamics. For example, angular dependence SHG of magnetic LaSrMnO_3 and ferroelectric PbZrTiO_3 bilayers indicates the symmetry and magnetization as we vary thicknesses of the magnetic and ferroelectric layers and its implication to magnetoelectric coupling.

1:03PM Q18.00008 Mn valences in $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$ Heterostructures, JINLING ZHOU, SRINIVAS POLISETTY, EVAN WOLFE, CHARLES FRYE, DISHENG CHEN, MIKEL HOLCOMB, West Virginia University, CATHERINE JENKINS, ANDREAS SCHOLL, Lawrence Berkeley National Lab, YING-HAO CHU, National Chiao Tung University — Magnetoelectric (ME) coupling—the electrical control of magnetic properties or vice versa—has promising applications in computer memory and logic, magnetic sensing and energy scavenging. Understanding the coupling mechanisms in a variety of magnetoelectric material systems is an important step as it will allow us to design better magnetoelectric systems. Our group studies the interfacial properties of the known magnetoelectric system of a ferromagnetic $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (LSMO) and a ferroelectric $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$ (PZT). Through photoemission electron microscopy imaging, ME coupling was confirmed at the interface. X-ray absorption spectroscopy of Mn was taken across wedged samples of varying ferroelectric and ferromagnetic thicknesses. Here, we will show the changes of Mn valences at different thicknesses of LSMO and PZT, which helps to understand ME coupling and impact of thickness on the ME properties.

1:15PM Q18.00009 Magnetic coupling at vertical perovskite-spinel epitaxial interface, QING HE, ELKE ARENHOLZ, Advanced Light Source, JAN-CHI YANG, YING-HAO CHU, National Chiao Tung University — Interfaces in complex oxides have been the focus of scientists because of their intriguing and unique properties that cannot be found in bulk. Vertical nanostructure is one of the most interesting heterostructure that has been studied for interface phenomena due to its high interface-volume ratio. In this study, $(\text{La,Ca})\text{MnO}_3$ (LCMO) (perovskite, matrix) / CoFe_2O_4 (CFO) (spinel, pillars, 50-200 nm in size) vertical nanostructure has been taken as model system to investigate the interface magnetic coupling with X-ray absorption spectroscopy and photoemission electron microscopy (PEEM), taking the advantages of their element sensitivity and spatial resolution. Matrix and pillars were studied separated with the photon energy set to different absorption edges. The magnetic order and valence states as well as site occupancy in CFO pillars were characterized by XMCD measurements at Co and Fe L-edges with the application of external magnetic fields. In order to investigate the exchange coupling at the interface, we combined this XMCD study with angular dependent XMLD measurements at Fe and Mn L-edges, which give us the information of orbital order in LCMO, while CFO pillars are magnetized in different directions. Similarly, XMCD studies at the Mn L-edges provide detailed insights into the magnetic order of the LCMO matrix, the Mn valence state and elucidate the impact of the CFO pillars. In addition, PEEM measurement provides spatially resolved XMCD/XMLD images that give more insight of the magnetic coupling at the matrix-pillar interface.

1:27PM Q18.00010 Transport Properties of Films of Prussian Blue Analogues and Manganites¹, P.A. QUINTERO, D.M. GRANT, E.S. KNOWLES, M.F. DUMONT, J.H. JEEN, A. BISWAS, M.W. MEISEL, Dept. Phys. and NHMFL, Univ. Florida, D.R. TALHAM, Dept. Chem., Univ. Florida — The CoFe Prussian blue analogue (PBA) is a coordination polymer, $\text{A}_x\text{Co}_k[\text{Fe}(\text{CN})_6]$ ($\text{A} = \text{K}, \text{Rb}, \text{Cs}$), that exhibits a photoinduced charge transfer.² The resulting changes in the magnetization and in the lattice parameter have been used to successfully apply stress on other pressure-sensitive materials, achieving photocontrol of the magnetic response.³ The metal-to-insulator transition (MIT) is a prominent feature of the manganites, whose transition temperature can be tuned by applying various stimuli such as pressure or magnetic field.⁴ By coupling a layer of PBA over a thin film of manganite, the temperature for the MIT can be altered by the light-induced changes in the CoFe PBA.

¹Supported by the NSF DMR-0804452 (AB), DMR-1005581 (DRT), DMR-0654118 (NHMFL) and the UF DSR-ROF.

²O. Sato *et al.*, Science **272** (1996) 704.

³D.M. Pajerowski *et al.*, J. Am. Chem. Soc. **132** (2010) 4058.

⁴H. J. Jeen and A. Biswas, Phys. Rev. B **83** (2011) 064408.

1:39PM Q18.00011 Enhanced magnetoresistivity of modulation-doped manganite superlattices

, P.V. WADEKAR, Q.Y. CHEN¹, H.J. HUNAG, S.W. YEH, C.F. CHANG, L.W. TU, H. CHOU, N.J. HO, National Sun-Yat Sen University, Kaohsiung, Taiwan, O. LOZANO, D. WIJESUNDERA, W.K. CHU, Texas Center for Superconductivity, University of Houston, TX, USA — Modulation-doped epitaxial superlattices of $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ and $\text{La}_{1-y}\text{Ca}_y\text{MnO}_3$ layers alternating with $x=1/3$ and $y=1/2$ on (001) LaAlO_3 substrates have been grown by magnetron sputtering. The magnetoresistivity (MR) has been greatly enhanced over a wide temperature range in comparison with the parent compounds. The MR is -50% at 0.5 Tesla and -90% at 4 Tesla. At low temperatures, a quantum interference effect (QIE) was observed, as manifested by a resistivity minimum considered to be incurred by the 3D e-e interactions. The modulation-doping approach is an enabling strategy to boost the sensitivity of colossal magnetoresistive oxides in response to an applied magnetic field.

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1:51PM Q18.00012 Induced magnetism at complex oxide interfaces

, JACOBO SANTAMARIA, J. TORNOS, F.A. CUELLAR, J. GARCIA-BARRIOCANAL, Z. SEFRIQUI, A. RIVERA, C. LEON, GPMC. Depto. Fisica Aplicada III. U. Complutense. 28040 Madrid, M. BIBES, A. BARTHÉLÉMY, Unite Mixte de Physique CNRS/Thales, Campus de Polytechnique, 1, Avenue A. Fresnel, 91767 Palaiseau and Université Paris-Sud, 91045 Orsay, France, M.R. FITZSIMMONS, Los Alamos National Laboratory, Los Alamos NM 87545 USA, Y.H. LIU, S.G.E. TE VELTHUIS, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA, M. VARELA, S.J. PENNYCOOK, Condensed Matter Sciences Division Oak Ridge National Laboratory, Tennessee 37831-6031, USA, N.M. NEMES, M. GARCIA HERNANDEZ, Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC). 28049 Cantoblanco. Madrid — Modified bonding at complex oxide interfaces may be at the bottom of the appearance of interesting novel behaviours not appearing in the bulk constituents. The possibility of tailoring the electronic structure of interfaces has driven an important effort towards the design of interfaces with specific functionalities. We have examined novel interfacial magnetic states originating at the modification of the orbital occupancy resulting from the modified bonding at the interface. We discuss the effect of these low dimensional magnetic states in determining the macroscopic magnetic response and in tailoring specific functionalities of heterostructures.

2:03PM Q18.00013 Photostriction-Magnetostriction Coupled Epitaxial Nanostructures

, YING-HAO CHU, National Chiao Tung University — Extensive research on complex oxide thin films and heterostructures suggest new possibilities to create and design devices with tantalizing functionalities by taking the advantages of the interplay between lattice, charge, orbital, and spin degrees of freedom. Recently, the self-assemble vertical nanostructures have drawn considerable attentions due to the strong coupling mediated by high interface-to-volume ratio to tailor the properties of oxide nanostructures. However, most studies have been stressing on the controllability of heterostructures through external electric or magnetic fields. In this study, we have synthesized SrRuO_3 (SRO)- CoFe_2O_4 (CFO) nanostructures to introduce light as other external control parameter, where the light-controlled properties are enabled by ultrafast photostriction of SRO and the magnetostriction of CFO. Through a combination of ultrafast-optics, magnetic force microscopy, and soft X-ray absorption spectroscopy, the coupling between SRO and CFO is clearly revealed. When illuminating CFO-SRO nanostructures, SRO matrix inflates its volume via expanding its c-axis; the elongated SRO matrix relaxes the out-of-plane compressive strain in CFO pillars effectively reduces the magnetic anisotropy thereof; the reduce magnetic anisotropy resets the preferred magnetization direction of CFO pillars; after removing the illumination, the magnetic anisotropy is re-installed and CFO pillars choose to reverse their magnetization. Our study paves a way to ultrafast optical-coupled functionalities.

Wednesday, February 29, 2012 11:15AM - 2:15PM –

Session Q19 FHP: Invited Session: The Scientific Legacy of Edward Purcell (1912-2012) 253AB

11:15AM Q19.00001 Purcell and NMR

, NICOLAAS BLOEMBERGEN, College of Optical Sciences, University of Arizona — In 1946 and 1947 the author carried out research at Harvard University under the guidance of Professor Edward M. Purcell. The results were communicated in a frequently cited paper, often referred to as BPP, after the authors Bloembergen, Purcell and Pound. The same material appeared in my 1948 Ph. D. Leiden thesis “Nuclear Magnetic Relaxation.” Some personal interactions with Ed Purcell and Bob Pound in these early and in later years at Harvard will be recounted.

11:51AM Q19.00002 Purcell and the Development of Radioastronomy

, DOC EWEN, Special Projects Team, LLC — “Join me for a ride on an electron, as we fly through electric and magnetic fields.” With those words, Ed Purcell began a course in Electromagnetic Theory. I had a front row seat. Ken Bainbridge recommended I take the course and get to know Ed. Ed’s wisdom and lucidity of thought soon gave the course, and Ed, a special place in my learning experience. I did not take notes in class. I was in awe at Ed’s ability to present the subject with such clarity and simplicity. Ed’s broad scope of interests and ability to present simple solutions to complex issues quickly led to my identification of Ed as the supreme mentor on any and all subjects. While working with Norman Ramsey to obtain an external beam from the Harvard Cyclotron, I consulted with Ed on the subject of available options. He suggested I scatter the beam off a target that could be remotely positioned, and catch it in a tunnel shielded from the magnetic field of the Cyclotron. When I had a problem with implementation I would, “Ask Ed.” During a visit to the Lab by Fermi, he commented on the simplicity of the solution. He was not surprised to learn that Purcell provided critical guidance. When I suggested Meteorology as a subject for my Oral Test, Purcell said it was not a science and I should pick another subject. I argued it was a science. Ed asked that I loan him some books on the subject and the Oral would be in two weeks. When I walked into the room for the Oral, I noticed that Ed had invited all seven authors of the books I had loaned to him. A simple Purcell answer to a problem. When I asked about his recommendations concerning doctorate dissertation topics, he said the selection must be based on my interests not his. I provided a brief summary: Mathematics, Quantum Mechanics, Meteorology, and Astronomy. Within two weeks, Ed proposed I look into the Hydrogen Line. After a joint review of the papers by Van de Hulst and Shklovski we concluded that: van de Hulst had clearly shown the line was undetectable, Shklovski had claimed the line was detectable, however, there was an error in his calculations. We noted, however, that the topic fit my interests. Purcell had a simple solution. I would proceed with a “negative thesis,” the goal to measure the level of non-detectability. As with all other joint ventures, Ed was always there when I needed help. His guidance was always simple and embarrassingly obvious. For my doctorate oral exam, Ed invited Van de Hulst as the only other participant. Purcell began by asking if I had any questions. I asked Van de Hulst why the line was detectable. Purcell then announced that I had my doctorate and could leave at any time, while he and Van de Hulst worked on the answer to my question. Many of us became terribly alone on March 7, 1997, when we learned we could no longer “Ask Ed.”

12:27PM Q19.00003 On small things in water moving around: Purcell’s contributions to biology

, HOWARD BERG, Departments of Molecular & Cellular Biology and of Physics, Harvard University — I went to see Purcell after finishing my course work for the Ph.D. (1961) to ask whether I might join his group. “But I don’t have any graduate students,” he said. “Why is that?” I asked. “I can’t think of anything to do,” he replied. That was a wipe out. After I had finished my Ph.D. with Ramsey on the hydrogen maser (1964), Ed and I came up with an idea that led to work on sedimentation field-flow fractionation (PNAS 1967). We had hoped this method would be useful for biology, but problems of adsorption of proteins to surfaces stood in the way. Then I moved over to the biology department and got interested in the motile behavior of bacteria (1968). Here was a subject that I thought Ed would really enjoy. There were wonderful movies made by Norbert Pfennig of experiments done by Theodor Engelmann in the 1880’s. We found a 16-mm projector and looked at these movies on Ed’s office wall. Ed’s first comment proved seminal, “How can such a small cell swim in a straight line?” We thought about how cells count molecules in their environment and wrote “Physics of chemoreception,” (*Biophys. J.*, 1977). In the meantime, Ed gave a memorable lecture at Viki Weisskopf’s retirement symposium, his classic “Life at low Reynolds number” (*Am. J. Phys.* 1977). Ed really wanted to understand what it would be like to swim like a bacterium! He wasn’t very interested in what the literature had to say about such a problem, he wanted to think it through for himself. My role was straight man. I very much enjoyed the ride.

1:03PM Q19.00004 Purcell's Work Helping the Government, RICHARD GARWIN, IBM Fellow Emeritus at IBM T.J. Watson Research Center, Yorktown Hts, NY 10598 — I worked closely with Ed Purcell from 1956 through 1975 or so, largely through our joint membership on and consulting with the President's Science Advisory Committee (PSAC) and working with the "Land Panel" on reconnaissance satellites. Purcell's work with the government had begun long before, with his 5-year service at the MIT Radiation Laboratory, and his advisory role had included, in particular, important work of the Technological Capabilities Panel (TCP) of the predecessor to PSAC. I will try to capture the flavor of Ed's contributions and the context of the times in which he was involved. His style and impact are well characterized by this quote from the book of Eisenhower's Science Advisor and PSAC Chair, James R. Killian, "When Eisenhower was later to speak in memorable tribute of 'my scientists' he was surely recalling among others this quiet, modest, lucid man. Robert Kreidler [one of Killian's staff], in an interview I had with him in preparing for this memoir spoke almost with awe of his [Purcell's] impact on PSAC, 'Ed Purcell did not speak often,' he said, 'but when he did there would be enormous silence in the room, because everybody knew that whatever he said was going to be worth listening to with careful attention.'" I give some examples why it was so worthwhile listening to Ed Purcell.

1:39PM Q19.00005 Purcell the Teacher: In and Out of the Classroom, JOHN RIGDEN, Washington University in St. Louis — As a high school student Edward Purcell read articles by K.K. Darrow from his series, "Advances in Contemporary Physics." Many years later, Purcell, referring to those articles, said they remind us "that great teaching does not require a classroom..." Many of Purcell's choices were motivated by his devotion to teaching: the undergraduate courses he preferred to teach at Harvard, the textbooks and pedagogical papers he wrote, and the professional activities he engaged in. He delighted in explaining complex phenomena in simple ways — a mark of a great teacher.

Wednesday, February 29, 2012 11:15AM - 2:15PM — Session Q20 FIAP: Invited Session: Robust Energy Storage with Engineered Si 253C

11:15AM Q20.00001 Silicon Nanowire Anodes: Materials and Composites, CANDACE CHAN, Arizona State University — Silicon nanowires (SiNWs) have the potential to perform as anodes for lithium-ion batteries with a much higher energy density than graphite. Previously, we have shown that reversible capacities $>3,000$ mAh/g can be obtained by using an electrode geometry consisting of SiNWs grown on metallic current collector substrates using the CVD-based vapor-liquid-solid (VLS) method. These electrodes consisted of SiNWs directly attached and vertically oriented off of the current collector. SiNWs can be synthesized in large quantities using the supercritical-fluid-solid (SFLS) method. Slurries were prepared composed of silicon nanowires synthesized using the SFLS method mixed with amorphous carbon or carbon anotubes and binder and coated onto Cu foil. Recent results regarding the cycling behavior of the SiNWs using different experimental conditions will be presented. The performance of these composite electrodes will also be compared with our previous work using the VLS SiNWs to determine how the electrode architecture affects the electrochemical performance.

11:51AM Q20.00002 Strain-tolerant High Capacity Silicon Anodes via Directed Lithium Ion Transport for High Energy Density Lithium-ion Batteries, JASON GOLDMAN, University of Illinois at Urbana Champaign — Energy storage is an essential component of modern technology, with applications including public infrastructure, transportation systems, and consumer electronics. Lithium-ion batteries are the preeminent form of energy storage when high energy / moderate power densities are required. Improvements to lithium-ion battery energy / power density through the adoption of silicon anodes—with approximately an order of magnitude greater gravimetric capacity than traditional carbon-based anodes—have been limited by $\sim 300\%$ strains during electrochemical lithium insertion which result in short operational lifetimes. In two different systems we demonstrated improvements to silicon-based anode performance via directed lithium ion transport. The first system demonstrated a crystallographic-dependent anisotropic electrochemical lithium insertion in single-crystalline silicon anode microstructures. Exploiting this anisotropy, we highlight model silicon anode architectures that limit the maximum strain during electrochemical lithium insertion. This self-strain-limiting is a result of selecting a specific microstructure design such that during lithiation the anisotropic evolution of strain, above a given threshold, blocks further lithium intercalation. Exemplary design rules have achieved self-strain-limited charging capacities ranging from 677 mAhg $^{-1}$ to 2833 mAhg $^{-1}$. A second system with variably encapsulated silicon-based anodes demonstrated greater than 98% of their initial capacity after 130+ cycles. This anode also can operate stably at high energy/power densities. A lithium-ion battery with this anode was able to continuously (dis)charge in 10 minutes, corresponding to a power / energy density of ~ 1460 W/kg and ~ 243 Wh/kg—up to 780% greater power density and 220% higher energy density than conventional lithium-ion batteries. Anodes were also demonstrated with areal capacities of 12.7 mAh/cm ^{2} , two orders of magnitude greater than traditional thin-film silicon anodes.

In collaboration with Michael W. Cason and Ralph G. Nuzzo.

12:27PM Q20.00003 Understanding the Degradation of Silicon Electrodes for Lithium-Ion Batteries Using Acoustic Emission and Fracture Mechanics¹, CLAUD DANIEL, Oak Ridge National Laboratory and University of Tennessee — Silicon is a promising anode material for lithium-ion battery application due to its high specific capacity, low cost, and abundance. However, when silicon is lithiated at room temperature, it can undergo a volume expansion in excess of 280%, which leads to an extensive fracturing. This is thought to be a primary cause of the rapid decay in cell capacity routinely observed. We have developed a special cell design which allows us to monitor acoustic emissions stemming from mechanical events in the cell and allow for detailed structural analysis using X-ray diffraction with an internal standard. The combined result from acoustic emissions and X-ray diffraction allow for a first of its kind detailed look at how silicon anodes degrade and together with presented theories of fracture mechanics enable a material engineering approach to optimize its long term behavior. In collaboration with Kevin Rhodes and Sergiy Kalnaus.

Parts of this research were performed at the High Temperature Materials Laboratory, a national user facility sponsored by the same office.

¹This research at Oak Ridge National Laboratory, managed by U.T. Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725 was sponsored by the Vehicle Technologies program for the Office of Energy Efficiency and Renewable Energy.

1:03PM Q20.00004 Reversible Cycling of Silicon and Silicon Alloys¹, MARK OBROVAC, Dalhousie University

— Lithium ion batteries typically use a graphite negative electrode. Silicon can store more lithium than any other element and has long been considered as an attractive replacement for graphite. The theoretical lithium storage capacity of silicon is nearly ten times higher than graphite volumetrically and three times higher gravimetrically. The equilibrium Si-Li binary system is well known. Completely new phase behaviors are observed at room temperature. This includes the formation of a new phase, Li₁₅Si₄, which is the highest lithium containing phase at room temperature [1]. The formation of Li₁₅Si₄ is accompanied by a 280 percent volume expansion of silicon. During de-alloying this phase contracts, forming amorphous silicon. The volume expansion of alloys can cause intra-particle fracture and inter-particle disconnection; leading to loss of cycle life. To overcome issues with volume expansion requires a detailed knowledge of Li-Si phase behavior, careful design of the composition and nanostructure of the alloy and the microstructure of the negative electrode [2]. In this presentation the phase behavior of the Li-Si system will be described. Using this knowledge alone, strategies can be developed so that silicon can be reversibly cycled in a battery hundreds of times. Further increases in energy density and efficiency can be gained by alloying silicon with other elements, while controlling microstructure [2]. Coupled with negative electrode design strategies, practical negative electrodes for lithium ion cells can be developed based on bulk materials, with significant energy density improvement over conventional electrodes.

[1] M.N. Obrovac and L.J. Krause, J. Electrochem. Soc., 154 (2007) A103.

[2] M.N. Obrovac, Leif Christensen, Dinh Ba Le, and J.R. Dahn, J. Electrochem. Soc., 154 (2007) A849

¹Reversible Cycling of Silicon and Silicon Alloys

1:39PM Q20.00005 Pair Distribution Function Analysis and Solid State NMR Studies of Silicon Electrodes for Lithium Ion Batteries: Understanding the (De)lithiation Mechanisms, BARIS KEY, Argonne National Laboratory

— The crystalline-to-amorphous phase transition that occurs on electrochemical Li insertion into crystalline Si, during the first discharge, hinders attempts to link the structure with electrochemical performance. We apply a combination of local structure probes, in situ and ex situ ⁷Li nuclear magnetic resonance (NMR) studies, and pair distribution function (PDF) analysis of X-ray data to investigate the changes in short-range order that occur during the initial charge and discharge cycles. The distinct electrochemical profiles observed subsequent to the first discharge have been shown to be associated with the formation of distinct amorphous lithiated silicide structures. The first process seen on the second discharge is associated with the lithiation of the amorphous Si, forming small clusters. These clusters are broken in the second process to form isolated silicon anions. The (de)lithiation model helps explain the hysteresis and the steps in the electrochemical profile observed during the lithiation and delithiation of silicon. At deep discharge states a highly reactive lithium excess Li₁₅Si₄ phase is detected by in situ NMR which undergoes a self-discharge process in electrolyte.

Wednesday, February 29, 2012 11:15AM - 2:15PM –

Session Q21 DCMP: Novel Superconductivity in New and Low Dimensional Materials 254A

11:15AM Q21.00001 Superconductivity in ThCoC₂¹, TED GRANT, University of California Irvine, ANTONIO J.S.

MACHADO, EEL-USP Brazil, ZACHARY FISK, University of California Irvine — We report bulk superconductivity in the metallic carbide compound ThCoC₂. This compound crystallizes in the orthorhombic CeNiC₂ prototype structure, a non-centrosymmetric system. Despite the presence of Cobalt and the lack of inversion symmetry, we find bulk superconductivity with a critical temperature of T_c = 2.6 K. Details of the superconducting state with specific heat, magnetization, and resistivity measurements will be presented. This study was made possible by the generous support of AFOSR MURI "Search for New Superconductors for Energy and Power Applications."

¹Supported by AFOSR-MURI

11:27AM Q21.00002 Superconductivity in ScGa₃ and LuGa₃¹, ETERI SVANIDZE, EMILIA MOROSAN, Physics and Astronomy Department, Rice University

— We are reporting low-temperature superconductivity in single crystals of ScGa₃ and LuGa₃. While the latter compound had been listed as a superconductor before, superconductivity in the former compound had never been observed, and characterization of the low-temperature state was lacking in both compounds. By measurements of magnetization, specific heat and resistivity, we show that RGa₃ (R = Sc and Lu) are conventional BCS superconductors with T_c around 2.3 K and the upper critical field less than 240 Oe. The experimental results agree with band structure calculation estimate of the critical temperature.

¹NSF DMR 0847681

11:39AM Q21.00003 Physical properties of single crystalline SrSn₄ and BaSn₅ superconductors¹

, XIAO LIN, SERGEY BUD'KO, Department of Physics and Astronomy, Iowa State University and Ames Laboratory, GERMAN SAMOLYUK, Materials Science & Technology Division, Oak Ridge National Laboratory, MILTON TORIKACHVILI, Department of Physics, San Diego State University, PAUL CANFIELD, Department of Physics and Astronomy, Iowa State University and Ames Laboratory — We present the growths and detailed thermodynamic and transport measurements on single crystals of the recently discovered binary intermetallic superconductors, SrSn₄ and BaSn₅. Their superconducting transition temperatures T_c are found to be 4.8 K and 4.4 K respectively. Both materials are strongly-coupled, possibly multi-band superconductors. Hydrostatic pressure causes a decrease in the superconducting transition temperature at the rate of ≈ -0.068 K/kbar for SrSn₄, and ≈ -0.053 K/kbar for BaSn₅. Band structure and upper superconducting critical field anisotropy of SrSn₄ suggest complex, multi-sheet Fermi surface formed by four bands. De Hass-van Alphen oscillations are observed in BaSn₅, which indicates a more complex topology of Fermi surface.

¹Work was supported by AFOSR-MURI grant FA9550-09-1-0603; the DMSE, Office of Basic Energy Sciences, US DOE contract # DE-AC02-07CH 11358; and NSF grant DMR-0805335.

11:51AM Q21.00004 Synthesis, Structure, Physical Properties of several Zirconium Chalcogenides, XIYU ZHU, BING LV, LIANGZI DENG, FENG YAN WEI, YANYI SUN, YUYI XUE, PAUL CHING-WU CHU, Texas Center for Superconductivity, University of Houston, Houston TX 77204-5002, USA

— Compounds of KxZr₂Se₆, RbxZr₂Se₆ and ZrTe_{1.3}As_{0.7} have been fabricated by high temperature solid state synthesis technique. All these compounds have the same space group Immm. They can be generally considered as the compounds derived from ZrSe₃ and ZrTe₃, which accommodate the quasi 2D type structure composed by (Zr₂Se₂)(Se₄) and (Zr₂Te₂)(Te₄) layers. KxZr₂Se₆ and RbxZr₂Se₆ could be considered as the anionic layers [(Zr₂Se₂)(Se₄)]^{x-} intercalated with alkali cations. One the other hand, ZrTe_{1.3}As_{0.7} isn't a layered compound. The compound has the same structure with NbPS, with disordered As and Te occupying the P sites. This structure could be considered as a derivative structure of ZrTe₃ with the retained (Zr₂Te₂) layers interspersed with linear (Te_{0.3}As_{0.7}) chains. We also measured the magnetic and transport properties of these samples. We shall present and discuss their interesting structural and physical properties.

12:03PM Q21.00005 Superconductivity in Pd, Ir, and Pt chalcogenide, YOON SEOK OH, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, JUNJIE YANG, Laboratory for Pohang Emergent materials, Postech, Korea, Y.J. CHOI, A. HOGAN, Y. HORIBE, S.-W. CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University — Large spin-orbit coupling in materials with heavy chalcogens can result in unique quantum states or functional properties such as topological insulator, giant thermoelectric power, and superconductivity. When materials contain heavy cations in addition to heavy chalcogens, spin-orbit coupling can be further enhanced. For these reasons, we have studied the superconductivity of Pd, Ir, and Pt tellurides and selenides. In the exploration of these chalcogenides, we have focused on the competition between superconductivity and charge density wave that is associated with superlattice reflections.

12:15PM Q21.00006 Elementary excitations and elusive superconductivity in palladium hydride – *ab initio* perspective. I. Paramagnons, P. BUCZEK, MPI Halle, Germany, V. BORISOV, MLU Halle-Wittenberg, Germany, C. BERSIER, MPI Halle, Germany, S. OSTANIN, MLU Halle-Wittenberg, Germany, L. SANDRATSKII, MPI Halle, Germany, J.B. STAUNTON, University of Warwick, United Kingdom, E.K.U. GROSS, MPI Halle, Germany, I. MERTIG, MLU Halle-Wittenberg, Germany, A. ERNST, MPI Halle, Germany — Motivated by a experimental reports on possible high temperature superconductivity in palladium hydride [Tripodi *et al.*, *Physica C* **388-389**, 571 (2003)], we present a first principle study of spin fluctuations, electron-phonon coupling and critical temperature in PdH_x , $0 \leq x \leq 1$. A prerequisite for any qualitative study of exchange-enhanced materials is the knowledge of spin flip fluctuation spectrum. It is generally believed [Berk & Schrieffer, *Phys. Rev. Lett.*, **17**, 433 (1966)] that the ferromagnetic-like paramagnons of Pd are destructive for the conventional, i.e. *s*-wave, superconductivity. We describe them using linear response time dependent density functional theory, recently implemented to study complex metals [Buczek *et al.*, *Phys. Rev. Lett.* **105**, 097205 (2010)]. We find that hydrogenation suppresses the intense spin fluctuations of pure Pd, driving it away from a magnetic critical point. Under the assumption of *s*-wave pairing, this could lead to the formation of the superconducting state. The *ab-initio* estimated electron-phonon coupling is strong enough to support superconductivity. Please look for the complementary contribution of Christophe Bersier.

12:27PM Q21.00007 Elementary excitations and elusive superconductivity in palladium hydride – *ab initio* perspective. II. Phonons, CHRISTOPHE BERSIER, PAWEŁ BUCZEK, MPI Halle, Germany, VLADISLAV BORISOV, SERGEY OSTANIN, MLU, Halle-Wittenberg, Germany, LEONID SANDRATSKII, MPI Halle, Germany, JULIE B. STAUNTON, University of Warwick, United Kingdom, E.K.U. GROSS, MPI Halle, Germany, I. MERTIG, MLU, Halle-Wittenberg, Germany, ARTHUR ERNST, MPI Halle, Germany — Motivated by a experimental reports on possible high temperature superconductivity in palladium hydride [Tripodi *et al.*, *Physica C* **388-389**, 571 (2003)], we present a first principle study of spin fluctuations, electron-phonon coupling and critical temperature (T_c) in PdH_x , $0 < x < 1$. Our results described in terms of (i) electronic structure, (ii) phonon density of states and (iii) Eliashberg function show that the hydrogenation of Pd clearly enhance the electron-phonon coupling in this material. Assuming phonons to be the driving force for superconductivity, fcc Pd features a vanishingly small T_c , while for the stoichiometric $x = 1$ PdH the resulting T_c is around 10K in agreement with experiment. It is generally believed [Berk & Schrieffer, *Phys. Rev. Lett.*, **17**, 433 (1966)] that intense spin-&flip fluctuations of Pd are destructive for the conventional, i.e. *s*-wave, superconductivity. However, the H doping leads to a drastic reduction of spin-flip scattering. Please look for complementary presentation of Paweł Buczek.

12:39PM Q21.00008 Structural and Electronic properties of the 2D Superconductor CuS covellite with 113-valent Copper, IGOR MAZIN, Naval Research Laboratory — Hexagonal CuS has recently been reported to superconduct at 40 K. At the same time, earlier experiments had found superconductivity at 1.5 K. Some authors reported local magnetic moments in this compound, while others observe pure Pauli paramagnetism. It exhibits a rather unusual for a good metal symmetry-lowering transition at 55 K of unknown origin. Even the Cu valency in CuS has been debated, with suggested ionic models such as $(\text{Cu}^{+1})_3(\text{S}_2^{-2})(\text{S}^{-1})$ and $(\text{Cu}^{+1})_3(\text{S}_2^{-1})(\text{S}^{-2})$, as well as noninteger valencies. To gain more insight, we've performed DFT calculations and found that the actual valency of Cu is $4/3$ (2), so that the Cu d band is not sufficiently ionized in the ideal compound to provide enough proximity to Mott dielectric for either local moments or unconventional superconductivity. On the other hand, the reason that Cu is not divalent here is that some sulfurs form covalent S_2 molecules with the effective S_2^{-2} valency. If some of these covalent S-S bonds are broken, local moments *can* form, and in that case superexchange in the hexagonal lattice can induce *f*-wave pairing. Finally, regarding the structural transition, it is well reproduced in DFT calculations. Possible microscopic origin of this transition will be discussed in the talk.

12:51PM Q21.00009 Moving Beyond Quantum Mechanics in Search for a Generalized Theory of Superconductivity, GODFREY AKPOJOTOR, Delta State University, ALEXANDER ANIMALU, International Centre for Basic Research — Though there are infinite number of theories currently in the literature in the search for a generalized theory of superconductivity (SC), there may be three dominating mechanisms for the Cooper pair formation (CPF) and their emergent theories of SC. Two of these mechanisms, electron-phonon interactions and electron-electron correlations which are based on the quantum theory axiom of action-at-a distance, may be only an approximation of the third mechanism which is contact interaction of the wavepackets of the two electrons forming the Cooper pair as envisaged in hadronic mechanics to be responsible for natural bonding of elements. The application of this hydronic –type interaction to the superconducting cuprates, iron based compounds and heavy fermions leads to interesting results. It is therefore suggested that the future of the search for the theory of SC may be considered from this natural possible bonding that at short distances, the CPF is by a nonlinear, nonlocal and nonhamiltonian strong hadronic-type interactions due to deep wave-overlapping of spinning particles leading to Hulthen potential that is attractive between two electrons in singlet couplings while at large distances the CPF is by superexchange interaction which is purely a quantum mechanical affairs.

1:03PM Q21.00010 Material Specific Design for Room Temperature Superconductivity¹, O-PAUL ISIKAKU-IRONKWE², The Center for Superconductivity Technologies, (TCST), Department of Physics, Michael Okpara University of Agriculture, Umudiike, (MOUUAU), Nigeria, UKO OFE, TCST @ MOUUAU, CHIJOKE ORIAKU, DAN ASIEGBU, TCST@MOUUAU, EMEKA OGUZI, TCST and Department of Chemistry, FUTU, Owerri, Nigeria — The transition temperature, T_c , of superconductors has been increased sevenfold from 23K in Nb_3Ge to 164K in Hg-1223. A further two-fold increase would get us to above room temperature superconductivity. Studying high temperature superconductors (HTSCs), we have developed a formula that expresses T_c in terms of electronegativity, valence electrons, N_v , atomic number, Z , formula mass and a coupling constant, K_o . We observe an increasing linear relationship between T_c and K_o . K_o also correlates with formula mass and atomic number and the number of atoms in the compound. By our formula, Hg-1223 has $K_o = 70$. We propose, using our design algorithm, that room temperature superconductivity may be realized in a system with $K_o = 160$; electronegativity = 2.5, $N_v/\text{Sqrt } Z = 0.8$. We proceed to show combinations of oxides and elements that will yield the required parameters for synthesizing reproducible room temperature superconductivity.

¹Research support from Dr. M.J. Schaffer, General Atomics, San Diego, CA.

²and RTS Technologies, San Diego CA 92122

1:15PM Q21.00011 Thermopower and Resistivity in the Spin Density Wave- Metal co-existence regime of (TMTSF)2PF6, ARJUN NARAYANAN, PAUL CHAIKIN, Department of Physics, New York University — The organic conductor (TMTSF)2PF6 is studied in the pressure regime where it is believed to exhibit co-existence between Metallic and Spin Density Wave domains. In this pressure regime, an anisotropy in the superconductivity transition - seen previously in resistivity data on separate samples in different experimental runs - is here reproduced using both resistivity and thermopower as probes, on three slices of the same crystal measured simultaneously. The simultaneous use of these two measurements along the a, b and c axes, enables us to extract complementary information about the remarkable anisotropy in the superconducting transition and may shed light on the possibly inhomogeneous ground states in the co-existence regime of (TMTSF)2PF6.

1:27PM Q21.00012 Non-analytical Angular Dependence of the Upper Critical Magnetic Field in a Quasi-One-Dimensional Superconductor¹, OTAR SEPPER, ANDREI LEBED, University of Arizona — We have derived the so-called gap equation, which determines the upper critical magnetic field, perpendicular to conducting chains of a quasi-one-dimensional superconductor. By analyzing this equation at zero temperature, we have found that the calculated angular dependence of the upper critical magnetic field is qualitatively different than that in the so-called effective mass model. In particular, our theory predicts a non-analytical angular dependence of the upper critical magnetic field, $H_{c2}(0) - H_{c2}(\alpha) \sim \alpha^{3/2}$, when magnetic field is close to one of the crystallographic axes and makes an angle α with the axis. We discuss possible experiments on the superconductor (DMET)2I3 to discover this non-analytical dependence.

¹This work was supported by the NSF under Grant No. DMR-1104512

1:39PM Q21.00013 Hidden Reentrant and Larkin-Ovchinnikov-Fulde-Ferrell Superconducting Phases in a Magnetic Field in (TMTSF)2ClO4¹, ANDREI LEBED, Department of Physics, University of Arizona — We solve a long-standing problem about a theoretical description of the upper critical magnetic field, parallel to conducting layers and perpendicular to conducting chains, in (TMTSF)2ClO4 superconductor. In particular, we explain why the experimental upper critical field, $H_{c2}^b = 6\text{T}$, is higher than both the quasi-classical upper critical field and Clogston paramagnetic limit. We show that this property is due to the coexistence of the hidden Reentrant and Larkin-Ovchinnikov-Fulde-Ferrell phases in a magnetic field in a form of three plane waves with non-zero momentums of the Cooper pairs. Our results are in good qualitative and quantitative agreement with the recent experimental measurements of H_{c2}^b and support a singlet d-wave-like scenario of superconductivity in (TMTSF)2ClO4.

¹This work was supported by the NSF thru Grant # DMR-1104512.

1:51PM Q21.00014 ¹H NMR Spin-Lattice Relaxation Study of κ -(ET)2Cu[N(CN)2]Br, J.C. GEZO, TAK-KEI LUI, R.W. GIANNETTA, C.P. SLICHTER, Loomis Laboratory of Physics, University of Illinois at Urbana-Champaign, IL 61801, J.A. SCHLEUTER, Material Sciences Division, Argonne National Laboratory, Argonne IL 60439 — The discovery of an anomalous Nernst signal in the organic superconductor κ -(ET)2Cu[N(CN)2]Br suggests the presence of magnetic flux vortices above T_c ^[1]. Previous studies below the transition temperature have shown that the additional fluctuating field created by vortices dramatically increases the ¹H NMR spin-lattice relaxation rate^[2]. We revisit ¹H spin-lattice relaxation in κ -(ET)2Cu[N(CN)2]Br and provide new evidence of inhomogeneous behavior both above and below T_c . ^[1]M. S. Nam et al, Nature 449, 584-587 (2007) ^[2]H. Mayaffre et al, Phys. Rev. Lett. 76, 4951-4954 (1996) Work at UIUC supported by NSF DMR 10-05708 and the Center for Emergent Superconductivity, USDOE Award No. DE-AC0298CH1088. Work at Argonne supported by UChicago Argonne, LLC, Operator of Argonne National Laboratory, DOE Contract No. DE-AC02-06CH11357.

2:03PM Q21.00015 ¹³C NMR Study of Slow Motions in κ -(ET)2Cu[N(CN)2]Br¹, TAK-KEI LUI, JOSEPH C. GEZO, RUSSELL W. GIANNETTA, CHARLES P. SLICHTER, University of Illinois at Urbana-Champaign, IL 61801, JOHN A. SCHLEUTER, Material Sciences Division, Argonne National Laboratory, Argonne, IL 60439 — Like the high- T_c cuprates, the 2D organic superconductor κ -(ET)2Cu[N(CN)2]Br ($T_c = 11.9\text{ K}$) exhibits a pseudo-gapped phase above the superconducting transition, as indicated by the ¹³C spin-lattice relaxation rate ($1/T_1T$) peak at about 50 K. While ¹³C NMR has been used extensively to probe the pseudo-gapped regime, T_1 is only sensitive to fast motions in the MHz scale (Larmor frequency), and T_2 remains relatively constant in the pseudo-gapped regime. Neither T_1 nor T_2 give us any clue about any possible slow motions. We report measurements using the stimulated echo pulse sequence² which is capable of providing more detailed information on possible slow motions in the pseudo-gapped regime.

¹Work at UIUC supported by NSF DMR 10-05708, and Center for Emergent Superconductivity USDOE Award No. DE-AC02-98CH10886, Work at Argonne supported by UChicago Argonne, LLC, Operator of Argonne National Laboratory, DOE Contract No. DE-AC02-06CH11357

²L. R. Becerra, C. A. Klug, C. P. Slichter, and J. H. Sinfelt, J. Phys. Chem. **97**, 12014 (1993).

Wednesday, February 29, 2012 11:15AM - 2:15PM –
Session Q22 DMP DCOMP: Focus Session: Fe-based Superconductivity - Doped and Undoped BaFe2As2 254B

11:15AM Q22.00001 Nature of phase transitions in the parent and lightly electron doped BaFe2As2 compounds¹, MIN GYU KIM, R.M. FERNANDES, A. KREYSSIG, Ames Laboratory, Dept. of Physics and Astronomy, Iowa State University, Ames, IA, J.W. KIM, Advanced Photon Source, ANL, Argonne, IL, A. THALER, S.L. BUD'KO, P.C. CANFIELD, R.J. MCQUEENEY, J. SCHMALIAN, A.I. GOLDMAN, Ames Laboratory, Dept. of Physics and Astronomy, Iowa State University, Ames, IA — We present a combined high-resolution x-ray diffraction and x-ray resonant magnetic scattering study of as-grown BaFe2As2. The structural and magnetic transitions must be described as a two-step process. The undoped BaFe2As2 parent compound manifests a second-order structural transition from the high-temperature paramagnetic tetragonal structure to a paramagnetic orthorhombic phase and a first-order antiferromagnetic transition from the paramagnetic orthorhombic phase to an antiferromagnetic orthorhombic phase at slightly lower temperature. As electrons are introduced by Co or Rh, the phase transitions evolve toward second-order transitions. Using these results, we provide an estimate of the position of a tricritical point in the phase diagram of Ba(Fe1-xCox)2As2.

¹The work at the Ames Laboratory was supported by US DOE, Office of Basic Energy Sciences, DMSE, contract DE-AC02-07CH11358.

11:27AM Q22.00002 Neutron powder diffraction studies on $\text{Ba}_{1-x}\text{A}_x\text{Fe}_2\text{As}_2$ ($\text{A}=\text{Na}, \text{K}$)¹, SEVDA AVCI, DUCK-YOUNG CHUNG, HELMUT CLAUS, STEPHAN ROSENKRANZ, RAY OSBORN, Argonne National Laboratory, OMAR CHMAISSEM, Northern Illinois University and Argonne National Laboratory, MERCOURI KANATZIDIS, Northwestern University and Argonne National Laboratory, EUGENE GORE-MYCHKIN, ISIS, Rutherford Appleton Laboratory, UK — In the so-called 122 iron pnictide superconductors, the SDW is suppressed and superconductivity can be induced by various means including charge doping, pressure, and isovalent substitution. Using neutron powder diffraction and SQUID magnetization measurements, we have investigated the effects of both potassium and sodium substitution on superconductivity, structural transformation and magnetic ordering in $\text{Ba}_{1-x}\text{A}_x\text{Fe}_2\text{As}_2$ ($\text{A}=\text{K}, \text{Na}$) producing detailed phase diagrams of both systems. We present a comparison of the similarities and differences in the various internal atomic and magnetic structural parameters as a function of temperature and composition of these two hole-doped systems.

¹This work is supported by U.S. Department of Energy Office of Science under contract No. DE-AC02-06CH11357.

11:39AM Q22.00003 Neutron diffraction study of the development of incommensurate magnetic order in $\text{Ba}(\text{Fe}_{1-x}\text{M}_x)\text{As}_2$ ($\text{M} = \text{Co}, \text{Ni}, \text{Cu}$)¹, R.J. MCQUEENEY, M.-G. KIM, D.K. PRATT, Ames Laboratory, Iowa State University, Ames, IA 50011, T.W. HEITMANN, The Missouri University Research Reactor, University of Missouri, Columbia, MO 65211, J. LAMSAL, S.N. KHAN, Y.B. LEE, G.S. TUCKER, A. THALER, S. RAN, S.L. BUD'KO, P.C. CANFIELD, D.D. JOHNSON, B.N. HARMON, A. KREYSSIG, A.I. GOLDMAN, Ames Laboratory, Iowa State University, Ames, IA 50011 — We employ neutron diffraction and electronic structure calculations using both virtual crystal and coherent potential approximations to investigate the conditions for incommensurate magnetism in several electron-doped compounds $\text{Ba}(\text{Fe}_{1-x}\text{M}_x)\text{As}_2$ with $\text{M} = \text{Co}, \text{Ni}, \text{Cu}$. Incommensurate order is observed for $\text{M} = \text{Co}$ and Ni with $x \approx 0.06$ and 0.03 , respectively. Assuming each Co (Ni) ion donates one (two) additional electrons, the appearance of incommensurate magnetism in the Co and Ni doped systems occurs at similar electron concentrations. For $\text{M} = \text{Cu}$, Cu should donate three electrons and one expects that incommensurate magnetism will appear at $x \approx 0.02$. However, we find that the magnetism remains commensurate until it disappears at $x \approx 0.05$. Thus, Cu doping behaves differently than either Co or Ni , as can be explained from the electronic structure.

¹The work at the Ames Laboratory was supported by US DOE, Office of Basic Energy Sciences, DMSE, contract DE-AC02-07CH11358.

11:51AM Q22.00004 Magnetic moment in single crystalline $\text{BaFe}_{2-x}\text{Zn}_x\text{As}_2$, YANFENG GUO, International Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science, XIA WANG, JUN LI, KAZUNARI YAMAURA, Superconducting Materials Centre, National Institute for Materials Science, EIJI TAKAYAMA-MUROMACHI, International Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science — Nature of the magnetism for iron-based superconductors (FeSCs) has been actively studied since the discovery of this new family of compounds in 2008, largely owing to its significance for interpreting the pairing mechanism. The approach through impurity substitution to shed light into this issue is always one of major ways. The substitution shows distinct responses to species of impurities, where partially replacement of Fe in parent FeSCs with a variety of d -metals like Co , Ni , Ru , Rh , Pd , Ir , and Pt generally results in superconductivity, while recent progress in Zn doped FeSCs gives rather contrary result, where Zn severely degenerates the T_C . Herein we show the magnetic and electrical studies on $\text{BaFe}_{2-x}\text{Zn}_x\text{As}_2$ single crystals. Nonmagnetic Zn doping progressively suppresses the SDW without resulting in superconductivity, while it alternatively develops the spin-glass state, possibly suggestive of local magnetic moment around the Fe sites induced by Zn . The characterizations by X-ray diffraction, magnetic and electrical transport properties, specific heat capacity, and Hall coefficient have been done and the results will be discussed in detail.

12:03PM Q22.00005 75As-NMR studies on $\text{Ba}(\text{Fe}_{1-x}\text{Ni}_x)_2\text{As}_2$ single crystals, JIANLIN LUO, XIAODONG ZHANG, GUOZHI FAN, XIUNIAN JING, Institute of Physics, Chinese Academy of Sciences, CHENGLIN ZHANG, Department of Physics and Astronomy, The University of Tennessee — 75As nuclear magnetic resonance (NMR) were measured for $\text{Ba}(\text{Fe}_{1-x}\text{Ni}_x)_2\text{As}_2$ single crystals with $x = 0.05$ and $x = 0.1$ under 0 GPa and 1.5 GPa, respectively. For the optimal doped sample with $x = 0.05$, the superconducting transition temperature T_C is strongly suppressed from 18 K to 5 K, while for the over-doped sample with $x = 0.1$, it is turned from the superconducting ground state to a disordered paramagnetic state under 1.5 GPa. Our experimental results show that the antiferromagnetic spin fluctuations are suppressed as well as T_C . The experimental results can be explained with the two-band model. As a result, the electronic band is downward shifted with increase of pressure and the electrons become the dominant carriers in the system.

12:15PM Q22.00006 Do Transition Metal Substitutions Dope Carriers in Iron Based Superconductors?¹, TOM BERLIJN, Brookhaven National Laboratory, CHAI-HUI LIN, Stony Brook University, WEI KU, Brookhaven National Laboratory — We investigate the currently debated issue concerning whether transition metal substitutions dope carriers in iron based superconductors. From first-principles calculations of the configuration-averaged spectral function [1,2] of BaFe_2As_2 with disordered Co/Zn substitutions of Fe , important doping effects are found beyond merely changing the carrier density. While the chemical potential shifts suggest doping of a large amount of carriers, a reduction of the coherent carrier density was found due to the loss of spectral weight. Therefore, none of the change in the Fermi surface, density of states, or charge distribution can be solely used for counting doped coherent carriers, let alone presenting the full effects of the disordered substitutions. Our study highlights the necessity of including disorder effects in the studies of doped materials in general. [1] W. Ku, T. Berlijn. and C.-C. Lee, Phys. Rev. Lett. 104, 216401 (2010) [2] T. Berlijn, D. Volja and W. Ku, Phys. Rev. Lett. 106, 077005 (2011)

¹Work supported by DOE DE-AC02-98CH10886 and DOE CMCSN

12:27PM Q22.00007 X-ray absorption spectroscopy study in the BaFe_2As_2 family, YOONYOUNG KOH, YEONGKWAN KIM, Yonsei university, WANLI YANG, Advanced Light Source, CHANGYOUNG KIM, Yonsei university — One of the representative Fe-based superconductor families, BaFe_2As_2 ($T_C \approx 38\text{K}$) is a semimetal with the same number of hole and electron carriers, and is in a spin density wave state below 139K. It has been reported that various types of “doped” BaFe_2As_2 systems can be obtained by substitution of Ba , Fe , and As atoms. However, an important issue has been recently raised regarding whether each type of substitution indeed induces effective charge doping or not. It is essential to clarify whether each type of substitution indeed induce an effective doping in BaFe_2As_2 system. To clarify the carrier doping issue, we performed high resolution X-ray absorption spectroscopy experiment on $\text{Ba}(\text{Fe}, \text{Co})_2\text{As}_2$, $\text{Ba}(\text{Fe}, \text{Ru})_2\text{As}_2$, $\text{BaFe}_2(\text{As}, \text{P})_2$ which are representative “doped” BaFe_2As_2 systems.

12:39PM Q22.00008 Competing Magnetic Phases in $\text{Ba}(\text{Fe}_{0.925}\text{Mn}_{0.075})_2\text{As}_2$ ¹, G.S. TUCKER, D.K. PRATT, M.G. KIM, S. RAN, A. THALER, Ames Laboratory and Department of Physics & Astronomy, Iowa State University, G.E. GRANROTH, K. MARTY, Oak Ridge National Laboratory, W. TIAN, J.L. ZARESTKY, S.L. BUD'KO, P.C. CANFIELD, A. KREYSSIG, A.I. GOLDMAN, R.J. MCQUEENEY, Ames Laboratory and Department of Physics & Astronomy, Iowa State University — Inelastic neutron scattering measurements on $\text{Ba}(\text{Fe}_{0.925}\text{Mn}_{0.075})_2\text{As}_2$ show broad, diffusive spin fluctuations at two different propagation vectors corresponding to stripe magnetic order and conventional Néel antiferromagnetic order. Below $T = 80\text{K}$ long-range stripe magnetic ordering occurs and sharp spin wave excitations appear at the stripe propagation vector while diffusive spin fluctuations remain at the Néel propagation vector. These results suggest that low concentrations of Mn dopants introduce a competing magnetic phase that may prevent the development of superconductivity in $\text{Ba}(\text{Fe}_{1-x}\text{Mn}_x)_2\text{As}_2$.

¹The work at the Ames Laboratory was supported by US DOE, Office of Basic Energy Sciences, DMSE, contract DE-AC02-07CH11358.

12:51PM Q22.00009 Infrared pseudogap in P- and Co-doped BaFe₂As₂ superconductors , S.J.

MOON, A.A. SCHAFFGANS, Department of Physics, University of California, San Diego, S. KASAHARA, Research Center for Low Temperature and Materials Science, Kyoto University, T. SHIBAUCHI, Department of Physics, Kyoto University, T. TERASHIMA, Research Center for Low Temperature and Materials Science, Kyoto University, Y. MATSUDA, Department of Physics, Kyoto University, M.A. TANATAR, R. PROZOROV, A. THALER, P.C. CANFIELD, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, A.S. SEFAT, D. MANDRUS, Materials Science and Technology Division, Oak Ridge National Laboratory, D.N. BASOV, Department of Physics, University of California, San Diego — We investigated the in-plane electronic response of P- and Co-doped BaFe₂As₂ compounds using infrared spectroscopy. We found hallmarks of the normal-state pseudogap in the optical spectra of the BaFe₂As₂ system, which are very similar with those of the cuprates. Based on the evolution of the electronic response with doping and across the superconducting transition, we suggest that the antiferromagnetic fluctuations can be a possible origin of the infrared pseudogap in the iron pnictides. We will also discuss implications of our results for the origin of the pseudogap in the cuprates.

1:03PM Q22.00010 Effects of disordered isovalent substitution in Fe-based superconductor¹

, LIMIN WANG, TOM BERLIJN, Brookhaven National Laboratory, YAN WANG, University of Florida, CHAI-HUI LIN, Stony Brook University, Brookhaven National Laboratory, P.J. HIRSCHFELD, University of Florida, WEI KU, Brookhaven National Laboratory, Stony Brook University — Using a recently developed first-principles method for disordered materials [1-2], we investigate the effect of isovalent substitution in Fe-based superconductors, BaFe₂(As_{1-x}P_x)₂, FeTe_{1-x}Se_x, and Ba(Fe_{1-x}Ru_x)₂As₂. For anion substitutions (the first two cases) effects of impurity scattering are found mostly in the anion bands. By contrast, the Ru substitution introduces much stronger scattering in the Fe bands. Surprisingly, in all the cases, the pockets near the chemical potential are the least affected, due to the low density of states near the chemical potential. Together, our results suggest an interesting scenario of enhancing superconductivity.

[1] T. Berlijn, D. Volja, W. Ku, Phys. Rev. Lett. 106, 077005 (2011).

[2] W.Ku, T. Berlijn, CC. Lee, Phys. Rev. Lett. 104, 216401 (2010).

¹Work supported by DOE DE-AC02-98CH10886 and DOE CMCSN

1:15PM Q22.00011 Electron Injection and “Oxygen Effect” in BaFe₂As₂: Mössbauer Studies

, AIRAT KHASANOV, University of North Carolina at Asheville, DING HU, XINGYE LU, HUIQIAN LUO, Institute of Physics, Academy of Sciences, Beijing, China, JIANYI JIANG, ERIC HELLSTROM, Florida State University, AMAR NATH, University of North Carolina at Asheville, MATERIALS RESEARCH LAB TEAM, HIGH FIELD LAB TEAM, BEIJING NATIONAL LABORATORY OF CONDENSED MATTER PHYSICS TEAM — It is widely believed that a few percent substitution of Co (with d7) or Ni (with d8) for Fe (with d6) in BaFe₂As₂ results in donation of electrons, killing of magnetism, and thereby induction of superconductivity. We are exploring the possibility of injecting electrons by physico-chemical techniques instead of substitutions. We have also discovered that traces of chemisorbed oxygen can change drastically the magnetic behavior in polycrystalline BaFe₂As₂ at low temperatures. BaFe₂As₂ exhibits considerable hysteresis behavior as well that of thermal history.

1:27PM Q22.00012 ABSTRACT MOVED TO Y22.00013 —

1:39PM Q22.00013 Effects of annealing on Ba(Fe_{1-x}Co_x)₂As₂ and Ba(Fe_{1-x-y}Co_xTM_y)₂As₂ (TM=Mn,Cr) single crystals¹ , ALEX THALER, SHENG RAN, Iowa State University/Ames Lab, ALFRED KRACHER, Retired, WARREN STRASZHEIM, JIA YAN, SERGEY BUD'KO, PAUL CANFIELD, Iowa State University/Ames Lab — Single crystals of Ba(Fe_{1-x-y}Co_xTM_y)₂As₂ (TM=Cr, Mn) have been grown and characterized by structural, magnetic and transport measurements, both in the as-grown state (quenched from ~ 1000° C) as well as after post-growth annealing. This phase space has many parameters and is rich and complex, with superconducting transition temperatures depending upon x and y, as well as annealing temperature and time. In this talk, we will present T-x and T-y, as well as T-time and T-T (for annealing) phase diagrams and discuss the implications for future research into these complex materials.

¹Work at the Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

1:51PM Q22.00014 Infrared conductivity of BaFe₂As₂ superconductors: Effects of in-plane and out-of-plane doping , R.P.S.M. LOBO, LPEM, ESPCI, CNRS, Paris, France, Y.M. DAI, B. XU, B. SHEN, H.H. WEN, X.G. QIU, IOP, Chinese Academy of Sciences, Beijing, China — We measured the *in-plane* optical conductivity of a nearly optimally doped (*T*_c = 39.1 K) single crystal of Ba_{0.6}K_{0.4}Fe₂As₂. Upon entering the superconducting state the optical conductivity vanishes below ~ 20 meV, indicating a fully gapped system. A model with two different isotropic gaps is required to describe the optical response of this material. The temperature dependence of the gaps indicate a strong interband interaction, but no impurity scattering induced pair breaking is present. This contrasts to the large residual conductivity observed in optimally doped Ba(Fe_{1-x}Co_x)₂As₂ and strongly supports an *s*_± gap symmetry for both compounds.

2:03PM Q22.00015 Ultrafast Probing of Antiferromagnetism and Dynamic Critical Behaviors in Iron Pnictide , TIANQI LI, AARON PATZ, SHENG RAN, SERGEY BUD'KO, PAUL CANFIELD, JIGANG WANG, Department of Physics and Astronomy and Ames Laboratory-USDOE, Iowa State University, DEPARTMENT OF PHYSICS AND ASTRONOMY AND AMES LABORATORY-USDOE, IOWA STATE UNIVERSITY COLLABORATION — Iron pnictide superconductors and their parent compounds exhibit superconductivity, antiferromagnetism, poor conductivity in undoped phase, structural instabilities, and additional peculiarities. Much of the complexity originates from strong interactions among the spin, charge, lattice degrees of freedom, where correlated excitations and self-organization among them occur and cause exotic cooperative behaviors. Time-resolved magneto-optical spectroscopy has been developed as a power tool to dynamically disentangle various degrees of freedoms by exploring their responses to fs photoexcitation. Using femtosecond optical and magneto-optical technique, we were able to measure and decoupling dynamics of AFM, structure and electronic excitations in parent BaFe₂As₂ and also underdoped sample (Co=4.7%). The technique demonstrated provides an extremely powerful tool to reveal fs dynamics and critical behaviors of various order parameters in the iron pnictide system.

Wednesday, February 29, 2012 11:15AM - 2:15PM —

Session Q23 DCMP: Superconductivity Theory III: Mainly Cuprates 255

11:15AM Q23.00001 Grand-canonical variational study for the Gutzwiller-projected BCS wave function , TING-KUO LEE, CHUNG-PIN CHOU, Institute of Physics, Academia Sinica, Nankang, Taipei 11529, Taiwan, FAN YANG, Department of Physics, Beijing Institute of Technology, Beijing PRC — We study the Gutzwiller-projected BCS wave function in the 2D extended t-J model using a variational Monte Carlo method. To take into account the effect of Gutzwiller projection, a fugacity factor proposed by Laughlin and Anderson has been included into the coherence factor of the BCS state. We show that the ground-state energy and excitation spectra calculated in the grand-canonical picture are essentially the same as previous results in the canonical scheme if the free energy is used for minimization. Except for La-214 materials, we find that the doping dependence of chemical potential is consistent with experimental findings on several cuprates. We have investigated the asymmetry of tunneling conductance observed by scanning tunneling spectroscopy becomes much stronger as decreasing doping. A very huge enhancement of phase fluctuation in the underdoped regime has been found.

11:27AM Q23.00002 Fluctuating Bond Model of cuprate superconductivity. , JENHAO HSIAO, NTHU, R.A. NISTOR, Columbia University, G.J. MARTYNA, D.M. NEWNS, C.C. TSUEI, IBM Watson Research Center — The fluctuating bond model(FBM), an empirical model based on a strong, local coupling of electrons to the square of the planar oxygen vibrator amplitudes, provides explanations of the d-wave pairing mechanism¹ and the pseudogap² of cuprate superconductivity. The d-wave pairing is mediated by the anharmonic phonon (planar oxygen vibrator) which is also responsible for the pseudogap when the C4 symmetry of the oxygen vibrator is broken. Here we present calculations of gap and T_c in a unitary framework involving pseudogap as a competing order parameter, with the help of ab initio simulations.

¹Nature phys. 3, 184-191 (2007)

²Phys. Rev. B 83, 144503 (2011)

11:39AM Q23.00003 d-wave superconductivity from correlated hopping interactions determined by angle-resolved photoemission spectroscopy¹ , CHUMIN WANG, CESAR G. GALVAN, Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, LUIS A. PEREZ, Instituto de Fisica, Universidad Nacional Autonoma de Mexico — Starting from a generalized Hubbard model, in which correlated-hopping interactions are considered in addition to the on-site repulsive Coulomb one, we solve numerically two coupled integral equations [1] within the Bardeen-Cooper-Schrieffer formalism, in order to quantify the doping effects on the critical temperature (T_c), d-wave superconducting gap, and the electronic specific heat. Within the mean-field approximation, we have determined the single and correlated electron hopping parameters for $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ compound by using angle-resolved photoemission spectroscopy (ARPES) data [2]. The resulting parametrized Hubbard model is able to explain the experimental T_c variation as a function of the doping level (x). In addition, the observed power-law behavior of the superconducting specific heat is reproduced by this correlated-hopping Hubbard model without adjustable parameters. [1] L.A. Pérez, J.S. Millán, C. Wang, *Int. J. Mod. Phys. B* **24**, 5229-5239 (2010). [2] T. Yoshida, *et al.*, *Phys. Rev. B* **74**, 224510 (2006).

¹This work has been partially supported by CONACyT-131596, UNAM-IN102511, UNAM-IN107411. Computations have been performed at Bakliz and KanBalam of DGTIC, UNAM.

11:51AM Q23.00004 Role of the charge reservoir layer in cuprate superconductors , THEODORE GEBALLE, SRINIVAS RAGHU, Stanford University — The high pressure measurements of Jorgensen *et al.*, which show that T_c increases as the apical oxygen distance from the CuO_2 plane decreases, is at odds with current theoretical predictions of T_c . Furthermore, the unusually close T_c (and similar NMR signatures) of Hg and TI based families of cuprates, in addition to the facts that their T_c is significantly higher than superconductors without charge reservoir layers (CRLs), suggest that CRLs play a significant role in determining T_c . Based on recent studies of S. Raghu *et al.* on the effects of longer ranged interactions on unconventional superconductivity, we discuss the possibility of the generic role that the CRLs may have in enhancing T_c by considering their role in screening short-range repulsive Coulomb interactions within the CuO_2 plane.

12:03PM Q23.00005 Phase separation instabilities and pairing modulations in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$, ARMEN KOCHARIAN, California State University, Los Angeles, CA 90032, KUN FANG, GAYANATH FERNANDO, KALUM PALANDAGE, University of Connecticut, Storrs, CT 06269, ALEXANDER BALATSKY, Theoretical Division, LANL, Los Alamos, NM 87545 — There is a growing evidence that the unconventional spatial inhomogeneities accompanied with the pairing of electrons, subsequent quantum phase transitions (QPTs), and condensation control coherent states in doped high- T_c cuprate superconductors, iron pnictide and telluride materials. We show that these superconducting states can be obtained from the phase separation instabilities near the quantum critical points. We examine electron coherent and incoherent pairing instabilities using our results on exact diagonalization in pyramidal and octahedron Hubbard-like clusters under variation of chemical potential (or doping), interaction strength, temperature and magnetic field. We also evaluate the dependence of the energy gap function in the vicinity of the sign change (nodes) as a function of position of the apical oxygen atom, due to vibration of apical atom and variation of inter-site coupling. The developed approach provides a simple microscopic explanation of (correlation) supermodulation of the coherent pairing gap observed recently in the scanning tunneling microscopy experiments at atomic scale in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$.

12:15PM Q23.00006 Pairing Correlations in the two-layer attractive Hubbard Model , ALEKSANDER ZUJEV, PINAKI SENGUPTA, Nanyang Technological University, RICHARD SCALETTAR, UC Davis — Quantum Monte Carlo (QMC) is used to study pairing correlations in a two-layer Hubbard Model in which one layer is attractive ($U < 0$), and the other uncorrelated ($U = 0$). We provide a detailed characterization of how superconductivity in the $U < 0$ layer induces pairing in the $U = 0$ layer, as a function of the interlayer hopping, density, temperature, and on-site attraction strength in the $U < 0$ layer. QMC data are complemented by calculations within the Bogoliubov - de Gennes approximation.

12:27PM Q23.00007 Pair-Density-Wave Superconducting Order in Two-Leg Ladders , AKBAR JAEFARI, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — We show, using bosonization and Renormalization Group methods, that Pair Density Wave (PDW) state happens in the system of two extended Hubbard-Heisenberg models on two leg ladders. Two different models are discussed in detail. In even legged ladder system we find that PDW state is the dominant instability for certain filling factors and some range of parameters. We show that phase diagram of the spin gap regime is composed of two dual phases: PDW and uniform Superconducting (SC) states. The phase transition between uniform SC and PDW in this model is shown to be in the Ising universality class. The idea has been generalized to the case of other commensurate fillings where we find higher order commensurate PDW states. Then we consider a two leg ladder system with nonzero flux Φ per plaquette. This system is commensurate for wide range of the electron fillings when $\Phi = \pi$. We show that commensurate PDW and incommensurate CDW are some of the phases present in the phase diagram of this model. We show how formation of PDW order in the ladder embodies the notion of intertwined orders.

12:39PM Q23.00008 Numerical Investigations of Spontaneous Orbital Currents in the Three-Orbital Hubbard Model¹, CHENG-CHIEN CHEN, ALEXANDER KEMPER, Stanford Institute for Materials and Energy Science, SLAC National Accelerator Laboratory, CHUNJING JIA, Department of Applied Physics, Stanford University, RONNY THOMALE, Department of Physics, Stanford University, THOMAS DEVEREAUX, Stanford Institute for Materials and Energy Science, SLAC National Accelerator Laboratory — Recent experiments show that the pseudogap regime of the cuprate superconductors could be characterized by a phase where the time-reversal symmetry is spontaneously broken but the translational symmetry remains intact. One possible but still highly disputed theory involves a circulating current looping around the Cu and O atoms. To address this issue, we perform large-scale exact diagonalization using a three-orbital Hubbard model on a Cu8O16 cluster. We find that the current-current correlations fall off quickly and show no signs of particular orbital current patterns. We also extend our calculations by adding explicitly a perturbative orbital current term into the Hamiltonian to study its experimental consequences. Using the magnetic moment measured in neutron scattering to constrain the strength of this perturbation, we compute the dichroic signals of various photon-spectroscopies to provide experimental benchmarks to test the existence of such a circulating current phase.

¹This work is supported by the U.S. DOE under contract number DE-AC02-76SF00515.

12:51PM Q23.00009 Momentum-Resolved d-wave Eliashberg Calculation Using The Spin Excitation Spectrum for LSCO Superconductors, SEUNG HWAN HONG, HAN-YONG CHOI, SungKyunKwan University — We solve the momentum resolved d-wave Eliashberg equation employing the magnetic excitation spectrum from the inelastic neutron scattering on the LSCO superconductors reported by Vignolle et al. [1]. The magnetic excitation spectrum exhibits 2 peaks: a sharp incommensurate peak at 18 meV at momentum $(\pi, \pi \pm \delta)$ and $(\pi \pm \delta, \pi)$, and another broad peak near 40~70 meV at momentum (π, π) . Above 70 meV, the magnetic excitation spectrum has a long tail that is shaped into a circle centered at (π, π) with δ' . The sign of the real part of the total self-energy $\Sigma(\vec{k}, \omega) + X(\vec{k}, \omega)$ is determined by the momentum position of the peaks of the magnetic excitation spectrum and bare dispersion $\xi(\vec{k})$. We will discuss the effects of the each component of the magnetic excitation spectrum on the self-energy $\Sigma(\vec{k}, \omega)$ the renormalization of the band dispersion $X(\vec{k}, \omega)$, the pairing function $\phi(\vec{k}, \omega)$, and the spectral function $A(\vec{k}, \omega)$.

[1] B.Vignolle et.al., Nature Physics 3,163-167 (2007)

1:03PM Q23.00010 Superconducting Instabilities in Electronic Liquid Crystal Phases, RODRIGO SOTO GARRIDO, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — We discuss the superconducting instabilities in a two dimensional fermionic system in uniform electronic liquid crystal phases which cause the Fermi surfaces (FS) to become distorted. We study the case of fermions in a time-reversal broken nematic-like state with $l = 3$ in the charge channel, and the $l = 2$ state in the spin channel. We discuss the competition between singlet and triplet superconducting states with pair density wave states.

1:15PM Q23.00011 Odd-frequency triplet pairing in mixed-parity superconductors¹, MARIO CUOCO, PAOLA GENTILE, CANIO NOCE, ALFONSO ROMANO, GAETANO ANNUNZIATA, CNR-SPIN, I-84084 Fisciano (Salerno), Italy and Dipartimento di Fisica E. R. Caianiello, Università di Salerno I-84084 Fisciano (Salerno), Italy, JACOB LINDER, Department of Physics, Norwegian University of Science and Technology, N-7491 Trondheim, Norway — We show that mixed-parity superconductors may exhibit equal-spin pair correlations that are odd-in-time and can be tuned by means of an applied field. The direction and the amplitude of the pair correlator in the spin space turn out to be strongly dependent on the symmetry of the order parameter, and thus provide a tool to identify different types of singlet-triplet mixed configurations. We suggest that odd-in-time spin-polarized pair correlations can be generated without magnetic inhomogeneities in superconducting/ferromagnetic hybrids with non-centrosymmetric superconductor or when parity mixing is induced at the interface. Paola Gentile, Canio Noce, Alfonso Romano, Gaetano Annunziata, Jacob Linder, Mario Cuoco, arXiv:1109.4885

¹The research leading to these results has received funding from the FP7/2007-2013 under the grant agreement No. 264098 - MAMA

1:27PM Q23.00012 Common Fermi-liquid origin of T₂ resistivity and superconductivity in n-type SrTiO₃, DIRK VAN DER MAREL, DOOK VAN MECHELEN, University of Geneva, IGOR MAZIN, Naval Research Laboratory — SrTiO₃ is a semiconductor which, when doped with a low density of electrons, becomes a good conductor with relatively high mobility and strong temperature dependence of the electrical resistivity and the infrared optical conductivity. At low temperatures the material becomes superconducting with a maximum reported T_c below 1 K with a dome-shaped doping dependence of T_c, both in the 3D bulk material and at the 2D LaAlO₃/SrTiO₃ interface. The DC resistivity below 100 K has a T² temperature dependence. The quasiparticles are in the anti-adiabatic limit with respect to electron-phonon interaction, which renders the interaction mediated through phonons effectively non-retarded. We apply Fermi-liquid theory for the T² term in the resistivity, and combine this with expressions for T_c and with the Brinkman-Platzman-Rice (BPR) sum-rule to obtain Landau parameters of n-type SrTiO₃. These parameters are comparable to those of liquid ³He, indicating interesting parallels between these Fermi-liquids despite the differences between the composite fermions from which they are formed.

1:39PM Q23.00013 Time Reversal Invariant Topological Superconductor in Rashba System, SHO NAKOSAI, Dept. of Appl. Phys., Univ. of Tokyo, YUKIO TANAKA, Dept. of Appl. Phys., Nagoya Univ., NAOTO NAGAOSA, Dept. of Appl. Phys., Univ. of Tokyo, CMRG & CERG, ASI, RIKEN — Recently, topological superconductors (TSCs) have been intensively studied as one of the topologically nontrivial phases. TSCs are characterized by topological numbers classified by their symmetries and dimensions. In the previous proposals on TSCs in Rashba systems, Zeeman splitting is necessary and therefore time reversal symmetry (TRS) is broken. We consider instead a bilayer Rashba system, e.g., a two-interface system, where hybridization causes a band gap. As for the single layer case, it has been shown experimentally that at the interface of SrTiO₃/LaAlO₃, two dimensional electron gas with Rashba spin-orbit interaction and superconductivity is formed. We find that the hybridization in bilayer system leads to topological phase without breaking TRS. This system belongs to the class characterized by Z₂ index. We obtain the conditions for odd-parity pair potentials by analyzing relations between strength of interactions and types of pair potentials. TSCs are attained in the case when the system has an odd-parity pair potential and the Fermi energy lies in the hybridization gap. We analytically calculate a topological number in a bulk system, and explicitly confirm the bulk-edge correspondence by performing numerical calculation in a finite system with edges.

1:51PM Q23.00014 Pairing Theories in Very High Magnetic Fields: Effects of Condensed and Non-condensed Pairs, PETER SCHERPELZ, DAN WULIN, KATHRYN LEVIN, James Franck Institute and Department of Physics, University of Chicago, ATTIPAT RAJAGOPAL, Inspire Institute — In this talk we focus on the interplay of pseudogap effects with high magnetic fields. Our work is built on reformulating the Gor'kov equations in the non-linear regime into a Landau level basis. Here we explore two distinct fermionic pairing schemes associated with the Abrikosov lattice in real and reciprocal space. We show how both have antecedents in the literature and both can be extended to accommodate non-condensed pairs. With this formulation, we can calculate quantities including the local density of states and H_{c2} in this regime. Importantly, both pairing theories yield gapless excitations which should be relevant to cuprate magneto-oscillatory experiments. The additional implications for the high field diamagnetic susceptibility are discussed.

2:03PM Q23.00015 Quantum oscillations in vortex-liquids¹, SUMILAN BANERJEE, SHIZHONG ZHANG, MOHIT RANDERIA, Department of Physics, The Ohio State University, Columbus, OH 43210 — Motivated by observations of quantum oscillations in underdoped cuprates [1], we examine the electronic density of states (DOS) in a *vortex-liquid* state, where long-range phase coherence is destroyed by an external magnetic field H but the local pairing amplitude survives. We note that this regime is distinct from that studied in most of the recent theories, which have focused on either a Fermi liquid with a competing order parameter or on a d -wave vortex lattice. The cuprate experiments are very likely in a resistive vortex-liquid state. We generalize the s -wave analysis of Maki and Stephen [2] to d -wave pairing and examine various regimes of the chemical potential, gap and field. We find that the $(1/H)$ oscillations of the DOS at the chemical potential in a d -wave vortex-liquid are much more robust, i.e., have a reduced damping, compared to the s -wave case. We critically investigate the conventional wisdom relating the observed frequency to the area of an underlying Fermi surface. We also show that the oscillations in the DOS cross over to a $\sqrt{H}$ behavior in the low field limit, in agreement with the recent specific heat measurements. [1] L. Taillefer, J. Phys. Cond. Mat. **21**, 164212 (2009). [2] M. J. Stephen, Phys. Rev. B **45**, 5481 (1992).

¹Supported by DOE-BES grant DE-SC0005035

Wednesday, February 29, 2012 11:15AM - 2:15PM – Session Q24 FIAP: Fractional Quantum Hall Effect II 256

11:15AM Q24.00001 Fractional Quantum Hall Effect of Rydberg-Polaritons, FABIAN GRUSDT, MICHAEL FLEISCHHAUER, Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, JOHANNES OTTERBACH, Physics Department, Harvard University, Cambridge, Massachusetts — Dark-state-polaritons (DSP) are bosonic quasiparticles arising in the interaction of light with 3-level atoms under conditions of electromagnetically induced transparency (EIT). They can be exposed to artificial magnetic fields, strong enough to enter the lowest Landau level regime [Otterbach et. al., Phys. Rev. Lett. **104** (2010)]. We take into account interactions between the DSPs via Rydberg dipole-dipole interactions and discuss the realization of the $\nu = 1/2$ -Laughlin state and its anyonic excitations (quasiholes) in such systems. The DSPs can be prepared in the correct total angular-momentum subspace by using orbital angular momentum light beams. A numerical and semi-analytical evaluation of the quasihole-gap is presented.

11:27AM Q24.00002 Compressible and incompressible phases in lattice fractional quantum Hall systems¹, SHUO YANG, KAI SUN, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, MD 20742 — We study lattice fractional quantum Hall (FQH) systems in the presence of local potential traps using the exact diagonalization technique. By implementing an array of local potential traps, we show that the system undergoes a series of phase transitions. As the strength of potential traps is increased, the FQH state turns into a compressible metallic state, and then into a topologically trivial insulator. We present the phase diagram as well as convincing numerical evidences which we use to identify these phases and phase transitions, including the energy spectrum, the fidelity metric, the Chern number, and the entanglement spectrum. In addition, we also compare the topological trivial insulator observed in our systems with Anderson insulators, which are expected in ordinary fractional quantum Hall systems in 2D electron gases in the presence of strong impurities.

¹This work is supported by DARPA-QuEST, Microsoft Q, and CNAM.

11:39AM Q24.00003 Tailoring Fabry-Perot Interferometers for Fragile Fractional Quantum Hall States¹, DOUGLAS MCCLURE, PATRICK GALLAGHER, CHARLES MARCUS, Harvard University, LOREN PFEIFFER, KEN WEST, Princeton University — Depending on the relevance of Coulomb interactions, electronic Fabry-Perot interferometers can exhibit two qualitatively different types of interference, each of which can shed light on the unique physics of quantum Hall systems. Long observed in the integer quantum Hall (IQH) regime, the so-called “Coulomb-dominated” interference has only recently been confirmed in the fractional quantum Hall (FQH) regime, where its observation has remained limited to the simplest and most robust FQH states. Building on our recent observation and analysis of this type of interference at several fractional filling factors, we report on interferometer design improvements yielding greater visibility, most notably for weaker FQH states. We find that parameters such as the distance from the gates defining the interferometer to the 2DEG, gate layout, and wafer structure affect the visibility much more in the FQH regime than in the IQH regime. High sensitivity to such parameters is also a characteristic of the second type of interference, believed to arise from a pure Aharonov-Bohm effect, which has been clearly observed only in the IQH regime; we discuss efforts to observe this behavior in the FQH regime.

¹We acknowledge funding from Microsoft Project Q, Harvard CNS, and DOE.

11:51AM Q24.00004 Multipartite wavefunctions for the second Landau level FQHE, SREEJITH GANESH JAYA, The Pennsylvania State University, ARKADIUSZ WÓJS, Wrocław University of Technology, CSABA TOKE, Institute of Physics, University of Pecs, Hungary, JAINENDRA JAIN, The Pennsylvania State University — We study the multipartite wave functions of composite fermions, in which the composite fermions within each partition are correlated differently than those across partitions. These include the Pfaffian wave function at $5/2$ and the Rezayi-Read wave function at $13/5$. Neutral and charged excitations of this state are modeled as neutral and charged excitations created in the individual partitions. We investigate how accurate these wave functions are for certain model three and four body interactions, and whether they are adiabatically connected to the Coulomb solutions. In particular, $5/2$ state for an odd number of particles, which contains at least one unpaired composite fermion, will be considered. We also test how multiple degeneracy arises in this model for quasiparticles and quasiholes.

12:03PM Q24.00005 Excitons in FQH states, MARIA HERMANNNS, Princeton University, THOMAS KVORNING, THORS HANS HANSSON, Stockholm University — Fractional quantum Hall (FQH) states are the first experimentally realized systems that exhibit topological order. For a full understanding of these systems it is crucial to be able to describe not only their ground states and quasihole excitations, but in fact the full low-energy sector. The lowest energy excitations are believed to be neutral quasihole-quasielectron pairs. We present a description of these excitations for a wide range of FQH states. Our method allows us to variationally change the model states without changing any of their topological properties.

12:15PM Q24.00006 Geometrical Description of fractional quantum Hall quasiparticles¹, YEJE PARK, BO YANG, F.D.M. HALDANE, Princeton University — We examine a description of fractional quantum Hall quasiparticles and quasiholes suggested by a recent geometrical approach (F. D. M. Haldane, Phys. Rev. Lett. **108**, 116801 (2011)) to FQH systems, where the local excess electric charge density in the incompressible state is given by a topologically-quantized “guiding-center spin” times the Gaussian curvature of a “guiding-center metric tensor” that characterizes the local shape of the correlation hole around electrons in the fluid. We use a phenomenological energy function with two ingredients: the shear distortion energy of area-preserving distortions of the fluid, and a local (short-range) approximation to the Coulomb energy of the fluctuation of charge density associated with the Gaussian curvature. Quasiparticles and quasiholes of the $1/3$ Laughlin state are modeled as “punctures” in the incompressible fluid which then relax by geometric distortion which generates Gaussian curvature, giving rise to the charge-density profile around the topological excitation.

¹Supported by DOE DE-SC0002140

12:27PM Q24.00007 Model wavefunctions for fractional quantum Hall collective modes¹, BO YANG, F.D.M. HALDANE, ZIXIANG HU, ZLATKO PAPIĆ, Princeton University — We examine the collective modes of primary fractional quantum Hall states which can be represented by Jack polynomial wavefunctions, in particular the $\nu = 1/3$ Laughlin and the $\nu = 1/2$ (or $5/2$) Moore-Read states. Using the extension of Jack Polynomial states (B. A. Bernevig and F. D. M. Haldane, Phys. Rev. Lett. 102, 066802 (2009)) to describe states with excited quasiparticles as well as quasiholes, we model the collective mode as a dipole formed by the combination of a single elementary quasiparticle with a single quasihole. In the Laughlin case, this neutral collective excitation is bosonic, while in the Moore-Read case, it has two forms, one bosonic and one fermionic. For small electric dipole moment (also small momentum and wavenumber) the (variational) energy of this mode lies above the threshold of the continuum of roton-pair (Laughlin) or neutral-fermion-pair (Moore-Read) excitations. In the long-wavelength limit the bosonic mode is a “spin-2” excitation that has an analogy to the “graviton” suggested by a recent geometric approach (F. D. M. Haldane, Phys. Rev. Lett. 108, 116801 (2011)) to FQH systems, while the neutral fermionic mode (present if the “odd-denominator rule” is violated) has “spin-3/2”, and has a possible analogy to the “gravitino”.

¹Supported by DOE DE-SC0002140

12:39PM Q24.00008 Determination of counter-propagating edge modes in the $\nu = 5/2$ fractional quantum Hall state, JENNIFER CANO, University of California, Santa Barbara, CHETAN NAYAK, University of California, Santa Barbara and Microsoft Station Q — Determining the wavefunction that describes the fractional quantum Hall state at $\nu = 5/2$ remains an unresolved question. Two main candidates are the Pfaffian and anti-Pfaffian states. A major difference between the two is the chirality of their neutral Majorana fermion modes, which in the former run parallel to the charged modes and in the latter, anti-parallel. We consider the recent experiment [Bid, A., et al. Nature, 466, 585-590 (2010)], in which counter-propagating, neutral edge modes in the $\nu = 5/2$ state were detected as a change in shot noise at an inter-edge quantum point contact (QPC) when current was injected at a point downstream of the QPC. We present a theoretical description of this experiment. We model the injection by coupling one edge to an external field and determine that the change in noise is incompatible with a parallel-propagating neutral mode. We also consider the injection as heat transfer to the neutral mode and reach the same conclusion. In agreement with experiment, these results are strong evidence in favor of any state with counter-propagating edge modes, such as the anti-Pfaffian, as a model for the $\nu = 5/2$ state.

12:51PM Q24.00009 Geometry of the fractional quantum Hall effect¹, F.D.M. HALDANE, Princeton University — Unlike the integer effect, the incompressible electron fluid that exhibits the fractional effect is *not* invariant under “area-preserving diffeomorphisms” of the guiding-center degrees of freedom. Instead (F. D. M. Haldane, Phys. Rev. Lett. 108, 116801 (2011)), it has a shear modulus that characterizes the energy cost of distortions of the correlation hole around the electrons, and a “guiding-center metric tensor” that exhibits quantum zero-point fluctuations around a preferred shape. In a simple (one-component) fluid, electronic charge-density fluctuations relative to the background set by the magnetic flux density are given by $\delta\rho = (e^*/2\pi)\bar{s}K$, where e^* is the elementary fractional charge, $\bar{s}$ is an integer or half-integer “guiding-center spin” that is topologically quantized by the Gauss-Bonnet theorem, and K is the local Gaussian curvature of the guiding-center metric. These results provide a simple explanation of the seminal 1985 results of Girvin, MacDonald and Platzman on the FQH structure factor and collective mode, which remained unexplained in previous proposed narrative explanations of FQH incompressibility (Ginzburg-Landau Chern-Simons theory, composite fermions, and non-commutative Chern-Simons field theory).

¹Supported by DOE DE-SC0002140

1:03PM Q24.00010 Microscopic nature of the backward propagating neutral edge modes of the “negative” flux FQHE states, YINGHAI WU, SREEJITH GANESH JAYA, JAINENDRA JAIN, The Pennsylvania State University — It is believed that FQHE states that require antiparallel vortex attachment, e.g. $2/3$, have neutral modes propagating in the backward direction. Recent experiments have observed signatures of such modes. We study the edge excitations of the fully spin polarized as well as spin singlet $2/3$ state both from exact diagonalization and from the microscopic composite fermion (CF) theory, to gain insight into the microscopic nature of the neutral edge modes. We investigate the validity of the CF theory for the edge modes, and also study the dependence on the form of the interaction and the background potential. We further evaluate the spectral weights and compare them with the predictions from the effective bosonic description.

1:15PM Q24.00011 Braiding statistics of the Gaffnian through the coherent state representation¹, JOHN FLAVIN, ALEXANDER SEIDEL, Washington University in St. Louis — Certain quantum Hall states have trial wave functions that can be connected to non-unitary conformal field theories, and arguments exist implying that such wave functions cannot describe gapped states. For these trial wave functions, the question arises whether braiding statistics may still be well defined through a formal Berry phase calculation. In essence, this corresponds to assuming an artificial gap to “non-zero modes” introduced by non-local terms in the Hamiltonian. The presence of long ranged correlations may still foil the emergence of well defined statistics. However, assuming that this is not the case, the question of what such statistics would be, and how they compare to those defined in terms of conformal block monodromies, can be analyzed using a recently developed coherent state Ansatz based on the thin torus limit. We report pertinent results for the Gaffnian state. Time and/or results permitting, we also present developments on the application of this method to a state by Thomale *et al.*, the associated conformal field theory of which is currently unknown. [References: S. Simon *et al.*, Phys. Rev. B 75, 075317 (2007), J. Flavin and A. Seidel, arXiv:1108.2734v1, N. Read, Phys. Rev. B 79, 045308 (2009)]

¹This work was supported by the National Science Foundation under NSF Grant No. DMR-0907793.

1:27PM Q24.00012 Gapless excitations in the Haldane-Rezayi state: The thin-torus limit¹, ALEXANDER SEIDEL, Department of Physics and Center for Materials Innovation, Washington University, St. Louis, MO 63130, USA, KUN YANG, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32306, USA — We study the thin-torus limit of the Haldane-Rezayi state. Eight of the ten ground states are found to assume a simple product form in this limit, as is known to be the case for many other quantum Hall trial wave functions. The two remaining states have a somewhat unusual thin-torus limit, where a “broken” pair of defects forming a singlet is completely delocalized. We derive these limits from the wave functions on the cylinder, and deduce the dominant matrix elements of the thin-torus hollow-core Hamiltonian. We find that there are gapless excitations in the thin-torus limit. This is in agreement with the expectation that local Hamiltonians stabilizing wave functions associated with non-unitary conformal field theories are gapless. We also use the thin-torus analysis to obtain explicit counting formulas for the zero modes of the hollow-core Hamiltonian on the torus, as well as for the parent Hamiltonians of several other paired and related quantum Hall states. [Reference: A. Seidel, K. Yang, PRB 84, 085122 (2011)]

¹This work was supported by the National Science Foundation under NSF Grant No. DMR-0907793 (AS) and NSF Grant No. DMR-1004545 (KY).

1:39PM Q24.00013 Dependence of pinning modes of 2D electron system on short-ranged alloy disorder , B.H. MOON, B.A. MAGILL, L.W. ENGEL, NHMFL/FSU, D.C. TSUI, L.N. PFEIFFER, K.W. WEST, Princeton University — A 2D electron system (2DES) in a low Landau filling (ν) pinned Wigner solid state exhibits a striking resonance in its rf or microwave spectrum. The resonance is understood as a pinning mode, in which the electrons oscillate about their pinned positions, and the frequency (f_{pk}) increases for larger disorder. We report on microwave spectroscopy of the low- ν Wigner solids in $\text{Al}_x\text{Ga}_{1-x}\text{As}-\text{Al}_{0.1}\text{Ga}_{0.9}\text{As}$ heterojunctions with $x=0.4$ and 0.8% . The 2DES resides mainly in the dilute $\text{Al}_x\text{Ga}_{1-x}\text{As}$, and the alloy disorder has been shown to be randomly distributed [1]. We compare the pinning modes of the samples as density (n , controlled by backgates) and magnetic field are varied. For example, with densities around $n \sim 6.5 \times 10^{10} \text{cm}^{-2}$ (in sample state with no indication of a $1/5$ fractional quantum Hall effect) $f_{pk} \approx 5.93$ and 8.55 GHz at $\nu \sim 0.2$ for $x=0.4$ and 0.8% respectively.

[1] W. Li *et al.*, Appl. Phys. Lett., 83, 2832 (2003).

1:51PM Q24.00014 Local Thermometry of Neutral Modes on the Quantum Hall Edge , SEAN HART, VIVEK VENKATACHALAM, Harvard University, LOREN PFEIFFER, KEN WEST, Princeton University, AMIR YACOBY, Harvard University — A system of electrons in two dimensions and strong magnetic fields can be tuned to create a gapped 2D system with one dimensional channels along the edge. Interactions among these edge modes can lead to independent transport of charge and heat, even in opposite directions. Measuring the chirality and transport properties of these charge and heat modes can reveal otherwise hidden structure in the edge. Here, we heat the outer edge of such a quantum Hall system using a quantum point contact. By placing quantum dots upstream and downstream along the edge of the heater, we can measure both the chemical potential and temperature of that edge to study charge and heat transport, respectively. We find that charge is transported exclusively downstream, but heat can be transported upstream when the edge has additional structure related to fractional quantum Hall physics.

2:03PM Q24.00015 Real Space Entanglement Spectrum of Fractional Hall States , EDWARD REZAYI¹, CSU Los Angeles, JEROME DUBAIL², NICHOLAS READ³, Yale University — The entanglement spectrum has been shown by Li and Haldane to provide a reliable tool to detect the topological order of Hall states. For example, bi-partitioning the system in orbital space produces the signature count of Hall edge states. The spectrum, however, appears to bear no resemblance to the linear spectrum conjectured by Kitaev and Preskill analogous to the actual edge mode dispersion. Here we employ two types of cuts: a real space and a modified particle bi-partitioning. On the sphere, we obtain the entanglement spectrum for the Laughlin, Moore-Read and Read-Rezayi states for both. We also consider the filled Landau level with a real space cut and show that the Laughlin state for $\nu=1/3$ has the same count of levels, which agrees with the chiral CFT (for up to $\Delta M = N/2$, $\Delta M = L_{\text{max}} - L_z$). Moreover, the entanglement spectrum of the Laughlin state approaches a linear spectrum, similar to the filled Landau level, as the size of the system increases.

¹supported by DOE grant no. DE-SC0002140

²Supported by Yale Postdoctoral Prize Fellowship

³Supported by NSF grant no. DMR-1005895

Wednesday, February 29, 2012 11:15AM - 2:03PM —
Session Q25 DCOMP GSCCM DMP: Focus Session: Simulation of Matter at Extreme Conditions - Phase Transitions 257A

11:15AM Q25.00001 Metallization of FeO at High Temperatures and Pressures: DFT-DMFT Computations and Comparisons with Experiments , R.E. COHEN, Geophysical Laboratory, Carnegie Institution, KRISTJAN HAULE, Dept. Physics, Rutgers University — DFT+Dynamical Mean Field Theory (DMFT) was applied to FeO as a function of pressure and temperature. We use an LAPW basis set, and the lattice terms are evaluated using the WIEN2K LAPW code. The impurity model is solved using continuous time quantum Monte Carlo (CTQMC). Temperature enters explicitly, so we made special efforts to understand high temperature behavior. The computations are fully self-consistent, including the impurity levels and crystal field splitting, and the total energy is evaluated using the full potential and charge density of the lattice plus impurity models. We find with increasing pressure in paramagnetic FeO in a cubic lattice and $U=8$ eV a high-spin low-spin transition, with a wide transition region between characterized by intermediate occupancies of the t_{2g} and e_g states between. We find that at 300K cubic FeO remains insulating to a factor of two compression (over 600 GPa), except for a small region of high spin metal. However, at high temperatures (e.g. 2000K) a metallic state is found. We find excellent agreement with recent high temperature high pressure experiments (Ohta et al.). We are now studying the antiferromagnetic ordering and effects of lattice strain.

11:27AM Q25.00002 ABSTRACT WITHDRAWN —

11:39AM Q25.00003 Finite-temperature solid phases and melting of denser lithium¹ , SABRI ELATRESH, Department of Physics, Dalhousie University, Halifax, NS, B3H 3J5, Canada, STANIMIR BONEV, Department of Physics, Dalhousie University, Halifax, NS, B3H 3J5, Canada; Lawrence Livermore National Laboratory, Livermore, California 94550 — There has been a lot of recent interest in lithium at high pressure, in particular, in relation to deviations from simple metallic behavior, non-intuitive structural changes, and its anomalous melting curve. Most of the theoretical studies have been limited to 0 K static lattices and liquid properties with classical ions. In this talk, we will present results for the stability of lithium up to 250 GPa and finite temperature, as well as its melting curve. Comparison with experimental measurements and the significance of quantum ion dynamics for the observed properties will be discussed.

¹Work supported by NSERC, Acenet, and LLNL under Contract DE-AC52-07NA27344.

11:51AM Q25.00004 Study on the release process of γ and α phase transition in cerium material , XIAOMIAN HU, HAO PAN, National Key Laboratory of Computational Physics, Institute of Applied Physics and Computational Mathematics, Beijing 100088, China, CHENGDA DAI, QIANG WU, Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, China Academy of Engineering Physics, Mianyang 621900, China, NATIONAL KEY LABORATORY OF COMPUTATIONAL PHYSICS, INSTITUTE OF APPLIED PHYSICS AND COMPUTATIONAL MAT TEAM, LABORATORY FOR SHOCK WAVE AND DETONATION PHYSICS RESEARCH, INSTITUTE OF FLUID PHYSICS, CHINA ACADEMY COLLABORATION — Cerium has lots of phase transition in high pressure and temperature. A volume change of about 15% occurs when Cerium is subject to high pressure (~ 0.7 GPa) and $\gamma \rightarrow \alpha$ phase change takes place. The phase transition and constitutive model of Cerium can be respectively obtained by calculating the experiment results and taking account of the multi-phase equation of state (EOS). The calculated results indicate that in loading condition the phase transition pressure of Cerium is higher than quasi-static compression. The calculated results indicate that the phase transition under release is difficultly described because the $\alpha \rightarrow \gamma$ phase reversal is great influenced by plastic flow. Based on multi-phase equation of state, constitutive model and non-equilibrium phase transition equation, introducing quasi-elastic unloading rule simulated the phase transition under release. The calculated result is according with the experiment.

12:03PM Q25.00005 Stability of dense liquid carbon dioxide¹, BRIAN BOATES, Lawrence Livermore National Laboratory, Dalhousie University, AMANUEL TEWELDEBERHAN, Lawrence Livermore National Laboratory, STANIMIR BONEV, Lawrence Livermore National Laboratory, Dalhousie University — We have used first-principles molecular dynamics to identify a transition from molecular liquid CO₂ to a new polymeric liquid phase under compression. The phase transition is first-order and unlike other such transitions, is not accompanied by metallization. The region near the liquid-liquid-solid triple point is particularly interesting as it coincides with pressure-temperature conditions inside the Earth's mantle. We have characterized the stability of CO₂ under these conditions; contrary to previous studies, our calculations show that CO₂ does not phase separate into carbon and oxygen. Comparisons with and alternative interpretations of previous measurements will be presented. Routes for experimental detection of our predictions will also be discussed.

¹Work supported by NSERC, LLNL, CFI, and Killam Trusts. Prepared by LLNL under Contract DE-AC52-07NA27344.

12:15PM Q25.00006 On the stability of body-centered cubic Fe at Earth's core conditions, VEKILOVA OLGA, SIMAK SERGEI, ABRIKOSOV IGOR, Linköping University, Linköping, Sweden — Elucidation of Earth's core content and structure is extremely important for understanding Earth's behavior influencing human life, from geodynamics to earthquakes. Though cosmochemical and geochemical studies strongly suggest that solid Fe is the main constituent of the inner core, its exact content and crystal structure are still a matter of debate. The recent experiments reported controversial results of phase stability. Dubrovinsky *et al.* showed stabilization of the body centered cubic (bcc) phase of Fe alloyed with 10 at. % of Ni at pressures above 225 GPa and temperatures over 3400 K [1]. Tateno *et al.* on pure Fe at up to 377 GPa and 5700 K, no bcc phase was observed [2]. We offer a resolution of this contradiction based on finite temperature first-principles molecular dynamics calculations of elastic properties of both bcc Fe and Fe₉₀Ni₁₀ alloy at high-temperature high-pressure conditions. We indicate the stability range for the bcc phase of high-pressure high-temperature Fe and show how experimental conditions may cause diverse phase stabilization. REFERENCES [1] L. S. Dubrovinsky *et al.* Body-centered cubic iron-nickel alloy in Earth's core. *Science* **316**, 1880-1883 (2007). [2] S. Tateno, K. Hirose, Y. Ohishi, Y. Tatsumi. The structure of iron in Earth's inner core. *Science* **330**, 359-361 (2010).

12:27PM Q25.00007 Thermoelastic Properties of Olivine and its High Pressure Polymorphs at High Pressures and Temperatures: A First-Principles Study¹, MARIBEL NÚÑEZ VALDEZ, School of Physics and Astronomy, University of Minnesota, ZHONGQIN WU, School of Earth and Space Sciences, University of Science and Technology of China, YOUNGGANG YU, Department of Chemical Engineering and Materials Science, University of Minnesota, RENATA WENTZCOVITCH, Department of Chemical Engineering and Materials Science, Minnesota Supercomputing Institute (MSI), University of Minnesota — We combine density functional theory (DFT) within the local density approximation (LDA), the quasi-harmonic approximation (QHA), and a model of vibrational density of states (VDoS) to calculate aggregate elastic moduli and sound velocities of olivine (α -phase) (Fe_xMg_{1-x})₂SiO₄, and its high pressure polymorphs, wadsleyite (β -phase) and ringwoodite (γ -phase), the most abundant minerals of the Earth's upper mantle (UM) and transition zone (TZ). Comparison of results with high-pressure and room-temperature data and ambient-pressure and high-temperature data shows very good agreement. Using our findings, we investigate the discontinuities in elastic moduli and velocities associated with the α to β and β to γ transformations at pressures and temperatures relevant to seismic discontinuities near 410 km and 520 km depth. This information offers clearly defined reference values to advance understanding of the role that chemical composition and temperature play in these mantle boundary layers.

¹Research supported by NSF/EAR-1019853 and EAR-0810272. Computations used the VLab cyberinfrastructure at the MSI

12:39PM Q25.00008 Fate of MgSiO₃ post-perovskite at multi-Mbar pressures¹, KOICHIRO UMEMOTO, University of Minnesota, SHUNQING WU, Iowa State University and Xiamen University, China, MIN JI, CAI-ZHUANG WANG, KAI-MING HO, Iowa State University, RENATA WENTZCOVITCH, University of Minnesota — The discovery of the post-perovskite (PPV) transition of MgSiO₃ in 2004 invited a new question: What would be the next phase transition from the PPV phase? The importance of this question has increased, since many terrestrial exoplanets with masses of a few to 10 times Earth's (super-Earth) have been recently discovered. Here we predict the new class of phase transitions of MgSiO₃ PPV under ultrahigh pressure by first-principles calculations combined with the adaptive genetic algorithm, which is a powerful tool for blind structural searches for systems with the large number of atoms. We discuss implications of these new phase transitions in modeling of interiors of terrestrial exoplanets.

¹KU, SQW, JM, CZW, and KMH was supported by the US Department of Energy, Basic Energy Sciences, Division of Materials Science and Engineering, under Contract No. DE-AC02-07CH11358/ KU and RMW was supported by NSF grants ATM-0426757 (VLab) and EAR-1047629.

12:51PM Q25.00009 Raman study of the Verwey transition in Magnetite at high-pressure and low-temperature; effect of Al doping¹, LEV GASPAROV, Z. SHIRSHIKOVA, T.M. PEKAREK, J. BLACKBURN, Department of Physics, University of North Florida, Jacksonville, FL, STRUZHUKIN, A. GAVRILIUK², Geophysical Laboratory, Carnegie Institution of Washington, Washington D.C., R. RUECKAMP, University of Cologne, Institute of Physics 2, Cologne, Germany, H. BERGER, Ecole Polytechnique Fédérale de Lausanne, Switzerland — We report high-pressure low-temperature Raman measurements of the Verwey transition in pure and Al-doped magnetite (Fe₃O₄) Al-doped magnetite Fe_{2.8}Al_{0.2}O₄ (T_V=116.5K) displays a nearly linear decrease of the transition temperature with an increase of pressure yielding dP/dT_V=-0.096±0.013 GPa/K. In contrast pure magnetite displays a significantly steeper slope of the PT equilibrium line with dP/dT_V = -0.18±0.013 GPa/K. Contrary to earlier high pressure resistivity reports we do not observe quantum critical point behavior at 8 GPa in the pure magnetite. Our data indicates that Al doping leads to a smaller entropy change and larger volume expansion at the transition. The trends displayed by the data are consistent with the mean field model of the transition that assumes charge ordering in magnetite.

¹Supported by NSF DMR0805073, DMR0958349, DMR0706593, ONR 000140610133, MaNEP of the Swiss NSF, Russian Fnd. for Basic Res. and Min. of Sc 090201527a, 110200291a, 11000636a, 16.518.11.7021

²Russian Academy of Sciences Institute for High Pressure Physics, Troitsk, and Institute of Crystallography, Moscow.

1:03PM Q25.00010 Magnetic and Thermal Fluctuations in Fe and (Fe,Ni) alloys at Earth Core Conditions¹, SUFIAN ALNEMRAT, BORIS KIEFER, New Mexico State University — Several lines of evidence suggest that the earth's inner core is dominated by an iron rich (Fe,Ni) alloy. In this study we address the influence of magnetic and thermal fluctuations as driving forces for phase transitions in Fe and Fe₇Ni structures at inner core pressure and temperature conditions. Bcc iron is stable at ambient conditions due to its ferromagnetic nature which highlights the importance of magnetism for structural stability. *Ab-initio* electronic structure calculations are used to study the thermal and magnetic fluctuations in Fe and (Fe,Ni) alloys up to pressures and temperatures expected in the earth's inner core. The variable cell shape molecular-dynamics simulations include the magnetic moment and thermal fluctuations. Our preliminary results show a phase transformation in hcp-Fe₇Ni alloy that occurs after 2.5 ps, well after equilibration. The correlation of magnetic and thermal fluctuations suggests that the residual magnetism is too weak to induce the observed transition. Instead, large thermal fluctuations at the onset of the transition provide a likely driving force.

¹The authors gratefully acknowledge funding from NSF through grant EAR-0636075.

1:15PM Q25.00011 Mechanism of body-centered cubic phase stabilization in Fe and He at high pressure and temperature, ANATOLY BELONOSHKO, KTH Royal Institute of Technology, Stockholm, Sweden, SERGIU ARAPAN, Uppsala University, Uppsala, Sweden, LOVE KOCL, AWA Patent AB, Stockholm, Sweden, ANDERS ROSENGREN, KTH Royal Institute of Technology, Stockholm, Sweden — We have investigated the stabilization of the body-centered cubic phase in Fe and He at high P and T by means of *ab initio* and classical molecular dynamics. These phases are dynamically unstable at high P and low T, however, they become dynamically stable at high T. We calculated the phonon density of states for Fe and He phases and observed that the bcc PDOS contains long-wavelength phonon states (absent in the close packed phases) that contribute to the free energy. This observation is consistent with the mechanism of stabilization proposed earlier (P. Loubeyre, J.-P. Hansen, PRB 31, 634 (1985); B. L. Holian et al., JCP 59, 5444 (1973)). Direct *ab initio* simulations of Fe crystallization and classical co-existence simulations for He indicate that the bcc phase is a submelting phase at high P. Previous calculations of the free energy in the bcc phase have been performed on small samples and could not adequately take the long-wavelength correlated motion into account.

1:27PM Q25.00012 ABSTRACT WITHDRAWN —

1:39PM Q25.00013 Computation of free energy of liquids and its application to melting of CO₂ and N¹, AMANUEL TEWELDEBRHAN, Lawrence Livermore National Lab, BRIAN BOATES, STANIMIR BONEV, Dalhousie University and Lawrence Livermore National Lab — A computationally efficient method is proposed to compute the free energy of liquids with accuracy comparable to *ab initio* thermodynamic integration. The method has been applied to predict melting curves of CO₂ and N over a wide range of pressure using the solid-liquid phase coexistence approach. The calculated melting lines are compared with available experimental data and the crossing of the geotherm and melting line of CO₂ is determined.

¹Work supported by LLNL, ACEnet, NSERC, and CFI. Prepared by LLNL under Contract DE-AC52-07NA27344.

1:51PM Q25.00014 Melting behaviour of high pressure Na. An *ab initio* study, DAVID J. GONZALEZ, Dpt Fisica Teorica, Universidad de Valladolid, Valladolid, LUIS E. GONZALEZ, Dpt Fisica Teorica, Universidad de Valladolid, Valladolid — The melting curve of sodium for a pressure range up to 120 GPa has been evaluated by the orbital free *ab initio* molecular dynamics method. This method uses the electronic density as the basic variable and scales almost linearly with system size which allows to perform simulations with a large number of particles and for long simulation times. For various pressures and temperatures we have calculated some static properties (pair distribution functions, static structure factors and short-range order parameters), dynamic properties (mean square displacement, velocity autocorrelation functions and dynamic structure factors) and transport coefficients (self-diffusion, adiabatic sound velocities and shear viscosities). The calculated melting curve reproduces the main qualitative features found in the experiment.

Wednesday, February 29, 2012 11:15AM - 2:15PM —

Session Q26 DCOMP: Focus Session: Computational Frontiers in Quantum Spin Systems I

257B

11:15AM Q26.00001 Computing Entanglement Entropy in Quantum Monte Carlo, ROGER MELKO, University of Waterloo — The scaling of entanglement entropy in quantum many-body wavefunctions is expected to be a fruitful resource for studying quantum phases and phase transitions in condensed matter. However, until the recent development of estimators for Renyi entropy in quantum Monte Carlo (QMC), we have been in the dark about the behaviour of entanglement in all but the simplest two-dimensional models. In this talk, I will outline the measurement techniques that allow access to the Renyi entropies in several different QMC methodologies. I will then discuss recent simulation results demonstrating the richness of entanglement scaling in 2D, including: the prevalence of the “area law”; topological entanglement entropy in a gapped spin liquid; anomalous subleading logarithmic terms due to Goldstone modes; universal scaling at critical points; and examples of emergent conformal-like scaling in several gapless wavefunctions. Finally, I will explore the idea that “long range entanglement” may complement the notion of “long range order” for quantum phases and phase transitions which lack a conventional order parameter description.

11:51AM Q26.00002 Scaling of entanglement entropy in the 2D Heisenberg ground state, ANN KALLIN, University of Waterloo, HYEJIN JU, University of California, Santa Barbara, PAUL FENDLEY, University of Virginia, Microsoft Station Q, MATTHEW HASTINGS, Duke University, Microsoft Station Q, ROGER MELKO, University of Waterloo — We use a Loop-Ratio Valence Bond quantum Monte Carlo algorithm to study the scaling of the bipartite Renyi entanglement entropy in the 2D Heisenberg ground state. We uncover the surprising result that finite-size scaling supports a logarithmic correction to the entropic area law even with the absence of corners in the entangled region. In addition, examining the scaling within a single system, we observe an aspect-ratio dependent scaling term resembling the “conformal distance” term that appears in one-dimensional systems with conformal symmetry.

12:03PM Q26.00003 Entanglement scaling of the 2D RVB wavefunction, HYEJIN JU, University of California, Santa Barbara, ANN KALLIN, University of Waterloo, PAUL FENDLEY, University of Virginia, Microsoft Station Q, MATTHEW HASTINGS, Duke University, Microsoft Station Q, ROGER MELKO, University of Waterloo — The resonating valence bond (RVB) state on a two-dimensional lattice is a superposition of all permutations of singlet spin pairs. This wavefunction was first proposed by Anderson as a simple spin liquid ground state, showing no long range order at T=0. Using a loop-algorithm Monte Carlo method that samples all nearest-neighbor singlet pairs, we examine the entanglement entropy of the nearest neighbor SU(2) RVB wavefunction on the square lattice. In addition to the area law, we show that the entanglement entropy splits into two branches, due to the different topological sectors of the RVB wavefunction. These branches individually scale with a logarithmic dependence on the size of the entangled region, the functional form of which appears to be similar to the conformal distance observed in scaling at conformal critical points in 1D. We comment on the implication for the search for topological order, and on generalizations of this wavefunction, including models involving SU(N) spins.

12:15PM Q26.00004 Entanglement entropy at the quantum critical point of the 2D transverse field Ising model, STEPHEN INGLIS, ROGER MELKO, University of Waterloo, RAJIV SINGH, University of California, Davis, ANDERS SANDVIK, Boston University — Entanglement entropy is a quantity that is desirable to examine at quantum critical points in condensed matter systems, because it is expected that sub-leading scaling terms should contain universal coefficients. In dimensions higher than one, these universal coefficients (that are sub-leading to the area law) may possibly be used to identify the universality class of the quantum critical point, much like the central charge in 1D systems. The recent development of zero temperature projector methods for the transverse field Ising model in combination with replica methods for stochastic series expansion quantum Monte Carlo (QMC) allows us to examine this idea, using measurements of Renyi entanglement entropies. We compare zero- and finite- temperature QMC results with series expansion, and discuss the scaling of the Renyi entropies at the 2D critical point in the transverse field Ising model.

12:27PM Q26.00005 Finite entanglement scaling at novel phase transitions in the Bose-Hubbard model with pairing terms

MICHAEL ZALETEL, ROGER MONG, JOEL MOORE, University of California, Berkeley — With the introduction of pair hopping, the 1+1D Bose-Hubbard model contains string like defects and half vortices in addition to the familiar vortices that drive the Kosterlitz - Thouless (KT) transition. Recent work [1] proposed the existence of a novel phase transition directly from the insulating to superfluid phase which is partly of an Ising, rather than KT type, contrary to expectations based on symmetry. To characterize the transition we demonstrate an approach to the study of 1+1D critical phenomena using infinite matrix product state algorithms (iMPS), in which critical fluctuations are cut off not by a finite system size, but by the finite entanglement of the iMPS ansatz. Starting from the “finite entanglement” scaling of the correlation length [2], we show that scaling and correlation functions also admit a universal “finite entanglement” collapse, avoiding boundary effects and validating an elegant alternative to finite size scaling methods for critical phases.

[1] Shi, Lamacraft and Fendley, arxiv:1108.5744v1

[2] Pollmann, Mukerjee, Turner and Moore, Phys. Rev. Lett. 102, 255701 (2009)

12:39PM Q26.00006 Renormalization of tensor-network states¹

TAO XIANG, HUI-HAI ZHAO, Institute of Physics, Chinese Academy of Sciences, ZHI-YUAN XIE, QIAO-NI CHEN, Institute of Theoretical Physics, Chinese Academy of Sciences, ZHONG-CHAO WEI, Institute of Physics, Chinese Academy of Sciences — We have discussed the tensor-network representation of classical statistical or interacting quantum lattice models, and given a comprehensive introduction to the numerical methods we recently proposed for studying the tensor-network states/models in two dimensions. A second renormalization scheme is introduced to take into account the environment contribution in the calculation of the partition function of classical tensor network models or the expectation values of quantum tensor network states. It improves significantly the accuracy of the coarse grained tensor renormalization group method. In the study of the quantum tensor-network states, we point out that the renormalization effect of the environment can be efficiently and accurately described by the bond vector. This, combined with the imaginary time evolution of the wave function, provides an accurate projection method to determine the tensor-network wave function. It reduces significantly the truncation error and enables a tensor-network state with a large bond dimension, which is difficult to be accessed by other methods, to be accurately determined.

¹This work was supported by the NSF-China and the National Program for Basic Research of MOST, China.

12:51PM Q26.00007 Cluster update for tensor network states¹

LING WANG, FRANK VERSTRAETE, Faculty of Physics, University of Vienna, IQI TEAM — We propose a novel recursive way of updating the tensors in projected entangled pair states by evolving the tensor in imaginary time evolution on clusters of different sizes. This generalizes the so-called simple update method of Jiang et al. [Phys. Rev. Lett. 101, 090603 (2008)] and the updating schemes in the single layer picture of Pizorn et al. [Phys. Rev. A 83, 052321 (2011)]. A finite-size scaling of the observables as a function of the cluster size provides a remarkable improvement in the accuracy as compared to the simple update scheme. We benchmark our results on the hand of the spin 1/2 staggered dimerized antiferromagnetic model on the square lattice, and accurate results for the magnetization and the critical exponents are determined. Reference L. Wang and F. Verstraete, arXiv:1110.4362.

¹This project is supported by the EU Strep project QUEVADIS, the ERC grant QUERG, and the FWF SFB grants FoQuS and ViCoM.

1:03PM Q26.00008 The spin 1/2 J1-J2 Antiferromagnetic Heisenberg model on Square Lattice

FRANK VERSTRAETE, LING WANG, Faculty of Physics, University of Vienna, ZHENG-CHENG GU, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, XIAO-GANG WEN, Department of Physics, Massachusetts Institute of Technology, ANDERS SANDVIK, Department of Physics, Boston University, VERSTRAETE'S GROUP COLLABORATION, WEN'S GROUP COLLABORATION, SANDVIK'S GROUP COLLABORATION — We studied the spin 1/2 J1-J2 Heisenberg antiferromagnets on square lattice using the recently proposed cluster update for tensor network states [arXiv:1110.4362]. Ground state wavefunction with tensor network bond dimension upto $D = 9$ was obtained. Through a finite size scaling analysis, we observe a second order phase transition from an antiferromagnetic ordered state to a paramagnetic phase with plaquette valence bond order at a coupling constant ratio $J_2/J_1 \approx 0.44$. The ground state energies in the thermodynamic limit are in the order of $10^{-3} J_1$ per site difference from the state of art exact diagonalization study [Eur. Phys. J. B 73, 117 (2010)].

1:15PM Q26.00009 The spin-1/2 $J_1 - J_2$ Heisenberg antiferromagnet on a square lattice: a plaquette renormalized tensor network study¹

YING-JER KAO, JI-FENG YU, Department of Physics, National Taiwan University — We apply the plaquette renormalization scheme of tensor network states [Phys. Rev. E, 83, 056703 (2011)] to study the spin-1/2 frustrated Heisenberg J_1 - J_2 model on an $L \times L$ square lattice with $L=8, 16$ and 32 . By treating tensor elements as variational parameters, we obtain the ground states for different J_2/J_1 values, and investigate staggered magnetizations, nearest-neighbor spin-spin correlations and plaquette order parameters. In addition to the well-known Néel-order and collinear-order at low and high J_2/J_1 , we observe a plaquette-like order at $J_2/J_1 \approx 0.5$. A continuous transition between the Néel order and the plaquette-like order near $J_2^{c1} \approx 0.40 J_1$ is observed. The collinear order emerges at $J_2^{c2} \approx 0.62 J_1$ through a first-order phase transition.

¹This work was partly supported by the NSC in Taiwan through Grants No. 100-2112-M-002 -013 -MY3, 100-2120-M-002-00

1:27PM Q26.00010 MERA Study of Spatially Anisotropic Triangular Antiferromagnets

KENJI HARADA, Graduate School of Informatics, Kyoto University, Japan, NAOKI KAWASHIMA, Institute for Solid State Physics, University of Tokyo, Japan — We report variational calculations for the ground states in the spatially anisotropic triangular antiferromagnets. The variational wave function is based on the tensor network with an entanglement renormalization [1]. The entanglement renormalization improves the ability of describing a quantum state. We construct a three-dimensional MERA tensor network for the triangular lattice models. The model in this study has two groups of the antiferromagnetic Heisenberg couplings on a triangular lattice: one on links along a lattice axis and the other on other links. J_1 and J_2 denote the coefficient of their couplings, respectively. We calculate the ground states of finite lattices ($N = 114, 2166$) and an infinite lattice. We confirm a magnetic phase in the region of $0.7 < J_2/J_1 \leq 1$. The magnetic structure is incommensurate, and the wave vector is not consistent with that of a classical model except for $J_1 = J_2$.

[1] G. Vidal, Phys. Rev. Lett. 99, 220405 (2007).

1:39PM Q26.00011 General framework of non-Abelian $SU(N)$ symmetries for matrix product states, ANDREAS WEICHSELBAUM, JAN VON DELFT, Ludwig Maximilians University, Munich, Germany — We present a generic numerical framework for the treatment of an arbitrary set of non-abelian quantum symmetries within the matrix product states (MPS) approach and generalization thereof. The framework is based on the simple observation that Clebsch Gordan coefficient spaces can be split off as tensor products for all objects relevant within MPS [1]. As such it is applicable, for example, to the numerical as well as the density matrix renormalization group (NRG or DMRG, respectively). The framework is applied to a generalized $SU(3)$ channel-symmetric Anderson impurity model within the NRG. This model of a fully screened spin $S = \frac{3}{2}$ Anderson model has been suggested recently as the effective microscopic Kondo model for Fe impurities in gold or silver [2]. Results are presented on the explicit treatment of $U(1) \otimes SU(2) \otimes SU(3)$ for charge, spin, and channel, respectively. This is compared to the alternative description in terms of $SU(2)^{\otimes 4}$ symmetries for total spin and particle-hole symmetry in every channel.

[1] Singh et al, PRA **82**, 050301 (2010)

[2] Costi et al, PRL **102**, 056802 (2009).

1:51PM Q26.00012 Reducing Memory Cost of Exact Diagonalization using Singular Value Decomposition, MARVIN WEINSTEIN, SLAC National Accelerator Laboratory, RAVI CHANDRA, ASSA AUERBACH, Technion, Haifa — We present a modified Lanczos algorithm to diagonalize lattice Hamiltonians with dramatically reduced memory requirements. In contrast to variational approaches and most implementations of DMRG, Lanczos rotations towards the ground state do not involve incremental minimizations, (e.g. sweeping procedures) which may get stuck in false local minima. The lattice of size N is partitioned into two subclusters. At each iteration the rotating Lanczos vector is compressed into two sets of n_{svd} small subcluster vectors using singular value decomposition. For low entanglement entropy S_{ee} , (satisfied by short range Hamiltonians), the truncation error is bounded by $\exp(-n_{\text{svd}}^{1/S_{ee}})$. Convergence is tested for the Heisenberg model on Kagomé clusters of 24, 30 and 36 sites, with no lattice symmetries exploited, using less than 15GB of dynamical memory. Generalization of the Lanczos-SVD algorithm to multiple partitioning is discussed, and comparisons to other techniques are given. Reference: arXiv:1105.0007

2:03PM Q26.00013 An efficient basis for the modeling of doped and undoped $S=1/2$ antiferromagnet¹, BAYO LAU, Department of Physics, Columbia University, NY, NY, MONA BERCIU, GEORGE A. SAWATZKY, Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia, V6T 1Z1 — We formulate an efficient numerical basis to model both doped and undoped $S=1/2$ Heisenberg antiferromagnet (AFM) with two-dimensional periodic boundary condition (2DPBC). Using a linear combination of Slater determinants with total-spin symmetries, a variational approach is developed to systematically and combinatorially decreases the Hilbert space of the problems, allowing the application of exact diagonalization to record-breaking system sizes. We can now model explicitly the wavefunction of an undoped 64-spin AFM square lattice with 2DPBC. For the doped scenarios, we solve a half-filled lattice with 32 coppers and 64 oxygens with one or two electrons removed. This allows, for the first time, a direct comparison of 32-unit-cell exact diagonalization between multi-band model and the t-J model, quantifying several oxygen-specific properties relevant to the lightly doped cuprate structures.

¹This work is funded by CFI, CIFAR, CRC and NSERC. Part of the computation was performed on the Westgrid.

Wednesday, February 29, 2012 11:15AM - 2:15PM –
Session Q27 DCMP: Invited Session: DCMP Prize Session: Buckley, Isakson, MGM 258AB

11:15AM Q27.00001 Oliver E. Buckley Condensed Matter Prize Lecture: Topological Insulators¹, CHARLES KANE, University of Pennsylvania — A topological insulator is a material that is an insulator on its interior, but has special conducting states on its surface. These surface states are unlike any other known two dimensional conductor. They are characterized by a unique Dirac type dispersion relation and are protected by a topological property of the material's underlying electronic band structure. In this talk we will outline our path to the theoretical discovery of this phase and describe the physical properties of the two dimensional topological insulator - also known as a quantum spin Hall insulator - as well as its three dimensional generalization. We will then go on to discuss more recent developments, including the topological classification of point and line defects in topological insulators and superconductors. The latter may provide a venue for observing Majorana fermion states and for realizing proposals for topological quantum computation.

¹Supported by NSF grant DMR-0906175.

11:51AM Q27.00002 HgTe as a Topological Insulator, LAURENS W. MOLENKAMP, Physics Institute(EP3), Wuerzburg University — HgTe is a zincblende-type semiconductor with an inverted band structure. While the bulk material is a semimetal, lowering the crystalline symmetry opens up a gap, turning the compound into a topological insulator. The most straightforward way to do so is by growing a quantum well with (Hg,Cd)Te barriers. Such structures exhibit the quantum spin Hall effect, where a pair of spin polarized helical edge channels develops when the bulk of the material is insulating. Our transport data provide very direct evidence for the existence of this third quantum Hall effect, which now is seen as the prime manifestation of a 2-dimensional topological insulator. To turn the material into a 3-dimensional topological insulator, we utilize growth induced strain in relatively thick (ca. 100 nm) HgTe epitaxial layers. The high electronic quality of such layers allows a direct observation of the quantum transport properties of the 2-dimensional topological surface states.

12:27PM Q27.00003 Oliver E. Buckley Condensed Matter Prize Lecture: Topological insulators and superconductors¹, SHOUCHENG ZHANG, Stanford University — In this talk I shall briefly review the basic concepts of topological insulators and superconductors, and recall the history of the discovery of the first topological insulator in nature, the HgTe material. I will then describe some striking physical properties of topological insulators and their possible applications.

X. L. Qi, S. C. Zhang, Phys. Today **63**, 33 (2010).

X. L. Qi, S. C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011).

¹Work supported by the Department of Energy, the National Science Foundation, Darpa, ARO and the Keck Foundation

1:03PM Q27.00004 Frank Isakson Prize for Optical Effects in Solids Lecture: Infrared nano-spectroscopy and nano-imaging of Dirac plasmons in graphene, DMITRI BASOV, UCSD — We have applied antenna-based infrared (IR) nano-spectroscopy and nano-imaging to investigate Dirac plasmons in monolayer graphene. This experimental technique enables IR imaging with nano-scale spatial resolution, and also allows one to investigate electromagnetic phenomena at wave-vectors on the order of the Fermi wave-vector in gated graphene. Nano-spectroscopy and nano-imaging experiments have uncovered rich optical effects associated with the Dirac plasmons of graphene [Fei *et al.* *Nano Letters* 2011]. We were able to directly image Dirac plasmons propagating over sub-micron distances and reflecting from the edges of graphene flakes, all with a spatial resolution far exceeding the plasmon wavelength. Furthermore, we employed new IR nano-optics capabilities to demonstrate the gate-tunable plasmonic properties of graphene and to investigate the coupling between Dirac plasmons and the phonon modes of polar substrates.

1:39PM Q27.00005 Maria Goeppert Mayer Award Lecture: Spectroscopy of Hybrid Superconductor-Carbon Nanostructure Systems, NADYA MASON, University of Illinois at Urbana-Champaign — The electronic properties of carbon nanotubes and graphene have excited much interest, for both fundamental science and technological applications. In this talk, I will discuss how coupling superconductors to these carbon nanostructures can enable new spectroscopic tools. In particular, I will discuss our experiments demonstrating that superconducting probes on carbon nanotube quantum dots can enhance weak spectroscopic features. I will also show how superconducting tunnel probes enable direct measurements of electron-electron interactions in carbon nanotubes. Finally, I will present data showing that connecting graphene to superconductors allows for the spectroscopy of individual, tunable superconducting (Andreev) bound states.

Wednesday, February 29, 2012 11:15AM - 2:15PM – Session Q28 FIAP: Applications of Semiconductors, Dielectrics, Complex Oxides 258C

11:15AM Q28.00001 Anatomy of a Nanoscale Conduction Channel Reveals the Mechanism of a High-Performance Memristor, FENG MIAO, JOHN PAUL STRACHAN, J. JOSHUA YANG, WEI YI, ILAN GOLDFARB, M.-X. ZHANG, ANTONIO C. TORREZAN, Hewlett-Packard Laboratories, Palo Alto, CA, PETER ESCHBACH, RONALD D. KELLEY, Hewlett-Packard, Corvallis, OR, GILBERTO MEDEIROS-RIBEIRO, R. STANLEY WILLIAMS, Hewlett-Packard Laboratories, Palo Alto, CA — Two major challenges for resistance memory devices (memristors) based on conductivity changes in oxide materials are better performance and understanding of the microscopic picture of the switching. After researchers' relentless pursuit for years, tantalum oxide-based memristors have rapidly risen to be the top candidate, showing fast speed, high endurance and excellent scalability. While the microscopic picture of these devices remains obscure, by employing a precise method for locating and directly visualizing the conduction channel, here we observed a nanoscale channel consisting of an amorphous Ta(O) solid solution surrounded by crystalline Ta₂O₅. Structural and chemical analyses of the channel combined with temperature dependent transport measurements revealed a unique resistance switching mechanism: the modulation of the channel elemental composition, and thus the conductivity, by the cooperative influence of drift, diffusion and thermophoresis, which seem to enable the high switching performance observed. (Miao*, Strachan*, Yang* *et al.*, *Advanced Materials*. DOI: 10.1002/adma.201103379 (2011))

11:27AM Q28.00002 Low-frequency noise properties in nanodiodes, SHAHRIR R. KASJOO, CLAUDIO BALOCCO, ARUN K. SINGH, LINQING Q. ZHANG, YASAMAN ALIMI, AIMIN M. SONG, School of Electrical and Electronic Engineering, University of Manchester, Manchester M13 9PL, United Kingdom — Terahertz (THz) detection by a novel type of unipolar nanodiodes, known as self-switching diodes (SSDs), has recently been demonstrated at room temperature up to 1.5 THz (App. Phys. Lett. Vol. 98, 223501, 2011). Since noise property is also of great importance for THz detection, here we have fabricated thousands of SSDs connected in parallel in order to increase the signal-to-noise ratio. Because of the planar nature of the SSDs, no specific metal interconnects are needed, and hence the device speed and voltage sensitivity are unaffected. We study the low-frequency noise spectra and noise equivalent power (NEP) at room and elevated temperatures. The exceptional possibility for the SSD to have an intrinsic zero threshold voltage enables very low noise at frequencies below 1 kHz, without being much affected by $1/f$ noise. We find that the NEP is comparable to the commercial Schottky diode detector. The activation energy extracted from the temperature dependence is approximately 0.27 eV, which we will compare with the barrier height in the SSD channel as well as the conduction band offset in the InGaAs/InAlAs structure used in this work. We show evidence that the observed $1/f$ noise properties at room and elevated temperatures seem to support Hooge's mobility fluctuation theory.

11:39AM Q28.00003 Understanding the resistive switching in thin-film Ta-O memristors by their d.c. switching characteristics, WEI YI, GILBERTO MEDEIROS-RIBEIRO, FENG MIAO, ILAN GOLDFARB, MAX ZHANG, J. JOSHUA YANG, MATTHEW D. PICKETT, JOHN PAUL STRACHAN, R. STANLEY WILLIAMS, Hewlett-Packard Laboratories, 1501 Page Mill Road, MS1123, Palo Alto, CA 94304, USA, HEWLETT-PACKARD LABORATORIES TEAM — Tantalum oxide (Ta-O) memristor is a promising candidate for resistive switching memory (RRAM) technology as they have demonstrated outstanding features such as high endurance, high speed, and low power. However, the responsible mechanisms remain vague partly due to difficulties in characterizing the amorphous film structure, nanoscale active regions, coupled ionic and electronic transport, and intertwined electrochemical and thermochemical processes. Rich information about Ta-O memristors has been revealed by microscopic structural and chemical characterizations of Ta-O conduction channels combined with temperature-dependent transport measurements. As an alternative approach, we took perspectives from a statistical study of the switching behavior under d.c. excitation. We identified distinctive behaviors in device switching characteristics depending on the chemical compositions of conductance channel, and found close correlations with previous temperature-dependent transport measurements and X-ray photoemission (XPS) characterizations. We were able to gather further insight into the microscopic switching mechanisms based on these observations, revealing the granularity of the switching phenomena.

11:51AM Q28.00004 *In-situ* MBE and ALD deposited HfO₂ on In_{0.53}Ga_{0.47}As¹, W.C. LEE, C.A. LIN, M.L. HUANG, J. KWO, Dept. Phys., Natl Tsing Hua Univ., Hsinchu 30013, Taiwan, Y.H. CHANG, P. CHANG, Dept. Mat. Sci. and Eng., Natl Tsing Hua Univ., Hsinchu 30013, Taiwan, T.D. LIN, M. HONG, Dept. Phys., Natl Taiwan Univ., Taipei 10617, Taiwan — The semiconductor industry is calling for innovative devices offering high performance with low power consumption. High- κ dielectrics/metal gates on high carrier mobility channels are now strong contenders in the post Si CMOS application. Hafnium-based oxide has been employed as the gate dielectric in Si CMOS since 45 nm node and InGaAs is a leading candidate for channel materials. However, reports of HfO₂ on InGaAs are scant, and surface treatments using H₂S or trimethylaluminum are claimed to be required for achieving high quality HfO₂(high- κ)/InGaAs interface. In this work, HfO₂ has been *in-situ* deposited on *n*- and *p*-In_{0.53}Ga_{0.47}As using both molecular-beam-epitaxy (MBE) and atomic-layer-deposition (ALD), without using any interfacial passivation layer or surface treatments. The HfO₂/In_{0.53}Ga_{0.47}As metal-oxide-semiconductor capacitors (MOSCAPs) all exhibit outstanding thermal stabilities ($> 800^{\circ}\text{C}$), low leakage currents ($\sim 10^{-8}$ A/cm² at 1 MV/cm), and good CV characteristics. Moreover, the MOSCAPs have shown spectra of interfacial trap densities (D_{it} 's) with no discernible peaks at mid-gap, confirmed by temperature-dependent conductance method.

¹This work has been supported by Nano National Program (NSC 100-2120-M-007-010) of the NSC of Taiwan, and the AOARD of the US Air Force.

12:03PM Q28.00005 *In-situ* photoemission analyses of ALD-oxide/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ (001) interfaces

, M.L. HUANG, Dept. Phys., Natl Tsing Hua Univ., Hsinchu, Taiwan, Y.H. CHANG, Dept. Mat. Sci. and Eng., Natl Tsing Hua Univ., Hsinchu, Taiwan, T.D. LIN, Dept. Phys., Natl Taiwan Univ., Taipei, Taiwan, W.C. LEE, Dept. Phys., Natl Tsing Hua Univ., Hsinchu, Taiwan, T.H. CHIANG, Dept. Mat. Sci. and Eng., Natl Tsing Hua Univ., Hsinchu, Taiwan, C.A. LIN, H.Y. LIN, Dept. Phys., Natl Tsing Hua Univ., Hsinchu, Taiwan, T.-W. PI, Natl Synchrotron Rad. Res. Ctr, Hsinchu, Taiwan, M. HONG, Dept. Phys., Natl Taiwan Univ., Taipei, Taiwan, J. KWO, Dept. Phys., Natl Tsing Hua Univ., Hsinchu, Taiwan — High- κ dielectrics on high carrier mobility channels, such as $\text{In}_x\text{Ga}_{1-x}\text{As}$, are now being considered for CMOS technology beyond 15 nm node. The initial bonding of high- κ /InGaAs determines the value and the distribution of interfacial density of states (D_{it}) within the $\text{In}_x\text{Ga}_{1-x}\text{As}$ band gap, key to the device performance. In this work, atomic layer deposited (ALD) HfO_2 and Al_2O_3 on MBE-grown $\text{In}_x\text{Ga}_{1-x}\text{As}$ (001) have been *in-situ* and *ex-situ* carried out to investigate the initial stage of interfacial reactions by high resolution photoemission spectroscopy using synchrotron radiation and monochromatic Al K α x-ray sources. Comparing the results with the corresponding electrical measurements (C-V and G-V at various temperatures), Fermi level unpinning in the oxide/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ hetero-structure may be attributed to the exclusion of the As-As and the As-O bonding during the initial interfacial formation.

12:15PM Q28.00006 High Temperature Seebeck Coefficient and Electrical Resistivity of $\text{Ge}_2\text{Sb}_2\text{Te}_5$ Thin Films

, LHACENE ADNANE, FARUK DIRISAGLIK, MUSTAFA AKBULUT, University of Connecticut, YU ZHU, CHUNG LAM, IBM T. J. Watson Research Center, ALI GOKIRMAK, HELENA SILVA, University of Connecticut — Phase-change memory (PCM) is a promising memory technology in which a small volume of a chalcogenide material can be reversibly and rapidly switched between amorphous and crystalline phases by an electrical pulse that brings it above crystallization (~ 150 -200 C) or melting (~ 700 C) temperature. The large temperature levels involved and small dimensions of PCM devices give rise to very large temperature gradients (~ 10 K/nm and higher) which result in strong thermoelectric effects. High-temperature characterization of the temperature-dependent thermoelectric properties of these materials is therefore critical to understand for the operation of these devices but to date there is only limited experimental data available. We have performed simultaneous measurements of Seebeck coefficient and electrical resistance of thin films of GST with different thicknesses, deposited on silicon dioxide, from room temperature to ~ 600 C, under small temperature gradients. Two-point current-voltage (I-V) measurements were performed using a semiconductor parameter analyzer. The resistance of the material and the Seebeck voltage (open-circuit voltage) are calculated from the slope and intercept of the I-V characteristics. The details of the measurements and S(T) and R(T) results for the GST thin film samples will be presented and discussed.

12:27PM Q28.00007 Thermoelectric Effects in Simulations of Phase Change Memory Mushroom Cells

, AZER FARACLAS, GOKHAN BAKAN, ALI GOKIRMAK, HELENA SILVA, University of Connecticut — Phase change memory is a potential candidate for the future of high-speed non-volatile memory, however significant improvements in cell design is crucial for its success in the mainstream market. Due to the asymmetric geometry of phase change mushroom cells and the high temperature gradients generated, thermoelectric effects play a key role in determining energy consumption, cell performance, and reliability. In this study, rotationally symmetric 2D finite element simulations using COMSOL Multiphysics are implemented for GeSbTe (GST). Temperature dependent material parameters (electrical conductivity, thermal conductivity, heat capacity, and Seebeck coefficient) are included in the model for accuracy. Switching the direction of current shows a large change in peak molten volume within the cell, as well as current and power consumption.

12:39PM Q28.00008 Light-controlled plasmon switching using hybrid metal-semiconductor nanostructures¹

, HARI PAUDEL, MICHAEL LEUENBERGER, University of Central Florida — We show a method for the dynamic control over the plasmon resonance frequencies in a hybrid metal-semiconductor nanoshell structure with silver core and TiO_2 coating. We temporarily change the dielectric function of TiO_2 using pump laser pulse operating at bandgap or above. This generates free electron-hole pairs in TiO_2 that alter the dielectric environment for the silver core. The probed surface plasmon frequency lying below bandgap appears to be blue-shifted due to the altered dielectric environment. We calculate the magnitude of the plasmon resonance wavelength shift as a function of electron-hole pair density and obtain shifts up to 126 nm at wavelengths of around 460 nm. Using these results, we propose a model of a light-controlled surface plasmon polariton (SPP) switch.

¹We acknowledge support from NSF (Grant No. ECCS-0901784), AFOSR (Grant No. FA9550-09-1-0450), and NSF (Grant No. ECCS-1128597).

12:51PM Q28.00009 Direct-bandgap infrared light emission from tensilely strained germanium nanomembranes¹

, JOSE SÁNCHEZ-PÉREZ, University of Wisconsin Madison, CICEK BOZTUG, Boston University, FENG CHEN², University of Wisconsin Madison, FAISAL SUDRADJAT, Boston University, DEBORAH PASKIEWICZ, R.B. JACOBSON, University of Wisconsin Madison, ROBERTO PAIELLA, Boston University, MAX LAGALLY, University of Wisconsin Madison — Silicon, germanium, and related alloys, which provide the leading materials platform of electronics, are extremely inefficient light emitters because of their indirect fundamental energy bandgap. This basic materials property has so far hindered the development of group-IV photonic active devices, including diode lasers, thereby significantly limiting our ability to integrate electronic and photonic functionalities at the chip level. We show that Ge nanomembranes can be used to overcome this materials limitation. Theoretical studies have predicted that tensile strain in Ge lowers the direct energy bandgap relative to the indirect one. We demonstrate [1] that mechanically stressed nanomembranes allow for the introduction of sufficient biaxial tensile strain to transform Ge into a direct-bandgap, efficient light-emitting material that can support population inversion and therefore provide optical gain.

[1] J. R. Sánchez-Pérez, C. Boztug, F. Chen, F. Sudradjat, D. M. Paskiewicz, R.B. Jacobson, M. G. Lagally, and R. Paiella, PNAS web published Nov, 14, 2011

¹Research supported in part by NSF and DOE.

²currently at Applied Materials China

1:03PM Q28.00010 A Tunable Terahertz Detector Based On Self Assembled Plasmonic Structure on a GaAs 2DEG

, CHEJIN BAE, DEEPU GEORGE, ROHIT SINGH, ANDREA MARKELZ, University at Buffalo (SUNY) Department of Physics — The use of tunable gated gratings on 2DEG structure has been well known methods for compact frequency sensitive THz detection based on the resonant absorption of the 2D Plasmon. The resonant frequency is dependent on system dimension and the tunability of that dimension by depletion gating. Here we attempt to improve detector sensitivity, tunability and remove polarization dependence through the development of a gated grid design. To satisfy the requirement for imaging applications of device dimensions on the order of < 1 micron over a detector area of 4 mm^2 , we have fabricated gated grid plasmonic structure on 2DEG material by using nanosphere self-assembly lithography. This fabrication method has not been widely developed for III-V processing but allows us to achieve large area sensitive detectors with tunability in the 1-4 THz range. In this paper we will discuss the characterization of the devices as a function of gate bias, magnetic field, and temperature using FTIR and THz time domain measurements.

1:15PM Q28.00011 Time-resolved second harmonic generation study of buried semiconductor heterointerfaces using soliton-induced transparency, Y.D. GLINKA¹, Department of Physics, University of Texas at Austin, Austin, Texas 78712, USA, N.H. TOLK, Department of Physics and Astronomy, Vanderbilt University, Nashville, Tennessee 37235, USA, J.K. FURDYNA, Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556, USA — The transient second harmonic generation (SHG) and linear optical reflectivity (LOR) signals measured simultaneously in reflection from GaAs/GaSb/InAs and GaAs/GaSb heterostructures revealed a new mechanism for creating self-induced transparency in narrow bandgap semiconductors at low temperatures, which is based on the dual-frequency electro-optic soliton propagation. The mechanism takes account of the photo-Dember field solitary wave, which traps both the fundamental and SHG pulses, slowing their velocity down to that of the solitary wave. The trapped light pulses maintain the amplitude of the solitary wave and hence create a condition, at which the self-reinforcing nonlinear optical polarization (dual-frequency electro-optic soliton) can propagate through the semiconductor. This allows the ultrafast carrier dynamics at buried semiconductor heterointerfaces to be studied.

¹Institute of Physics, National Academy of Sciences of Ukraine, Kiev, 03028, Ukraine

1:27PM Q28.00012 Room temperature ballistic transport in InSb quantum well structures, ADAM GILBERTSON, LESLEY COHEN, Imperial College, PHIL BUCKLE, Cardiff University, TIM ASHLEY, Warwick University, STUART SOLIN, Washington University in St. Louis, ANDOR KORMANYOS, COLIN LAMBERT, Lancaster University — We report significant advancements in InSb/AlInSb quantum well (QW) heterostructures for room temperature nanoelectronic applications. InSb/AlInSb heterostructures have phenomenally high room temperature mobility but display intrinsic parallel conduction in the buffer layer limiting exploitation for nanostructured devices where deep isolation etch processing is impractical. We demonstrate a strategy to reduce the parasitic conduction by the insertion of a pseudomorphic barrier layer of wide-band-gap alloy below the QW.¹ Mesoscopic geometric nanocrosses fabricated from such material clearly demonstrate ballistic transport at room temperature, as evidenced by very significant negative bend resistance (NBR). We have studied the interplay between sidewall and bulk scattering at 300K in relation to quantum calculations. DC measurements in the non-equilibrium (hot carrier) regime reveal that electrons remain ballistic at current densities in excess of 10^6 A/cm².

¹A.M. Gilbertson, P.D. Buckle, T. Ashley, L.F. Cohen, Phys Rev B **84**, 075474 (2011).

1:39PM Q28.00013 Spectral and Spatial Response of Sulfur-Hyperdoped n+/p Silicon Photodiodes¹, DAVID HUTCHINSON, Rensselaer Polytechnic Institute, DANIEL RECHT, Harvard University, JOSEPH SULLIVAN, Massachusetts Institute of Technology, JEFFREY WARRENDER, US Army - ARDEC, Benet Laboratories, MICHAEL AZIZ, Harvard University, TONIO BUONASSISI, Massachusetts Institute of Technology, PETER PERSANS, Rensselaer Polytechnic Institute — Pulsed laser melting of implanted silicon can enable doping well above equilibrium concentrations. Sulfur doping leads to a deep donor state that may form an impurity band at high enough concentrations. Photodiodes formed from sulfur-hyperdoped n+ layers on a p-type wafer have shown external quantum efficiency of much greater than 100%, as well as enhanced infrared response. In this paper we report on optoelectronic characterization of diodes prepared by implantation of $10^{15} - 10^{16}$ sulfur/cm² into a p-type wafer, followed by nanosecond pulsed laser melting and recrystallization. Experimental results from wavelength-dependent diode response, spatial quantum efficiency mapping, intensity dependent efficiency, and current-voltage techniques will be reported. We will also discuss potential models for the observed behavior.

¹Research at Rensselaer was supported by the Army Research Office. Research at Harvard was supported by the US Army ARDEC. D.R. was supported in part by a National Defense Science and Engineering Graduate fellowship.

1:51PM Q28.00014 The mesoscopic chaotic cavity as a rectifying heat engine, ANDREW JORDAN, University of Rochester, BJÖRN SOTHMANN, University of Geneva, RAFAEL SÁNCHEZ, Instituto de Ciencia de Materiales de Madrid, MARKUS BUTTIKER, University of Geneva — We present an exactly solvable model of a mesoscopic heat engine that works using the principle of rectifying thermal fluctuations applied to a nonlinear system. The system is a chaotic mesoscopic cavity where the contact transmission to leads is energy-dependent. This energy-dependence is generic in mesoscopic conductors, and leads to an intrinsic nonlinearity. The cavity is coupled capacitively to another conductor, held at a different temperature. The nonlinear cavity rectifies the thermal fluctuations, leading to a hot spot rectified electrical current that is proportional to the asymmetry in the energy-dependence of the contacts, and to the temperature difference. We will discuss the maximum power produced by the system, as well as the efficiency of the engine by comparing it to the heat current that passes between the coupled systems. Possible practical energy-harvesting applications will be proposed.

2:03PM Q28.00015 Thermal properties of CuGaS₂ from first principles¹, ALDO H. ROMERO, CINVESTAV, Unidad Queretaro, Mexico, MANUEL CARDONA, REINHARD KREMER, MPI, Stuttgart, ALEXANDER SCHINDLER, NETZSCH-Geratebau GmbH, ALFONSO MUÑOZ, Departamento de Física, Universidad de la Laguna, Spain — We have investigated in the past the specific heats of monatomic and binary semiconductors and their dependence on temperature and isotopic mass, both experimentally and theoretically. The theoretical calculations were performed *ab initio* with LDA exchange correlations. We are at present carrying over these investigations to ternary materials, in particular to those with chalcopyrite structure. We present here results involving the dependence of the specific heat and other physical properties (lattice parameters, volume thermal expansion, phonon dispersion) of the chalcopyrite CuGaS₂ on temperature and on the isotopic masses of the three constituent atoms. Particular emphasis is paid to the maxima of C_p/T^3 found at low temperatures which correspond to the deviation of Debye's law related to transverse acoustic phonons near the zone boundary. The calculations were performed with the ABINIT and VASP codes within the local density approximation for exchange and correlation. The results are shown to be in excellent agreement with the experimental data. Correlation with similar compounds such as CuAlS₂ and CuInS₂ is discussed.

¹Supported by CONACYT projects J-152153-F and Binational collaboration TAMU-CONACYT

Wednesday, February 29, 2012 11:15AM - 2:15PM – Session Q29 GQI: Focus Session: Topologically Protected Qubits II 259A

11:15AM Q29.00001 Topological superconducting states and protected qubit manipulations¹, SUMANTA TEWARI, Physics and Astronomy, Clemson University, Clemson, SC 29634 — Topological superconducting states supporting Majorana fermion excitations have been recently proposed as platforms for topological quantum computation. Of particular importance are semiconductor-superconductor and topological insulator-superconductor heterostructures, which have been shown to support Majorana fermions at order parameter defects under appropriate external conditions. Here I will focus on topologically non-trivial properties of two-dimensional semiconductors and one-dimensional quantum wires placed adjacent to superconductors, and discuss the possible protected qubit manipulations that may eventually lead to topological quantum computation.

¹Work done at Clemson University and at CMTC, UMD in collaboration with Sankar Das Sarma. Work supported by DARPA-MTO, DARPA QuEST, JQI-NSF-PFC, and Microsoft Q.

11:51AM Q29.00002 Majorana Zero Modes in 1D Quantum Wires Without Long-Ranged Superconducting Order, LUKASZ FIDKOWSKI, ROMAN LUTCHYN, CHETAN NAYAK, Microsoft Station Q, MATTHEW FISHER, University of California, Santa Barbara — We show that long-ranged superconducting order is not necessary to guarantee the existence of Majorana fermion zero modes at the ends of a quantum wire. We formulate a concrete model which applies, for instance, to a semiconducting quantum wire with strong spin-orbit coupling and Zeeman splitting coupled to a wire with algebraically-decaying superconducting fluctuations. We solve this model by bosonization and show that it supports Majorana fermion zero modes. We argue that a large class of models will also show the same phenomenon. We discuss the implications for experiments on spin-orbit coupled nanowires coated with superconducting film and for LaAlO₃/SrTiO₃ interfaces.

12:03PM Q29.00003 Coulomb stability of the 4π -periodic Josephson effect of Majorana fermions, FABIAN HASSLER, Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany, BERNARD VAN HECK, ANTON R. AKHMEROV, C.W.J BEENAKKER, Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands — The Josephson energy of two superconducting islands containing Majorana fermions is a 4π -periodic function of the superconducting phase difference. If the islands have a small capacitance, their ground state energy is governed by the competition of Josephson and charging energies. We calculate this ground state energy in a ring geometry, as a function of the flux Φ enclosed by the ring, and show that the dependence on the Aharonov-Bohm phase $2e\Phi/\hbar$ remains 4π -periodic regardless of the ratio of charging and Josephson energies—provided that the entire ring is in a topologically nontrivial state. If part of the ring is topologically trivial, then the charging energy induces quantum phase slips that restore the usual 2π -periodicity [B. van Heck, F. Hassler, A. R. Akhmerov, and C. W. J. Beenakker, Phys. Rev. B **84**, 180502(R) (2011)].

12:15PM Q29.00004 Unconventional Josephson signatures of Majorana bound states, LIANG JIANG, DAVID PEKKER, GIL REFAEL, Department of Physics, Caltech, JASON ALICEA, Department of Physics and Astronomy, University of California, Irvine, YUVAL OREG, Department of Condensed Matter Physics, Weizmann Institute of Science, FELIX VON OPPEN, Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin — A junction between two topological superconductors containing a pair of Majorana fermions exhibits a ‘fractional’ Josephson effect, 4π periodic in the superconductors’ phase difference. An additional fractional Josephson effect, however, arises when the Majoranas are spatially separated by a superconducting barrier. This new term gives rise to a set of Shapiro steps which are essentially absent without Majorana modes and therefore provides a unique signature for these exotic states. Other new signatures associated with Majorana fermions will also be discussed.

12:27PM Q29.00005 Signature of Majorana Fermions in Charge Transport in Semiconductor Nanowires¹, CHUNLEI QU, YONGPING ZHANG, LI MAO, CHUANWEI ZHANG, Department of Physics and Astronomy, Washington State University, Pullman, WA 99164 — We investigate the charge transport in a semiconductor nanowire that is subject to a perpendicular magnetic field and in partial contact with an s-wave superconductor. We find that Majorana fermions, existing at the interface between superconducting and normal sections of the nanowire within certain parameter region, can induce resonant Andreev reflection of electrons at the interface, which yields a zero energy peak in the electrical conductance of the nanowire. The width of the zero energy conductance peak for different experimental parameters is characterized. While the zero energy peak provides a signature for Majorana fermions in one dimensional nanowires, it disappears in a two-dimensional semiconductor thin film with the same experimental setup because of the existence of other edge states in two dimensions. The proposed charge transport experiment may provide a simple and experimentally feasible method for the detection of Majorana fermions in semiconductor nanowires.

¹This work is supported by DARPA-MTO (FA9550-10-1-0497), DARPA-YFA (N66001-10-1-4025), and NSF-PHY (1104546).

12:39PM Q29.00006 Searching for Majorana Zero-Energy Modes in Semiconductor Nanowires, PETER O'MALLEY, PEDRAM ROUSHAN, BORZOYEH SHOJAEI, UC Santa Barbara, ROMAN LUTCHYN, Microsoft Station Q, CHRIS PALMSTROM, JOHN MARTINIS, UC Santa Barbara — Majorana fermions are proposed elementary particles with the unique property of being their own antiparticle, whose discovery remains elusive. Because of their non-Abelian statistics, Majorana fermions provide a promising opportunity to realize fault-tolerant topological quantum computation. Recently, semiconductor nanowires have been proposed as a possible platform for realizing Majorana physics in solid state systems. An s-wave superconductor inducing the proximity effect in a one-dimensional semiconductor nanowire would create chiral p-wave superconductivity in the nanowire; this superconductor would have Majorana modes as zero-energy excitations. We use nanofabrication techniques to create such nanowires out of MBE-grown two-dimensional electron gas formed in III-V semiconductor heterostructures. We present measurements which show the promise of this approach to creating and controlling Majorana excitations.

12:51PM Q29.00007 Majorana fermions in superconducting helical magnets, IVAR MARTIN, LANL, ALBERTO MORPURGO, University of Geneva — In a variety of rare-earth based compounds singlet superconductivity coexists with helical magnetism. Here we demonstrate that surfaces of these system are expected to generically host a finite density of zero-energy Majorana modes. When confined to a wire geometry, a discrete number of Majorana modes can be isolated, in close analogy with the Rashba superconductors proposed recently as a framework for topological quantum computing. In contrast to the latter systems, however, the larger characteristic energy scales for superconductivity and magnetism, as well as the lack of need for fine-tuning, make helical magnetic superconducting compounds favorable for the observation and experimental investigation of Majorana fermions.

1:03PM Q29.00008 Stability of Majorana fermions in proximity-coupled topological insulator nanowires¹, ASHLEY COOK, MARCEL FRANZ, University of British Columbia — It has been shown previously [1] that a finite-length topological insulator nanowire, proximity-coupled to an ordinary bulk s-wave superconductor and subject to a longitudinal applied magnetic field, realizes a one-dimensional topological superconductor with an unpaired Majorana fermion localized at each end of the nanowire. Here we show that the unpaired Majorana fermions persist in this system for any value of the chemical potential inside the bulk band gap of order 300 meV in Bi₂Se₃, and, remarkably, also outside this gap in smaller domains, by computing the Majorana number. From this calculation, we also show that the unpaired Majorana fermions persist when the magnetic flux through the nanowire cross-section deviates significantly from half flux quantum. Lastly, we demonstrate that the unpaired Majorana fermions persist in strongly disordered wires with fluctuations in the on-site potential ranging in magnitude up to the size of the bulk band gap. These results suggest this solid-state system should exhibit the elusive Majorana particles under conditions accessible enough for their long sought-after experimental realization.

[1] A. Cook and M. Franz, Phys. Rev. B (in press, arXiv:1105.1787)

¹This work was supported by NSERC and CIFAR.

1:15PM Q29.00009 Josephson current in finite-length nanowire SNS junctions with Majorana fermions, RAMON AGUADO, ELSA PRADA, ICM-CONICET, Consejo Superior de Investigaciones Científicas, PABLO SAN JOSE, ICM-CONICET, Consejo Superior de Investigaciones Científicas — The dc Josephson effect (JE) through infinite-length junctions of one-dimensional topological superconductors exhibits an anomalous 4π periodic phase (ϕ) dependence which originates from a parity-protected level crossing of zero-energy Majorana bound states (MBS) at $\phi = \pi$. This “fractional” JE provides an important experimental detection tool for MBS. In this talk, I will discuss the JE in more realistic SNS junctions of arbitrary transparency and when both the normal and the nanowire regions are of finite length, namely beyond the short-junction and infinite topological superconductor limits. In general, the spectrum of Andreev bound states can become rather intricate and dense as opposed to the infinite-length case. Moreover, the low-energy spectrum around $\phi = \pi$ shows always anticrossings, originated from hybridization of four MBS, which may preclude the experimental observation of the fractional JE. At finite bias voltages, Landau-Zener dynamics involving the MBS and quasi-continuum Andreev levels gives rise to a nontrivial ac Josephson current. Interestingly, the ac current phase diagram as a function of the Josephson frequency/normal transmission shows fractional JE regions which are tunable through bias/gate voltages.

1:27PM Q29.00010 Detecting a Majorana-Fermion Zero Mode Using a Quantum Dot¹, DONG E. LIU, HAROLD U. BARANGER, Duke University — We propose an setup for detecting a Majorana zero mode consisting of a spinless quantum dot coupled to the end of a p-wave superconducting nanowire [1]. The conductance through the dot is monitored by adding two external leads. We find that the Majorana bound state at the end of the wire strongly influences the conductance through the quantum dot: driving the wire through the topological phase transition causes a sharp jump in the conductance by a factor of 1/2. In the topological phase, the zero temperature peak value of the dot conductance (i.e. on resonance and symmetric coupling) is $e^2/2h$. In contrast, if the wire is in its trivial phase, the peak is e^2/h , or if a regular fermionic zero mode occurs, the conductance is 0. We also consider coupling the dot to both ends of the wire (two MBS), with a magnetic flux Φ through the loop. The conductance as a function of phase shows peaks at $\Phi/\Phi_0 = (2n+1)\pi$ which can be used to tune Flensberg’s qubit system [PRL (2011)] to the energy degeneracy point.

[1] D. E. Liu and H. U. Baranger, PRB in press (2011); arXiv/1107.4338.

¹Supported by the U.S. Dept. of Energy (Materials Sciences and Engineering, DE-SC0005237).

1:39PM Q29.00011 Majorana chain coupled to a microwave cavity, MIRCEA TRIF, YAROSLAV TSERKOVNYYAK, Department of Physics and Astronomy, University of California, Los Angeles, California 90095, USA — We study the Majorana end-states in a one-dimensional Kitaev model in the presence of a microwave cavity. We analyze both the resonant and off-resonant coupling to the cavity for different cavity states. In the resonant regime, we find that the topology of the system can be modified depending on the number of photons in the cavity, while in the off-resonant regime (large detuning), the cavity could be used to detect the topological transition from a non-trivial to trivial state, being thus an optical alternative to the transport-based detection of the transition point. We also analyze the effects of the coupling to the cavity on the braiding of the emerging Majoranas.

1:51PM Q29.00012 Majorana modes in time-reversal invariant s-wave topological superconductors, SHUA DENG, LORENZA VIOLA, Dartmouth College, GERARDO ORTIZ, University of Indiana, Bloomington — We present a time-reversal invariant s-wave superconductor supporting Majorana edge modes. The multi-band character of the model together with spin-orbit coupling are key to realizing such a topological superconductor. We characterize the topological phase diagram by using a partial Chern number sum, and show that the latter is physically related to the parity of the fermion number of the time-reversal invariant modes. By taking the self-consistency constraint on the s-wave pairing gap into account, we also establish the possibility of a direct topological superconductor-to-topological insulator quantum phase transition.

2:03PM Q29.00013 Majorana Fermions in Disordered Quasi-One-Dimensional Topological Superconductors, ANDREW POTTER, PATRICK LEE, MIT — Majorana fermions have long been predicted to emerge in certain quantum Hall states and other naturally occurring p-wave superconductors. However, these materials are quite delicate and consequently the experimental realization of Majorana fermions remains elusive. The possibility of engineering 1D networks of topological superconducting wires from conventional materials offers a promising alternative route to realize Majorana fermions and probe their predicted non-Abelian statistics. In practice, it is impossible to fabricate perfectly clean and strictly one-dimensional structures; how do these non-idealities affect the proposed Majorana states? This talk will show that Majorana end states are robust away from the strict 1D limit, so long as the sample width is not much larger than the superconducting coherence length. The effects of disorder are potentially more severe, as impurity scattering is generally pair-breaking and tends to suppress the gap protecting the Majorana modes. Finally, we propose new candidate materials and geometries that greatly simplify the experimental setup and mitigate the harmful effects of disorder.

Wednesday, February 29, 2012 11:15AM - 2:15PM –
Session Q30 GQI: Focus Session: Superconducting Qubits: Architecture, Tunable, and Static Coupling 259B

11:15AM Q30.00001 Coupling superconducting qubits and resonators, JOEL STRAND, Syracuse University — The performance of superconducting qubits has evolved rapidly in recent years, with coherence times now often measured in tens of microseconds. This makes superconducting qubits a promising candidate for a scalable quantum computing architecture and for modeling quantum systems. To realize this potential, consideration must be given to coupling multiple qubits to a system of microwave resonators in a way that balances coherence times, control and readout times, crosstalk, and space constraints. We compare three methods of coupling qubits to resonators: inductive coupling through a shared kinetic inductance with the resonator, capacitive coupling to a voltage antinode, and coupling to a three-dimensional superconducting cavity. We will also present designs and measurements of samples incorporating both inductively and capacitively coupled qubits on the same coplanar resonator. Lastly, we discuss a three-qubit/two-resonator system with one qubit bridging the two resonators that could serve as the building block of a large-scale architecture.

11:51AM Q30.00002 Inductive coupling to the fluxonium qubit¹, N.A. MASLUK, A. KAMAL, I. POP, Z.K. MINEV, Yale University, V.E. MANUCHARYAN, Harvard University, J. KOCH, Northwestern University, L.I. GLAZMAN, M.H. DEVORET, Yale University — Fluxonium is a highly anharmonic artificial atom, which utilizes an inductance formed by an array of large Josephson junctions to shunt the junction of a Cooper-pair box. The first excited state transition frequency is widely tunable with flux, and due to interactions of transitions to the second excited state with the readout cavity, a dispersive readout is possible over the entire five octave range. Previous fluxonium samples relied on a capacitive coupling to the readout cavity, but there is evidence that dielectric losses in these capacitors contributes significantly to relaxation [1]. We present a new method of coupling to the cavity through a mutual inductance, reducing relaxation through dielectric loss.

[1] V. E. Manucharyan et al., arXiv:1012.1928v1 (2010).

¹Work supported by IARPA, ARO and NSF.

12:03PM Q30.00003 A dc SQUID Phase Qubit with Controlled Coupling to the Microwave Line¹, R.P. BUDOYO, B.K. COOPER, JQI and CNAM, University of Maryland, V. ZARETSKEY, Laboratory for Physical Sciences and University of Maryland, C.J. BALLARD, JQI and CNAM, University of Maryland, Z. KIM, JQI, University of Maryland, H. KWON, J.R. ANDERSON, C.J. LOBB, F.C. WELLSTOOD, JQI and CNAM, University of Maryland — We have designed and fabricated a Al/AIO_x/Al dc SQUID phase qubit on a sapphire substrate with a qubit junction area of 0.4 μm^2 . The qubit junction is shunted with a 1 pF interdigitated capacitor, and is isolated from the bias leads by an LC filter and an inductive isolation network using a larger Josephson junction. Our previous device (A. Przybysz *et al.*, IEEE Trans. on Appl. Supercond., 2011) with similar parameters had its relaxation time T_1 limited by coupling to the microwave line. To reduce this coupling, we adopted a coplanar stripline design and verified the coupling strength using finite element model microwave simulations. We will discuss our design, the microwave simulations, estimates for the overall coherence time due to losses and noise from various sources, the device fabrication process, and progress towards testing the device.

¹Acknowledgement: LPS, CNAM, JQI

12:15PM Q30.00004 Large tunable inductance of the decorated Josephson chain, IVAN SADOVSKYY, MATTHEW BELL, LEV IOFFE, Rutgers University, ALEXEI KITAEV, California Institute of Technology, MICHAEL GERSHENSON, Rutgers University — We discuss the new design of a tunable superconductive inductance made from the decorated frustrated Josephson junction chains frustrated by magnetic field. We show that for the optimal choice of parameters the inductance of this chain varies in a very wide range as a function of the magnetic field. The resulting plasma frequency may exceed the value of quantum resistance, $\sqrt{L/C} \gg h/(2e)^2$ that characterizes superinductance. The important distinction of this design from the chain of dc-SQUIDs loops is the absence of phase slips at all magnetic fields. We present the results of the extensive numerical simulations that confirm these expectations.

12:27PM Q30.00005 Driven dynamics of a qubit tunably coupled to a harmonic oscillator¹, SIMON GUSTAVSSON, JONAS BYLANDER, FEI YAN, POL FORN-DIAZ, Massachusetts Institute of Technology, VLAD BOLKHOVSKY, DANIELLE BRAJE, STEVEN SPECTOR, BEN TUREK, PAUL B. WELANDER, MIT Lincoln Lab, FUMIKI YOSHIHARA, NEC, DAVID. G. CORY, University of Waterloo, YASUNOBU NAKAMURA, NEC, WILLIAM D. OLIVER, Massachusetts Institute of Technology, MIT Lincoln Lab — We have investigated the driven dynamics of a superconducting flux qubit that is tunably coupled to a microwave resonator. We find that the qubit experiences an additional oscillating field mediated by off-resonant driving of the resonator, leading to unanticipated, strong modifications of the qubit Rabi frequency. Low-frequency noise in the coupling parameter translates to an effective noise in the amplitude of the drive field, causing a reduction of the coherence time during driven evolution. The noise can be mitigated with the rotary-echo pulse sequence, which, for driven systems, is analogous to the Hahn-echo sequence.

¹This work is sponsored by the Department of the Air Force under contract number FA8721-05-C-0002. Opinions, interpretations, conclusions, and recommendations are those of the author(s) and are not necessarily endorsed by the United States government.

12:39PM Q30.00006 Phase gate operation on a flux qubit via the readout SQUID line¹, X.Y. JIN, S. GUSTAVSSON, J. BYLANDER, F. YAN, Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, F. YOSHIHARA, S. NAKAMURA, The Institute of Physical and Chemical Research (RIKEN), Wako, Saitama 351-0198, Japan, W.D. OLIVER, MIT Lincoln Laboratory, 244 Wood Street, Lexington, Massachusetts 02420 — Detuning a superconducting qubit from its rotating frame is one means to implement a phase gate operation. For superconducting flux qubits, this detuning can be realized by changing the magnetic flux threading the qubit loop, e.g., by the mutual coupling from a nearby microwave antenna. In this work, we demonstrate an alternative approach: we implement a phase gate by pulsing a current through the readout DC SQUID. While the DC SQUID acts as a qubit flux sensor for readout, we in turn may use it as an actuator to impose the phase-gate flux shift. Using this pulsed current approach, we demonstrated Ramsey-type free-induction with more than 20 oscillation periods. We also studied the impact of the first phase gate on subsequent, sequential phase gates.

¹This work is sponsored by the Department of the Air Force under contract number FA8721-05-C-0002. Opinions, interpretations, conclusions, and recommendations are those of the author(s) and are not necessarily endorsed by the United States government.

12:51PM Q30.00007 Progress towards a metastable superconducting qubit¹, ANDREW KERMAN, WILLIAM OLIVER, VLADIMIR BOLKHOVSKY, MARK GOUKER, MIT Lincoln Laboratory — We will report on progress towards the demonstration of a metastable RF SQUID (MRFS) qubit, which has the potential to exhibit excited-state lifetimes many orders of magnitude longer than present-day superconducting qubits, while retaining long enough coherence times to allow gate error rates as low as $\sim 10^{-5}$. These properties result from the two main characteristics of the MRFS qubit: (i) its two lowest levels are essentially macroscopically distinct persistent-current states, which can be strongly decoupled from high-frequency electromagnetic fluctuations (in contrast to most superconducting qubits whose levels are approximately those of a nonlinear LC oscillator and are thus strongly coupled); and (ii) its extremely large inductance makes it only weakly sensitive to low-frequency magnetic flux noise.

¹This work is sponsored under Air Force Contract Number FA8721-05-C-0002. Opinions, interpretations, conclusions, and recommendations are those of the authors and are not necessarily endorsed by the United States Government.

1:03PM Q30.00008 Quantum gates by qubit frequency modulation in circuit QED, FELIX BEAUDOIN, Universite de Sherbrooke, MARCUS P. DA SILVA, BLAKE R. JOHNSON, THOMAS A. OHKI, ZACHARY DUTTON, Disruptive Information Processing Technologies Group, Raytheon BBN Technologies, ALEXANDRE BLAIS, Universite de Sherbrooke — Several types of two-qubit gates have been realized experimentally in circuit QED. These are based, for example, on tuning the pair of qubits in resonance with each other [Majer, Nature 449, 443-447 (2007)] or on a microwave pulse on one qubit at the transition frequency of a second qubit [Chow, Phys. Rev. Lett. 107, 080502 (2011)]. Another realization is based on a sequence of blue-sideband transitions generated by microwave pulses [Leek, Phys. Rev. B 79, 180511(R) (2009)]. Here, we propose a different approach relying on oscillations of the qubit frequency using a flux-bias line. We explain how frequency modulation leads to tunable qubit-resonator and qubit-qubit interactions. We also show how this form of quantum control leads to faster (first-order) sideband transitions and consider applications to two-qubit gates.

1:15PM Q30.00009 Transmon qubit coupled to a quasi-lumped element resonator, B. SURI, S. NOVIKOV, V. ZARETSKEY, Dept. of Physics, University of Maryland, College Park, B.S. PALMER, Lab for Physical Sciences, College Park, Maryland, F.C. WELLSTOOD, JQI, CNAM, Dept. of Phys, Univ of MD, College Park — We report on the design, fabrication and measurement of an Al/AIO_x/Al transmon qubit coupled to a quasi-lumped element superconducting resonator. Our resonator, which has a resonant frequency of ≈ 5.4 GHz, and a loaded quality factor $Q_l \approx 30,000$ is, in turn, coupled to a transmission line. The qubit is designed to have $E_J/E_C > 30$ to significantly decrease the sensitivity to low-frequency charge noise. The coupling of the qubit to the resonator is designed to be $g/2\pi > 100$ MHz. We report and discuss preliminary spectroscopic measurements and coherence measurements of the qubit.

1:27PM Q30.00010 Fast, coherent control of the tunable coupling qubit, SRIKANTH SRINIVASAN, ANTHONY HOFFMAN, YANBING LIU, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544, JAY GAMBETTA, IBM T.J. Watson Research Center, Yorktown Heights, New York 10598, ANDREW HOUCK, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544 — We present results of time domain measurements on a tunable coupling qubit (TCQ) coupled to a superconducting coplanar waveguide resonator. The TCQ has the benefit of independently tunable qubit frequency and cavity-qubit coupling. We show that the TCQ's frequency and coupling can be dynamically controlled in tens of nanoseconds by using two on-chip flux control lines. Using this dynamic control, Rabi oscillations were measured at various coupling strengths showing that the coupling can be reduced by a factor greater than 1500. To measure qubit coherence at low coupling, the TCQ was tuned to a high coupling region, excited by a synchronized pi-pulse and then returned to the zero coupling region where the qubit state was measured. Coherence times of several microseconds were measured and are comparable to other superconducting qubits

1:39PM Q30.00011 Transferring the state of a quantum register to a single oscillator: a simple circuit verses numerical optimization¹, KURT JACOBS, XIAOTING WANG, University of Massachusetts at Boston, FREDERICK STRAUCH, Williams College — We consider the problem of swapping a quantum state between a register of qubits and a single quantum oscillator. We design a mesoscopic quantum circuit to do this, using an off-resonant interaction, based on the concept of coherent feedback control. We consider an explicit realization of this circuit, and perform simulations of its performance. We then take a different approach, in which we couple the register directly to the resonator, including inter-qubit couplings and local controls, and use numerical optimization to search for a control protocol that will achieve the swap with very high fidelity. Our results show that the protocols found using numerical searches are superior in speed and fidelity to the manually-designed circuit. We also explore how the time and complexity of the protocols increases with the problem size.

¹Research supported by the NSF under grant nos. PHY-0902906 and PHY-1005571

1:51PM Q30.00012 Gradiometric persistent current flux qubit with tunable tunnel coupling¹, F. DEPPE, M. SCHWARZ, J. GOETZ, A. BAUST, M. HAEBERLEIN, E. HOFFMANN, E.P. MENZEL, F. WULSCHNER, L. ZHONG, A. MARX, R. GROSS, Walther-Meissner-Institute and TU Munich, Garching, Germany — The persistent current flux qubit is a Josephson junction based superconducting circuit exhibiting a strong anharmonicity in combination with excellent coherence times of more than 10 μ s. However, quantum coherence decreases drastically away from an optimal point and a controlled design of the transition frequency at this point is demanding with respect to fabrication stability. Here, we present the spectroscopic analysis of a gradiometric flux qubit, where the tunnel coupling can be tuned from a few hundreds of Megahertz to several Gigahertz.

¹Supported by the DFG via SFB 631 and by the German Excellence Initiative via NIM.

2:03PM Q30.00013 Large dispersive shift in superconducting flux qubit, TSUYOSHI YAMAMOTO, NEC Corporation, KUNIHIRO INOMATA, RIKEN, YASUNOBU NAKAMURA, JAW-SHEN TSAI, NEC Corporation — We study dispersive readout in superconducting flux qubits which are capacitively coupled to a superconducting cavity with ~ 10 GHz resonant frequency f_r . To discriminate the state of the qubit precisely, large magnitude of the dispersive shift χ is desirable. For the two-level system, χ is given by g^2/Δ where g is the coupling strength and Δ is the detuning between the qubit and the cavity. For the multilevel system such as superconducting qubits, however, this formula is modified due to the contributions from higher levels [1]. It has been pointed out that if f_r lies between 01 and 12 transition frequencies of the qubit (f_{01} and f_{12} , respectively), $|\chi|$ becomes large because of constructive contributions from different levels [1]. Our flux qubit has $f_{01} = 5$ GHz and $f_{12} = 15$ GHz at the optimal flux bias, thus satisfying this condition. Moreover, because of the large anharmonicity ($|f_{12} - f_{01}|$) of the flux qubit, we can easily make g as large as ~ 100 MHz, while staying in the deep dispersive limit. Both of these enhance $|\chi|$ and we have obtained χ of 80 MHz at the optimal flux bias, which agrees well with the prediction by the energy band calculation. [1] J. Koch et al., PRA 76, 042319 (2007)

Wednesday, February 29, 2012 11:15AM - 2:15PM – Session Q31 GMAG DMP: Focus Session: Topological Insulators - Edge States 260

11:15AM Q31.00001 Electrical control of spin in topological insulators, KAI CHANG, SKLSM, Institute of Semiconductors, Chinese Academy of Science, Beijing, China — All-electrical manipulation of electron spin in solids becomes a central issue of quantum information processing and quantum computing. The many previous proposals are based on spin-orbit interactions in semiconductors. Topological insulator, a strong spin-orbit coupling system, make it possible to control the spin transport electrically. Recent calculations proved that external electric fields can drive a HgTe quantum well from normal band insulator phase to topological insulator phase [1]. Since the topological edge states are robust against local perturbation, the controlling of edge states using local fields is a challenging task. We demonstrate that a p-n junction created electrically in HgTe quantum wells with inverted band structure exhibits interesting intraband and interband tunneling processes. We find a perfect intraband transmission for electrons injected perpendicularly to the interface of the p-n junction. The opacity and transparency of electrons through the p-n junction can be tuned by changing the incidence angle, the Fermi energy and the strength of the Rashba spin-orbit interaction (RSOI). The occurrence of a conductance plateau due to the formation of topological edge states in a quasi-one-dimensional p-n junction can be switched on and off by tuning the gate voltage. The spin orientation can be substantially rotated when the samples exhibit a moderately strong RSOI [2]. An electrical switching of the edge-state transport can also be realized using quantum point contacts in quantum spin Hall bars. The switch-on/off of the edge channel is caused by the finite size effect of the quantum point contact and therefore can be manipulated by tuning the voltage applied on the split gate [3,4]. The magnetic ions doped on the surface of 3D TI can be correlated through the helical electrons. The RKKY interaction mediated by the helical Dirac electrons consists of the Heisenberg-like, Ising-like, and Dzyaloshinskii-Moriya (DM)-like terms, which can be tuned by changing the gate voltage. It provides us a new way to control surface magnetism electrically. The gap opened by doped magnetic ions can lead to a short-range Bloembergen-Rowland interaction. The competition among the Heisenberg, Ising, and DM terms leads to rich spin configurations and an anomalous Hall effect on different lattices [4]. There are many proposals for quantum computation scheme are based on the spin in semiconductor quantum dots. Topological insulator quantum dots display a very different behavior with that of conventional semiconductor quantum dots [5]. In sharp contrast to conventional semiconductor quantum dots, the quantum states in the gap of the HgTe QD are fully spin-polarized and show ring-like density distributions near the boundary of the QD and optically dark. The persistent charge currents and magnetic moments, i.e., the Aharonov-Bohm effect, can be observed in such a QD structure. This feature offers us a practical way to detect these exotic ring-like edge states by using the SQUID technique.
Refs: [1] W. Yang, Kai Chang, and S. C. Zhang, Phys. Rev. Lett. 100, 056602 (2008); J. Li and Kai Chang, Appl. Phys. Lett. 95, 222110 (2009). [2] L. B. Zhang, Kai Chang, X. C. Xie, H. Buhmann and L. W. Molenkamp, New J. Phys. 12, 083058 (2010). [3] L. B. Zhang, F. Cheng, F. Zhai and Kai Chang, Phys. Rev. B 83 081402(R) (2011); Z. H. Wu, F. Zhai, F. M. Peeters, H. Q. Xu and Kai Chang, Phys. Rev. Lett. 106, 176802 (2011). [4] J. J. Zhu, D. X. Yao, S. C. Zhang, and Kai Chang, Phys. Rev. Lett. 106, 097201 (2011). [5] Kai Chang, and Wen-Kai Lou, Phys. Rev. Lett. 106, 206802 (2011).

11:51AM Q31.00002 Conductance of the Quantum Spin Hall Edge in HgTe Quantum Wells ,

VIVEK VENKATACHALAM, SEAN HART, Harvard University, MATHIAS MÜHLBAUER, CHRISTOPH BRÜNE, LAURENS MOLENKAMP, Würzburg University, AMIR YACOBY, Harvard University — A two-dimensional electron system with band inversion due to spin-orbit interactions can support counterpropagating edge channels, each with one unit of conductance. Unlike the conventional quantum Hall effect, however, these channels can back scatter into each other in the presence of magnetic impurities (or other time-reversal breaking scattering sources). With topgates, we can create 1 μm edges of these QSH states and characterize their transmission. In some regions, we are able to see the quantized conductance that is expected of the QSH effect. In other regions, we see a higher resistance corresponding to a nonzero amount of scattering in the channel.

12:03PM Q31.00003 Inelastic electron backscattering in a generic helical edge channel ,

THOMAS L. SCHMIDT, Department of Physics, Yale University, 217 Prospect Street, New Haven, CT 06520, USA and Department of Physics, University of Basel, Switzerland, STEPHAN RACHEL, Department of Physics, Yale University, 217 Prospect Street, New Haven, CT 06520, USA, FELIX VON OPPEN, Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany, LEONID I. GLAZMAN, Department of Physics, Yale University, 217 Prospect Street, New Haven, CT 06520, USA — We calculate the low-temperature conductance of a generic one-dimensional helical liquid which exists at the edge of a two-dimensional topological insulator (quantum spin Hall insulator). In a generic case, the S_z spin-symmetry is absent, which opens a possibility of single-particle inelastic electron backscattering. We show that although time-reversal invariance is preserved, inelastic backscattering gives rise to a temperature-dependent deviation from the quantized conductance, $\delta G \propto T^4$. In addition, δG is sensitive to the position of the Fermi level in the gap of the insulator. We present an effective model for this type of helical liquid and determine its parameters explicitly from numerical solutions of microscopic models for two-dimensional topological insulators in the presence of Rashba spin-orbit coupling.

12:15PM Q31.00004 Gate controlled Rotating Spin Wave and chiral FFLO Superconducting phases in Quantum Spin Hall edge ,

QINGLEI MENG, TAYLOR HUGHES, MATTHEW GILBERT, SMITHA VISHVESHVARA, UIUC — We explore the phases exhibited by an interacting quantum spin Hall edge state in the presence of finite chemical potential (applied gate voltage) and spin imbalance (applied magnetic field). We find that the helical nature of the edge state gives rise to orders that are expected to be absent in non-chiral one-dimensional electronic systems. For repulsive interactions, the ordered state has an oscillatory spin texture whose ordering wavevector is controlled by the chemical potential. We analyze the manner in which a magnetic impurity provides signatures of such oscillations. For attractive interactions, finite spin-imbalance, which acts to set up a finite current in unordered QSH edges, results in superconducting order that is characterized by FFLO-type oscillations.

12:27PM Q31.00005 Phonon induced backscattering in helical edge states ,

JAN CARL BUDICH, Institute for Theoretical Physics and Astrophysics, University of Würzburg, FABRIZIO DOLCINI, Dipartimento di Fisica del Politecnico di Torino, Torino Italy, PATRIK RECHER, BJOERN TRAUZETTEL, Institute for Theoretical Physics and Astrophysics, University of Würzburg, MESOSCOPIC PHYSICS GROUP TEAM — A single pair of helical edge states as realized at the boundary of a quantum spin Hall insulator is known to be robust against elastic single particle backscattering as long as time reversal symmetry is preserved. However, there is no symmetry preventing inelastic backscattering as brought about by phonons in the presence of Rashba spin orbit coupling. In this work, we show that the quantized conductivity of a single channel of helical Dirac electrons is protected even against this inelastic mechanism to leading order. We further demonstrate that this result remains valid even when Coulomb interaction is included in the framework of a helical Tomonaga Luttinger liquid.

12:39PM Q31.00006 Optically engineering the topological properties of helical edge states ,

JÉRÔME CAYSSOL¹, Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany, BALÁZS DÓRA, FERENC SIMON, Department of Physics, Budapest University of Technology and Economics, Budafoki út 8, 1111 Budapest, Hungary, RODERICH MOESSNER, Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — Time-periodic perturbations can be used to engineer topological properties of matter by altering the Floquet band structure. This is demonstrated for the helical edge state of a spin Hall insulator in the presence of monochromatic circularly polarized light. We first demonstrate that the inherent spin structure of the edge state is influenced by the Zeeman coupling and not by the orbital effect. The photocurrent (and the magnetization along the edge) develops a finite, helicity dependent expectation value and turns from dissipationless to dissipative with increasing radiation frequency, signalling a change in the topological properties. The connection with Thouless' charge pumping and non-equilibrium Zitterbewegung is discussed, together with possible experiments. B. Dora, J. Cayssol, F. Simon, and R. Moessner, Optically engineering the topological properties of a spin Hall insulator, arXiv:1105.5963

¹Also affiliated at: LOMA (UMR-5798), CNRS and University Bordeaux 1, F-33045 Talence, France

12:51PM Q31.00007 ABSTRACT WITHDRAWN —

1:03PM Q31.00008 Fingerprints of a bidimensional topological insulator in Bismuth nanocontacts ,

JUAN JOSE PALACIOS, Universidad Autonoma de Madrid, DANIEL GOSALBEZ, CARLOS SABATER, Universidad de Alicante, JOAQUIN FERNANDEZ-ROSSIER, International Iberian Nanotechnology Laboratory, CARLOS UNTIEDT, Universidad de Alicante — We report on experimental and theoretical work of the electronic transport in Bismuth nanocontacts as created by repeated breaking and indentation using scanning tunneling microscopy techniques. The conductance exhibits a number of unusual features, not shared by normal metals, one of the most striking ones being the presence of plateaus at fractional values of the quantum of conductance at low temperatures. We understand this phenomenon on the basis of the formation of a bilayer of Bismuth (a predicted bidimensional topological insulator) which supports a maximum of a quantum of conductance as expected for its odd number of gapless edge modes. Theoretical transport results based on an atomistic tight-binding model with disorder and spin-orbit coupling permit us to associate the fractional-valued plateaus to the final stages of the breaking of the bilayer.

1:15PM Q31.00009 Spin Josephson effect at the quantum spin Hall edge ,

VASUDHA SHIVAMOGGI, QINGLEI MING, TAYLOR HUGHES, Department of Physics, University of Illinois, MATTHEW GILBERT, Department of Electrical and Computer Engineering, University of Illinois, SMITHA VISHVESHVARA, Department of Physics, University of Illinois — We study a spin Josephson effect in a ferromagnetic junction at the quantum spin Hall (QSH) edge. The helical nature of the QSH edge states has striking consequences for the transport properties of such a junction. We derive an expression for the spin current through the junction as a function of the change in magnetization, similar to the current-phase relation of a Josephson junction. We discuss the novel transport properties of the junction that result from fractionally charged excitations hosted by the QSH edge.

1:27PM Q31.00010 Equality of certain bulk wave functions and edge correlations in $d = 2$ and $d = 3^1$, RAMAMURTI SHANKAR, Yale University, ASHVIN VISHWANATH, University of Californian Berkeley — Ground state wavefunctions and gapless edge physics provide two complementary approaches to the study of quantum Hall liquids. Seminal work of Read and Moore establishes a connection between wavefunctions and 1+1 D Conformal Field Theories, which also describe edge states. Here we provide a transparent derivation of the edge correlation-wavefunction *equality* for certain topological superconductors - theories with edge states, where charge is not conserved. By studying the 2+1 D $p + ip$ superconductor in some detail, we show that the only necessary ingredient is an approximate Lorentz invariance. We are therefore able to extend the derivation to other dimensions, for example an analogous equality of bulk wavefunctions and edge correlations is derived for superfluid $^3\text{He} - B$ in $d = 3$. A key realization is that ground state wavefunctions can be extracted by considering Euclidean partition functions with a time dependent chemical potential. We also demonstrate that the method works for interacting phases, by studying a “fractional” topological superconductor using the parton construction. This connection may help identify novel topological phases in various dimensions.

¹We are grateful for NSF for grants DMR- 0645691 (AV), and DMR-0103639 (RS). RS is grateful to the Department of Physics at UC Berkeley for hosting his sabbatical in Spring 2011, which made this work possible.

1:39PM Q31.00011 Transport on the Surface of Weak Topological Insulators, ROGER MONG, JENS H. BARDARSON, JOEL E. MOORE, University of California, Berkeley — Weak topological insulators have an even number of Dirac cones in their surface spectrum and are thought to be unstable to disorder, which leads to an insulating surface. Here we argue that the presence of disorder alone will not localize the surface states, rather, the presence of a time-reversal symmetric mass term is required for localization. Through numerical simulations, we show that in the absence of the mass term the surface always flow to a stable metallic phase and the conductivity obeys a one-parameter scaling relation, just as in the case of a strong topological insulator surface. With the inclusion of the mass, the transport properties of the surface of a weak topological insulator follow a two-parameter scaling form.

1:51PM Q31.00012 Coherent transport of topological insulator surface states, PIERRE ADROGUER, DAVID CARPENTIER, EDMOND ORIGNAC, Laboratoire de physique, Ecole Normale Supérieure de Lyon, France, JEROME CAYSSOL, LOMA, University Bordeaux-1, France — Topological insulators (TIs) are a new state of matter recently predicted theoretically^{1,2} and realized experimentally. In 3D they are characterized by the presence of gapless surface states which exhibit a linear dispersion, typical of Dirac fermions. Moreover, contrary to conventional materials, these Dirac cones occur in an odd number of Dirac fermions at the surface: ARPES experiments^{3,4} have found a single Dirac cone at the surface of Bi₂Se₃, Bi₂Te₃. This work focuses on the electronic transport properties calculations in the diffusive limit of a single Dirac cone. Specificities of the TI surface states, like the hexagonal warping coupling are taken into account.

¹C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 226801 (2005).

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³Y. Xia, D. Qian, D. Hsieh, L. Wray, A. Pal, H. Lin, A. Bansil, D. Grauer, Y. S. Hor, R. J. Cava, and M. Z. Hasan, Nature Physics 5, 398 (2009).

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2:03PM Q31.00013 Spin polarized multi-terminal transport in helical edge states, SUMATHI RAO, Harish-chandra Research Institute, SOURIN DAS, Delhi University — We propose a three-terminal spin polarized scanning tunneling microscope setup for probing the helical nature of the edge states that appear in the quantum spin Hall system. We show that the three-terminal tunneling conductance depends on the magnetic anisotropy, i.e., the angle between the magnetization of the tip and the local orientation of the electron spin on the edge. We show that chiral injection of an electron into the helical Luttinger liquid is associated with fractionalization of the spin and charge of the injected electron. Finally, we show that the magnetic anisotropy of the probe also leads to Fabry-Perot like two-terminal resonances in charge transport.

Wednesday, February 29, 2012 11:15AM - 2:15PM –
Session Q32 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides - Multiferroics and Magnetoelectrics 261

11:15AM Q32.00001 Skyrmions in Multiferroics, SHINICHIRO SEKI, Department of Applied Physics, University of Tokyo, XIUZHEN YU, RIKEN CMRG/CERG, SHINTARO ISHIWATA, YOSHINORI TOKURA, Department of Applied Physics, University of Tokyo — Magnetic skyrmion is a topologically stable particle-like object, which appears as nanometer-scale vortex-like spin texture in a chiral-lattice magnet. In metallic materials, electrons moving through skyrmion spin texture gain a nontrivial quantum Berry phase, which provides topological force to the underlying spin texture and enables the current-induced manipulation of magnetic skyrmion. Such electric controllability, in addition to the particle-like nature, is a promising advantage for potential spintronic device applications. In this talk, we report the experimental discovery of magnetoelectric skyrmion in an insulating chiral-lattice magnet Cu₂OSeO₃. We find that the skyrmion can magnetically induce electric polarization through the relativistic spin-orbit interaction, which implies possible manipulation of the skyrmion by external electric field without loss of joule heating. The present finding of multiferroic skyrmion may pave a new route toward the engineering of novel magnetoelectric devices with high energy efficiency.

11:27AM Q32.00002 Dynamical matrix in magnetoelectrics¹, RAFFAELE RESTA, Physics Dept., Univ. of Trieste — In ordinary dielectrics the dynamical matrix at the zone center is a nonanalytic function of degree zero in the wavevector $\mathbf{q}$. Its expression (for a crystal of arbitrary symmetry) is well known and is routinely implemented in first principle calculations. The nonanalytic behavior occurs in polar crystals and owes to the coupling of the macroscopic electric field $\mathbf{E}$ to the lattice. In magnetoelectric crystals both electric and magnetic fields, $\mathbf{E}$ and $\mathbf{H}$, are coupled to the lattice, formally on equal footing. I provide the general expression for the zone center dynamical matrix in a magnetoelectric, where the $\mathbf{E}$ and $\mathbf{H}$ couplings are accounted for in a symmetric way. As in the ordinary case, the dynamical matrix is a nonanalytic function of degree zero in $\mathbf{q}$, and is exact in the harmonic approximation. Besides the above major result, I will also discuss other related issues: (i) The Lyddane-Sachs-Teller relationship for MEs, where the fields $\mathbf{E}$ and $\mathbf{H}$ are (once more) dealt with in a symmetric way; (ii) The microscopic origin of the coupling of magnetic fields to the lattice, which may look counterintuitive; (iii) The relationship to first-principle implementations, where in the simplest cases $\mathbf{E}$ and $\mathbf{B}$ (not $\mathbf{H}$) are zero.

¹Partially supported by ONR Grant N00014- 11-1-0145.

11:39AM Q32.00003 Multiferroic behavior in $\text{Lu}_2\text{MnCoO}_6$, VIVIEN ZAPF, E.-D. MUN, B.G. UELAND, J.D. THOMPSON, J. SINGLETON, Los Alamos National Laboratory, Los Alamos, NM, J. GARDNER, NIST Center for Neutron Research National Institute of Standards and Technology, Gaithersburg, MD, S. YÁÑEZ-VILAR, M. SÁNCHEZ-ANDÚJAR, M.A. SEÑARIS-RODRIGUEZ, Dpto. Química Fundamental, U. Coruna, Coruna (Spain), J. MIRA, Dpto. Física Aplicada, U. Santiago de Compostela, Santiago de Compostela (Spain), N. BISKUP, Dpto. Tecnologías de la Información, Inst. de Ciencia de Materiales, Madrid (Spain), C.D. BATISTA, Los Alamos National Laboratory, Los Alamos, NM — $\text{Lu}_2\text{MnCoO}_6$ is a new member of the multiferroics with coupling between net magnetization and net electric polarization. Similar to $\text{Ca}_3\text{MnCoO}_6$, an up-up-down-down order of the magnetic spins is found that breaks spatial-inversion symmetry and creates an electric polarization. Unlike $\text{Ca}_3\text{MnCoO}_6$, the Co and Mn ions are both in a $S = 3/2$ state, the ordering temperature is 42 K, and the magnetic field needed to suppress electric polarization is 2 T. We present an experimental study of the multiferroic properties and spin structure including neutron diffraction, electric polarization, magnetization, dielectric constant, and specific heat measurements.

11:51AM Q32.00004 Structural and Magnetic Properties of $\text{Ln}_2\text{CoMnO}_6$ ($\text{Ln} = \text{Dy}$ and La) Produced by Combustion Synthesis¹, PEDRO LINHARES C. FILHO, UFPE, PETRUCIO BARROZO, UFS, N.R. DILLEY, Quantum Design, J. ALBINO AGUIAR, UFPE, UFPE TEAM, UFS COLLABORATION, QUANTUM DESIGN COLLABORATION — The lanthanum manganites have been intensively studied in recent years. These compounds present a wide variety of properties of great technological and scientific interest. The half-doped lanthanum manganite with Co in Mn site have ferroelectric and ferromagnetic properties with critical temperatures close to room temperature. The mechanisms responsible for magnetoelectric coupling in these materials are not yet understood. In this work we study the effect of Dy doping at La site in the structural and magnetic properties of lanthanum manganite half-doped with Co obtained by combustion method. The dark powder obtained was heat-treated in air and cooled slowly in the oven. The samples were characterized structurally by X-ray diffractometry with Rietveld refinement analysis. Magnetization measurements as a function of temperature and the magnetic field were carried out on the SQUID magnetometer in temperature interval of 5 - 300 K and in magnetic fields up to 7T. The results show an decreases of the magnetic transition temperature when we substitute the La by Dy.

¹Work financed by CAPES, CNPq and FACEPE (Grant 0589-1.05/08).

12:03PM Q32.00005 Emergence of a new order reconciling ferroelectric and antiferrodistortive instabilities in EuTiO_3 , JONG-WOO KIM, PHILIP RYAN, Argonne National Laboratory, PAUL THOMPSON, SIMON BROWN, XMaS, European Synchrotron Radiation Facility, France, PETER NORMILE, Universidad de Castilla-la Mancha, Spain, ANKE WEIDENKAFF, University of Bern, Swiss — Control of magnetic moments with electric field or electric polarization with magnetic field can open new possibilities to develop future applications of low power sensors, data storages and spintronics. However, in general this magnetoelectric coupling is extremely small for device application. Although, a substantial change of the dielectric constant under magnetic field was observed in the EuTiO_3 system. This finding offers an insight into how the electric polarization couples with the magnetism through phonon modes to the spin of the Eu atoms. We present recent x-ray diffraction data on a single crystal EuTiO_3 providing the direct proof of antiferrodistortive (AFD) TiO_6 octahedral rotations correlated with the quantum paraelectric state. Forming an incommensurate AFD order mediates the competition between antiferroelectric and AFD order. We discuss the origin of magnetoelectric coupling based on the interplay of AFD order and antiferromagnetic interactions.

12:15PM Q32.00006 Spin-phonon coupling in the rare-earth orthoferrite DyFeO_3 , ANDREW LAFORGE, University of California, Santa Cruz, JEFFREY WHALEN, THEO SIEGRIST, Florida State University, ARTHUR RAMIREZ, ZACK SCHLESINGER, University of California, Santa Cruz — The rare-earth orthoferrite (RFeO_3) canted antiferromagnets are known to exhibit a wide array of magnetic properties, including spin reorientation transitions and compensation points between the rare-earth and iron sublattices. Furthermore, strong magnetoelastic coupling has been observed to lead to field-induced multiferroism with a large dielectric polarization. Here we present an infrared optical study of DyFeO_3 , focusing on the evolution of the phonon structure with temperature. Polarized single-crystal reflectance measurements are supplemented with magnetization and dielectric constant measurements to illuminate the role of spin-phonon coupling in the lattice dynamics.

12:27PM Q32.00007 A first principles investigation of a hexagonal ferrite LuFeO_3 , HENA DAS, Postdoctoral Research Associate, CRAIG J. FENNIE, Assistant Professor — The multiferroic hexagonal manganites RMnO_3 ($\text{R}=\text{Dy-Lu,Y}$), are a fascinating class of materials that display an unusual, complex interplay between structural, polar and magnetic domains. For example, the electric polarization in these compounds are found to be a by-product of a trimerized (zone-boundary) lattice distortion, arising from the ionic size mismatch between R^{+3} and Mn^{+3} ions. As a direct consequence of this improper ferroelectric transition, the ferroelectric and structural trimer domains are locked; rotation of structural distortion at a structural domain not only flips the polarization, but also rotates the spins. The hexagonal ferrites RFeO_3 ($\text{R}=\text{Lu,Er-Tb}$) crystallize in the same polar structure as the manganite counterparts. However, unlike the $\text{M}=0$, non-collinear antiferromagnetism in manganites, the ferrites have recently been shown to display weak ferromagnetic behaviour[1], the underlying microscopic mechanism of which so far is not understood. In the present study, using first principles density functional calculations, we investigate the structural and magnetic properties of LuFeO_3 , one of the members of this ferrite series.

[1] A. R. Akbashev, A. S. Semisalova, N. S. Perov and A. R. Kaul, Appl. Phys. Lett **99**, 122502 (2011).

12:39PM Q32.00008 Atomic Resolution Valence Mapping in LuFe_2O_4 in an Aberration Corrected STEM¹, J.A. MUNDY, Cornell University, C.M. BROOKS, R. MISRA, P. SCHIFFER, Pennsylvania State University, D.A. MULLER, D.G. SCHLOM, Cornell University — LuFe_2O_4 is a multiferroic with the simultaneous existence of ferroelectricity and ferrimagnetism at the highest temperature of any known material. The improper ferroelectricity is attributed to charge ordering in the Fe-O layers, however, a direct measure of the Fe valence on individual columns in the crystal remains elusive. Scanning Transmission Electron Microscopy (STEM) in combination with Electron Energy Loss Spectroscopy (EELS) allows for spatially resolved, chemically sensitive investigation of oxide materials. We used a Nion 5th-order aberration corrected 100 keV dedicated STEM to collect spectroscopic images from a thin film of LuFe_2O_4 on MgAl_2O_4 to map the two-dimensional concentrations of every atomic species in the film. The Fe valence on individual columns was measured, however, no statistically significant modulation—as would be consistent with charge ordering—was observed. Finally, changes in the fine structure in the EELS O atoms in the Lu-O and Fe-O planes, was mapped in two-dimensions.

¹Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0002334

12:51PM Q32.00009 Anisotropy in the magnetic and multiferroic properties of $\text{LuFe}_2\text{O}_{4-\delta}$ single crystals with varying oxygen stoichiometry, G. BALAKRISHNAN, R.A. MCKINNON, M.R. LEES, Department of Physics, University of Warwick, Coventry CV4 7AL, UK — LuFe_2O_4 is a multiferroic, where the origin of the ferroelectricity is attributed to electron correlations and directly linked to the charge ordering of Fe^{2+} and Fe^{3+} in the lattice. The multiferroic properties of this system are known to be sensitive to the oxygen stoichiometry. Large single crystals of $\text{LuFe}_2\text{O}_{4-\delta}$ with varying oxygen stoichiometry have been produced by the floating zone technique. Detailed magnetic susceptibility, dielectric constant and polarization measurements have been carried out along specific crystallographic axes of the single crystals over a wide temperature range to study the anisotropic properties. The effect of altering the $\text{Fe}^{2+}/\text{Fe}^{3+}$ stoichiometry on the physical properties of $\text{LuFe}_2\text{O}_{4-d}$ is discussed.

1:03PM Q32.00010 Charge dynamics in a frustrated charge ordered multiferroic system, MAKOTO NAKA, SUMIO ISHIHARA, Department of Physics, Tohoku University — Electronic ferroelectricity is known as phenomena where the electric polarization is caused by the electronic charge order without inversion symmetry. This is seen in some transition metal oxides, e.g. LuFe_2O_4 , and organic salts. It is suggested from the theoretical work [1] that large charge fluctuation and frustration are responsible for the electric polarization. This charge fluctuation is expected to govern dynamical properties. Actually, the measurements of the low frequency dielectric dispersion and the optical conductivity indicate that the large charge fluctuation remains in charge ordered phase in LuFe_2O_4 . Motivated by these experimental results, we study charge dynamics in charge ordered system on the layered triangular lattice. We adopt the V-t model where the inter-site electron transfers and the inter-site Coulomb interactions are taken into account. We analyze this model by utilizing the exact diagonalization method and focus on effects of frustration in the charge dynamics. In the 3-fold charge ordered phase associated with the electric polarization, the optical conductivity shows multiple-peak structure in a wide energy range. In finite temperature, the low frequency oscillator strength of the optical conductivity and the dynamical charge correlation functions in 3-fold charge ordered phase decrease slower than those in the non-polar 2-fold charge ordered phase. These results imply the strong charge fluctuation in the 3-fold charge ordered phase due to the geometrical frustration. [1] M. Naka et al. Phys. Rev. B. **77** 224441.

1:15PM Q32.00011 Multiferroic M-type hexaferrites with room-temperature conical spin structure, Y. TAGUCHI, Y. TOKUNAGA, CMRG and CERG, RIKEN ASI, Japan, Y. KANEKO, ERATO MF, JST, Japan, D. OKUYAMA, CMRG and CERG, RIKEN ASI, Japan, S. ISHIWATA, Dept. of Appl. Phys., Univ. of Tokyo, Japan, T. ARIMA, Dept. of Adv. Mat. Sci., Univ. of Tokyo, Japan, S. WAKIMOTO, K. KAKURAI, Japan Atomic Energy Agency, Japan, Y. TOKURA, CMRG and CERG, RIKEN ASI, ERATO MF, JST, Univ. of Tokyo, Japan — Magnetic and magnetoelectric properties have been investigated for single crystals of Sc-doped M-type hexaferrites [1]. Magnetization and neutron diffraction studies have indicated that a longitudinal conical state is stabilized up to room temperature by tuning the Sc concentration. Magnetoelectric measurements have shown that electric polarization can be induced by applying a transverse magnetic field at lower temperatures, and that the spin helicity is nonvolatile and endurable up to near the transition temperature from conical to collinear state. In addition, the behavior of the polarization vector upon the reversal of magnetization varies with temperature, thereby allowing us to control the relation between spin helicity and magnetization vectors with magnetic field and temperature. This work was in part supported by FIRST program on "Quantum Science on Strong Correlation" from JSPS. [1] Y. Tokunaga, Y. Kaneko, D. Okuyama, S. Ishiwata, T. Arima, S. Wakimoto, K. Kakurai, Y. Taguchi, and Y. Tokura, Phys. Rev. Lett. **105**, 257201 (2010)

1:27PM Q32.00012 The magnetoelectric effect in the $\text{RAl}_3(\text{BO}_3)_4$ ($\text{R}=\text{Tb, Ho, Er, and Tm}$), K.-C. LIANG, R. P. CHAUDHURY, B. LORENZ, TCSUH and Department of Physics, University of Houston, Houston, TX 77204, USA, L.N. BEZMATERNYKH, V.L. TEMEROV, Institute of Physics, Siberian Division, Russian Academy of Sciences, Krasnoyarsk, 660036, Russia, C.W. CHU, TCSUH and Department of Physics, University of Houston, Houston, TX 77204, USA — We study the magnetoelectric (ME) effect of the rare earth aluminum borates, $\text{RAl}_3(\text{BO}_3)_4$ ($\text{R}=\text{Tb, Ho, Er, and Tm}$). The magnetic, magnetoelectric, and magnetostrictive properties were investigated between 2K and 300K with different orientation of fields up to 70kOe. A giant magnetoelectric polarization, $3600 \mu\text{C}/\text{m}^2$, is found in $\text{HoAl}_3(\text{BO}_3)_4$ while a 70kOe transverse magnetic geometry field is applied. This value is significantly larger than that previously reported in all other bulk crystalline linear magnetoelectric or multiferroic materials. Furthermore, the ME polarization decreases with increasing magnetic anisotropy of the rare earth moment. The magnetostrictive measurements show that there is a strong coupling between the 4-f moments and the lattice. Our data further imply that the field-induced ionic displacements in a unit cell give rise to a change of structural symmetry from non-polar to polar symmetry.

1:39PM Q32.00013 Polar Nanodomains and Giant Converse Magnetoelectric Effect in Charge-Ordered Fe_2OBO_3 , HUAIXIN YANG, HUANFANG TIAN, YUANJUN SONG, YUANBIN QIN, Institute of Physics, Chinese Academy of Sciences, YONGGANG ZHAO, Department of Physics, Tsinghua University, CHAO MA, JIANQI LI, Institute of Physics, Chinese Academy of Sciences — Charge ordering (CO) is considered to be an important issue that leads to metal-insulator transitions in numerous materials and also shows possible correlations to many notable physical phenomena, such as colossal magnetoresistance, superconductivity and multiferroics. In recent investigations, oxyborate Fe_2OBO_3 has been found to show certain structural and physical features in connection with a continuous CO transition [1, 2]. By using *In-situ* TEM technique, we revealed that the charge-ordering transition characterized by an incommensurate modulation could evidently result in remarkable polar nanodomains at low temperatures. This kind of nanodomain could play a critical role in triggering a high dielectric constant and notable dielectric dispersion as observed in Fe_2OBO_3 . Moreover, measurements of the magnetoelectric coupling under electrical field demonstrate the existence of giant electrically induced changes in magnetization around the magnetic transition [1, 2]. 1.Y. J. Song et al., Phys. Rev. B **81**, 020101(R) (2010). 2.H. X. Yang et al., Phys. Rev. Lett. **106**, (2011) 016406.

1:51PM Q32.00014 Ferroelectric Phase Transition in $\text{Pb}_5\text{Cr}_3\text{F}_{19}$ and Coupling of Electric Polarization and Magnetization, ZVONKO TRONTELJ, Physics Department, IMFM, Ljubljana, DAMIR PAJIC, Department of Physics, University of Zagreb, Croatia, MARKO JAGODIC, Physics Department, IMFM, Ljubljana, PAVEL CEVC, Josef Stefan Institute, Ljubljana, Slovenia — The ferroelectric fluoride $\text{Pb}_5\text{Cr}_3\text{F}_{19}$ with ferroelectric/paraelectric phase transition at 545 K offers a possibility of multiferroic behavior. The paramagnetic Cr^{3+} ion with electronic spin 3/2 has two inequivalent positions in the unit cell and is responsible for magnetic properties. These properties were measured with a SQUID magnetometer from 2 K to 630 K in addition to our earlier EPR measurements. At the ferroelectric/paraelectric phase transition the lattice parameters (c and a unit cell dimensions) experience relatively big changes leading to alteration of magnetic dipole-dipole and exchange interactions. The temperature dependence of magnetic susceptibility times temperature around the phase transition was analyzed following the usual free energy expansion. We obtained that a coupling between the electric polarization and the magnetization is quadratic. A magnetic anomaly was observed below 25 K.

2:03PM Q32.00015 The origin and coupling mechanism of magnetoelectric effect in $\text{TMCl}_2\cdot 4\text{SC}(\text{NH}_2)_2$ ($\text{TM} = \text{Ni and Co}$), E. MUN, National High Magnetic Field Laboratory (NHMFL), Los Alamos National Lab (LANL), Los Alamos, NM, J. WILCOX, J. MANSON, Department of Chemistry and Biochemistry Eastern Washington University Cheney, WA 99004 USA, B. SCOTT, MPA-MC, LANL, Los Alamos, NM, P. TOBASH, E. BAUER, MPA-CMMS, LANL, Los Alamos, NM, P. SENGUPTA, Nanyang Technological Institute, Singapore, C. BATISTA, Theory division, LANL, Los Alamos, NM, V. ZAPF, National High Magnetic Field Laboratory (NHMFL), Los Alamos National Lab (LANL), Los Alamos, NM — Most research on multiferroics and magnetoelectric effects to date has focused on inorganic oxides. Metal organic frameworks (MOF) are a new field in which to search for ferroelectricity and explore new coupling mechanisms between electricity and magnetism. We will present the magnetic and electric properties of $\text{NiCl}_2\cdot 4\text{SC}(\text{NH}_2)_2$, DTN, and $\text{CoCl}_2\cdot 4\text{SC}(\text{NH}_2)_2$, DTC, compounds as a function of temperature, magnetic, and electric field. We gain insights into the coupling mechanism by observing that in DTN the electric polarization closely tracks the magnetic ordering whereas in DTC it does not. For DTN, all electrically polar thiourea, $\text{SC}(\text{NH}_2)_2$, molecules are tilted in the same direction along the c-axis, breaking spatial inversion symmetry, whereas for DTC, two thiourea molecules are pointing up and the other two thiourea molecules are pointing down direction with respect to c-axis, perfectly canceling the net electrical polarization. Thus the magnetoelectric coupling mechanism is likely magnetostrictive adjustments of the thiourea molecule orientation in response to magnetic order.

Wednesday, February 29, 2012 11:15AM - 2:15PM –

Session Q33 GIMS: Focus Session: X-ray and Neutron Instruments and Measurement Science

11:15AM Q33.00001 Science Enabled by the Advanced Photon Source Upgrade¹, G. BRIAN STEPHENSON, Argonne National Laboratory — The Advanced Photon Source (APS) at Argonne National Laboratory is embarking on a major Upgrade that will significantly enhance capabilities for research using high brilliance, high energy synchrotron x-ray beams. The APS is a DOE Office of Science user facility that provides access to x-ray scattering, spectroscopy, and imaging instruments through an open, peer-reviewed proposal process. Currently 64 simultaneously operating beamlines are used by more than 4000 researchers each year across the full range of science and technology fields. The APS Upgrade project will provide major improvements to the x-ray sources as well as more than a dozen new or upgraded beamlines. Key areas of emphasis are using penetrating, high energy x-rays for atomic-scale studies of real materials in real time under real conditions, imaging of hierarchical structures on length scales from millimeters to nanometers, and ultrafast studies of chemical and physical processes on time scales down to picoseconds. I will illustrate the science enabled by the APS Upgrade using examples such as developing synthesis of new materials with outstanding properties and probing picosecond dynamics in energy conversion systems.

¹Work supported by the Dept. of Energy, Office of Basic Energy Sciences under contract DE-AC02-06CH11357.

11:51AM Q33.00002 Initial Results and Future Plans for the Soft X-ray Instrument for Materials at the Linac Coherent Light Source (LCLS), WILLIAM SCHLOTTER, Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, CA, OLEG KRUPIN, European XFEL, Hamburg, Germany, MICHAEL MINITTI, JOSHUA TURNER, Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, CA — For two years ultrafast high intensity x-ray pulses have been available at the Linac Coherent Light Source, the x-ray free electron laser at the SLAC National Accelerator Laboratory. The soft x-ray instrument (SXR) operates at an energy range from 480eV-2000eV and features a plane grating monochromator as well as a bendable refocusing mirror system. The measured performance of the instrument will be presented as well as the future direction for instrumentation development.

Acknowledgement: This research was carried out on the SXR Instrument at the Linac Coherent Light Source (LCLS), a division of SLAC National Accelerator Laboratory and an Office of Science user facility operated by Stanford University for the U.S. Department of Energy. The SXR Instrument is funded by a consortium whose membership includes the LCLS, Stanford University through the Stanford Institute for Materials Energy Sciences (SIMES), Lawrence Berkeley National Laboratory (LBNL), University of Hamburg through the BMBF priority program FSP 301, and the Center for Free Electron Laser Science (CFEL).

12:03PM Q33.00003 Microfocusing options for sector 3 of the Advanced Photon Source upgrade project¹, A.M. ALSMADI, Umm Al-Qura University, A. ALATAS, J. ZHAO, L. YAN, L. GAO, E.E. ALP, Argonne National Laboratory — Synchrotron radiation from third generation, high-brilliance rings is an ideal source for x-ray microbeams. The aim of this report is to describe a microfocusing scheme that combines both a toroidal mirror and a Kirkpatrick-Baez (KB) mirrors for upgrading the existing optical system for inelastic x-ray scattering experiments at sector 3 at the Advanced photon Source (APS). Shadow ray tracing simulations show that this combination can provide beam sizes of $4.5 \mu\text{m}$ (H) $\times$ $0.6 \mu\text{m}$ (V) (FWHM) at the end of the existing D-station (66 m from the source) with a transmission of up to 59 % and a beam size of $3.7 \mu\text{m}$ (H) $\times$ $0.46 \mu\text{m}$ (V) (FWHM) at the front end of proposed E-station (68 m from the source) with a transmission of up to 57 %. With this new setup, experiments that combine high pressure, low temperature and external magnetic field can be done.

¹We would like to thank the IAEA for providing Dr. A. M. Alsmadi with a supported fellowship to stay at the APS for 6 months during this project.

12:15PM Q33.00004 Advances in X-ray Raman spectroscopy at Stanford Synchrotron Radiation Lightsource, DIMOSTHENIS SOKARAS, DENNIS NORDLUND, TSU-CHIEN WENG, ROBERTO ALONSO MORI, UWE BERGMANN, SLAC National Accelerator Laboratory — We present a state-of-the-art x-ray Raman spectroscopy end-station recently developed, installed, and operated at the Stanford Synchrotron Radiation Lightsource. The end-station consists of two multichannel Johann type spectrometers arranged on a Rowland circle of 1m. The first one, positioned at the forward scattering angles (low-q), consists of 40 diced and spherically bended Si(110) crystals of 4" of diameter providing a large solid angle of detection as well as an overall energy resolution of about 270 meV at 6462.20 eV. The second spectrometer, consisting of 14 spherically bent Si(110) crystal analyzers, is positioned at the backward scattering angles (high-q) enabling the study of non-dipole transitions. These features, in particular the improved total resolution with a substantial increase in solid angle, positions the instrumentation as a unique alternative to soft x-ray absorption for difficult sample conditions and bulk sensitive measurements, which allows a systematic implementation of this photon-in/photon-out hard x-ray technique on emerging research of multidisciplinary scientific fields in energy-related science, physics, and material science. Preliminary results and prospects will be presented and discussed, in particular for applications in Energy Science.

12:27PM Q33.00005 Facility Overview and Double-Focusing Thermal Triple-Axis Spectrometer at the NCNR, JEFFREY LYNN, National Institute of Standards and Technology — We will briefly overview the neutron scattering instrumentation at the NCNR, but will focus the talk on the capabilities of the new thermal triple-axis spectrometer is located at the BT-7 beam port [1]. This spectrometer takes full advantage of the large 165 mm diameter reactor beam to tailor the dual $20 \times 20 \text{ cm}^2$ double-focusing monochromator system to provide monochromatic fluxes exceeding $10^8 \text{ n/cm}^2/\text{s}$ onto the sample. The two monochromators installed are PG(002) and Cu(220), which provide incident energies for 5 meV to above 500 meV. The computer controlled analyzer system offers six standard modes of operation, including a diffraction detector, a position-sensitive detector (PSD) in diffraction mode, horizontal energy focusing analyzer with detector, a Q-E mode employing a flat analyzer and PSD, a constant-E mode with the analyzer crystal system and PSD, and a conventional mode with a selection of Söller collimators and detector. Additional configurations for specific measurement needs are also available. The capabilities and performance will be discussed and examples of published data presented.

[1] J. W. Lynn, Y. Chen, S. Chang, Y. Zhao, S. Chi, W. Ratcliff, II, B. G. Ueland, and R. W. Erwin, J. Research NIST 117 (in press).

1:03PM Q33.00006 ABSTRACT WITHDRAWN —

1:15PM Q33.00007 Advanced Thermal Neutron Detectors, GRAHAM SMITH, JACK FRIED, GIANLUIGI DE GERONIMO, GEORGE MAHLER, DON MAKOWIECKI, JOE MEAD, VELJKO RADEKA, NEIL SCHAKNOWSKI, EMERSON VERNON, BO YU, Brookhaven National Laboratory — With the advent of new high intensity spallation sources, there is a vital need for development of advanced position sensitive detectors. Using neutron conversion in helium 3, which yields a large signal with excellent background rejection capability, our research program focuses on improving the rate capability, resolution, efficiency and long term stability of detectors for neutron scattering studies. We have developed a suite of detectors using proportional chambers, the latest being an array of curved, multi-wire segments with interpolating cathode strip electrodes operating simultaneously and seamlessly in a single gas volume. With rate capability of nearly 1 million per sec, this instrument has significantly advanced the state-of-the-art for protein crystallography. To attain even higher count rates, a new concept based on operation in the ionization mode is being explored, in which direct ionization from a neutron conversion is collected with unity gain on one of many pads that form the anode plane. Each pad is implemented with charge sensitive electronics, using purpose-designed application specific integrated circuits. A prototype device with 48 by 48 pads has been successfully developed. Examples of measurements at major neutron user facilities will be presented.

1:27PM Q33.00008 ABSTRACT WITHDRAWN —

1:39PM Q33.00009 The wetting behavior of electrolytes at charged carbon electrode materials probed using neutron scattering¹, JOSE LEO BAÑUELOS, PASQUALE FULVIO, GERNOT ROTHER, LAWRENCE ANOVITZ, JIM BROWNING, Oak Ridge National Laboratory — Breakthroughs in the performance of energy storage technologies come from efficient combinations of novel electrolytes and electrode materials. Knowledge of the structure of these materials under applied electric fields is necessary to better tailor them to our energy needs. Neutron scattering, as a structural probe to investigate the ordering of electrolytes at an interface, or the effects of confinement on an electrolyte in a nanoporous matrix, is well suited since the electrolytes commonly used contain hydrogen and the host matrix can often contain active sites that are difficult to discern without the use of contrast matching via isotopic substitution. We present small angle neutron scattering results, conducted at the EQ-SANS (ORNL) instrument and at the Low-Q Diffractometer (LANL), from in situ electrochemical measurements of a deuterated ionic liquid, and of aqueous electrolytes, in a mesoporous carbon membrane at different applied potentials over time. Recent neutron reflectometry measurements (LR, SNS) complement the observed behavior from SANS. We observe a higher electrolyte density near the electrode material surface, compared to without an applied potential. Furthermore, this high density region persists long after the applied potential is removed.

¹This work supported by the U.S. DOE, BES, as part of an Energy Frontier Research Center. Neutron scattering was conducted at the Lujan Neutron Scattering Center and Spallation Neutron Source, sponsored by the Div. of Sci. User Facilities, U.S. DOE.

1:51PM Q33.00010 Combined X-Ray and Neutron Powder Diffraction Studies of Nanoscale $\text{Ca}_{5-x}\text{Fe}_x(\text{PO}_4)_3\text{OH}$ Systems, A. KYRIACOU, TH. LEVENTOURI, Florida Atlantic University, B.C. CHAKOUMAKOS, V.O. GARLEA, C.D. CRUZ, Neutron Scattering Science Division, Oak Ridge National Laboratory, A.J. RONDINONE, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, K.D. SORGE, Florida Atlantic University — Multi-substituted hydroxyapatite (HAp) with crystallite size 4-130 nm is the major mineral phase in physiological apatites. Substitutions at all ionic sites affect their physicochemical properties. Fe is one of the minor substitutions at the Ca sites of HAp. It is important because it reduces the solubility of HAp, functioning as a cavities preventive agent, whereas Fe overload leads to a decreased mechanical strength and osteoporosis. Powder x-ray and neutron diffraction methods as well as energy-filtered transmission electron microscopy were used to study the effect of Fe substitution on the crystal structure properties of the $\text{Ca}_{(5-x)}\text{Fe}_x(\text{PO}_4)_3\text{OH}$ systems. Single phase HAp is identified in systems with $x \leq 0.1$. Hematite is formed for higher x . Simultaneous Rietveld refinement of the x-ray and neutron diffraction patterns reveals an unexpected increase of the a-lattice constant. It is attributed to the increase of the Ca1-O3 and Ca2-O1 interatomic distances indicating a local lattice relaxation. Fe substitutes in both Ca1 and Ca2 sites with a preference to the Ca2 site and an occupancy up to 0.05 for $x=0.3$. Magnetic measurements reveal a transition from the diamagnetic state of the HAp to the paramagnetic of the Fe-doped systems.

2:03PM Q33.00011 Profile retrieval using Spin-Echo Resolved Grazing Incidence Scattering combined with dynamical scattering theory¹, RANA ASHKAR, Physics Department, Indiana University Bloomington, ROGER PYNNE, Physics Department, Indiana University Bloomington and Neutron Science Directorate, Oak Ridge National Laboratory — Spin-echo Resolved Grazing Incidence Scattering (SERGIS) is a novel neutron scattering technique that provides lateral and in-depth characterization of density correlations in thin films and at interfaces. The method can be used to study the self-assembly of materials in a periodic array of nano-channels such as a diffraction grating. Since scattering from such periodic structures is dominated by dynamical effects that are not accounted for in approximate scattering theories, we developed a dynamical theory (DT) model, based on a Parratt formalism, and tested it on SERGIS data collected from a set of nanostructured gratings with different profiles in various scattering geometries. The model shows good agreement with all the data sets obtained so far. We found that the SERGIS technique is very sensitive to slight variations in the scattering geometry and the sample profile and the DT calculations accurately reproduce this sensitivity. This is a very promising step in combining a neutron scattering technique with an exact theory to retrieve profile information of periodic samples with unknown structures and to probe the morphology of self-assemblies in periodic nano-confinements.

¹This work was supported by the Department of Energy through its Office of Basic Energy Sciences, Division of Material Science and Engineering (Grant No. DE-FG02-09ER46279).

Wednesday, February 29, 2012 11:15AM - 2:15PM – Session Q34 DCP: Focus Session: Nano IV: Nanocatalysis 107A

11:15AM Q34.00001 Cluster size effects on chemical and physical properties of model catalysts, SCOTT ANDERSON, University of Utah — Model catalysts are prepared by deposition of size- and energy-selected metal clusters on well characterized solid supports in an ultrahigh vacuum system. The system provides capabilities to probe the physical properties of the samples by X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS), ion neutralization spectroscopy (INS), and low energy ion scattering (ISS). The chemical properties can be probed by a variety of pulsed, temperature-programmed, and constant temperature mass spectrometric methods, and resulting changes in physical properties from interactions with adsorbates are probed by XPS, UPS, INS, and or ISS. Recently, capabilities for in situ electrochemical characterization were added. Results from several systems will be presented, including gas-surface reactions over Pd/alumina and Pd/titania, and solution phase oxygen reduction over Pt/glassy carbon.

11:51AM Q34.00002 CO Oxidation on Copper Oxide Cluster Ions, MASAHIKO ICHIHASHI, Toyota Technological Institute, SHINICHI HIRABAYASHI, Genesis Research Institute, Inc., YOSHIYUKI KAWAZOE, Tohoku University — We investigated the reaction of CO and O_2 on size-selected copper cluster ions, Cu_n^+ ($n=4-18$) and Cu_n^- ($n=4-11$), by use of a tandem mass-spectrometer equipped with octopole ion guides. A coadsorbing product, $\text{Cu}_n\text{O}_2(\text{CO})^+$, was observed in the reaction of Cu_nO_2^+ with CO, and it was found that CO adsorbs onto Cu_nO_2^+ more efficiently than onto Cu_n^+ in $n \geq 9$. This shows the cooperative coadsorption of O_2 and CO. On the other hand, in the reaction of Cu_nO_2^- with CO, a reduced product, Cu_nO^- , was obtained instead of the coadsorbing product, $\text{Cu}_n\text{O}_2(\text{CO})^-$. In particular, Cu_5O_2^- and Cu_9O_2^- have relatively high efficiency for the production of Cu_nO^- . This result suggests the production of CO_2 by the oxidation of CO on Cu_nO_2^- . The DFT calculation indicates that the activation energy in the reaction of $\text{Cu}_5\text{O}_2(\text{CO})^- \rightarrow \text{Cu}_5\text{O}(\text{CO}_2)^-$ is only 0.79 eV while that of the corresponding cation is 1.79 eV. The structure of Cu_n^- is more flexible than that of Cu_n^+ probably because of its excess electron. It is concluded that the stabilization of the transition state and the decrease of the activation energy make the CO oxidation proceed on Cu_nO_2^- .

12:03PM Q34.00003 Effective rate constants for nanostructured heterogeneous catalysts, SHAUN HENDY, NICOLA GASTON, PHILIP ZHANG, Industrial Research Ltd, NAT LUND, Victoria University of Wellington — There is currently a high level of interest in the use of nanostructured materials for catalysis. For instance, gold, which is largely inert in the bulk, can exhibit strong catalytic activity when in nanoparticle form. With precious metal catalysts such as Pt and Pd in high demand, the use of these materials in nanoparticle form can also substantially reduce costs by exposure of more surface area for the same volume of material. When reactants are plentiful, the effective activity of a nanoparticulate catalyst will increase roughly with its surface area. However, under diffusion-limited conditions, the reactant must diffuse to active sites on the catalyst, so a high surface area and a high density of active sites may bring diminishing returns if reactant is consumed faster than it arrives. Here we apply a mathematical homogenisation approach to derive simple expressions for the effective reactivity of a nanostructured catalyst under diffusion limited conditions that relate the intrinsic rate constants of the surfaces presented by the catalyst to an effective rate constant. When highly active catalytic sites, such as step edges or other defects are present, we show that distinct limiting cases emerge depending on the degree of overlap of the reactant depletion zone about each site. In gases, the size of this depletion zone is approximately the mean free path, so the effective reactivity will depend on the structure of the catalyst on that scale. We discuss implications for the optimal design of nanoparticle catalysts.

12:15PM Q34.00004 Towards a Molecular Level Understanding of CO and H₂ Adsorption and Dissociation on Cobalt Nanoparticles, EMILY LEWIS, APRIL JEWELL, GEORGIOS KYRIAKOU, CHARLES SYKES, Tufts University — The development of sustainable energy technologies, including the production of synthetic fuels, is of global importance. Fischer-Tropsch synthesis (FTS) has recently gained increased attention as it involves the formation of hydrocarbons via the catalytic conversion of syngas (CO and H₂), which can be derived from renewable sources. FTS is often performed using Co-based catalysts that are greatly affected by the adsorption state of reactants, as well as nanoparticle shape and size. Here we have used low-temperature scanning tunneling microscopy (LT-STM) to study the interaction of syngas with well-defined Co nanoparticles grown onto Cu {111}, an inert metal for FTS. Hydrogen adsorbs dissociatively on the Co surfaces, resulting in three unique coverage-dependent phases. We demonstrate that these phases can resolve crystal packing ambiguities of the underlying Co nanoparticles, a question that has been debated in the literature. Simultaneous exposure of the Co to H₂ and CO results in segregated islands of the adsorbates on the nanoparticle surface at 80 K, and we propose that atomic H blocks CO adsorption, causing the build-up of CO at the nanoparticle step edges. With increasing CO coverage, a two-dimensional phase compression of H by CO is observed, providing the *first direct* visualization of this phenomenon in a catalytically relevant system. Our data suggest that FTS reactivity may be dominated by the interface length between the adsorbates and be subject to unforeseen kinetic restraints as a function of particle size.

12:27PM Q34.00005 Cooperative Effects in the Oxidation of CO by Palladium Oxide Cations¹, ARTHUR C. REBER, SHIV N. KHANNA, Department of Physics, Virginia Commonwealth University, ERIC C. TYO, CHRISTOPHER L. HARMON, A. WELFORD CASTLEMAN JR., Departments of Chemistry and Physics, Penn. State University — It is shown that cooperative reactivity plays an important role in the oxidation of CO to CO₂ by palladium oxide cations. Comprehensive studies including guided-ion-beam mass spectrometry and theoretical investigations reveal the reaction products and profiles of PdO₂⁺ and PdO₃⁺ with CO through oxygen radical centers and dioxygen complexes bound to the Pd atom. We find that the O radical centers are more reactive than the dioxygen complexes, and experimental evidence of both direct and cooperative CO oxidation with the adsorption of two CO molecules are observed. The binding of multiple electron withdrawing CO molecules is found to increase the barrier heights for reactivity due to decreased binding of the secondary CO molecule, however reactivity is enhanced by the increase in kinetic energy available to hurdle the barrier. We examine the effect of oxygen sites, cooperative ligands, and spin including two-state reactivity.

¹This material is based upon work supported by the Air Force Office of Scientific Research (AFOSR) Award: FA9550-08-01-0400.

12:39PM Q34.00006 Design of nanocatalysts for improved selectivity and stability, FRANCISCO ZAERA, University of California — Several examples from ongoing work in our laboratory on the use of self-assembly to prepare heterogeneous catalysts with novel architectures will be discussed in this presentation. In one case, catalysts consisting of dispersed platinum metal nanoparticles with narrow size distributions and well-defined shapes were prepared and tested for the selective promotion of carbon-carbon double-bond cis-trans isomerization reactions in olefins. It was shown that the selective formation of the cis isomer could be controlled by using tetrahedral particles with exposed (111) facets. In a second example, catalysts based on small platinum nanoparticles of well-defined sizes were made by using dendrimers as scaffolding structures. The organic framework in that case can provide new functionality, including chirality as a way to introduce enantioselectivity. The third example involves the control of metal nanoparticle sintering by covering those with a layer of mesoporous silica grown on top. The final case to be discussed is one where yolk@shell metal-semiconductor constructs are being developed for increase stability in oxidation and photocatalytic applications.

1:15PM Q34.00007 Towards Catalysis by Gold Clusters: reaction cycles and poisons, ELIZABETH C. BERET, LUCA M. GHIRINGHELLI, MATTHIAS SCHEFFLER, Fritz-Haber-Institut, D-14195, Berlin — Nanosized gold particles are good catalysts in a variety of oxidation reactions. These reactions, for which oxidation of CO to CO₂ serves as a paradigm, imply a transition in the total spin and therefore do not occur spontaneously in the gas phase. In the catalytic process, the catalyst clusters are exposed to an atmosphere of gas-phase O₂ and CO reactants at finite temperature and pressure. We have thus modeled free gold clusters in contact with an atmosphere composed of O₂ and CO by means of DFT calculations (PBE functional), and accounted for both temperature and pressure effects employing *ab initio* atomistic thermodynamics. On the basis of this analysis, we could recognize the thermodynamic driving force of the catalytic CO oxidation process and single out the possible (*p*, *T*)-dependent reaction cycles and those paths leading to stable structures that poison the catalytic process. This as a useful (exploratory) theoretical step, before taking chemical reaction kinetics into consideration. In the proposed reaction paths, the total spin is conserved in each elementary step, and it is the adsorption of an incoming O₂ molecule that drives the catalyst cluster from the singlet to the triplet spin state, and *vice versa*.

1:27PM Q34.00008 Breaking Carbonyl Bonds in Formaldehyde via Complementary Active Sites¹, SHIV N. KHANNA, ARTHUR C. REBER, Department of Physics, Virginia Commonwealth University, W. HUNTER WOODWARD, JORDAN C. SMITH, A. WELFORD CASTLEMAN JR., Departments of Chemistry and Physics, Pennsylvania State University — We had recently shown that the complementary active sites in homonuclear clusters may stimulate the breaking of polar bonds enabling an atomic level control of reactivity. However, such bond cleavage has only been observed in hydroxyl bonds. In this work, we present experimental and theoretical evidence that demonstrates that the stronger C=O carbonyl bond of formaldehyde is split by complementary active sites on size selective aluminum cluster anions. The resonance structure in which the carbonyl is reduced to a single bond is stabilized by the paired active sites establishing the potential use of these geometrically driven centers in devising precursors for synthesizing chemicals or radicals that might find use in production of fine chemicals.

¹We gratefully acknowledge financial support from Air Force Office of Scientific Research through grants #FA9550-10-1-0071 and FA9550-09-1-0371.

1:39PM Q34.00009 Morphological, electronic, and catalytic properties of Pt nanoclusters on defective graphene, IOANNA FAMPIOU, ASHWIN RAMASUBRAMANIAM, University of Massachusetts Amherst — The synthesis of well dispersed, size-controlled Pt nanoclusters on carbon supports is highly desirable since such clusters have been shown to possess enhanced catalytic activity and selectivity in a variety of chemical reactions. However, these nanoclusters interact rather weakly with defect-free carbon supports and can coarsen over time leading to loss of surface area and thence catalytic activity. Defects in carbon supports play an important role in enhancing Pt-carbon bonding, thereby reducing the propensity for cluster coalescence. Using a combination of density functional theory and empirical potential simulations, we examine the interaction of Pt nanoclusters with point defects in graphene. We focus on the role of the support defects in controlling the morphology, electronic structure, and CO-tolerance of Pt nanoparticles. Our results suggest possible avenues for controlling the dispersion and activity of Pt nanoclusters on carbon supports via defect engineering.

1:51PM Q34.00010 Controlled Catalytic Properties of Platinum Clusters on Strained Graphene, GYUBONG KIM, Korea Institute of Science and Technology, YOSHIYUKI KAWAZOE, Tohoku University, KWANG-RYEOL LEE, Korea Institute of Science and Technology — We employed biaxially strained graphene as the supporting material for Pt clusters (Pt_x , $x=1, 4$ or 6) and studied the molecular adsorption behaviors of H_2 , CO and OH on the cluster using ab initio calculations. It was shown that the applied strain enhances binding of the Pt cluster on the graphene, which lowers the average energy of Pt d electron (d-band center). The binding energies of H_2 , CO and OH on Pt_1 /graphene are strongly correlated with the d-band center modulated by the graphene strain. The calculations with small Pt clusters (Pt_4 and Pt_6) also show that the d-band center is a substantial factor for the catalytic activity of the Pt_x /graphene system. We also found that the stability of the Pt clusters was enhanced by applying the strain on the graphene support.

2:03PM Q34.00011 Composition-Dependent Size and Shape Changes of Pt-Rh Alloy Nanoparticles on $\alpha-Al_2O_3(0001)$ during CO Oxidation Reactions¹, UTA HEJRAL, PATRICK MUELLER, University of Siegen - Germany, OLIVIER BALMES, DIEGO PONTONI, European Synchrotron Radiation Facility (ESRF) - France, ANDREAS STIERLE, University of Siegen - Germany — Pt-Rh nanoparticles are widely used in chemical industry and in automotive exhaust control where they catalyze among other reactions the oxidation of CO. Major attention has in recent years been paid to the study of alloy nanoparticles with the aim to identify systems that allow to control the catalyst selectivity and to enhance its activity and lifetime [1]. Sintering is regarded as one of the major causes of catalyst deactivation and it is of utmost scientific and economic interest to find ways to prevent it. Here we present concentration-dependent size and shape changes of epitaxial Pt-Rh alloy nanoparticles on $\alpha-Al_2O_3(0001)$ substrates observed in-situ during CO oxidation at near atmospheric pressures. The experiments were carried out in a flow-reactor at the high energy beamline ID15A (ESRF) by means of grazing incidence x-ray diffraction ($E=78.8$ keV), x-ray reflectivity measurements and in-situ mass-spectrometry [2]. During the experiments the O_2 pressure ranged between 0 and 14 mbar while the temperature and CO pressure were kept at 550 K and 20 mbar, respectively. Our results demonstrate that a higher Rh concentration reduces sintering significantly.

[1] J.Y. Park et al., Nano Lett. 8 673 (2008)

[2] R. v. Rijn et al., Rev. Sci. Instr. 81 014101 (2010)

¹BMBF Project NanoXCat

Wednesday, February 29, 2012 11:15AM - 2:03PM – Session Q35 DCP: Focus Session: DFT VI: New Functional Developments 107B

11:15AM Q35.00001 Some thoughts about old and new density functionals, MIGUEL MARQUES, LPMCEN, Université Lyon I and CNRS — The only theoretical approximation that lies at the heart of DFT appears is the (in)famous exchange-correlation functional. It is therefore not surprising that this quantity has been extensively studied, and that more than 150 different approximations have been put forward in the past 50 years. In this talk I will show some results concerning different families of functionals. The first concerns hybrid functionals, and in particular the role of the mixing parameter. This is commonly assumed to be fixed at a value around 0.2-0.3. However, by noting the similarities between the hybrid functionals and screened Hartree-Fock and ultimately GW theories, we can relate this parameter to the screening properties of the system. In this way we can build a recipe that allows for a considerable improvement on the results obtained by traditional hybrid functionals for solids. As a second topic, I will discuss if it is possible to completely get rid of the Slater integrals present in both Hartree-Fock, hybrid functionals or OEP approaches, and anyway get a proper description of the exchange in terms of reduced densities. I will pay particular attention to the new meta-GGA functionals for the exchange potentials, like, e.g., the Becke-Johnson potential and its more recent variations, like the Tran and Blaha or the Rasanen, Pittalis, and Proetto functionals.

11:51AM Q35.00002 Self-interaction corrected Kohn–Sham potentials, VIKTOR STAROVEROV, Department of Chemistry, The University of Western Ontario, London, Ontario N6A 5B7, Canada — Exchange-correlation potentials derived from conventional density-functional approximations fail to exhibit the slow Coulombic decay—a problem that is related to the self-interaction error in the potential. We show how the self-interaction error of standard semilocal approximations can be effectively reduced by employing modified electron densities to construct the corresponding Kohn–Sham potentials. Using this correction scheme in the framework of adiabatic time-dependent density-functional theory we obtain significantly improved electronic excitation energies, especially for Rydberg states.

12:03PM Q35.00003 Density-on-wave-function mapping beyond the Hohenberg-Kohn theorem, KLAUS CAPELLE, Federal University of ABC (UFABC) — Density-functional theory is based on the Hohenberg-Kohn theorem, establishing a one-on-one mapping between ground-state densities and wave functions. That theorem does not, however, make a direct statement on whether two wave functions that are in some sense close are mapped on two densities that are also close, and vice versa. In this work, a metric is defined that allows to quantify the meaning of “close” in the preceding sentence. This metric stratifies Hilbert space into concentric spheres on which maximum and minimum distances between states can be defined and geometrically interpreted. Numerical calculations for the Helium atom, Hooke's atom and a lattice Hamiltonian show that the mapping between densities and ground states, which is highly complex and nonlocal in the coordinate description, in metric space becomes a monotonic and nearly linear mapping of vicinities onto vicinities. In this sense, the density-on-wave-function mapping is not only simpler than expected; it is as simple as it could be.

I. D'Amico, J. P. Coe, V. V. França, and K. Capelle, Phys. Rev. Lett. 106, 050401 (2011) and Phys. Rev. Lett. 107, 188902 (2011). See also E. Artacho, Phys. Rev. Lett. 107, 188901 (2011).

12:15PM Q35.00004 Finding density functionals with machine learning¹, JOHN SNYDER, University of California, Irvine, MATTHIAS RUPP, Eidgenössische Technische Hochschule, Zurich, KATJA HANSEN, KLAUS MUELLER, Technische Universität, Berlin, KIERON BURKE, University of California, Irvine — Using standard methods from machine learning, we introduce a novel technique for density functional approximation. We use kernel ridge regression with a Gaussian kernel to approximate the non-interacting kinetic energy of 1-dimensional multi-electron systems. With fewer than 100 training densities, we can achieve mean absolute errors of less than 1 kcal/mol on new densities. We determine densities for which our new functional will fail or perform well. Finally, we use principle component analysis to extract accurate functional derivatives from our functional, enabling an orbital-free minimization of the total energy to find a self-consistent density. This empirical method has two parameters, set via cross-validation, and requires no human intuition. In principle, this general technique can be extended to multi-dimensional systems, and can be used to approximate exchange-correlation density functionals.

¹We thank NSF (CHE-0809859), DFG (MU 987/4-2) and EU (PASCAL2) for support.

12:27PM Q35.00005 New Density Functionals with Broad Applicability in Chemistry (SOGGA11, SOGGA11-X, M11, M11-L) and Approaches to Open-Shell DFT¹, DONALD TRUHLAR, University of Minnesota — The accuracy of density functional theory for practical applications is determined by the quality of the necessarily approximate exchange-correlation functional (“density functional”) being used, and the goal of functional development in chemical physics is to obtain a functional that is accurate for a broad range of chemistry and physics. In our work we consider molecular structures and solid-state lattice constants and band gaps, but we emphasize energetics for main-group and transition-metal chemistry, including thermochemistry and barrier heights, noncovalent interaction energies, and excitation energies. This lecture will discuss four new density functionals, each optimized to give the best across-the-board performance for a broad range of chemistry in their class of functional: SOGGA11, a generalized gradient approximation (GGA); SOGGA11-X, a global hybrid GGA; M11: a range-separated hybrid meta-GGA, and M11-L, a meta-GGA. SOGGA11 and M11-L are local functionals, and SOGGA11-X and M11 include some nonlocal Hartree-Fock exchange. To the extent that time permits, I may also discuss recent progress in the treatment of open-shell systems by density functional theory, including time-dependent DFT, open-shell SCF, and noncollinear DFT. This invited lecture is based on collaborative research carried out with Roberto Peverati, Sijie Luo, Ke Yang, Boris Averkiev, Yan Zhao, and Rosendo Valero.

¹This work is supported in part by the AFOSR and the NSF.

1:03PM Q35.00006 Self-Interaction Free and Analytic Treatment of the Coulomb Energy in Kohn-Sham Density Functional Theory¹, MARKUS DAENE, ANTONIOS GONIS, Lawrence Livermore National Laboratory, DON M. NICHOLSON, G. MALCOLM STOCKS, Oak Ridge National Laboratory — We have developed a new treatment of the LDA functional in Kohn-Sham density functional theory which is expressed in terms of the pair density of a non-interacting system of particles, thus avoiding from the outset self-interaction effects. The pair density is expressed explicitly in terms of the density using a orthonormal and complete basis expressed as a functional of the density. This allows its functional differentiation with respect to the density and therefore the determination of the self-interaction free Coulomb potential by analytic means. The method is illustrated with numerical results for the atom series.

¹This material is based upon work supported as part of the Center for Defect Physics, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

1:15PM Q35.00007 Electronic structure via potential functional approximations, ATTILA CANGI, Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany, DONGHYUNG LEE, Department of Chemistry, Rice University, 6100 Main Street, Houston, TX 77005-1892, USA, PETER ELLIOTT, Department of Physics and Astronomy, Hunter College and the City University of New York, 695 Park Avenue, New York, New York 10065, USA, KIERON BURKE, Department of Chemistry, University of California, 1102 Natural Sciences 2, Irvine, California 92697-2025, USA, E.K.U. GROSS, Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany — The universal functional of Hohenberg and Kohn is given as a coupling-constant integral over the density as a functional of the potential [1]. Conditions are derived under which potential-functional approximations are variational. Construction via this method and imposition of these conditions are shown to greatly improve the accuracy of the non-interacting kinetic energy needed for orbital-free Kohn-Sham calculations. This result provides a direct route to a self-consistent, orbital-free theory for the electronic structure of matter within the Kohn-Sham framework. It solely requires an approximation to the non-interacting density as a functional of the potential, which, so far, has been derived for simple systems [2,3].

[1] A. Cangi, D. Lee, P. Elliott, K. Burke, E. K. U. Gross, *Phys. Rev. Lett.* 106, 236404, (2011).

[2] A. Cangi, D. Lee, P. Elliott, K. Burke, *Phys. Rev. B* 81, 235128, (2010).

[3] P. Elliott, D. Lee, A. Cangi, K. Burke, *Phys. Rev. Lett.* 100, 256406, (2008).

1:27PM Q35.00008 Self-Consistent Random Phase Approximation, DANIEL ROHR, Rice University, Houston, TX, MARIA HELLGREN, E.K.U. GROSS, Max-Planck-Institute, Halle, Germany — We report self-consistent Random Phase Approximation (RPA) calculations within the Density Functional Theory. The calculations are performed by the direct minimization scheme for the optimized effective potential method developed by Yang et al. [1]. We show results for the dissociation curve of H_2^+ , H_2 and LiH with the RPA, where the exchange correlation kernel has been set to zero. For H_2^+ and H_2 we also show results for RPAX, where the exact exchange kernel has been included. The RPA, in general, over-correlates. At intermediate distances a maximum is obtained that lies above the exact energy. This is known from non-self-consistent calculations and is still present in the self-consistent results. The RPAX energies are higher than the RPA energies. At equilibrium distance they accurately reproduce the exact total energy. In the dissociation limit they improve upon RPA, but are still too low. For H_2^+ the RPAX correlation energy is zero. Consequently, RPAX gives the exact dissociation curve. We also present the local potentials. They indicate that a peak at the bond midpoint builds up with increasing bond distance. This is expected for the exact KS potential.

[1] W. Yang, and Q. Wu, *Phys. Rev. Lett.*, 89, 143002 (2002)

1:39PM Q35.00009 On the Hohenberg-Kohn and Levy-Lieb Constrained Search Proofs of Density Functional Theory, VIRAH T SAHNI, Brooklyn College CUNY, XIAO-YIN PAN, Ningbo University — In HK, a 1-1 relationship between the density $\rho(\mathbf{r})$ and the potential $v(\mathbf{r})$ is established. (The relationship between $v(\mathbf{r})$ and the ground state Ψ is 1-1.) The proof, valid for v -representable densities, shows $\rho(\mathbf{r})$ to be a basic variable. The LL proof is independent of $v(\mathbf{r})$, and is valid for N -representable densities. In¹ we have proved that in an external magnetic field $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$, there is a 1-1 relationship between $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$, with $\mathbf{j}(\mathbf{r})$ the physical current density, and the potentials $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$. (The relationship between $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ and Ψ is *many-to-one*.) This proves that $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ are the basic variables. The LL proof independent of $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ follows readily. However, such a proof also follows if $\{\rho(\mathbf{r}), \mathbf{j}_p(\mathbf{r})\}$, with $\mathbf{j}_p(\mathbf{r})$ the paramagnetic current density, are considered the basic variables. As such knowledge of the basic variables as determined via HK is a pre-requisite to any LL type proof.

¹Pan and Sahni, *IJQC* 110, 2833 (2010)

1:51PM Q35.00010 Efficient van der Waals energy calculations via a continuum mechanics approach, TIM GOULD, JOHN F. DOBSON, Qld Micro- and Nanotechnology Centre, Griffith University, Nathan, Qld 4111, Australia, ILYA V. TOKATLY, IKERBASQUE, Basque Foundation for Science, E-48011, Bilbao, Spain — Recent developments in continuum mechanics (CM) [Tao *et al*, PRL103,086401] enable the calculation of density response functions from groundstate properties only. Using the direct Random Phase Approximation (dRPA) we develop this CM approach into a third-rung van der Waals energy functional, which we dub the CM-dRPA. The functional requires as input the groundstate Kohn-Sham potential $V^{\text{KS}}(\vec{r})$, density $n^0(\vec{r})$ and a kinetic stress tensor $T^0(\vec{r})$ defined via $T_{\mu\nu}^0 = \text{Re} \sum_{i\text{occ}} \psi_{i,\mu}^* \psi_{i,\nu} - n_{\mu,\nu}^0/4$ where ψ_i is an orbital. We present efficient algorithmic schemes for its evaluation in bulk and molecular systems using the full eigen-solutions of the bare CM equation and a second, simpler evaluation to find the interacting eigenvalues. These eigen-solutions are then used to calculate the correlation energy via a simple summation. The CM-dRPA is *significantly* faster than a full dRPA calculation in systems with many electrons. We then apply the CM-dRPA functional to metallic, slab-like 2D-homogeneous jellium systems and periodic solids, with good results for vdW dispersion. In the metallic case most efficient vdW functionals would fail qualitatively.

Wednesday, February 29, 2012 11:15AM - 2:15PM – Session Q36 DCP: Water and Ice 107C

11:15AM Q36.00001 Ionic force field optimization and modified ion-pair mixing rules, MARIA FYTA, Physics Department (T37) Technical University of Munich, ROLAND R. NETZ, Fachbereich Physik, Freie Universitaet Berlin, 14195 Berlin, Germany — We propose an optimization scheme to obtain good ionic force fields for classical simulations of salt solutions, also of biological relevance. Our work is based on Molecular Dynamics simulations with explicit (SPC/E) water for different halide and alkali ions forming salt solutions at finite ion concentration. The force field derivation technique we propose is based on a simultaneous optimization of single-ion and ion-pair properties and the determination of the cation-anion interaction parameters (traditionally given by the mixing rules). From the finite-concentration simulations, thermodynamic properties of the salt solutions are derived, using the Kirkwood-Buff theory of solutions, and compared to relevant experimental data. For the rather size-symmetric salt solutions involving bromide and chloride ions, this scheme using the standard mixing rules works fine. For the iodide and fluoride solutions, corresponding to the largest and smallest anion we have considered, a rescaling of the mixing rules was necessary. In this respect, we have introduced scaling factors for the cation-anion Lennard-Jones interaction that quantify deviations from the standard mixing rules. We discuss the efficiency and complications of the proposed ionic force field optimization scheme.

11:27AM Q36.00002 Effects of Applied Electric Field on the Dynamics of Nano-Confined Water¹, SOULEYMANE DIALLO, EUGENE MAMONTOV, Spallation Neutron Source, NOBUO WADA, Nagoya University — We present quasi-elastic neutron scattering measurements of the proton diffusion in water confined in silica nanopores (FSM), with average pore diameters of 16 Å and 39 Å. The measurements were performed on the high resolution backscattering silicon spectrometer (BaSiS) at the Spallation Neutron Source (SNS). From the data, we determine the self diffusion constants, and the translational and rotational relaxation times, as a function of temperature from 300 K down to 200 K. We observe a significant slowing down of the proton diffusion as the temperature is lowered, and a remarkable effect of confinement of the translational motion. Recent results on the effects of applied electrical field on these dynamical processes will be reported.

¹Work at ORNL and SNS is sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, US DOE.

11:39AM Q36.00003 Competing Nuclear Quantum Effects and van der Waals Interactions in Water, JEFFREY MCMAHON, Department of Physics, University of Illinois, Urbana-Champaign, IL 61801, MIGUEL MORALES, Lawrence Livermore National Laboratory, Livermore, California 94550, USA, DAVID CEPERLEY, Department of Physics, University of Illinois, Urbana-Champaign, IL 61801 — Water plays a central role in many scientific disciplines, and a number of studies have been performed to understand its properties. However, providing an accurate ab initio description is a significant challenge, and because of this, many of water's properties remain elusive. In particular, the description of hydrogen bonding and the importance of van der Waals (vdW) interactions and nuclear quantum effects are still matters of debate. Recent computational advancements have been made that allow for the accurate and efficient modeling of such effects. We present results from path integral molecular dynamics simulations based on density functional theory employing exchange and correlation functionals capable of accounting for vdW interactions (so-called vdW-DF, vdW-DF2, and optB88-vdW). We demonstrate that, contrary to expectation, the interaction between nuclear quantum effects and vdW interactions hardens the structure of water. These results suggest that ad hoc methods to account for these effects, such as temperature rescaling of simulations employing classical nuclei, are insufficient to describe water, and that fully ab initio calculations must be performed. We discuss the implications of these results for understanding the local structure and hydrogen bonding in water.

11:51AM Q36.00004 BSE/GW calculations of liquid and solid H₂O¹, JOHN VINSON, J.J. KAS, F.D. VILA, J.J. REHR, University of Washington, E.L. SHIRLEY, NIST, Gaithersburg MD — We have calculated both the UV/VIS and Oxygen K-edge x-ray spectra of model ice and water systems within many-body perturbation theory using state-of-the-art Bethe-Salpeter equation (BSE) and GW self-energy approximations [1], as implemented in the valence- and core-excitation codes OCEAN and AI2NBSE [2]. While the various phases of crystalline ice have well-characterized structures, the local environment and fluctuations of liquid water remain subjects of debate. Due in part to limitations of previous theoretical models, the interpretation of experimental probes has been controversial. We find that the BSE approach, which provides an accurate treatment of core-hole interactions, is vital for a quantitative agreement between experiment and theory. Likewise the effects of self-energy corrections within the GW approximation are needed to explain the observed band-stretching and damping of the spectra. Prospects for further improvements are briefly discussed.

[1] J. Vinson, J. J. Kas, F. D. Vila, J. J. Rehr, and E. L. Shirley, arXiv:1010.0025 (2011).

[2] J. Vinson et al., Phys. Rev. B 83, 115106 (2011); H. M. Lawler et al., Phys. Rev. B 78, 205108 (2008).

¹Supported by DOE BES Grant DE-FG03-97ER45623 and facilitated by DOE CMCSN Grant DE-SC0005180.

12:03PM Q36.00005 Effect of hydrogen bond cooperativity on the phase behavior of water, KEVIN STOKELY, Boston University Physics Department — Four scenarios have been proposed for the low-temperature phase behavior of liquid water, each predicting different thermodynamics. The physical mechanism which leads to each is debated. Moreover, it is still unclear which of the scenarios best describes water, as there is no definitive experimental test. Here we address both open issues by analyzing a microscopic cell model within a mean-field limit. We show that a common physical mechanism underlies each of the four scenarios, and that two key physical quantities determine which of the four scenarios describes water: (i) the strength of the directional component of the hydrogen bond and (ii) the strength of the cooperative component of the hydrogen bond. The four scenarios may be mapped in the space of these two quantities. Using estimates from experimental data for H bond properties, the model predicts that the low-temperature phase diagram of water exhibits a liquid-liquid critical point at positive pressure.

12:15PM Q36.00006 Structure and dynamics of the liquid water-ZnO(10 $\bar{1}$ 0) interface from first principles, GABRIELE TOCCI, ANGELOS MICHAELIDES, London Centre for Nanotechnology & University College London, Department of Chemistry — Liquid water-metal oxide interfaces are of fundamental and technological interest. In this context, the water-ZnO(10 $\bar{1}$ 0) interface is an extensively studied system, which is also relevant for instance to the field of heterogeneous catalysis and photocatalysis. Yet, whether or not water dissociates at this surface at coverages exceeding one monolayer is still a matter of debate. Likewise questions about proton transfer to the surface, water diffusion and rearrangement within the hydrogen-bonded network remain unanswered. Here we report the first density functional theory (DFT) molecular dynamics study of a liquid water film on ZnO(10 $\bar{1}$ 0) and of water at monolayer coverages. The water structure obtained for the first layer in the liquid simulation differs quite significantly from that at monolayer coverage. Hydrogen bonding between the first layer and the water overlayer plays a crucial role in the stabilisation of the new adsorption structure. Rapid proton transfer and rattling within the hydrogen bonding network at the interface is observed and analysed in detail. On the whole, this study provides considerable new insight into water structure and dynamics and proton transfer at ZnO(10 $\bar{1}$ 0) and in the field of liquid water-metal oxides interfaces in general.

12:27PM Q36.00007 Density fluctuations and dielectric constant of water in low and high density liquid states, ERIK LASCARIS, Boston University, CUI ZHANG, GIULIA A. GALLI, University of California, Davis, GIANCARLO FRANZESE, Universitat de Barcelona, H. EUGENE STANLEY, Boston University — The hypothesis of a liquid-liquid critical point (LLCP) in the phase diagram of water, though first published many years ago, still remains the subject of a heated debate. According to this hypothesis there exists a critical point near $T \approx 244$ K, and $P \approx 215$ MPa, located at the end of a coexistence line between a high density liquid (HDL) and a low density liquid state (LDL). The LLCP lies below the homogenous nucleation temperature of water and it has so far remained inaccessible to experiments. We study a model of water exhibiting a liquid-liquid phase transition (that is a liquid interacting through the ST2 potential) and investigate the properties of dipolar fluctuations as a function of density, in the HDL and LDL. We find an interesting correlation between the macroscopic dielectric constants and the densities of the two liquids in the vicinity of the critical point, and we discuss possible implications for measurements close to the region where the LLCP may be located.

12:39PM Q36.00008 The role of quantum nuclear effects in hydrogen bonded crystals and their calculated NMR shielding constants¹, KJARTAN THOR WIKFELDT, London Centre for Nanotechnology, University College London, CHRIS PICKARD, Department of Physics and Astronomy, University College London, ANGELOS MICHAELIDES, London Centre for Nanotechnology, University College London — Because of its ubiquity in nature the hydrogen atom plays a very important role in computational materials science. As the lightest element, hydrogen nuclei are also the most strongly affected by quantum nuclear effects (QNEs). The path integral (PI) formalism provides a rigorous approach to obtain equilibrium quantum static properties, but PI simulations in conjunction with electronic structure calculations are rarely used due to high computational requirements. This contribution will discuss *ab initio* PI simulations aimed at elucidating the role of QNEs in hydrogen bonded crystals and how these impact upon experimental observables such as nuclear magnetic resonance (NMR) shielding constants and chemical shifts. We find that *ab initio* PI simulations improve the agreement with experimental chemical shifts compared to simulations with classical nuclei and that the influence of QNEs is very sensitive to the strength of the hydrogen bonds in the crystal.

¹This work was supported by the European Research Council. Computational resources from the London Centre for Nanotechnology as well as U.K.'s national high-performance computing service HECToR are gratefully acknowledged.

12:51PM Q36.00009 Selective mode analysis of nuclear quantum effects for liquid water using non-Markovian thermostats, SRIRAM GANESHAN, MARIVI FERNÁNDEZ-SERRA, Stony Brook University — Simulating nuclear quantum effects in liquid water using both DFT and force fields has been an active area of research in recent years. Recently, Ceriotti et. al [1] introduced a comprehensive framework to use a custom-tailored Langevin equation with correlated-noise in the context of molecular-dynamics simulations. One of the interesting applications of these thermostats is that, such a framework can be used to selectively damp normal modes whose frequency falls within a prescribed range. In this work we study how the flexible force field models respond to the selective mode thermostating using the delta-like memory kernels. We apply this delta thermostat to the molecular dynamics of TIP4P/F water force field [2], a model explicitly fitted with the lack of zero point ionic vibrations. We address the question of whether thermostating each mode to its zero point temperature is enough to generate the nuclear quantum effects in water and similar systems. This work also provides a way to identify the dominant modes for which the quantum effects are important. [1] M. Ceriotti, G. Bussi, and M. Parrinello, Phys. Rev. Lett. 103, 030603 (2009). [2] S. Habershon, T. E. Markland, and D. E. Manolopoulos, J. Chem. Phys. 131, 024501 (2009).

1:03PM Q36.00010 ABSTRACT WITHDRAWN —

1:15PM Q36.00011 Anomalous nuclear quantum effects in ice¹, BETÜL PAMUK, Stony Brook University, JOSE M. SOLER, Universidad Autonoma de Madrid, PHILIP B. ALLEN, MARIVI FERNÁNDEZ-SERRA, Stony Brook University — The lattice parameters of light (H₂O) and heavy (D₂O) ice at 10 K differ by 0.09%. [1] The larger lattice constant is that of the heavier isotope. This isotope shift with anomalous sign is linked to the zero point energy of phonons in ice. To determine the origin of this anomaly, we use *ab initio* density functional theory to compute the free energy of ice within the quasiharmonic approximation. As expected, the frozen lattice constant at $T = 0$ K is smaller than the quantum lattice constant, independent of the isotopic substitution. We find that, the heavy isotope D gives more zero point expansion than H, whereas the heavy isotope ¹⁸O gives normal zero point expansion, i.e smaller than ¹⁶O. Relative to the classical result, the net effect of quantum nuclei (H and O) on volume has the conventional (positive) sign at $T = 0$ but it becomes negative above 70 K, indicating that it may be also relevant for liquid water. These results are not reproduced by state of art polarizable empirical potentials. [2] [1] B. K. Röttger et. al., Acta Cryst. B 50, 644-648 (1994). [2] C. P. Herrero and R. Ramírez, J. Chem. Phys. 134, 094510 (2011).

¹This work is supported by DOE award numbers DE-FG02-08ER46550, DE-SC0003871.

1:27PM Q36.00012 Mechanism of sessile water droplet evaporation, HADI GHASEMI, CHARLES WARD, University of Toronto — The energy transport mechanisms during the evaporation of sessile water droplets have been investigated. Steady-state evaporation experiments were conducted on substrates of Cu, Au(111) and PDMS. The buoyancy-driven convection was suppressed by maintaining the droplets' base temperature just less than 4°C while evaporation cooled the liquid-vapor interface to lower temperatures. The temperature fields were measured in solid (only in Au(111) experiments), liquid and vapor phases. On all three substrates, the energy balance at the liquid-vapor interface showed that thermocapillary convection transported the major portion of the energy required for the evaporation. It transported up to 98% for Cu, up to 87% for Au(111) and up to 72% for PDMS. The role of thermocapillary convection is dominant close to three-phase contact line where most of the evaporation occurs. The experiment on Au (111) showed that of the energy supplied by the solid substrate, only a small portion is transported perpendicular to the solid-liquid interface to the bulk liquid phase. A much larger proportion is conducted through the adsorbed layer at the solid-liquid interface to the three-phase contact line where it is distributed by thermocapillary convection over the liquid-vapor interface and consumed by the phase change process.

1:39PM Q36.00013 Theory and Simulation of Droplet Wetting on Patterned Surfaces¹, AZAR SHAHRAZ, ALI BORHAN, KRISTEN FICHTHORN, Penn State University — Liquid droplets can have multiple wetting modes on physically patterned surfaces, each corresponding to a (meta)stable state. For example, in the Cassie mode, the droplet resides on top of the pattern, while in the Wenzel mode, the droplet penetrates into the pattern. In this work, we study the wetting of patterned surfaces on two different length scales: on the nano-scale using molecular dynamics (MD) and on the macro-scale by minimizing free-energy expressions for various droplet wetting modes. We find that surface topography, size, and initial position of the droplet strongly affect the wetting states and contact angles. In the small Bond-number (small droplet) regime, the surface topography can be scaled by the droplet size, such that the preferred wetting modes and contact angles become independent of droplet size for surfaces with the same scaled topography. MD simulations and theory are in good agreement for small Bond numbers. For moderate to large Bond numbers, gravity plays an important role and MD simulations cannot accurately describe wetting. We create wetting phase diagrams and find that our predictions are in good agreement with experiment. The resulting wetting phase diagrams may serve as a guideline in creating surfaces with desired wettability.

¹Sponsored by NSF CBET 0730987

1:51PM Q36.00014 Freezing of Water next to Solid Surfaces Probed Using Sum-Frequency Generation Spectroscopy¹, EMMANUEL ANIM-DANSO, ANISH KURIAN, LIEHUI GE, University of Akron, AZAR ALIZADEH, General Electric, ALI DHINOJWALA, University of Akron — The control of ice formation next to solid surfaces is important in many technological applications such as de-icing for aircrafts and generation of power using wind turbines. We have studied the water-ice transition next to sapphire surface to understand the freezing transition and nucleation of ice. The infrared-visible sum frequency generation spectroscopy is sensitive to the structure and orientation of water molecules next to the solid interface and provides direct information on transition kinetics at the interface. The differences in the nucleation kinetics will be discussed for water in contact with hydrophilic and hydrophobic surfaces.

¹Funded by National Science Foundation

2:03PM Q36.00015 Charging and transmission of low energy particles through Amorphous Solid Water films, YONATAN HOROWITZ, MICHA ASSCHER, Institute of Chemistry, Edmund J. Safra Campus, Givat-Ram, The Hebrew University of Jerusalem, Israel — The interaction of charged particles with condensed water films has drawn significant attention in recent years due to its importance in biological and atmospheric processes. We have studied low energy electrons (3-25 eV) and positive argon ions (55 eV) charging and transmission effects while striking Amorphous Solid Water (ASW) films, 240-1080 ML thick, deposited on ruthenium single crystal substrate, utilizing contact potential difference (CPD) measurements. Charging by both species has shown a plate capacitor-like behaviour. L-defects energetically located just below the conduction band of ice, are likely to stabilize them. The incoming electrons kinetic energy dictates the maximal CPD by retardation of any further electrons from adding up to the already accumulated charges. Electron transmission measurements (0.5-1.5 microamps) have shown that the maximal and stable CPD values were obtained only following a relatively slow change that has developed within the ASW structure. Upon film stabilization, the spontaneous discharge was measured over a period of up to three hours. UV laser photo-emission study of the charged films has suggested that the negative charges tend to reside primarily at the ASW-vacuum interface, in good agreement with a study of charged water nano-clusters.

Wednesday, February 29, 2012 11:15AM - 1:15PM – Session Q37 FIAP FEd: Focus Session: Students, Physics and Innovation 108

11:15AM Q37.00001 Physicists and Economic Growth: Preparing the Next Generation, DOUGLAS ARION, Carthage College — For many years it has been recognized that many physicists are “hidden” – deep in the industrial world or holding positions not named “physicist.” In parallel with this phenomenon is the recognition that many new and innovative product ideas are, in fact, generated by physicists. There are many more ideas that could be brought to market to the benefit of both society and the inventor, but physicists don’t often see themselves as the innovators and inventors that they actually are. A number of education programs have arisen to try to address this issue and to engender a greater entrepreneurial spirit in the scientific community. The *ScienceWorks* program at Carthage College was one of the first to do so, and has for nearly twenty years prepared undergraduate science majors to understand and practice innovation and value creation. Other programs, such as professional masters degrees, also serve to bridge the technical and business universes. As it is no doubt easier to teach a scientist the world of business than it is to teach a businessperson the world of physics, providing educational experiences in innovation and commercialization to physics students can have tremendous economic impact, and will also better prepare them for whatever career direction they may ultimately pursue, even if it is the traditional tenure-track university position. This talk will discuss education programs that have been effective at preparing physics students for the professional work environment, and some of the positive outcomes that have resulted. Also discussed will be the variety of opportunities and resources that exist for faculty and students to develop the skills, knowledge and abilities to recognize and successfully commercialize innovations.

11:51AM Q37.00002 Teaching Innovation Through Undergraduate Research¹, JOHN R. BRANDENBERGER, Department of Physics, Lawrence University, Appleton, WI 54911 — A three-year investigation into the use of ongoing research programs to incubate innovative behavior among undergraduates is underway. Inspired by the 2005 report, *Rising Above the Gathering Storm*, this investigation embraces the claim that more innovation in the US should help arrest the current slippage in US competitiveness. Believing that the development of approaches to teach innovation is timely, physicists at Lawrence University are employing a five-step strategy that spans ten summer weeks to boost innovative attitudes and behavior among physics majors. We are also attempting to inculcate fifteen character traits associated with successful innovators. Recent progress in this investigation will be discussed.

¹Supported by NSF/CCLI/TUES.

12:03PM Q37.00003 The Innovation Hyperlab - Linking Student Innovation at University and Pre-College Levels, RANDALL TAGG, University of Colorado Denver — We have created a laboratory environment to support collaboration between university and pre-college students on innovation and entrepreneurship projects. Called the “Innovation Hyperlab,” this facility is located in a K-12 complex called VistaPEAK schools in Aurora, Colorado. The lab is supported by four elements: a research-grade technical infrastructure of supplies and equipment for technical prototyping, a developing curriculum of “learning modules on demand” for rapid assimilation of technical skills, mentors from universities / medical schools / industry, and innovation projects stimulated by connections with the regional community. A current focus of projects is on medical technology development, linking tenth graders with university undergraduate research students and coordinated with the University of Colorado Denver’s medical school. The Innovation Hyperlab is a work in progress and we will describe challenges that arise in connecting such a collaboration with traditional curriculum at both the university and pre-college levels.

12:15PM Q37.00004 The Physics Entrepreneurship Program - 11 Years of Teaching and Practicing Innovation and Entrepreneurship to Graduate Students and Beyond, EDWARD CANER, Case Western Reserve University — The Physics Entrepreneurship Program (PEP) at Case Western Reserve University is a MS in Physics, Entrepreneurship Track that teaches physics, business, and innovation. PEP admitted its first class in 2000 with the original goal of empowering physicists to be successful entrepreneurs. Since Y2K, much has happened in the world's economies and markets, and we have shifted our goals to include a strong innovation component. For instance, our metrics have changed from "companies created" to "capital raised by our students" (i.e., grants and investment in innovation), which allows our students to participate in an apprentice-type relationship with a more experienced entrepreneur before venturing out on their own (which could take many years before they are ready). We will describe the program, how we teach innovation, student and alumni activities and how difficult it is to operate a sustainable graduate program in this arena.

12:27PM Q37.00005 The Story of a Typical Atypical Graduate of the Physics Entrepreneurship Program at Case Western Reserve University, ADELE LUTA, Adjuvat Biosciences — An entrepreneurial perspective to life can lead to wearing a myriad of hats. Long gone is the stereotypical start-up role. Entrepreneurs now hold physics degrees and procure innovation when called upon. An alumni of the Physics Entrepreneurship Program, Adele Luta has spent the last 5 years at NASA developing an innovative approach to spacesuit sizing. Previously, she founded Eleda International consulting firm and is currently working with Adjuvat Biosciences, on a proprietary treatment pancreatic cancer.

12:39PM Q37.00006 Developing affordable multi-touch technologies for use in physics¹, MARK POTTER, CAROLINA ILIE, DAMIAN SCHOFIELD, DAVID VAMPOLA, State University of New York at Oswego — Physics is one of many areas which has the ability to benefit from a number of different teaching styles and sophisticated instructional tools due to it having both theoretical and practical applications which can be explored. The purpose of this research is to develop affordable large scale multi-touch interfaces which can be used within and outside of the classroom as both an instruction technology and a computer supported collaborative learning tool. Not only can this technology be implemented at university levels, but also at the K-12 level of education. Pedagogical research indicates that kinesthetic learning is a fundamental, powerful, and ubiquitous learning style [1]. Through the use of these types of multi-touch tools and teaching methods which incorporate them, the classroom can be enriched to allow for better comprehension and retention of information. This is due in part to a wider range of learning styles, such as kinesthetic learning, which are being catered to within the classroom.

[1] Wieman, C.E, Perkins, K.K., Adams, W.K., "Oersted Medal Lecture 2007: Interactive Simulations for teaching physics: What works, what doesn't and why," *American Journal of Physics*. **76** 393-99.

¹Trio: Ronald E. McNair Postbaccalaureate Achievement Program, SUNY Oswego Student/Faculty Collaborative Challenge Grant

12:51PM Q37.00007 Wolfram technologies as an integrated scalable platform for interactive learning, VITALIY KAUROV, Wolfram Research — We rely on technology profoundly with the prospect of even greater integration in the future. Well known challenges in education are a technology-inadequate curriculum and many software platforms that are difficult to scale or interconnect. We'll review an integrated technology, much of it free, that addresses these issues for individuals and small schools as well as for universities. Topics include: Mathematica, a programming environment that offers a diverse range of functionality; natural language programming for getting started quickly and accessing data from Wolfram|Alpha; quick and easy construction of interactive courseware and scientific applications; partnering with publishers to create interactive e-textbooks; course assistant apps for mobile platforms; the computable document format (CDF); teacher-student and student-student collaboration on interactive projects and web publishing at the Wolfram Demonstrations site.

1:03PM Q37.00008 Promoting Conceptual Coherence in Quantum Learning through Computational Models¹, HEE-SUN LEE², University of California, Santa Cruz — In order to explain phenomena at the quantum level, scientists use multiple representations in verbal, pictorial, mathematical, and computational forms. Conceptual coherence among these multiple representations is used as an analytical framework to describe student learning trajectories in quantum physics. A series of internet-based curriculum modules are designed to address topics in quantum mechanics, semiconductor physics, and nano-scale engineering applications. In these modules, students are engaged in inquiry-based activities situated in a highly interactive computational modeling environment. This study was conducted in an introductory level solid state physics course. Based on in-depth interviews with 13 students, methods for identifying conceptual coherence as a function of students' level of understanding are presented. Pre-post test comparisons of 20 students in the course indicate a statistically significant improvement in students' conceptual coherence of understanding quantum phenomena before and after the course, Effect Size = 1.29 SD. Additional analyses indicate that students who responded to the modules more coherently improved their conceptual coherence to a greater extent than those who did less to the modules after controlling for their course grades.

¹This work is supported by the NSF (DUE-0802532). Any opinions, findings, or recommendations in this paper do not necessarily reflect the views of the NSF.

²Charles Xie, Concord Consortium; Gey-Hong Gweon, UC-Santa Cruz

Wednesday, February 29, 2012 11:15AM - 2:03PM –
Session Q39 DMP DBIO DPOLY: Focus Session: Materials and Functional Structures for Biological Interfaces - Micro and Nanofluidics 109B

11:15AM Q39.00001 Integration of Materials and Functions in Microfluidic Devices, MARCELLA CHIARI, National Research Council of Italy — The physical and chemical properties of a surface determine how that surface interacts with its surrounding environment. Despite the large number of potential schemes feasible for surface modification, the covalent attachment of polymers remains the most promising approach to tailor important properties of lab-on-chip (LOC) devices such as adhesion, wettability and biocompatibility. This presentation deals with "surface related" issues that must be addressed in the development of LOC systems. An innovative approach that allows the attachment of polymer molecules to surfaces of different composition such as glass, silicon and polymer materials will be presented. Examples of interfaces modified by "smart coatings" able to give an appropriate and predictable response to outside conditions and decorated with biologically relevant biomolecules will be discussed.

11:51AM Q39.00002 Dynamic micromolds to fabricate multi-layered hydrogel microstructures, HALIL TEKIN, Department of Electrical Engineering and Computer Science, MIT, TONIA TSINMAN, Department of Biological Engineering, MIT, JEFFERSON G. SANCHEZ, Department of Chemical Engineering, MIT, BRIANNA J. JONES, Department of Physics, MIT, ROBERT LANGER, Department of Chemical Engineering, MIT, ALI KHADEMHOSEINI, Center for Biomedical Engineering, Brigham and Women's Hospital, Harvard Medical School — Hydrogel microstructures can be used to mimic living systems and create drug carriers. Living materials can be encapsulated within multi-layered microgels to replicate native tissues. Furthermore, multiple drugs can be immobilized within different layers of microgels to create multifunctional drug carriers. Photolithography is a commonly used method to create these multi-layered microgels, but it is not applicable to non-photocrosslinkable materials. Also, conventional micromolding methods do not allow creating multi-layered microgels due to the static environment of the microstructures. Herein, we created dynamic micromolds by exploiting the thermoresponsiveness of poly(N-isopropylacrylamide). These micromolds allowed sequential molding of microgels at different temperatures. Different cell types were spatially immobilized in different layers of microgels to replicate native tissue complexity. Furthermore, fluorescent microbeads were spatially immobilized within different microgel layers to show a concept of drug carriers which could encapsulate various drugs. These dynamic micromolds could be potentially useful in creating multi-layered hydrogel microstructures in order to mimic biological systems and fabricate multifunctional drug carriers.

12:03PM Q39.00003 Implementation of a Peltier-based cooling device for localized deep cortical deactivation during in vivo object recognition testing, KYLE MARRA, Boston College, BRETT GRAHAM, SAMANTHA CAROUSO, DAVID COX¹, Rowland Institute — While the application of local cortical cooling has recently become a focus of neurological research, extended localized deactivation deep within brain structures is still unexplored. Using a wirelessly controlled thermoelectric (Peltier) device and water-based heat sink, we have achieved inactivating temperatures (<20 °C) at greater depths (>8 mm) than previously reported. After implanting the device into Long Evans rats' basolateral amygdala (BLA), an inhibitory brain center that controls anxiety and fear, we ran an open field test during which anxiety-driven behavioral tendencies were observed to decrease during cooling, thus confirming the device's effect on behavior. Our device will next be implanted in the rats' temporal association cortex (TeA) and recordings from our signal-tracing multichannel microelectrodes will measure and compare activated and deactivated neuronal activity so as to isolate and study the TeA signals responsible for object recognition. Having already achieved a top performing computational face-recognition system, the lab will utilize this TeA activity data to generalize its computational efforts of face recognition to achieve general object recognition.

¹Visual Neuroscience Group, Rowland Institute, Harvard University

12:15PM Q39.00004 Droplet Microfluidics for Artificial Lipid Bilayers, SRIKOUNDINYA PUNNAMARAJU, ANDREW STECKL, Nanoelectronics Laboratory, University of Cincinnati — Droplet interface bilayer is a versatile approach that allows formation of artificial lipid bilayer membrane at the interface of two lipid monolayer coated aqueous droplets in a lipid filled oil medium. Versatility exists in the form of voltage control of DIB area, ability of forming networks of DIBs, volume control of droplets and lipid-oil, and ease of reformation. Significant effect of voltage on the area and capacitance of DIB as well as DIB networks are characterized using simultaneous optical and electrical recordings. Mechanisms behind voltage-induced effects on DIBs are investigated. Photo induced effect on the DIB membrane porosity is obtained by incorporating UVC-sensitive photo-polymerizable lipids in DIB. Photo-induced effects can be extended for in-vitro studies of triggered release of encapsulated contents across membranes. A droplet based low voltage digital microfluidic platform is developed to automate DIB formation, which could potentially be used for forming arrays of lipid bilayer membranes.

12:27PM Q39.00005 Density fluctuations in nanochannel-confined DNA, JOSHUA CARPENTER, ALENA KARPUSENKO, CHUNDA ZHOU, SHUANG FANG LIM, JUNHAN PAN, ROBERT RIEHN, Department of Physics, NC State University — The dynamic behavior of a polymer chain in dense solution is typically described within the framework of reptation, which assumes that polymers primarily move along tubes formed by other chains. We have studied the dynamic density fluctuations of single DNA molecules confined to nanofabricated channels that mimic reptation tubes, and found that the classical harmonic spring model yields a satisfactory description. In particular, we have recovered the expected dispersion relationship. By looking at fluctuation amplitudes, we have also found that the description demands a minimum spring length approximately equal to the size of self-avoiding DeGennes blobs.

12:39PM Q39.00006 Extension and Diffusion of DNA in Nanochannels, DOUGLAS TREE, University of Minnesota, YANWEI WANG, Soochow University, KEVIN DORFMAN, University of Minnesota — Nanochannels are an ideal platform for studying the basic physics of confined polymers, using DNA as the model polymer. While the scaling laws for strong (Odijk) and weak (de Gennes) confinement were established decades ago, recent experiments have illuminated the complex physics arising between these limiting cases. We will first present Monte Carlo simulation data on the extension of DNA in nanochannels. Our results provide clear evidence for the existence of two transition regimes between the Odijk and de Gennes regimes, thereby resolving the apparent contradiction between these scaling theories and the corresponding experiments by Austin and coworkers. We will then present results for the diffusivity of DNA in nanochannels and explain their connection to the different regimes of extension. By using Monte Carlo sampling of the Kirkwood diffusivity and a numerical solution for the confined Green's function, we have calculated the diffusivity for DNA contour lengths ranging over three orders of magnitude and nanochannel sizes over two orders of magnitude. By using a DNA model that accurately reproduces the free solution radius of gyration and diffusivity over a range of molecular weights, we can directly connect the simulation data and experiments.

12:51PM Q39.00007 DNA conformation and dynamics in quasi-2D and -1D confinement, YENG-LONG CHEN, Institute of Physics, Academia Sinica — We investigate the structure and correlation length of DNA molecules in sub-100nm quasi-2D slits and 1D square channels. In strong slit confinement, the segmental correlation length of DNA molecules separates into two components – in the confined and unconfined dimensions. In the confined dimension, the segmental correlation length is controlled by the slit height. In the unconfined dimension, the segmental correlation length increases as the slit height decreases. In the nano-channel, segmental correlation length increases beyond the chain contour length as channel height decreases below channel persistence length. We generalize how this affects the entropic elasticity of confined DNA molecules and how it affects chain thermodynamic properties.

1:03PM Q39.00008 Mapping the yeast genome by melting in nanofluidic devices, ROBERT L. WELCH, ILJA CZOLKOS, McGill University, ROB SLADEK, Genome Quebec Innovation Centre, WALTER REISNER, McGill University — Optical mapping of DNA provides large-scale genomic information that can be used to assemble contigs from next-generation sequencing, and to detect re-arrangements between single cells. A recent optical mapping technique called denaturation mapping has the unique advantage of using physical principles rather than the action of enzymes to probe genomic structure. The absence of reagents or reaction steps makes denaturation mapping simpler than other protocols. Denaturation mapping uses fluorescence microscopy to image the pattern of partial melting along a DNA molecule extended in a channel of cross-section ~100nm at the heart of a nanofluidic device. We successfully aligned melting maps from single DNA molecules to a theoretical map of the yeast genome (11.6Mbp) to identify their location. By aligning hundreds of molecules we assembled a consensus melting map of the yeast genome with 95% coverage.

1:15PM Q39.00009 Spatially Varying Nanoconfinement as a Probe of Polymer Physics, ALEXANDER KLOTZ, WALTER REISNER, McGill University — Complex nanofluidic systems have the capability to unveil a rich landscape of new polymer physics. One-dimensional channels and two-dimensional slits have been used for precise measurements of persistence length and to verify scaling laws. Recently, devices with spatially varying confinement have been used to gain further control over single molecule polymer conformation. We use a system consisting of a nanofluidic slit embedded with a lattice of pits acting as entropic traps. Single DNA polymers in this system self-organize into discrete conformational states. We have shown that this system can be used to define stable DNA configurations at equilibrium and to fine-tune diffusion to a local minimum corresponding to stable conformational states. Measurements of mean occupancy with varying device parameters can be fit to theory, giving information about the confinement free energy of DNA in a nanoslit (a subject of controversy) and the strength of excluded volume interactions. Measurements of the excluded volume interaction provide information about the strength of intersegmental repulsive electrostatic interactions, quantified by the notion of effective width. The scaling of width with respect to salt concentration is observed in single DNA molecules for the first time.

1:27PM Q39.00010 The Nanofluidic Staircase: A Brownian Motor for Polymer Characterization and Transport, FREDERICK PHELAN JR., National Institute of Standards and Technology (NIST), CHRISTOPHER FORREY, Food and Drug Administration (FDA), JON GEIST, SAMUEL STAVIS, ELIZABETH STRYCHALSKI, National Institute of Standards and Technology (NIST) — A coarse-grained molecular dynamics simulation is used to study the motion of a polymer chain in a nanofluidic staircase (Stavis et al., Nanotechnology, 20(16), 2009), a device which consists of a collection of nanoslits of increasing depth arranged in step-like fashion in a fluidic channel. The slit depths span the Odijk ($H < L_k$) and de Gennes ($L_k < H < R_g$) regimes, where H is the slit depth, L_k is the polymer Kuhn length, and R_g is the radius of gyration. Simulation results show that the model captures the 1-D biased diffusion of chains from regions of high to low confinement that has been measured in recent experiments (Strychalski et al., 14th Int. Conf. on Min. Sys. for Chem. and Life Sci., 2010). The drift velocity increases with increasing step size but also decays more rapidly; stiffer chains drift at a higher rate than softer chains. For all cases, the overall diffusion rates are higher than those calculated for chains in free solution, indicating that the chains gain a "push" as they migrate through the staircase, a manifestation of entropic forces. The staircase system therefore acts as a Brownian motor, which transfers energy from an external source (the polymer free energy) into directed transport using only thermal fluctuations and the biased structural features of the device.

1:39PM Q39.00011 ABSTRACT WITHDRAWN —

1:51PM Q39.00012 Geometrically induced polarization and alignment of cells on nanopillar arrays, YOLANDA VASQUEZ, MICHAEL BUCARO, BENJAMIN HATTON, JOANNA AIZENBERG, Harvard University — Topological features at the nano and microscale can trigger mammalian cell growth and differentiation. In this work, we describe geometrical tuning of ordered arrays of nanopillars and micropillars that elicit specialized morphologies in adherent cells. Systematic analysis of the effects of the pillar radius, height, and spacing reveals that stem cells assume either flattened, polarized, or stellate morphologies in direct response to interpillar spacing. Notably, on patterns of pitch near a critical spacing ($d_{crit} = 2 \text{ }\mu\text{m}$ for C3H10T1/2 cells), cells exhibit rounding of the cell body, pronounced polarization, and extension of narrow axon-like cell projections aligned with the square or hexagonal lattice of the NP array. This morphology persists for various stem cell lines and primary mesenchymal stem cells. The neuron-like morphological characteristics suggest that NP arrays can be utilized in tissue engineering applications that require directed axon growth. The ability of nano and micropillars to support various morphogenetic trends will allow rational design of scaffolds that may be useful for stem cell lineage specification, formation of patterned neural networks, and enhancement of implant integration with adjoining tissue.

Wednesday, February 29, 2012 11:15AM - 2:15PM —

Session Q40 DBIO GSNP: Focus Session: Systems Biology and Biochemical Networks III 156A

11:15AM Q40.00001 TBD, TING LU, —

11:51AM Q40.00002 Fold-change detection and scalar symmetry of sensory input fields, OREN SHOVAL, Weizmann Institute of Science, LEA GOENTORO, California Institute of Technology, YUVAL HART, AVI MAYO, Weizmann Institute of Science, EDUARDO SONTAG, Rutgers University, URI ALON, Weizmann Institute of Science — Recent studies suggest that certain cellular sensory systems display fold-change detection (FCD): a response whose entire shape, including amplitude and duration, depends only on fold-changes in input, and not on absolute changes. We show that FCD is necessary and sufficient for sensory search to depend only on the spatial profile of the input, and not on its amplitude. Such amplitude scalar symmetry occurs in a wide range of sensory inputs, such as source strength multiplying diffusing chemical fields sensed in chemotaxis, ambient light multiplying the contrast field in vision, and protein concentrations multiplying the output in cellular signaling systems. We present a wide class of mechanisms that have FCD, including certain nonlinear feedback and feedforward loops. In addition, we find that bacterial chemotaxis displays feedback within the present class, and has indeed recently been shown to exhibit FCD. This can explain experiments in which chemotaxis searches are insensitive to attractant source levels. This study thus suggests a connection between properties of biological sensory systems and scalar symmetry stemming from physical properties of their input fields.

12:03PM Q40.00003 Network architectural conditions for prominent and robust stochastic oscillations, JAEWOOK JOO, JINMYUNG CHOI, University of Tennessee — Understanding relationship between noisy dynamics and biological network architecture is a fundamentally important question, particularly in order to elucidate how cells encode and process information. We analytically and numerically investigate general network architectural conditions that are necessary to generate stochastic amplified and coherent oscillations. We enumerate all possible topologies of coupled negative feedbacks in the underlying biochemical networks with three components, negative feedback loops, and mass action kinetics. Using the linear noise approximation to analytically obtain the time-dependent solution of the master equation and derive the algebraic expression of power spectra, we find that (a) all networks with coupled negative feedbacks are capable of generating stochastic amplified and coherent oscillations; (b) networks with a single negative feedback are better stochastic amplified and coherent oscillators than those with multiple coupled negative feedbacks; (c) multiple timescale difference among the kinetic rate constants is required for stochastic amplified and coherent oscillations.

12:15PM Q40.00004 Properties of gene expression including the non-functional binding of transcription factors to DNA, ANAT BURGER, University of California San Diego, ALEKSANDRA WALCZAK, Ecole Normale Supérieure, PETER WOLYNES, Rice University — Many eukaryotic transcription factors bind to DNA sequences with a remarkable lack of specificity. This suggests that non-functional binding between transcription factors and DNA might not have the detrimental effect on regulation one would naively assume results from competition for binding. In fact, if binding to DNA protects transcription factors from degradation, the number and binding affinity of these 'decoy' binding sites should have no influence on the copy number of transcription factors available for regulation. We calculate the influence of adding decoy binding sites on several important aspects of gene expression including the noise, the time to reach steady state, and bimodal switch rates. Analyzing these effects could shed some light on how a gene functions in the 'dressed' environment of a genomic background.

12:27PM Q40.00005 Single promoters as regulatory network motifs, CHRISTOPHER ZOPF, NARENDRA MAHESHWRI, Massachusetts Institute of Technology — At eukaryotic promoters, chromatin can influence the relationship between a gene's expression and transcription factor (TF) activity. This additional complexity might allow single promoters to exhibit dynamical behavior commonly attributed to regulatory motifs involving multiple genes. We investigate the role of promoter chromatin architecture in the kinetics of gene activation using a previously described set of promoter variants based on the phosphate-regulated PHO5 promoter in *S. cerevisiae*. Accurate quantitative measurement of transcription activation kinetics is facilitated by a controllable and observable TF input to a promoter of interest leading to an observable expression output in single cells. We find the particular architecture of these promoters can result in a significant delay in activation, filtering of noisy TF signals, and a memory of previous activation – dynamical behaviors reminiscent of a feed-forward loop but only requiring a single promoter. We suggest this is a consequence of chromatin transactions at the promoter, likely passing through a long-lived “primed” state between its inactive and competent states. Finally, we show our experimental setup can be generalized as a “gene oscilloscope” to probe the kinetics of heterologous promoter architectures.

12:39PM Q40.00006 Towards a principled way of making kinetic models from data¹, STEVE PRESSE, UCSF — Kinetic model extraction from noisy data is the basic route to mechanistic insight in biology. I will show how the tools of Maximum Caliber (the dynamical analog of Maximum Entropy) can be used to infer -and not fit- models in a way which is driven by the structure and limitations of the data. For instance, the typical output of an experiment in systems biology is the stochastic expression of one reporter gene. Master equations used to model the regulatory process underlying the stochastic gene expression require knowledge of a circuit topology and rates. However rates and topology are often fit as these are rarely all independently determinable from the limited data. Our goal is to build a kinetic model from the data available with no adjustable parameter using the tools of Maximum Caliber. We apply our method to infer the statistics of rare stochastic switching events in the genetic toggle switch from fluctuations on shorter measurable timescales. In addition, we discuss how these tools can be used to infer kinetic models from real single molecule data drawn from anomalous folding kinetics of phosphoglycerate kinase and RNA hairpin zipping-unzipping time traces.

¹NIH, FQRNT

12:51PM Q40.00007 Reaction kinetics in the cell membrane: confining domains lead to reaction bursts, ZIYA KALAY, TAKAHIRO FUJIWARA, AKIHIRO KUSUMI, Kyoto University - Inst. for Integrated Cell-Material Sciences — Our goal is to reveal the effects of confining domains such as those observed in cell membranes on the kinetics of reversible reactions in two-dimensions. During the last two decades, single molecule tracking experiments showed that proteins and lipids are temporarily confined in the compartments of a meshwork induced by the actin cytoskeleton, while diffusing laterally in the plasma membrane. It has been clearly demonstrated that the presence of these compartments significantly hinders the diffusion of membrane molecules. Nevertheless, how confinement affects the interaction between membrane molecules and the regulation of signaling has still not been clarified. Using Monte Carlo simulations and the mathematical theory of diffusion, we showed that the presence of compartments leads to reaction bursts, during which the number of reactions an individual molecule experiences rises sharply, but briefly. Surprisingly, we found that the mean reaction rate does not depend on whether compartments exist or not. However, our results show that the variance of the rate depends strongly on the presence of confinement effects, which turns out to be an indicator of a profound change in the temporal pattern of reaction events: bursts of reactions instead of constant but low yield.

1:03PM Q40.00008 Inference of Mechanical Network Parameters in Epithelial Tissue Development, KEVIN CHIOU, Department of Physics, UCSB, LARS HUFNAGEL, EMBL Heidelberg, BORIS SHRAIMAN, KITP, UCSB — Mechanical stress in cells has been linked to biochemical networks that influence cell structure and function. Yet direct *in vivo* measurements of mechanical forces in epithelial tissues remain a serious experimental challenge. I will present an alternative approach based on a computational analysis of high resolution images of epithelial tissues. Assuming that epithelial cell layers are close to mechanical equilibrium, we use the observed geometry of the two dimensional cell array to infer interfacial tensions and intracellular pressures. I will present applications of this mechanical parameter inference algorithm in the context of several developmental processes involving epithelial cell layers.

1:15PM Q40.00009 Regulatory dynamics and stability in discrete and continuous models¹, FAKHTEH GHANBARNEJAD, KONSTANTIN KLEMM, Bioinformatics Group, Institute for Computer Science, University of Leipzig — Biological processes such as cell deviation, cell differentiation and so on are regulated dynamics. These dynamics are often described by continuous rate equations for continuously varying chemical concentrations. Binary discretization of state space and time leads to another class of models, Boolean dynamics, which are dealing with larger systems, higher complexity and less computational details. Here we study the reaction of discrete and continuous dynamics to perturbations. When asking if a gene-regulatory system reproduces a prescribed trajectory despite noise, large perturbations are to be considered in the case of low copy numbers of regulatory molecules and bursty stochastic response. Small perturbations, however, are more appropriate when modelling systems with large copy numbers and an integrative response to filter out bursts. In Boolean networks, the dynamics has been called unstable if flip perturbations lead to damage spreading. We find that this stability classification strongly differs from the stability properties of the original continuous dynamics under small perturbations of the state vector. In particular, random networks of nodes with large sensitivity yield stable dynamics under small perturbations and chaotic regime disappears.

¹Physical Review Letters 107, 188701 (2011)

1:27PM Q40.00010 Polarization and molecular information transmission in the cell, ADRIANO VALDEZ-GOMEZ, GUILLERMO RAMIREZ-SANTIAGO, Instituto de Fisica, Universidad Nacional Autonoma de Mexico — During chemotaxis, pseudopodia are extended at the leading edge and retracted at the back of the cell. Efficient chemotaxis is the result of a refined interplay between signaling modules to transmit and integrate spatial information such as PtdIns(3,4,5)P₃. The localization of PtdIns(3,4,5)P₃ is expected to depend on the distributions or activities of PI3Ks, PTEN, and 5-phosphatases. The spatial signals spread relatively slowly so that high local concentrations of PIP₃ in the plasma membrane appear in patches. These gradients induce localization of PIP₃ and PTEN to the front and back of the cell, respectively. To simulate this polarization process that involves the action of seven reaction-channels inside the cell we carried out extensive stochastic simulations using Gilliespie algorithm. The simulations were done on a square cell with ten thousand sites (100 × 100) emulating a square cell with side 10 μm long. We found that there are localized patches of PIP₃ at the active receptors and segregation of PTEN on the opposite side of the cell. When we block the reaction-channel, $PTEN + PIP_3 \rightarrow PIP_2$ that involves the production of PIP₂ we obtained a five-fold increase in the concentration of PIP₃. This finding appears to be consistent with the o

1:39PM Q40.00011 Energy Flow in Neuronal Systems, ZRINKA GREGURIC FERENCEK, JOHN ROBERT CRESSMAN, ZAID OBADA, George Mason University — We will present results from a computational model designed to investigate the physical underpinnings of neuronal systems. Most neuronal models assume that the ionic flow across neuronal membranes is too small to effect the ionic composition inside and outside of cells. However neurons exhibiting high levels of activity can produce ionic redistributions large enough to cause significant changes to cellular excitability. Furthermore, physically-accurate neuronal models must obey conservation of mass and energy. Energy is injected into these cells through the consumption of ATP, stored in electrochemical gradients, and dissipated through ionic flow down these gradients. Our model incorporates essential biological mechanisms required to reproduce this energy flow and storage. We will discuss the advantages and limitations of this dynamic system in the context of neuronal function.

1:51PM Q40.00012 Rhythm-Induced Spike-Timing Patterns Characterized by 1D Firing Map, JAN ENGELBRECHT, RENNIE MIROLLO, Boston College — A basic problem in neuroscience is to understand how the dynamic mechanisms that govern the responses of nerve cells to stimuli, which are both non-linear and noisy, still produce reliable collective activity. We study patterning in the responses of neurons subjected to periodic rhythms. These patterns are governed by simple, low-dimensional mathematical structures independent of modeling detail. We show both theoretically and in whole-cell recordings that the 1D map generated from successive spike times is such a construct. As expected, the stable periodic points of this 1D map cause a neuron's entrainment or phase-locking to a periodic rhythm. But our work has also revealed a complementary and unexpected patterning in the spike-timing of un-entrained neurons in the form of repeated sequences of reliable spike-phase advances, which cannot be characterized simply as a noisy perturbation near the stable periodic points of the noise-free return map. This new patterning appears to require both noise and a sufficiently steep return map.

2:03PM Q40.00013 The Effects of Intrinsic Noise on an Inhomogeneous Lattice of Chemical Oscillators¹, MICHAEL GIVER, Brandeis University, ZAHERA JABEEN, University of Michigan, BULBUL CHAKRABORTY, Brandeis University — Intrinsic or demographic noise has been shown to play an important role in the dynamics of a variety of systems including biochemical reactions within cells, predator-prey populations, and oscillatory chemical reaction systems, and is known to give rise to oscillations and pattern formation well outside the parameter range predicted by standard mean-field analysis. Motivated by an experimental model of cells and tissues where the cells are represented by chemical reagents isolated in emulsion droplets, we study the stochastic Brusselator, a simple activator-inhibitor chemical reaction model. Our work extends the results of recent studies on the zero and one dimensional system to the case of a non-uniform one dimensional lattice using a combination of analytical techniques and Monte Carlo simulations.

¹This work was supported by the NSF MRSEC DMR-0820492.

Wednesday, February 29, 2012 11:15AM - 2:03PM – Session Q41 DFD: Biofluids 156B

11:15AM Q41.00001 Fool's Gold Footprinting: microfluidic probing of nucleic acids¹, CHRISTOPHER D. JONES, Cornell University, School of Applied & Engineering Physics, JOERG C. SCHLATTERER, Albert Einstein College of Medicine, Department of Biochemistry, MICHAEL BRENOWITZ, Albert Einstein College of Medicine, LOIS POLLACK, Cornell University — We describe a microfluidic device containing a mineral matrix capable of rapidly generating hydroxyl radicals that enables high-resolution structural studies of nucleic acids. Hydroxyl radicals cleave the solvent accessible backbone of DNA and RNA; the cleavage products can be detected with as fine as single nucleotide resolution. Protection from hydroxyl radical cleavage (footprinting) can identify sites of protein binding or the presence of tertiary structure. Here we report preparation of micron sized particles of iron sulfide (pyrite) and fabrication of a microfluidic prototype that together generate enough hydroxyl radicals within 20 ms to cleave DNA sufficiently for a footprinting analysis to be conducted. This prototype enables the development of high-throughput and/or rapid reaction devices with which to probe nucleic acid folding dynamics and ligand binding.

¹This work was supported by the NSF through the IDBR program and the Cornell NanoScale Facility, a member of the National Nanotechnology Infrastructure Network.

11:27AM Q41.00002 Dislocation dynamics and bacterial growth, ARIEL AMIR, DAVID NELSON, Harvard University — Recent experiments have revealed remarkable phenomena in the growth mechanisms of rod-shaped bacteria: proteins associated with the cell wall growth move at constant velocity in circles oriented approximately along the cell circumference (Garner et al., Science 2011, Domínguez-Escobar et al., Science 2011, Deng et al., PNAS 2011). We view these dislocations in the partially ordered peptidoglycan structure, and study theoretically the dynamics of these interacting dislocations on the surface of a cylinder. The physics of the nucleation of these dislocations and the resulting dynamics within the model show surprising effects arising from the cylindrical geometry, which are predicted to have important implications on the growth mechanism. We also discuss how long range elastic interactions affect the dynamics of the fraction of active dislocations in the environment.

11:39AM Q41.00003 Signal Relay During Cell Migration, CAN GUVEN, Department of Physics, University of Maryland, ERIN RERICHA, School of Medicine, Vanderbilt University, EDWARD OTT, WOLFGANG LOSERT, Department of Physics, University of Maryland — We developed a signal relay model to quantify the effect of intercellular communication in presence of an external signal, during the motion of groups of Dictyostelium discoideum cells. A key parameter is the ratio of amplitude of the cAMP (cyclic adenosine monophosphate) a signaling chemical secreted from individual cells versus the external cAMP field, which defines a time scale. Another time scale is set by the degradation rate of the cAMP. In our simulations, the competition between these two time scales results rich dynamics including uniform motion, as well as streaming and clustering instabilities. The simulations are compared to experiments for a wide range of different external signal strengths for both cells that secrete cAMP and a mutant which cannot relay cAMP. Under different strength of external linear cAMP gradient, the wild type cells form streams and exhibit clustering due to the intercellular signaling through individual cAMP secretion. In contrast, cells lacking signal relay move relatively straight. We find that the model captures both independent motion and the formation of aggregates when cells relay the signal.

11:51AM Q41.00004 Intracellular Transport in Beta Cells - from Anti-Corellated to Active, STANISLAV BUROV, ALI TABELI, AARON DINNER, NORBERT SCHERER, University of Chicago — The intracellular transport along micro-tubules is the main focus of this research. We study the transport of insulin granules inside Beta cells. By developing new technique for the analysis of single 2D trajectories we observe a transition in the transport behavior from anti-correlated to active as a function of time. We further use the observed effect in order to discriminate between possible scenarios of active transport through disordered media as models of efficient intracellular transport.

12:03PM Q41.00005 Acoustic streaming in the cochlea under compressive bone conduction excitation, KATHERINE AHO, MEGHA SUNNY, TAOUFIK NABAT, JENNY AU, CHARLES THOMPSON, University of Massachusetts Lowell — This work examines the acoustic streaming in the cochlea. A model will be developed to examine the steady flow over a flexible boundary that is induced by compressive excitation of the cochlear capsule. A stokeslet based analysis of oscillatory flows was used to model fluid motion. The influence of evanescent modes on the pressure field is considered as the limit of the aspect ratio epsilon approaches zero. We will show a uniformly valid solution in space.

12:15PM Q41.00006 Subtle exchange model of flow depended on the blood cell shape to enhance the micro-circulation in capillary¹, IATNENG CHAN, Physics Group, Faculty of Science and Technology, University of Macau — In general the exchange of gases or other material in capillary system is conceptualized by the diffusion effect. But in this model, we investigate a micro-flow pattern by simulation and computation on a micro-exchange model in which the blood cell is a considered factor, especially on its shape. It shows that the cell benefits the circulation while it is moving in the capillary. In the study, the flow detail near the cell surface is mathematically analyzed, such that the Navier-Stokes equations are applied and the viscous factor is also briefly considered. For having a driven force to the motion of micro-circulation, a breathing mode is suggested to approximately compute on the flow rate in the blood capillary during the transfer of cell. The rate is also used to estimate the enhancement to the circulation in addition to the outcome of diffusion. Moreover in the research, the shape change of capillary wall under pressure influence is another element in the beginning calculation for the effect in the assistance to cell motion.

¹Funded by the research grant of the University of Macau

12:27PM Q41.00007 Modeling fluid diffusion in cerebral white matter with random walks in complex environments, AMICHAÏ LEVY, GABRIEL CWILICH, SERGEY V. BULDYREV, Department of Physics, Yeshiva University, VAN J. WEEDEN, Athinoula A. Martinos Center for Biomedical Imaging, Harvard Medical School — Recent studies with diffusion MRI have shown new aspects of geometric order in the brain, including complex path coherence within the cerebral cortex, and organization of cerebral white matter and connectivity across multiple scales. The main assumption of these studies is that water molecules diffuse along myelin sheaths of neuron axons in the white matter and thus the anisotropy of their diffusion tensor observed by MRI can provide information about the direction of the axons connecting different parts of the brain. We model the diffusion of particles confined in the space of between the bundles of cylindrical obstacles representing fibrous structures of various orientations. We have investigated the directional properties of the diffusion, by studying the angular distribution of the end point of the random walks as a function of their length, to understand the scale over which the distribution randomizes. We will show evidence of qualitative change in the behavior of the diffusion for different volume fractions of obstacles. Comparisons with three-dimensional MRI images will be illustrated.

12:39PM Q41.00008 Adhesion of a Cylindrical Bacterium in the Presence of DLVO Potential, JIAYI SHI, SINAN MUFTU, APRIL GU, KAI-TAK WAN, Northeastern university — A single cigar shape bacterium attaches to a rigid substrate (e.g. sand surface). In the presence of electrostatic double layers and van der Waals attraction according to the Derjaguin-Landau-Verwey-Overbeek (DLVO) theory, the bacterium glycoprotein shell deforms and may settle in either the primary or secondary energy minimum depending on whether it has sufficient energy to overcome the repulsive energy barrier. The adhesion-detachment mechanics is derived using a computational approach, and the followings are obtained: (i) relation between the applied load and contact area with the substrate, (ii) deformed profile at equilibrium, (iii) mechanical stress distribution in the shell, (iv) critical compressive load to force the shell going from secondary energy minimum to primary, and (v) “pull-off” forces to detach the shell from substrate. The model leads to better understanding of bacteria adhesion-aggregation-transportation, and has significant relevance to environmental and medical sciences.

12:51PM Q41.00009 Hydrodynamic behavior of tumor cells in a confined model microvessel, ZEINA S. KHAN, SIVA A. VANAPALLI, Department of Chemical Engineering, Texas Tech University — An important step in cancer metastasis is the hydrodynamic transport of circulating tumor cells (CTCs) through microvasculature. In vivo imaging studies in mice models show episodes of confined motion and trapping of tumor cells at microvessel bifurcations, suggesting that hydrodynamic phenomena are important processes regulating CTC dissemination. Our goal is to use microfluidics to understand the interplay between tumor cell rheology, confinement and fluid forces that may help to identify physical factors determining CTC transport. We use leukemia cells as model CTCs and mimic the in vivo setting by investigating their motion in a confined microchannel with an integrated microfluidic manometer to measure time variations in the excess pressure drop during cell motion. Using image analysis, variations in excess pressure drop, cell shape and cell velocity are simultaneously quantified. We find that the throughput of the technique is high enough (~100 cells/min) to assess tumor cell heterogeneity. Therefore, in addition to measuring the hydrodynamic response of tumor cells in confined channels, our results indicate that the microfluidic manometer device could be used for rapid mechanical phenotyping of tumor cells.

1:03PM Q41.00010 Flow and rupture of vesicles in narrow channels, ALISON HARMAN, MARTIN BERTRAND, BELA JOOS, University of Ottawa, Ontario, Canada — Small lipid bilayer vesicles, also known as liposomes, are used for drug delivery systems in vasculature. Consequently how they deform and when they become unstable and rupture (lose their inner contents) under capillary flow is of great interest. In addition vesicles with a filling fraction of 0.6 can be considered as a simple mechanical model of red blood cells. We use coarse-grained molecular dynamics (CGMD) simulations with explicit solvent to study lipid bilayer vesicles in 3D capillary flow with filling fractions of 1.0 and 0.6. The shapes of the vesicles obtained in these simulations compare well to other experimental and theoretical studies. Using CGMD allows the study of rupture. This is in contrast to the majority of other approaches which model the bilayer as a purely elastic surface and only allow the investigation of deformation. We look at the stress profiles of these vesicles as measured by the area expansion per lipid along the membrane, and determine the location and pressure of rupture for a given confinement ratio (diameter of the vesicle divided by diameter of the channel). We also discuss the subsequent loss of inner fluid content.

1:15PM Q41.00011 Simulations of cardiovascular blood flow accounting for time dependent deformational forces¹, AMANDA PETERS RANGLES, Harvard University, SIMONE MELCHIONNA, JONAS LATT, SAURO SUCCI, Consiglio Nazionale delle Ricerche, EFTHIMIOS KAXIRAS, Harvard University — Cardiovascular disease is currently the leading cause of death in the United States, and early detection is critical. Despite advances in imaging technology, 50% of these deaths occur suddenly and with no prior symptoms. The development and progression of coronary diseases such as atherosclerosis has been linked to prolonged areas of low endothelial shear stress (ESS); however, there is currently no way to measure ESS in vivo. We will present a patient specific fluid simulation that applies the Lattice Boltzmann equation to model the blood flow in the coronary arteries whose geometries are derived from computed tomography angiography data. Using large-scale supercomputers up to 294,912 processors, we can model a full heartbeat at the resolution of the red blood cells. We are investigating the time dependent deformational forces exerted on the arterial flows from the movement of the heart. The change in arterial curvature that occurs over a heartbeat has been shown to have significant impact on flow velocity and macroscopic quantities like shear stress. We will discuss a method for accounting for these resulting forces by casting them into a kinetic formalism via a Gauss-Hermite projection and their impact on ESS while maintaining the static geomtry obtained from CTA data.

¹Fellowship support provided by DOE CSGF program under grant DE-FG02-97ER2530.

1:27PM Q41.00012 Using vortex corelines to analyze the hemodynamics of patient specific cerebral aneurysm models, GREG BYRNE, FERNANDO MUT, JUAN CEBRAL, George Mason University — We construct one-dimensional sets known as vortex corelines for computational fluid dynamic (CFD) simulations of blood flow in patient specific cerebral aneurysm models. These sets identify centers of swirling blood flow that may play an important role in the biological mechanisms causing aneurysm growth, rupture, and thrombosis. We highlight three specific applications in which vortex corelines are used to assess flow complexity and stability in cerebral aneurysms, validate numerical models against PIV-based experimental data, and analyze the effects of flow diverting devices used to treat intracranial aneurysms.

1:39PM Q41.00013 Picoliter droplet-based digital peptide nucleic acid clamp PCR and dielectric sorting for low abundant K-ras mutations, HUIDAN ZHANG, RALPH SPERLING, ASSAF ROTEM, LIANFENG SHAN, JOHN HEYMAN, YIZHE ZHANG, DAVID WEITZ, School of Engineering and Applied Sciences, Department of Physics, Harvard University — Colorectal cancer (CRC) remains the second leading cause of cancer-related mortality in the US, and the 5-year survival of metastatic CRC (mCRC) is less than 10%. Although monoclonal antibodies against epidermal growth factor receptor (EGFR) provide incremental improvements in survival, approximately 40% of mCRC patients with activating KRAS mutations won't benefit from this therapy. Peptide nucleic acid (PNA), a synthetic non-extendable oligonucleotides, can bind strongly to completely complementary wild-type KRAS by Watson-Crick base pairing and suppress its amplification during PCR, while any mutant allele will show unhindered amplification. The method is particularly suitable for the simultaneously detection of several adjoining mutant sites, just as mutations of codons 12 and 13 of KRAS gene where there are totally 12 possible mutation types. In this work, we describe the development and validation of this method, based on the droplet-based digital PCR. Using a microfluidic system, single target DNA molecule is compartmentalized in microdroplets together with PNA specific for wild-type KRAS, thermocycled and the fluorescence of each droplet was detected, followed by sorting and sequencing. It enables the precise determination of all possible mutant KRAS simultaneously, and the precise quantification of a single mutated KRAS in excess background unmutated KRAS.

1:51PM Q41.00014 Liquid solution delivery through the pulled nanopipette combined with QTF-AFM system¹, SANGMIN AN, Seoul Nation University, COREY STAMBAUGH, National Institute of Standards and Technology, GUNN KIM, Sejong University, MANHEE LEE, Harvard University, YONGHEE KIM, KUNYOUNG LEE, WONHO JHE, Seoul Nation University — Nanopipette is a versatile fluidic tool for biochemical analysis, controlled liquid delivery in bio-nanotechnology. However, most of the researches have been performed in solution based system, thus it is challenge to study nanofluidic properties of the liquid solution delivery through the nanopipette in ambient conditions. In this work, we demonstrated the liquid ejection, dispersion, and subsequent deposition of the nanoparticles via a 30 nm aperture pipette based on the quartz tuning fork – atomic force microscope (QTF-AFM) combined nanopipette system.

¹This work is supported by NRF of Korea (OISE 0853104).

Wednesday, February 29, 2012 11:15AM - 2:03PM –
Session Q42 DBIO GSNP: Focus Session: Stochastic Population Dynamics II - Games and Spatial Dynamics 156C

11:15AM Q42.00001 Bacterial Games, ERWIN FREY, Ludwig-Maximilians-Universitaet Muenchen — Microbial laboratory communities have become model systems for studying the complex interplay between evolutionary selection forces, stochastic fluctuations, and spatial organization. Two fundamental questions that challenge our understanding of evolution and ecology are the origin of cooperation and biodiversity. Both are ubiquitous phenomena yet conspicuously difficult to explain since the fitness of an individual or the whole community depends in an intricate way on a plethora of factors, such as spatial distribution and mobility of individuals, secretion and detection of signaling molecules, toxin secretion leading to inter-strain competition and changes in environmental conditions. We discuss two possible solutions to these questions employing concepts from evolutionary game theory, nonlinear dynamics, and the theory of stochastic processes. Our work provides insights into some minimal requirements for the evolution of cooperation and biodiversity in simple microbial communities. It further makes predictions to be tested by new microbial experiments.

11:51AM Q42.00002 Evolutionary dynamics of range expansions with curved fronts and inflationary directed percolation, MAXIM LAVRENTOVICH, Harvard University, KIRILL KOROLEV, Massachusetts Institute of Technology, DAVID NELSON, Harvard University — We compare the evolutionary dynamics of populations expanding into a new territory with flat and curved fronts. When actively reproducing individuals confined to a thin, uniform population front experience deleterious mutations, the evolutionary dynamics fall into the directed percolation (DP) universality class. At the DP phase transition, the selective advantage of the fit individuals balances the deleterious mutation rate. Curvature in the front changes the dynamics: Sectors of the population become causally disconnected after a time $t_* = R_0/v$, where R_0 is the initial radius of the population and v is the radial front propagation speed. The reproducing population size increases, creating an inflationary effect that prevents the loss of fit individuals due to sector boundary diffusion and sector interactions. We develop a generalization of the Domany-Kinzel model on amorphous, isotropic lattices to simulate radial expansions. We find scaling functions characterizing the effects of inflation at criticality. We also discuss analytic results for two-point correlation functions and survival probabilities in the two limiting cases of no mutations (compact DP) and no selection.

12:03PM Q42.00003 Competition and cooperation in one-dimensional stepping stone models, KIRILL KOROLEV, Massachusetts Institute of Technology, DAVID NELSON, Harvard University — Mutualism and cooperation are major biological forces sustaining ecosystems and enabling complex evolutionary adaptations. Although spatial degrees of freedom and number fluctuations often significantly affect evolutionary dynamics, their effects on mutualism are not fully understood. We show that, even when mutualism confers a distinct selective advantage, it persists only in populations with high density and frequent migrations. When these parameters are reduced, number fluctuations lead to the local extinctions of one of the species, segregating the species in space and decreasing the size of regions where cooperation occurs. The segregated and mutualistic states are separated by a second order nonequilibrium phase transition. Generically, this transition is in the universality class of directed percolation (DP), but the phase diagram is strongly influenced by an exceptional symmetric directed percolation (DP2) transition. This influence is manifested in a strong increase in the resilience to number fluctuations of symmetric mutualism, when organisms benefit equally from interacting.

12:15PM Q42.00004 Range expansion of mutualists, MELANIE J.I. MULLER, Harvard University, KIRILL S. KOROLEV, Massachusetts Institute of Technology, ANDREW W. MURRAY, DAVID R. NELSON, Harvard University — The expansion of a species into new territory is often strongly influenced by the presence of other species. This effect is particularly striking for the case of mutualistic species that enhance each other's proliferation. Examples range from major events in evolutionary history, such as the spread and diversification of flowering plants due to their mutualism with pollen-dispersing insects, to modern examples like the surface colonisation of multi-species microbial biofilms. Here, we investigate the spread of cross-feeding strains of the budding yeast *Saccharomyces cerevisiae* on an agar surface as a model system for expanding mutualists. Depending on the degree of mutualism, the two strains form distinctive spatial patterns during their range expansion. This change in spatial patterns can be understood as a phase transition within a stepping stone model generalized to two mutualistic species.

12:27PM Q42.00005 Cooperation, cheating, and collapse in microbial populations , JEFF GORE, Massachusetts Institute of Technology — Natural populations can suffer catastrophic collapse in response to small changes in environmental conditions, and recovery after such a collapse can be exceedingly difficult. We have used laboratory yeast populations to study proposed early warning signals of impending extinction. Yeast cooperatively breakdown the sugar sucrose, meaning that there is a minimum number of cells required to sustain the population. We have demonstrated experimentally that the fluctuations in the population size increase in magnitude and become slower as the population approaches collapse. The cooperative nature of yeast growth on sucrose suggests that the population may be susceptible to cheater cells, which do not contribute to the public good and instead merely take advantage of the cooperative cells. We have confirmed this possibility experimentally by using a cheater yeast strain that lacks the gene encoding the cooperative behavior [1]. However, recent results in the lab demonstrate that the presence of a bacterial competitor may drive cooperation within the yeast population.

[1] Gore et al, *Nature* **459**, 253 – 256 (2009)

1:03PM Q42.00006 ABSTRACT WITHDRAWN —

1:15PM Q42.00007 Evolution of cooperation in microbial biofilms - A stochastic model for the growth and survival of bacterial mats , JOHANNES KNEBEL, JONAS CREMER, ANNA MELBINGER, ERWIN FREY, Ludwig-Maximilians University of Munich — Cooperative behavior is essential for microbial biofilms. The structure and composition of a biofilm change over time and thereby influence the evolution of cooperation within the system. In turn, the level of cooperation affects the growth dynamics of the biofilm. Here, we investigate this coupling for an experimentally well-defined situation in which mutants of the *Pseudomonas fluorescens* strain form a mat at the liquid-air interface by the production of an extra-cellular matrix [1]. We model the occurrence of cooperation in this bacterial population by taking into account the formation of the mat. The presence of cooperators enhances the growth of the mat, but at the same time cheaters can infiltrate the population and put the viability of the mat at risk. We find that the survival time of the mat crucially depends on its initial dynamics which is subject to demographic fluctuations [2]. More generally, our work provides conceptual insights into the requirements and mechanisms for the evolution of cooperation.

[1] P. Rainey et al., *Nature* **425**, 72 (2003).

[2] A. Melbinger et al., *PRL* **105**, 178101 (2010).

1:27PM Q42.00008 Bacterial Cheating Limits the Evolution of Antibiotic Resistance¹ , EUGENE YURTSEV, HUI XIAO CHAO, Department of Physics, Massachusetts Institute of Technology, MANOSHI DATTA, Computational and Systems Biology, Massachusetts Institute of Technology, TATIANA ARTEMOVA, JEFF GORE, Department of Physics, Massachusetts Institute of Technology — The emergence of antibiotic resistance in bacteria is a significant health concern. Bacteria can gain resistance to the antibiotic ampicillin by acquiring a plasmid carrying the gene beta-lactamase, which inactivates the antibiotic. This inactivation may represent a cooperative behavior, as the entire bacterial population benefits from removal of the antibiotic. The presence of a cooperative mechanism of resistance suggests that a cheater strain - which does not contribute to breaking down the antibiotic - may be able to take advantage of resistant cells. We find experimentally that a "sensitive" bacterial strain lacking the plasmid conferring resistance can invade a population of resistant bacteria, even in antibiotic concentrations that should kill the sensitive strain. We use a simple model in conjunction with difference equations to explain the observed population dynamics as a function of cell density and antibiotic concentration. Our experimental difference equations resemble the logistic map, raising the possibility of oscillations or even chaotic dynamics.

¹This research was supported by the National Science Foundation Graduate Research Fellowship under Grant no. 0645960.

1:39PM Q42.00009 Does fast migration imply well-mixing? , MICHAEL KHASIN, University of Michigan, EVGENIY KHAIN, Oakland University, LEONARD SANDER, University of Michigan — A popular assumption in population dynamics is that the population is well mixed, i.e., a spatial character of the interactions between the individuals can be neglected. A common justification of this assumption is that the rate of migration between the local possibly well-mixed population-dynamics domains is much larger than the rates of interactions within a domain. We consider a system of local well-mixed domains of varying carrying capacity. In the limit of infinite migration rate we calculate the stationary probability distribution of the total population and find that generally it is not equivalent to the stationary probability distribution of a single well-mixed domain with a large carrying capacity. This proves that fast migration does not generally justify the well-mixed population assumption.

1:51PM Q42.00010 Turing patterns and a stochastic individual-based model for predator-prey systems , SEIDO NAGANO, Ritsumeikan University — Reaction-diffusion theory has played a very important role in the study of pattern formations in biology. However, a group of individuals is described by a single state variable representing population density in reaction-diffusion models and interaction between individuals can be included only phenomenologically. Recently, we have seamlessly combined individual-based models with elements of reaction-diffusion theory. To include animal migration in the scheme, we have adopted a relationship between the diffusion and the random numbers generated according to a two-dimensional bivariate normal distribution. Thus, we have observed the transition of population patterns from an extinction mode, a stable mode, or an oscillatory mode to the chaotic mode as the population growth rate increases. We show our phase diagram of predator-prey systems and discuss the microscopic mechanism for the stable lattice formation in detail.

Wednesday, February 29, 2012 11:15AM - 2:15PM —

Session Q43 DBIO: Invited Session: Techniques to Study Dynamic Cellular Processes One Molecule at a Time (Including Delbruck Award Lecture) 157AB

11:15AM Q43.00001 Max Delbruck Prize in Biological Physics Lecture: Single-molecule protein folding and transition paths¹ , WILLIAM EATON, Laboratory of Chemical Physics, NIDDK, National Institutes of Health, Bethesda, MD — The transition path is the tiny fraction of an equilibrium molecular trajectory when a transition occurs by crossing the free energy barrier between two states. It is a uniquely single-molecule property, and has not yet been observed experimentally for any system in the condensed phase. The importance of the transition path in protein folding is that it contains all of the mechanistic information on how a protein folds. As a major step toward observing transition paths, we have determined the average transition-path time for a fast and a slow-folding protein from a photon-by-photon analysis of fluorescence trajectories in single-molecule FRET experiments. While the folding rate coefficients differ by 10,000-fold, surprisingly, the transition-path times differ by less than 5-fold, showing that a successful barrier crossing event takes almost the same time for a fast- and a slow-folding protein, i.e. almost the same time to fold when it actually happens.

¹This work was carried out in collaboration with Hoi Sung Chung.

11:51AM Q43.00002 ATP-induced helicase slippage reveals highly coordinated subunits, MICHELLE D. WANG, Cornell University — Helicases are vital enzymes that carry out strand separation of duplex nucleic acids during replication, repair and recombination. T7 helicase, a model hexameric motor, has been observed to use dTTP, but not ATP, to unwind dsDNA as it translocates along ssDNA. Whether and how different subunits of the helicase coordinate their chemo-mechanical activities and DNA binding during translocation is still under debate. Here we address this question using a single-molecule approach to monitor helicase unwinding. We found that T7 helicase does in fact unwind dsDNA in the presence of ATP and that the unwinding rate is even faster than that with dTTP. However, unwinding was repeatedly interrupted by sudden slippage events, ultimately preventing unwinding over a substantial distance. This behaviour was greatly reduced with the supplement of a small amount of dTTP. These findings presented an opportunity to use nucleotide mixtures to investigate helicase subunit coordination. Our results support a model where nearly all subunits coordinate their chemo-mechanical activities and DNA binding. Such subunit coordination may be general to many ring-shaped helicases and reveals a potential mechanism for regulation of DNA unwinding during replication.

12:27PM Q43.00003 Unraveling the motion of single-stranded DNA binding proteins on DNA using force and fluorescence spectroscopy, TAEKJIP HA, Department of Physics, University of Illinois at Urbana-Champaign — Single-stranded DNA binding (SSB) proteins bind to and control the accessibility of single stranded (ss) DNA generated as a transient intermediate during a variety of cellular processes. For subsequent DNA processing, however, such a tightly wrapped, high-affinity protein-DNA complex still needs to be removed or repositioned quickly for unhindered action of other proteins. Here we show, using single-molecule two- and three-colour fluorescence resonance energy transfer, that SSB can spontaneously migrate along ssDNA. Diffusional migration of SSB helps in the local displacement of SSB by an elongating RecA filament. SSB diffusion also melts short DNA hairpins transiently and stimulates RecA filament elongation on DNA with secondary structure. This observation of diffusional movement of a protein on ssDNA introduces a new model for how an SSB protein can be redistributed, while remaining tightly bound to ssDNA during recombination and repair processes. In addition, using an optomechanical tool combining single-molecule fluorescence and force methods, we probed how proteins with such a large binding site size (~ 65 nucleotides) can migrate rapidly on DNA and how protein-protein interactions and tension may modulate the motion. We observed force-induced progressive unravelling of ssDNA from the SSB surface between 1 and 6 pN, followed by SSB dissociation at ~ 10 pN, and obtained experimental evidence of a reptation mechanism for protein movement along DNA wherein a protein slides via DNA bulge formation and propagation. SSB diffusion persists even when bound with RecO, and at forces under which the fully wrapped state is perturbed, suggesting that even in crowded cellular conditions SSB can act as a sliding platform to recruit and carry its interacting proteins for use in DNA replication, recombination and repair.

1:03PM Q43.00004 Beholding the subcellular world in your PALM: nanometer resolution optical measurements of protein assemblies in cells¹, HARI SHROFF, National Institute of Biomedical Imaging and Bioengineering — Key to understanding a protein's biological function is the accurate determination of its spatial distribution inside a cell. Although fluorescent protein markers enable specific targeting with molecular precision, much of this utility is lost when the resultant fusions are imaged with conventional, diffraction-limited optics. In response, several imaging modalities that rely on the stochastic activation and bleaching of single molecules, and that are capable of resolution $10\times$ below the diffraction limit (250 nm for visible wavelengths), have emerged. This talk will cover superresolution imaging of biological structures using photoactivated localization microscopy (PALM). In addition to covering the theory, we will also discuss the use of the technique in understanding biological phenomena on the nanoscale, including the organization of bacterial chemoreceptors, the movement of actin in neuronal spines, and the stratification of focal adhesions.

¹This work was supported by the Intramural Research Programs of the National Institute of Biomedical Imaging and Bioengineering.

1:39PM Q43.00005 Single-molecule conductance measurements of biomolecule translocation across biomimetic nuclear pores¹, CEES DEKKER, Delft University of Technology — After a brief overview of our recent work on solid-state nanopores, I will present single-molecule transport data across biomimetic nanopores that contain the key regulating parts of the nuclear pore complex (NPC). The mechanism for the remarkable selectivity of NPCs has remained unclear in a large part due to difficulties in designing experiments that can probe the transport at the relevant length and time scales. Building and measuring on biomimetic NPCs provides new opportunities to address this long-standing problem. covalently tether the natively unfolded Phe-Gly rich domains (FG-domains) of human nuclear binding proteins to a solid-state nanopore (a 10-100 nm sized hole in a SiN membrane). Ionic current measurements provide a probe to monitor single molecules that traverse the pore. Translocation events are observed for transport receptors (Imp β), whereas transport of passive molecules (BSA) is found to be blocked. Interestingly, a single type of nuclear pore proteins appears already sufficient to form a selective barrier for transport. A translocation time of about 2.5 ms is measured for Imp β . This time is found to be similar for transport across Nup153 and Nup98 coated pores, although the observed ionic conductance differs between these two types of pores. We compare two simple models for the pore conductance and find, for both Nups, that the data fits best to a model with an open central channel and a condensed layer along the outer circumference of the pore. reproducing the key features of the NPC, our biomimetic approach opens the way to study a wide variety of nucleo-cytoplasmic transport processes at the single-molecule level in vitro.

¹Work carried out by my graduate student Stefan W. Kowalczyk at Delft and in collaboration with Larisa Kapinos and Roderick Y. H. Lim at the University of Basel.

Wednesday, February 29, 2012 11:15AM - 2:15PM –
Session Q44 DPOLY: Focus Session: Interparticle Interactions in Polymer Nanocomposites - Transport and Dynamics 157C

11:15AM Q44.00001 Multiscale structure, interfacial cohesion, adsorbed layers, miscibility and properties in dense polymer-particle mixtures, KEN SCHWEIZER, University of Illinois at Urbana-Champaign — A major goal in polymer nanocomposite research is to understand and predict how the chemical and physical nature of individual polymers and nanoparticles, and thermodynamic state (temperature, composition, solvent dilution, filler loading), determine bulk assembly, miscibility and properties. Microscopic PRISM theory provides a route to this goal for equilibrium disordered mixtures. A major prediction is that by manipulating the net polymer-particle interfacial attraction, miscibility is realizable via the formation of thin thermodynamically stable adsorbed layers, which, however, are destroyed by entropic depletion and bridging attraction effects if interface cohesion is too weak or strong, respectively. This and related issues are quantitatively explored for miscible mixtures of hydrocarbon polymers, silica nanospheres, and solvent using x-ray scattering, neutron scattering and rheology. Under melt conditions, quantitative agreement between theory and silica scattering experiments is achieved under both steric stabilization and weak depletion conditions. Using contrast matching neutron scattering to characterize the collective structure factors of polymers, particles and their interface, the existence and size of adsorbed polymer layers, and their consequences on microstructure, is determined. Failure of the incompressible RPA, accuracy of PRISM theory, the nm thickness of adsorbed layers, and qualitative sensitivity of the bulk modulus to interfacial cohesion and particle size are demonstrated for concentrated PEO-silica-ethanol nanocomposites. Temperature-dependent complexity is discovered when water is the solvent, and nonequilibrium effects emerge for adsorbing entangled polymers that strongly impact structure. By varying polymer chemistry, the effect of polymer-particle attraction on the intrinsic viscosity is explored with striking non-classical effects observed. This work was performed in collaboration with S.Y.Kim, L.M.Hall, C.Zukoski and B.Anderson.

11:51AM Q44.00002 Organically Modified Nanoclay-Reinforced Rigid Polyurethane Films, YONG TAE PARK, Department of Chemical Engineering and Materials Science, University of Minnesota, YUQIANG QIAN, Department of Chemistry, University of Minnesota, CHRIS LINDSAY, Huntsman Polyurethanes, ANDREAS STEIN, Department of Chemistry, University of Minnesota, CHRISTOPHER MACOSKO, Department of Chemical Engineering and Materials Science, University of Minnesota — The nanodispersion of vermiculite in polyurethanes was investigated to produce organoclay-reinforced rigid gas barrier films. Reducing gas transport can improve the insulation performance of closed cell polyurethane foam. In a previous study, the dispersion of vermiculite in polyurethanes without organic modification was not sufficient due to the non-uniform dispersion morphology. When vermiculite was modified by cation exchange with long-chain quaternary ammonium cations, the dispersion in methylene diphenyl diisocyanate (MDI) was significantly improved. Dispersion was improved by combining high intensity dispersive mixing with efficient distributive mixing. Polymerization conditions were also optimized in order to provide a high state of nanodispersion in the polyurethane nanocomposite. The dispersions were characterized using rheological, microscopic and scattering/diffraction techniques. The final nanocomposites showed enhancement of mechanical properties and reduction in permeability to carbon dioxide at low clay concentration (around 2 wt percent).

12:03PM Q44.00003 Shear viscosity of polymer nanocomposites from NEMD simulations, JAGANNATHAN T. KALATHI, SANAT K. KUMAR, Columbia University, GARY S. GREST, Sandia National Laboratories — Polymer nanocomposites (PNC) are preferred for a variety of applications since they offer excellent thermal, electrical, and mechanical properties. The viscosity of PNC is primarily a strong function of filler size. For micron-sized fillers, the shear viscosity increases with filler volume fraction following the well-known Einstein relationship. However as the particle size approaches the nanoscale, the viscosity is found to either increase or decrease depending on the strength of interactions between the particle and polymer. In this study, the shear viscosity of an entangled polymer melt of $N=400$ beads of diameter σ with and without fillers is estimated using NEMD simulations. The diameter of the nanoparticles ($1-10\sigma$) and volume fraction ($0.05-0.3$) are varied for shear rate from 10^{-2} to $10^{-6}\tau^{-1}$. The viscosity of PNC decreases when compared to pure melt for nanoparticles of size 1σ and recovers to the value of a pure melt when the size approaches 10σ , provided all the interactions are neutral. It thus appears that the increase in viscosity embodied in the Einstein relationship only manifests itself for large nanoparticle size $>10\sigma$.

12:15PM Q44.00004 Towards the Next Generation of Polymer Nanocomposites: More Rigid, Lighter Weight, Yet Easier to Process¹, JEONGJAE WIE, JONATHAN SEPPALA, MICHAEL MACKAY, University of Delaware, WOO JIN CHUNG, JEFFREY PYUN, University of Arizona — Polymer nanocomposites are attractive for their lightness in weight and excellent mechanical reinforcement. Current nanocomposites incorporate high aspect ratio fillers such as clays, carbon nanotubes (CNT), and graphenes. Exfoliation of clay, for example, is essential to obtain maximum mechanical reinforcement, yet this results in a 2 to 4 order of magnitude melt viscosity increase. This high viscosity leads to a reduction in the production rate and/or increased processing cost, which is undesirable. In order to obtain reduced melt viscosity without sacrificing the advantages of current nanocomposites, we prepared poly(styrene) (PS) nanocomposites by inclusion of various spherical nanoparticles using a technique that ensures good dispersion. Tensile tests demonstrated enhanced tensile modulus in the glassy state while a reduced melt viscosity was observed. The results show that nanoparticle geometry is extremely important and nanoscale effects can lead to the next generation of polymer nanocomposites.

¹This work has been supported by U.S. Army Research Office (ARO) under contract W911NF-09-1-0145.

12:27PM Q44.00005 A Comparative Study of Interfacial Slip in Polymer Blends with Nanoparticles and Diblock Copolymer Compatibilizers, JOSEPH ORTIZ, DILIP GERSAPPE, Department of Materials Science and Engineering, Stony Brook University — The interfacial region in polymer blends has been identified as a low viscosity region in which considerable slip can occur when the blend is subjected to shear forces. Here we use Molecular Dynamics simulations to establish and compare the roles that added nanoparticle fillers and diblock copolymers play in modifying the interfacial rheology. By choosing conditions under which the fillers and diblocks are localized, either in the two phases or at the interface, we can look at the interplay between their strengthening capabilities and the change in the interfacial slip behavior. We examine particle size, attraction between the particle and the polymer component, and the amount of filler in the material and compared this to systems including diblock copolymers at the same volume fraction. Our studies are performed, for a variety of shear values, both above and below the point at which the filler particles form a transient network in the blend.

12:39PM Q44.00006 The Effect of Elongational Flow on the Placement and Orientation of Nanorods in Polymer: Modeling and Experiments, JAY PARK, Cornell University, VIBHA KALRA, Drexel University, YONG JOO, Cornell University — Nanorods are often incorporated into a polymer to enhance its functionality. Gaining control over the placement of nanorods in polymer is important to improve the desired nanocomposite material property and for application like solar cell. First, we used coarse-grained molecular dynamics (CGMD) simulation to quantitatively examine the effect of elongational flow on the placement of model nanorods in homopolymer matrix. We have investigated how flow strength, concentration, interaction, and aspect ratio of nanorods affect its placement in homopolymer. As an analogous experiment, we have electrospun polyvinyl alcohol (PVA) in water with Au nanorods. The experimental result showed dispersion and alignment of Au nanorods, as predicted by the simulation. We also demonstrated selective placement of nanorods along the outer layer of fiber by co-axially electrospinning PVA/Au nanorods and pure PVA as shell and core, respectively. The material properties of the PVA/Au nanocomposite fiber are tested to show its potential application such as electromagnetic interference (EMI) shielding. The good agreements between simulation and experiment suggest that CGMD simulation can be used as a predictive tool for controlling nanorod placement in a polymer under extensional flow.

12:51PM Q44.00007 Directed Self-Assembly of Nanoparticles via Flexible-Blade Flow Coating¹, DONG YUN LEE, JONATHAN PHAM, JIMMY LAWRENCE, CHEOL HEE LEE, HYUN SUK KIM, CASSANDRA PARKOS, TODD EMRICK, ALFRED J. CROSBY, University of Massachusetts Amherst — We present a facile, non-lithographic, one-step method termed flexible-blade flow coating to direct the assembly of quantum dots. This versatile technique exploits the phenomenon known as the “coffee ring effect” coupled with confined convective flow and controlled stick-slip motion to fabricate ribbons and fabrics with a broad range of length scales of nearly any material. We achieve nanostripe dimensions of width below 300 nm, thickness of a single nanoparticle (~ 8 nm), and continuous length exceeding 5 cm. This multi-length scale control is facilitated by the use of a flexible blade, which allows capillary forces to self-regulate the uniformity of convective flow processes. We exploit solvent mixture dynamics and nanoparticle chemistry to enhance intra-assembly particle packing, leading to novel assembly properties including conductivity and free-standing mechanical flexibility and strength. This simple technique and the use of novel materials open up a new paradigm for integration of nanoscale patterns over large areas for various applications.

¹This material is based upon work supported as part of the PHaSE, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001087

1:03PM Q44.00008 Properties of Macroscopic Nanoparticle Assemblies Fabricated by Flexible Blade Flow Coating, JONATHAN T. PHAM, DONG YUN LEE, JIMMY LAWRENCE, CHEOL HEE LEE, TODD EMRICK, ALFRED J. CROSBY, University of Massachusetts Amherst — Nanoparticle assemblies have gained much interest for their potential in electronic, photonic, optical, chemical, and biological applications. Although one of the greatest challenges is the controlled positioning of nanoscale components into the desired multi-length scale structures, understanding the properties of nanoparticle assemblies has also remained elusive. We have developed a technique termed flexible blade flow coating to direct the assembly of nanoparticles into ribbons and fabrics with a broad range of length scales. Ribbons and fabrics constructed with photoreactive quantum dots are crosslinked by UV irradiation affording long, flexible and robust structures that allow for subsequent liftoff from the substrate by dissolution of a sacrificial underlayer. The structural integrity of freely floating fabrics and extremely high aspect ratio ribbons are observed through fluorescence microscopy. Physical properties of these assemblies are explored with varying dimensions and ligand chemistry. We find that nanoparticle ribbons and fabrics possess unique properties in comparison to continuous polymer thin films, such as spherical wrapping and two-dimensional flexibility.

1:15PM Q44.00009 Reversible Shear-Flow-Induced Polymer and Colloid Aggregates, HSIEH CHEN, ALFREDO ALEXANDER-KATZ, MIT — Using hydrodynamic simulations and a coarse-grained interaction model, we show that self-associating polymer and colloid mixtures can form reversible flow-induced aggregates in shear flow. We find that when increasing shear rates, the mixtures go through four distinct conformations from no aggregation to dense aggregates. The different conformations are verified by analyzing their radial distribution functions, $g(r)$, as well as by visual inspection. Furthermore, we find that the formation of the aggregates is reversible. That is, the shear-induced aggregates disappear when we decrease the shear rates, and reappear when we increase the shear rates again.

1:27PM Q44.00010 Impact of Carbon Nanoparticle Shape on Polymer Dynamics in Nanocomposites¹, BRAD MILLER, MARK DADMUN, Department of Chemistry, University of Tennessee, Knoxville — In forming quality nanocomposites of carbon-based nanoparticles (CNPs) in a polymer matrix, achieving and maintaining a high degree of dispersion is a crucial problem. One method to attain well-dispersed CNP nanocomposites is to incorporate non-covalent interactions between the CNP and matrix, which also impacts the dynamics of the polymer chain. In this work, T2 NMR relaxometry (T2 NMR) examines the effect on polymer chain dynamics of incorporating CNPs into polystyrene-co-acrylonitrile (SAN) random copolymer matrices. In SAN-CNP composites, the segmental-chain dynamics can be influenced by the non-covalent interactions formed with the nanoparticle (interacting), but are also influenced by the CNP steric bulk alone (non-interacting). The use of T2 NMR allows for the examination of the influence of the extent of non-covalent interactions on this segmental chain level. This segmental level view also allows for the distinction between relaxation dynamics of the interacting and non-interacting regimes. Current data indicates that increased acrylonitrile content in the copolymer results in increased non-covalent interactions and overall slowing of chain dynamics.

¹NSF, Oak Ridge National Laboratory, Department of Energy

1:39PM Q44.00011 Modifying Fragility and Length Scales of Polymer Glass Formation with Nanoparticles, BEATRIZ A. PAZMINO, Physics Dept., Wesleyan University, Middletown, CT, JACK F. DOUGLAS, Polymer Division, NIST, Gaithersburg, MD, FRANCIS W. STARR, Physics Dept., Wesleyan University, Middletown, CT — We investigate the effects of nanoparticles on glass formation in a model polymer melt by molecular dynamics simulations. The addition of nanoparticles allows us to change the glass transition temperature T_g , the fragility of glass formation, and both static and dynamical length scales in a controlled fashion. We contrast the length scales of static density changes with the length scale over which nanoparticles perturb the dynamics, as well as the length scale of cooperative string-like motion. Using the Adam-Gibbs approach, we show how the changes of fragility can be interpreted as a measure of the scale of cooperative string-like motion. We contrast the behavior along isobaric and isochoric paths to T_g , and find that changes along an isobaric path (most relevant experimentally) are much smaller than those along an isochoric path.

1:51PM Q44.00012 Glass transition temperature of polymer nano-composites with polymer and filler interactions, KATSUMI HAGITA, National Defense Academy, HIROSHI TAKANO, KEIO University, MASAO DOI, University of Tokyo, HIROSHI MORITA, AIST — We systematically studied versatile coarse-grained model (bead spring model) to describe filled polymer nano-composites for coarse-grained (Kremer-Grest model) molecular dynamics simulations. This model consists of long polymers, crosslink, and fillers. We used the hollow structure as the filler to describe rigid spherical fillers with small computing costs. Our filler model consists of surface particles of icosahedra fullerene structure C320 and a repulsive force from the center of the filler is applied to the surface particles in order to make a sphere and rigid. The filler's diameter is 12 times of beads of the polymers. As the first test of our model, we study temperature dependence of volumes of periodic boundary conditions under constant pressures through NPT constant Andersen algorithm. It is found that Glass transition temperature (T_g) decrease with increasing filler's volume fraction for the case of repulsive interaction between polymer and fillers and T_g weakly increase for attractive interaction.

2:03PM Q44.00013 Payne effect in model nanocomposite the role of polymer confinement, HELENE MONTES, FRANÇOIS LEQUEUX, ESPCI-Paristech, PAPON AURELIE TEAM — Payne effect is a non-linearity observed in polymer nanocomposites at small strain amplitudes, above the bulk glass transition temperature. The origin is the non-linear mechanical response of the polymer located near the solid fillers. However the exact nature of the mechanical response is still the object of debate. We have developed since ten years model nano-composite systems consisting in monodisperse spherical particles dispersed in an elastomer matrix. Thanks to NMR and Neutrons scattering, we have been able to determine precisely the amount of polymer confined between pairs of particles and with a modified dynamics. From that we have deduced that the Payne effect clearly originates in two mechanisms: i) around each particle, a glass transition temperature gradient ii) around this first layer, a modified topology of the polymer —originating itself in the glassiness of the polymer very near the particles. Hence, we are able to build a master curve for the Payne effect amplitude versus the number of particles connected to their neighbors by these two layers, that gathers measurements at various temperatures, volume fractions and frequencies.

**Wednesday, February 29, 2012 11:15AM - 2:15PM –
Session Q45 DPOLY: Elastomers and Gels 159**

11:15AM Q45.00001 Can a Rheological Experiment Distinguish Between a Gel and a Soft Glass? If yes, which Experiment?, HORST WINTER, University of Massachusetts Amherst — Generic rheological differences between gels and soft glasses appear most pronounced in the *immediate approach of the liquid-to-solid transition from the liquid side*. Two model systems of known linear viscoelasticity were chosen to exemplify the two material classes: a crosslinking PDMS represents gelation and a concentrated, aqueous suspension represents the soft glass transition. The longest relaxation time and the zero shear viscosity diverge for both materials, which look very similar in this way. However, the relaxation time spectrum and its expression as complex modulus, with components G' and G'' , provide a clear distinction between gelation and the soft glass transition. While the long-time component of the relaxation time spectrum follows a powerlaw in time for both, $\log H \sim n \log t$, their powerlaw exponent n is of different sign: negative n for the critical gel (material at the gel point) (Chambon et al. Polym Bull 13:499–503, 1985; Winter et al. J Rheology 30:367–382, 1986; Chambon et al. J Rheol 31:683–697, 1987) and positive n for the soft glass (Siebenbürger et al. J Rheology 53:707–720, 2009; Winter et al. Rheol Acta 48:747–753). The powerlaw spectrum is cut off by the diverging, longest relaxation time (called “alpha relaxation time” for the soft glass) in the approach of the liquid-to-solid transition. In summary, relaxation data provide a clear distinction between these two classes of materials.

11:27AM Q45.00002 Effects of crosslinker concentration and chemical disorder on the nonlinear mechanics of thermoreversibly associating networks, GLENN H. FREDRICKSON, University of California, Santa Barbara, ROBERT S. HOY, Yale University — We present simulation studies of thermoreversibly associating polymer networks that relate dramatic differences in nonlinear mechanics (e. g. creep and fracture) to differences in crosslinker placement and consequent differences in the equilibrium structure and quiescent dynamics of these systems. Our results illustrate how the greater structural and dynamical heterogeneity in systems possessing randomly placed crosslinkers leads to higher mobility, increased creep compliance and decreased fracture toughness in comparison to systems with uniformly spaced crosslinkers. Further quiescent-dynamical slowdown and mechanical property enhancement may be obtained through well-defined but nonuniform placement of crosslinkers. The variation of properties with crosslinker concentration c and parent chain length N is also investigated. Increasing characteristic chemical distances between crosslinkers decreases effects arising from network “loops,” the prevalence of which is closely associated with chemical order. At fixed c , while differences associated with chemical (dis)order decrease with increasing N , they remain dramatic in the $N \sim N_e$ regime which is often used in practical applications.

11:39AM Q45.00003 Mechanically induced oscillations in Belousov-Zhabotinsky gels, IRENE CHEN, Massachusetts Institute of Technology, OLGA KUKSENOK, VICTOR YASHIN, ANNA BALAZS, University of Pittsburgh, KRISTYN VAN VLIET, Massachusetts Institute of Technology — Belousov-Zhabotinsky (BZ) gels are a unique class of stimuli-responsive materials that exhibit periodic changes in both color and size due to the self-oscillating kinetics of the BZ reduction-oxidation reaction. Such oscillations last for several hours, ending when a steady-state is reached in which the chemical reactants have been depleted. Here, we demonstrate that a depleted, non-oscillating BZ gel can be mechanically resuscitated, extending the oscillatory functionality of the material. These results represent the first experimental demonstration of mechanically induced oscillations in N-isopropylacrylamide-Ru(bpy)₃ gels. We characterize this phenomenon by quantifying the critical stress required to trigger oscillations, and the dependence of period and amplitude for triggered oscillations as a function of malonic acid concentration. Lastly, we demonstrate sensor applications comprising arrays of discrete BZ gel discs in which individual gels oscillate in color upon compression and have the capacity to transmit chemical signals away from the deformation site.

11:51AM Q45.00004 Nonlinear Elasticity of Entangled Polymer Networks, OZAN SARIYER, University of North Carolina at Chapel Hill, SERGEY PANYUKOV, P. N. Lebedev Physics Institute, Russian Academy of Sciences, MICHAEL RUBINSTEIN, University of North Carolina at Chapel Hill — We develop a microscopic model for elasticity of entangled polymer networks. The classical models of rubber elasticity (affine network and phantom network models) take into account only the effect of cross-links, but not the entanglements between polymer chains. For uniaxial deformation, the entanglement effects can be characterized by the dependence of Mooney ratio on network deformation. Constrained network models (such as constrained-junction and diffused-constraint models), tube models (such as Edwards' tube and nonaffine tube models) as well as phenomenological models (such as Mooney-Rivlin model) have been proposed to capture the experimentally observed dependence of Mooney ratio on network deformation. One of the latest efforts in the field is the slip-tube model, in which the entanglements are represented by slip-rings that can glide along the network chains but elastically constrained in space. The model we study improves over the original slip-tube model by taking into account harmonic interactions along the chain between such slip-links. We analytically and numerically solve the new microscopic model and present our results in comparisons with experimental and simulation data for both uniaxial and biaxial deformation.

12:03PM Q45.00005 Coarse grain modeling of the high-rate stress-strain behavior for select model Poly[urethane urea] (PUU) elastomers, T.L. CHANTAWANSRI, Y.R. SLOZBERG, A. HSIEH, J.W. ANDZELM, Army Research Laboratory — Microphase-separated PUU, which consists of 4,4'-dicyclohexylmethane diisocyanate, diethyltoluenediamine and poly[tetramethylene oxide](PTMO), exhibits versatile mechanical properties making them an excellent choice for potential applications in the form of films, adhesives, coatings and matrix materials for composites. To elucidate the effects of composition, including the hard segment content & molecular weight of PTMO, on rate-dependent mechanical deformation in the high strain-rate regime ($>> 10^5/s$) the stress-strain behavior for PUU at various rates are calculated for four model systems using a coarse-grain model. Pair interactions between topologically non-connected particles are described by the standard truncated Lennard-Jones (LJ) pair potential, where bonded particles interact according to the standard FENE/LJ potential. An angle harmonic potential is also used to enforce the rigidity of the hard segments, and the system is evolved using molecular dynamics. Stress-strain curves are calculated at various strain-rates and qualitatively agree with experimental results when extrapolated to higher rate. Further analysis of the morphology is also performed to characterize the morphology and discern its connection to the calculated mechanical properties.

12:15PM Q45.00006 Swelling Behavior of Crosslinked Rubber: Does the Peak in Dilational Modulus Exist?¹, BEN XU, XIAOJUN DI, GREGORY B. MCKENNA, Department of Chemical Engineering, Texas Tech University — Previous work² has shown that when handled properly, Frenkel³-Flory-Rehner⁴(FFR) theory is an excellent model to explain swelling behavior with the exception of failing to describe the peak of the swelling activity parameter S , or dilational modulus. This peak was first observed by Gee et al.⁵ and has eluded explanations. In the present work, we explored the importance of fitting procedure to the isopiestic data on the presence of the peak of S . We found the peak in S disappears when using a FFR model based fit instead of the empirical or polynomial fits used previously. We take model material parameters and show that adding less than 1% random error to the theoretical curves can lead to the peak in S . Our findings suggest strongly that the “peak” in S is due to experimental errors that are amplified by the fitting method.

¹The authors thank the Office of Naval Research under grants N00014-06-1-0922 and N00014-11-1-0424 for support of this work.

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⁵G. Gee, J. B. M. Herbert, and R. C. Roberts, Polymer, 6, 541 (1965).

12:27PM Q45.00007 Microphase Separation and Dynamics of Elastomeric Polyureas¹, JAMES RUNT, ALICIA CASTAGNA, TAEYI CHOI, YOUMI JEONG, Penn State University — Polyureas, consisting of alternating polyether soft segments and urea-containing hard segments, are of interest for shock and other energy absorbing applications. The properties of these materials are strongly influenced by microphase separation of the hard and soft segments, which is rather incomplete. Bulk- and solution-polymerized polyureas based on oligomeric polytetramethylene oxide and methylene diphenyl diisocyanate were investigated, and the role of PTMO molecular weight was identified. The morphology was characterized using atomic force microscopy and quantitative degrees of phase separation were determined from small-angle X-ray scattering. Dielectric relaxation spectroscopy and dynamic mechanical analysis were used to probe the dynamics. Particular attention was paid to the segmental dynamics of the soft phase, which has been proposed to be a major contributor to shock energy absorption in these materials.

¹Supported by the Office of Naval Research.

12:39PM Q45.00008 Opening and Closing of Nanocavities under Stress in Soft Nanocomposites: A Real Time Small Angle X-ray Scattering (SAXS) Observation, HUAN ZHANG, JORDAN DE CREVOISIER, Soft Matter Science and Engineering, ESPCIParisTech-CNRS-UPMC, Paris, France, ARTHUR SCHOLZ, Materials Research Laboratory, UCSB, 93106-5121 CA, U.S.A., FABIEN VION-LOISEL, Michelin, EDWARD J. KRAMER, Departments of Materials and Chemical Engineering, UCSB, 93106-5050, COSTANTINO CRETON, Soft Matter Science and Engineering, ESPCIParisTech-CNRS-UPMC, Paris, France — Cavitation occurring at the nanometer length scale has been recently demonstrated conclusively in rubbers¹. Real time SAXS with synchrotron radiation is employed to probe the structure changes in carbon black filled styrene-butadiene rubber (SBR) under uniaxial tension. The scattering invariant $Q(\lambda)$, where λ is the extension ratio, increases sharply, which we attribute to void formation, above a critical true stress (~ 25 MPa) that is roughly independent of both filler content and crosslinking density. During step-cycle tests Q decreases on unloading to Q_0 , its value before any testing, and does not increase again until λ exceeds the maximum previous $\lambda = \lambda_{max}$, showing that the voids close upon unloading and only reappear upon reloading when $\lambda > \lambda_{max}$ (Mullins effect). We attribute the increase of the scattering invariant once λ exceeds λ_{max} to the creation of new voids rather than to the reopening of old ones. The scattering of the voids in the region $q < 0.1 \text{ nm}^{-1}$ can be separated from that of the carbon black particles and provides information on average void size and shape.

12:51PM Q45.00009 Reversible shape memory, SERGEI SHEIKO, JING ZHOU, SARAH WHITE, VALERIE ASHBY, University of North Carolina at Chapel Hill — An “Achilles’ heel” of shape memory materials is that shape transformations triggered by an external stimulus are usually irreversible. Here we present a new concept of reversible transitions between two well-defined shapes by controlling hierarchic crystallization of a dual-network elastomer. The reversibility was demonstrated for different types of shape transformations including rod bending, winding of a helical coil, and widening an aperture. The distinct feature of the reversible shape alterations is that both counter-shapes are infinitely stable at a temperature of exploitation. Shape reversibility is highly desirable property in many practical applications such as non-surgical removal of a previously inserted catheter and handfree wrapping up of an earlier unraveled solar sail on a space shuttle.

1:03PM Q45.00010 Inscribing dynamical patterns within heterogeneous self-oscillating gels., ANNA C. BALAZS, VICTOR V. YASHIN, Chemical Engineering Department, University of Pittsburgh, Pittsburgh, PA 15261, SEIICHI SUZUKI, RYO YOSHIDA, Department of Materials Engineering, Graduate School of Engineering, The University of Tokyo, Tokyo, 113-8656, Japan — Grafting the ruthenium catalyst to the network of swollen chemo-responsive polymer gel creates a new class of materials, which exhibit the autonomous, coupled chemical and mechanical oscillations induced by the ongoing Belousov-Zhabotinsky (BZ) reaction. The mechanical oscillations occur due to the hydrating effect of the oxidized Ru that causes the gel to swell and de-swell repeatedly. It was predicted previously that compartmentalization of BZ gels in a nonresponsive gel matrix would enable a researcher to create gel-based devices with the functionality inscribed by the configuration of the Ru-containing patches. Recently, the heterogeneous gels were fabricated that encompass the disk-shaped BZ patches. It was demonstrated experimentally for the first time that the direction of propagation of the chemo-mechanical waves in an array of the BZ patches can be controlled by varying the ruthenium content and size of the patches. Here, we present the results of computational modeling of such heterogeneous self-oscillating gels. We discuss how the catalyst concentration, patch size, and inter-patch distance affect the synchronization of oscillations in the neighboring BZ gels, and how the synchronization effects can be utilized to control the dynamical behavior of the entire system.

1:15PM Q45.00011 Swelling instabilities in patterned, microscale gels, RYAN TOOMEY, SAMUEL DUPONT, University of South Florida, NONE TEAM — Hydrogels facilitate reconfigurable structures with response integrated at the material level. Response is engendered by a competing mechanism: the elasticity of the network counterbalances expansion by the solvent. If the strength of expansion can be controlled by an environmental cue, the hydrogel can be adjusted in situ. The equilibrium state occurs when the osmotic stress exerted by the solvent in the gel equals the osmotic pressure of the solvent outside the gel. For a free structure, the equilibrium state corresponds to homogenous swelling. If a free surface of the gel is mechanically constrained, however, the dimensions available for the relief of the osmotic stress are reduced, resulting in non-uniform or inhomogeneous swelling. In this study, we demonstrate how mechanical constraints impose differential gel swelling and buckling in patterned gels. Depending on the initial geometry of the constrained gel, three general modes of swelling-induced deformation can be observed: lateral differential swelling, bulk sinusoidal buckling, and surface wrinkling. Through confocal microscopy and 3D image rendering, the mechanics of swelling has been evaluated in the context of linear elasticity theory.

1:27PM Q45.00012 Thermoresponsive hydrogels from ABC triblock terpolymers, CAN ZHOU, TIMOTHY LODGE, MARC HILLMYER, Department of Chemistry, University of Minnesota, Twin City — We have prepared novel thermoreversible ABC hydrogels from poly(ethylene-alt-propylene)-b-poly(ethylene oxide)-b-poly(N-isopropylacrylamide) (PEP-PEO-PNIPAm) triblock terpolymers. The terpolymers form micelles in water at low temperatures with hydrophobic PEP cores surrounded by hydrophilic PEO-PNIPAm coronas, and these micelles subsequently associate to form a hydrogel upon heating above the lower critical solution temperature (LCST) of PNIPAm. The separation of micellization and gelation leads to the formation of a two-compartment network with exclusively bridging conformations for the PEO midblocks. Therefore, gelation can be achieved at a much lower concentration, with better mechanical properties and a sharper sol-gel transition, when compared with ABA triblock copolymer hydrogels from PNIPAm-PEO-PNIPAm. The results highlight the intricate nanostructures and new properties available from ABC terpolymer hydrogels.

1:39PM Q45.00013 Single Quantum Dot Tracking in Heterogeneous Polyacrylamide Hydrogels, CHEOL HEE LEE, ALFRED CROSBY, RYAN HAYWARD, TODD EMRICK, University of Massachusetts Amherst — Structural heterogeneity within polymer gels plays an important role in determining their material properties, yet is difficult to characterize by established methods. Single particle tracking measurements can provide highly localized information on the diffusion dynamics of tracer particles, and therefore on the material properties of the medium. We use tailored core-shell quantum dots (QDs) with hydrophilic ligands to characterize polyacrylamide hydrogels with varying crosslink density. We find that QDs show sub-diffusive behavior and non-Gaussian displacement distributions, consistent with prior reports on diffusive behavior in other heterogeneous media. We also consider the distribution of particle caging times, which is dictated by the potential energy barriers to escape pores, and therefore provides insight into structural heterogeneity. Specifically, we find that gels with a higher density of crosslinks yield broader distributions of caging times, indicating greater heterogeneity of these networks.

1:51PM Q45.00014 Modeling Photo-Reconfiguration and Directed Motion of Spirobenzopyran- Containing Polymer Gels, OLGA KUKSENOK, ANNA C. BALAZS, University of Pittsburgh — We develop a computational model to simulate the behavior of photo-responsive polymer gels that contain spirobenzopyran (SP) chromophores. Using this model, we design three-dimensional samples with dynamically reconfigurable morphologies and photo-induced motility. In the dark, the SP moieties assume an open ring conformation and are hydrophilic; under illumination with blue light, the chromophores assume a closed ring conformation and are hydrophobic. This collapse of the gels is caused by the decrease in hydration due to conformational changes and not by a light-induced heating of the polymer network. We demonstrate that these gels can be effectively patterned remotely and reversibly with light by illuminating the sample through photomasks. We also show that by introducing variations in crosslink density within the gels during their preparation, as well as introducing temperature gradients, we have additional means of guiding the dynamic behavior of these versatile, responsive systems. Furthermore, we demonstrate that one can use a mobile light source to move multiple gel pieces to a specific location. The results point to a novel method for controlling the self-organization of soft, reconfigurable materials.

2:03PM Q45.00015 Gelation of Copolymers Photo-crosslinked by Pendent Benzophenones, SCOTT CHRISTENSEN, RYAN C. HAYWARD, UMass - Amherst Polymer Science and Engineering — Copolymers containing pendent benzophenone (BP) groups provide a simple and powerful route to crosslinkable polymer films. While the solution state photo-chemistry of BP is well established, and crosslinking of polymers blended with BP has been studied in detail, the process of crosslinking by covalently attached BP has received comparatively little attention. We have prepared copolymers of BP with several different monomers, and studied gelation as a function of BP content and degree of photochemical conversion. Understanding the influence of polymer chemistry on crosslinking efficiency allows the appropriate choice of materials for nanostructured photo-crosslinkable polymer films and reactive polymer blends.

Wednesday, February 29, 2012 11:15AM - 2:15PM – **Session Q46 GQI: Invited Session: Quantum Information Processing in Diamond 160AB**

11:15AM Q46.00001 Single spins in diamond: scalable quantum registers and nanoscale sensors, FEDOR JELEZKO, Institute of Quantum Optics, Ulm University — Ability to detect single atoms is a key element of several key technologies of including quantum information processing, communications as well as nanoscale imaging and sensing. Usually single atom control techniques are limited to low temperature operation. In this talk we will show that single spins associated with nitrogen-vacancy defects diamond (NV centers) can be used as nanoscale magnetic field sensor allowing detecting magnetic moment associated with single electrons under ambient conditions. We also show that coupled arrays of spins can be used as building blocks for scalable quantum registers.

11:51AM Q46.00002 Towards large-scale quantum computing using spins and photons on a chip, KAI-MEI FU, University of Washington — Nitrogen-vacancy (NV) centers in diamond are attractive candidates for quantum bits for quantum information processing. Theoretically it should be possible to build large-scale quantum optical networks with the NV-diamond system. We report HP Labs' recent results toward coupling chip-based optical cavities to negatively charged NV centers in two systems: all diamond micro-ring cavities coupled to native NV centers and GaP micro-ring cavities coupled to near surface centers formed by implantation and annealing. In both systems we observe an enhancement of the spontaneous emission rate into the NV zero-phonon line. Additionally we will discuss recent results in engineering the optical properties of near-surface NV centers suitable for photonic coupling.

12:27PM Q46.00003 Probing the motion of a mechanical resonator via coherent coupling to a single spin qubit, J.G.E. HARRIS, Departments of Physics and Applied Physics, Yale University, New Haven, CT, 06520, USA — Mechanical systems can be influenced by a wide variety of extremely small forces, ranging from gravitational to optical, electrical, and magnetic. If the mechanical resonator is scaled down to nanometer-scale dimensions, these couplings can be harnessed to monitor and control individual quantum systems. In this talk, I will describe experiments in which the coherent evolution of a single electronic spin associated with a Nitrogen Vacancy (NV) center in diamond is coupled to the motion of a magnetized mechanical resonator. Specifically, we have used coherent manipulation of the NV spin to sense the resonator's Brownian motion under ambient conditions. Potential applications of this technique include the detection of the zero-point fluctuations of a mechanical resonator, the realization of strong spin-phonon coupling at a single quantum level, and the implementation of quantum spin transducers.

1:03PM Q46.00004 Preparation, single-shot readout and long-distance coupling of solid-state quantum registers, HANNES BERNIEN, Kavli Institute of Nanoscience Delft — A key challenge in quantum science is to robustly control and to couple long-lived quantum states in solids. In this talk, we report on our latest advances towards realizing long-distance quantum networks with spins in diamond. First, we demonstrate preparation and single-shot measurement of a quantum register containing up to four quantum bits [1]. Projective readout of the electron spin of a single NV center in diamond is achieved by resonant optical excitation. In combination with hyperfine-mediated quantum gates, this readout enables us to prepare and measure the state of multiple nuclear spin qubits with high fidelity. We show compatibility with qubit control by demonstrating initialization, coherent manipulation, and single-shot readout in a single experiment on a two-qubit register, using techniques suitable for extension to larger registers. Second, we observe quantum interference of photons emitted by two spatially separated NV centers [2]. By using electrical tuning of the optical transition frequencies, we are able to observe such interference even for initially dissimilar centers, indicating a viable path for scaling towards a multi-node diamond-based quantum network. We will present these results, along with our most recent data, and discuss the prospects of realizing quantum networks with NV centers in diamond in the near future.

[1] Nature 477, 574 (2011)

[2] arXiv 1110.3329

1:39PM Q46.00005 Electrical tuning of single-photon emission in diamond devices¹, LEE C. BASSETT², Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — For quantum information applications, nitrogen-vacancy (NV) centers in diamond combine many of the advantages of atomic systems (optical access, millisecond spin-coherence times) with the engineering flexibility of solid-state devices. Recent demonstrations of coherent coupling between photons and individual NV-center spins [1,2] provide a route to integrating NV-center qubits within photonic networks and for on-demand generation of entangled single-spin/single-photon pairs. Such applications require the ability to tune the NV-center zero-phonon optical transitions, to compensate for natural sample inhomogeneities which perturb the electronic orbital states. Here we demonstrate the ability to electrically control the orbitals of individual NV centers by applying voltages to micron-scale surface gates [3]. Surprisingly, the local electric field experienced by an NV center is significantly enhanced by a photoinduced space charge resulting from photoionization of deep donor impurities within the diamond, even in high-purity single-crystal material (< 5 ppb nitrogen content). Since the photoinduced electric fields are reproducible as a function of gate voltage and are predominantly directed perpendicular to the diamond surface, we can harness them to obtain three-dimensional control of the local electric field vector with surface gates alone. To demonstrate this technique, we tune the excited-state orbital doublet of a strained NV center to degeneracy, as required for some spin-photon entanglement protocols [2], and then adjust the optical transition frequency, showing that we can tune multiple NV centers to have the same degenerate transition energy. This method should enable the coherent coupling of multiple NV center spins to indistinguishable photons within a scalable photonic network.

[1] B. B. Buckley, G. D. Fuchs, L. C. Bassett, and D. D. Awschalom, *Science* **330**, 1212 (2010).

[2] E. Togan *et al.*, *Nature* **466**, 730 (2010).

[3] L. C. Bassett, F. J. Heremans, C. G. Yale, B. B. Buckley, and D. D. Awschalom, *Phys. Rev. Lett.* (in press).

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²In collaboration with F. J. Heremans, C. G. Yale, B. B. Buckley, and D. D. Awschalom.

Wednesday, February 29, 2012 11:15AM - 2:15PM – **Session Q47 DPOLY DBIO: Focus Session: DNA-Coated Colloid Particles 160C**

11:15AM Q47.00001 Heterogeneous 3D Assembly of DNA-encoded Quantum Dots and Gold Nanoparticles¹, DAZHI “PETER” SUN, OLEG GANG, Center for Functional Nanomaterials, Brookhaven National Laboratory — We report the heterogeneous assembly of quantum dots (QDs) and gold nanoparticles (AuNPs) into three-dimensional (3D) superlattices by means of DNA encoding. CdSe/ZnS core-shell QDs were functionalized with stranded (ss) DNA to obtain a stable aqueous dispersion of QD-DNA conjugates, which maintains the optical properties of the original QDs. By introducing AuNPs modified by complementary ssDNA, QD-AuNP aggregates were assembled. Using synchrotron-based small angle X-ray scattering, we found that QD-AuNP assemblies form a body center cubic (BCC) lattice, while each nanoparticle type, QD and AuNP, are positioned in a simple cubic (SC) manner. Distance-dependent optical property of QDs in heterogeneous superlattices was studied by time-resolved fluorescence spectroscopy. The potential applications of the above optically-active nanosystems will also be discussed.

¹Research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

11:27AM Q47.00002 Self-Assembly of Octopus Nanoparticles into Pre-Programmed Finite Clusters¹, JONATHAN HALVERSON, ALEXEI TKACHENKO, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973 — The precise control of the spatial arrangement of nanoparticles (NP) is often required to take full advantage of their novel optical and electronic properties. NPs have been shown to self-assemble into crystalline structures using either patchy surface regions or complementary DNA strands to direct the assembly. Due to a lack of specificity of the interactions these methods lead to only a limited number of structures. An emerging approach is to bind ssDNA at specific sites on the particle surface making so-called octopus NPs. Using octopus NPs we investigate the inverse problem of the self-assembly of finite clusters. That is, for a given target cluster (e.g., arranging the NPs on the vertices of a dodecahedron) what are the minimum number of complementary DNA strands needed for the robust self-assembly of the cluster from an initially homogeneous NP solution? Based on the results of Brownian dynamics simulations we have compiled a set of design rules for various target clusters including cubes, pyramids, dodecahedrons and truncated icosahedrons. Our approach leads to control over the kinetic pathway and has demonstrated nearly perfect yield of the target.

¹Research carried out in whole at the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

11:39AM Q47.00003 DNA-induced 2D-to-1D Phase Transition of Nanoparticle Assemblies at Liquid-Vapor Interface¹, SUNITA SRIVASTAVA, DMYTRO NYKYPANCHUK, Center for Functional Nanomaterials, Brookhaven National Laboratory, MASAFUMI FUKUTO, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, OLEG GANG, Center for Functional Nanomaterials, Brookhaven National Laboratory — We have investigated the structure formation and development for two-dimensional assembly of DNA functionalized nanoparticles at liquid-vapor interface. The adsorption of negatively charged DNA-coated particle to the interface was triggered by a positively charged lipid layer. A normal and in-plane structure of the nanoparticle monolayer were probed using in-situ surface scattering methods, x-ray reflectivity and grazing incidence small angle x-ray scattering. We observed the formation of the hexagonally closed packed (HCP) 2D lattice of nanoparticles due to a combination of electrostatic surface-to-particle attraction and interparticle repulsion. Upon an onset of DNA hybridization between particles the phase transition from HCP order to 1D crystalline structure was observed. The control on the interparticle spacing and monolayer confinement were also examined by changing a salt concentration. Our studies demonstrate novel mechanism for transition from ordered 2D to ordered 1D structure due to the domination of DNA-induced attraction over an electrostatic repulsion and open a route for nano-structure manipulations at the interfaces.

¹Research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

11:51AM Q47.00004 Structural Diversity of DNA-Coated Particle Assemblies, FRANCIS W. STARR, Physics Dept., Wesleyan University, Middletown, CT — Custom designed nanoparticles (NP) or colloids with specific recognition offer the possibility to control the phase behavior and structure of particle assemblies for a range of applications. One approach to realize these new materials is by attaching DNA to a core particle; the hybridization of double-stranded DNA between particles results in the spontaneous assembly of higher-order structures. Control of the assembled state can be achieved by adjusting several parameters, including sequence selectivity, DNA link orientation, DNA length and flexibility, and the balance between the length of links and non-specific repulsive interactions. I will discuss the results of a coarse-grained molecular model for DNA-linked nanoparticles that helps to rationalize experimental findings and demonstrate new routes to control the assembled structure. We examine how the number and orientation of strands affects the structure, phase behavior, and dynamics. We show that it is possible to realize unusual phase diagrams with many thermodynamically distinct phases, both amorphous and crystal. We further examine the parameters that control the pathways of assembly, which are critical to avoid kinetic bottlenecks. Finally, we discuss strategies to create highly anisotropic structures using both isotropic and anisotropic core units.

12:27PM Q47.00005 DNA Mediated Nanoparticle Crystallization: Characterizing How Equilibrium is Reached¹, CHRISTOPHER KNOROWSKI, ALEX TRAVESSET, Department of Physics and Astronomy and Ames Laboratory, Iowa State University, Ames, IA — DNA programmed self-assembly is becoming one of the most powerful tools for designing nanoparticle crystals due to the exquisite control over lattice size and structure achievable. While in recent years the inventory of crystalline structures accessible through DNA programming has grown, our understanding of the dynamical processes that lead to crystallization is still limited. Using MD we simulate the nucleation and growth of DNA programmed nanoparticle crystallization and characterize the different processes that determine the relaxation times leading to equilibrium. In particular, we classify the topological defects and the processes leading to their annihilation. Implications for experiments as well as for achieving single crystals are also discussed.

¹This work has been supported by the DOE through Ames lab under Contract DE-AC02-07CH11358

12:39PM Q47.00006 Packing of DNA-assembled Nanocubes and Nanooctahedra¹, FANG LU, YUGANG ZHANG, KEVIN YAGER, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY, 11973, DANIEL VAN DER LELIE, Center for Agricultural and Environmental Biotechnology, Research Triangle Institute International, Research Triangle Park, NC, 12194, OLEG GANG, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY, 11973 — Nanoparticle shape has a profound effect on assembly behavior. However, the contribution of surface-attached molecules can significantly modulate the packing of nanoscale objects, inducing phases markedly different from the known packing rules of macroscopic objects. Our studies uncover the phase behavior of nanocubes and nanooctahedron assembled by DNA-mediated interactions into three-dimensional structures, which were probed in-situ by small angle x-ray scattering. We observed that the packing of these nanoscale anisotropic objects depends strongly on the details of the DNA linkages. Using electron microscopy and optical spectroscopy, we elucidate the factors that drive assembly and dictate the spatial organization of the nano-objects. The relationship between particle shape and the mechanism of phase formation for nanocubes has been also investigated.

¹Research was supported by the U.S. DOE Office of Science and Office of Basic Energy Sciences under contract No. DE-AC-02-98CH10886.

12:51PM Q47.00007 Making DNA competitive: a new strategy to improve the self-assembly properties of DNA-coated particles, MIRJAM LEUNISSEN¹, FOM Institute AMOLF, BORTOLO MOGNETTI², DAAN FRENKEL³, University of Cambridge — We present a new approach to widen the normally very narrow temperature window for equilibrium self-assembly (e.g. crystallization) of DNA-coated particles. Using Monte Carlo simulations, we first show that not only enthalpic but also entropic effects - due to the multi-bond character of the DNA-mediated interactions - play an important role in the overall binding properties of the particles. We then outline a new strategy that exploits the competition between different types of inter-particle DNA linkages to achieve a temperature-dependent switching of the dominant bond type. Depending on the length ratio of the DNA constructs, the bond switching is either energetically driven or controlled by a combinatorial entropy gain, which arises from the large number of possible binding partners for each DNA strand. Importantly, the resulting particle interaction is less strongly temperature dependent than in "conventional" systems with only one bond type, thus enhancing the experimental control over self-assembly. Finally, we will also show that in general stable gas-liquid separation is expected to occur only for particles smaller than a few tens of nanometers, which suggests that nanoparticles and micrometer-sized colloids will follow different routes to crystallization.

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1:03PM Q47.00008 DNA Regulated Clusters: Structure and Self-limiting Assembly¹, CHENG CHI, Center for Functional Nanomaterials, Brookhaven National Laboratory, FERNANDO VARGAS LARA, FRANCIS STARR, Physics Department, Wesleyan University, ALEXEI TKACHENKO, OLEG GANG, Center for Functional Nanomaterials, Brookhaven National Laboratory — We have investigated the structural details of nanoparticle clusters assembled by flexible DNA linkers in dimer clusters using electron microscopy, in-situ x-ray scattering and optical methods. The observed dependence of interparticle distance on a DNA length significantly deviates from the predictions for single chain linkages and previous measurements for superlattices. The observed effect is attributed to a large solid angle of interparticle contact, in agreement with computational results. Our studies further reveal the non-monotonic decrease of interparticle distance for the longer linkers; that suggests nanoparticles confinement by hybridized linkers from opposite particles' hemispheres. The effect is accompanied by inhibited development of nanoclusters and results in a self-limited cluster assembly. The mechanism of dimer formation was investigated in details using the optical methods.

¹Research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

1:15PM Q47.00009 Kinetics of the Association of DNA Coated Colloids, KUN-TA WU, LANG FENG, Center for Soft Matter Research, New York University, RUOJIE SHA, Chemistry Department, New York University, REMI DREYFUS, Complex Assemblies of Soft Matter, CNRS-Rhodia-UPenn UMI 3254, ALEXANDER GROESBERG, Center for Soft Matter Research, New York University, NADRIAN SEEMAN, Chemistry Department, New York University, PAUL CHAIKIN, Center for Soft Matter Research, New York University, CENTER FOR SOFT MATTER RESEARCH, NEW YORK UNIVERSITY TEAM, CHEMISTRY DEPARTMENT, NEW YORK UNIVERSITY COLLABORATION, COMPLEX ASSEMBLIES OF SOFT MATTER, CNRS-RHODIA-UPENN UMI 3254 COLLABORATION — The self-assembly of DNA coated colloidal particles opens a door to complex colloidal architecture. To understand how particles aggregate due to DNA hybridization between particles is the key to program colloidal aggregation. In this study, we investigate theoretically and experimentally the aggregation time of micron scale particles as a function of DNA coverage and the ion concentration I . Our particles coated with streptavidin can attach $\sim 70,000$ biotinylated DNA molecules, which have a double strand with 49 base pairs and an 11 base sticky end. At $I = 60$ mM, particles 100% fully covered with DNA show an aggregation time of $\tau = 6$ minutes. For 10% DNA covered particles at $I = 35$ mM, $\tau = 57$ hours. A simple model based on the reaction limited aggregation and electrical repulsion for DNA hybridization is developed and tested. These experiments and the model also allow us to use the microscopic colloidal aggregation to measure nanoscopic hybridization rates.

1:27PM Q47.00010 Phase Behavior and Magnetic Response of DNA-mediated Gold and Iron Oxide Nanoparticle Assemblies¹, YUGANG ZHANG, FANG LU, KEVIN G. YAGER, Center for Functional Nanomaterials, Brookhaven National Laboratory, DANIEL VAN DER LELIE, Center for Agricultural and Environmental Biotechnology, Research Triangle Institute International, OLEG GANG, Center for Functional Nanomaterials, Brookhaven National Laboratory — Gold nanoparticles (NPs) have long been long served as model systems to study phase behavior of DNA-assisted NP assemblies. Incorporation of different types of nano-objects into DNA-NP systems opens attractive possibilities for the material design. Furthermore, it also allows enriching a self-assembly behavior by an introduction of non-specific yet controllable interparticle interactions. Herein, we report the DNA-mediated assembly of a heterogeneous system comprising gold and superparamagnetic iron oxide (IO) NPs. We systematically studied the phase diagram of the assembled systems by varying a system's composition, DNA design and environmental conditions. Our studies show that by controlling a balance between non-specific and DNA-recognition interactions via system design the assembled phase can be switched between a face-centered cubic (fcc) structure of a IO assembly and a superlattice formed by Au-IO core-shells clusters. We also observed that structure of assemblies is responsive to the magnetic field.

¹Research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

1:39PM Q47.00011 Modeling of DNA-Directed Colloidal Self-Assembly and Crystallization, TING LI, RASTKO SKNEPNEK, ROBERT J. MACFARLANE, CHAD A. MIRKIN, MONICA OLVERA DE LA CRUZ, Northwestern University — A series of design rules have recently been developed for using gold nanoparticles conjugated with a dense layer of double stranded DNA chains to assemble a wide variety of nanoparticle superlattice structures [1]. Key design parameters for obtaining different structures in a binary system were shown to be the ratio of the hydrodynamic radii of the DNA-conjugated particles, the ratio of the number of DNA strands per particle, and the self- or non-self-complementary nature of the DNA sequences guiding the assembly process. Guided by those experiments, we have built a coarse grained model that faithfully mimics relative design parameters in the experimental system. Working with nanoparticles in the size range from 8nm to 15nm, overall DNA-nanoparticle hydrodynamic radii of 10nm to 30nm, and the number of DNA strands per particle between 30 and 100, we have developed a simulation method that confirms that these design rules can be used to assemble a variety of different crystal structures. In particular, we have identified FCC, BCC, CsCl, AlB_2 and Cr_3Si structures. With these data, we have constructed a detailed phase diagram that closely corresponds to the experimentally obtained phase diagram developed in ref. [1]. [1] R. J. Macfarlane, B. Lee, M. R. Jones, N. Harris, G.

1:51PM Q47.00012 DNA coated rods: pure Biological materials for self assembly studies, RAFAEL CABANAS, SETH FRADEN, Brandeis University, DR. ERIKA EISER GROUP CAMBRIDGE UNIVERSITY, UK. COLLABORATION — We will present a way of coating Fd virus, a model of colloidal liquid crystal, with DNA. The DNA coating provides new interesting tunable properties to control the liquid crystalline behavior.

2:03PM Q47.00013 Linear DNA-linked colloidal chains: a model to visualize polymer dynamics¹, SIBANI BISWAL, JULIE BYROM, DANIEL DU, Rice University — We present the development of synthetic materials consisting of chains of DNA-linked paramagnetic colloids that have rigidity and length specificity. These chains have demonstrated capability for folding and self-assembly. This is classic bead-spring-bead model can be a model system to visualize polymer dynamics. Here, I will describe the formation mechanism and stability of these DNA-linked magnetic particle chains. I will also describe a model that describes the total energy landscape that describes the inter-particle interactions and provides a workable theory toward the optimization of experimental parameters in synthesizing more stable and reliable colloidal assemblies. In addition to stability, we will also present the use of a colloidal worm-like chain (WLC) model system to describe chain dynamics. We measure bending rigidity by monitoring the thermal fluctuations of the chains. We show that the persistence length of the chains can be tuned from 1 to 50 nm ($L/LP = 0.002 - 0.1$), by changing the length of the DNA used to link adjacent particles from 75 to 15 bases. We also will show that the bending relaxation dynamics of these chains, which match well with theoretical predictions, further supporting the validity of using these colloidal chains as models for semiflexible polymer systems in both equilibrium and dynamic studies.

¹We acknowledge NSF CAREER CBET 0955003 for support

Wednesday, February 29, 2012 11:15AM - 2:03PM – Session Q48 DPOLY: Polymer Blends and Crystallization 161

11:15AM Q48.00001 How Pure Components Control Polymer Blend Miscibility¹, RONALD WHITE, JANE LIPSON, Dartmouth College, JULIA HIGGINS, Imperial College, London — We present insight into some intriguing relationships revealed by our recent studies of polymer mixture miscibility. Applying our simple lattice-based equation of state, we discuss some of the patterns observed over a sample of experimental blends. We focus on the question of how much key information can one determine from a knowledge of just the pure components only, and further, on the role of separate enthalpic and entropic contributions to the miscibility behavior. One interesting correlation connects the value of the difference in pure component energetic parameters with that of the mixed segment interactions, suggesting new possibilities for predictive modeling. We also show how in some cases these two parameter groupings act as separate controls determining the entropy and enthalpy of mixing. Also discussed are the different patterns exhibited for UCST-type and LCST-type blends, these being revealed in some cases by simple examination of the underlying microscopic parameters.

¹work supported by the National Science Foundation

11:27AM Q48.00002 Tailoring Co-continuous Nanostructured Morphologies in Polymer Blends, LE LI, SUNG-WOO HONG, XIAOBO SHEN, RYAN HAYWARD, THOMAS RUSSELL, University of Massachusetts Amherst — We describe a simple approach to prepare thin films of polymer mixtures with co-continuous morphologies having characteristic length scales down to tens of nanometers based on spinodal phase separation. The degree of immiscibility between polystyrene (PS) and poly(2-vinylpyridine) (P2VP) is tuned by incorporating styrene monomers into the P2VP backbone to yield a random copolymer, thereby tailoring the nonfavorable interactions between the two components. The size scale of the co-continuous morphology is controlled by varying the molecular weights of the components and the film thickness. This strategy is shown to be robust in that the process involves a simple solution-casting; the co-continuity of the morphology occurs provided the solvent dissolves both components; and the co-continuous morphology is insensitive to the substrate surface chemistry. Porous membranes with continuous channels and gradient co-continuous structures can also be generated from the phase separated blend films.

11:39AM Q48.00003 Structure and elasticity of crosslinked polymer blends, BING LU, University of Illinois at Urbana-Champaign, XIANGJUN XING, Shanghai Jiao Tong University, PAUL GOLDBART, Georgia Institute of Technology — We consider a blend of mutually incompatible homopolymer species, A and B, that are randomly crosslinked to form a network. In such a network there is a competition between the repulsion of the A and B polymers (which favors the demixing of the two species) and the crosslinking (which prohibits complete demixing) [1,2]. We treat the system by means of a model of flexible polymers, which are permanently crosslinked (with statistics modeled by the Deam-Edwards distribution) and have species-dependent excluded-volume interactions [3]. As expected, the model shows that at sufficiently low temperatures the demixing tendency drives microphase separation, with a characteristic scale set by the network localization length. It also shows that if the system is strained after crosslinking, correspondingly anisotropic microdomains are generated in the pattern of A-B polymer concentration fluctuations trapped in by the network and, furthermore, allows the impact of microphase separation on the elastic properties of the network to be determined.

[1] P.G. de Gennes, J. Phys. (Paris) Lett., 40 (1979) L-69.

[2] D.J. Read, M.G. Brereton and T.C.B. McLeish, J. Phys. II, 5 (1995) 1679.

[3] C. Wald et al., Europhys. Lett. 70, 843–849 (2005); J. Chem. Phys. 124, 214905 (2006).

11:51AM Q48.00004 Assessing the Strength Enhancement of Heterogeneous Networks of Miscible Blends of 1,2-Polybutadiene and Polyisoprene¹, CARL GILLER, American Society for Engineering Education, Washington, D.C., MIKE ROLAND, Chemistry Division, Code 6120, Naval Research Laboratory, Washington, D.C. — At typical crosslink densities of elastomers, failure properties vary inversely with mechanical stiffness, so that compounding entails a compromise between stiffness and strength. Our approach to circumvent this conventional limitation is by forming networks of two polymers that: (i) are thermodynamically miscible, so that the chemical composition is uniform on the nm level; and (ii) have markedly different reactivities for network formation. The resulting elastomer consists of one highly crosslinked component and one that is lightly or uncrosslinked. This disparity in crosslinking causes their respective contributions to the network mechanical response to differ diametrically. Earlier results showed some success with this approach for thermally vulcanized blends of 1,2-polybutadiene and polyisoprene, taking advantage of their differing reactivities to sulfur. In this work we explore networks of this miscible blend formed via UV irradiation with a photoinitiator. The vinyl group in 1,2-polybutadiene has a much greater photo-reactivity than the double bond in polyisoprene, resulting in a disparity in respective degrees of crosslinking, while the thermodynamic miscibility is retained. Mechanical properties of the radiation crosslinked blend are compared to conventional networks.

¹This work was supported by the Office of Naval Research. CG acknowledges an American Society for Engineering Education fellowship.

12:03PM Q48.00005 Compatibilization of polymer blends with star polymers containing a gamma-cyclodextrin core and polystyrene arms¹, C.M. BALIK, Dept. of Materials Science and Engineering, North Carolina State University, A.E. TONELLI, Dept. of Textile Engineering, Chemistry and Science, North Carolina State University, RYAN LIBERT, Dept. of Materials Science and Engineering, North Carolina State University — Cyclodextrins (CDs) are cyclic starch molecules having a hollow central cavity which can be threaded by a polymer to form an inclusion compound. This characteristic is exploited in a new type of compatibilizer: a star polymer with a gamma-CD (g-CD) core and polystyrene (PS) arms (CD-star). The mechanism of compatibilization involves threading of the CD core by a second polymer and solubilization of the threading polymer into a PS matrix by the PS star arms. In principle, the same CD-star polymer can be used to compatibilize blends of several different polymers with PS, provided that the second polymer is able to thread the CD core. We have taken the first step toward demonstrating the generality of this approach by producing compatibilized blends of PS with poly(dimethyl siloxane) (PDMS) or poly(methyl methacrylate) (PMMA) using the same CD-star polymer. Thin spun-cast films of these blends exhibit a nanoscale level of mixing, while spun-cast films of the same blends without CD-star exhibit large-scale phase separation. The number of CD-star molecules that must be threaded onto the polymer chain to achieve compatibilization is larger for PMMA than for PDMS.

¹Supported by grant M10-NS01 from the National Textile Center.

12:15PM Q48.00006 Theory of Hydrogen-Bonding in Diblock Copolymer/Homopolymer Blends, ASHKAN DEGHAN, AN-CHANG SHI, McMaster University — The phase behavior and physical properties of hydrogen-bonding diblock copolymer/ homopolymer (AB/C) blends are examined using self-consistent field theory. We consider two methods for modeling the formation of hydrogen bonds between polymer chains. The first using a large negative (attractive) interaction parameter and the second using polymer-polymer complexation. Despite the success of the first model in describing the phase behavior of the system, it fails to correctly predict the change in lamella spacing induced by addition of homopolymer chains, previously shown in many experiments. Using polymer-polymer complexation we were able to qualitatively show the order-order phase transitions and decrease in lamella spacing for the case of strong hydrogen bonding. Our analysis of both methods show that hydrogen bonding of polymer chains should be described by polymer-polymer complexation.

12:27PM Q48.00007 Effect of mid-block on the morphology and properties of PDLA-softblock-PDLA/PLLA Blends, SAHAS RATHI, E. BRYAN COUGHLIN, SHAW LING HSU, University of Massachusetts Amherst — A novel method to overcome the brittleness of PLLA is by kinetically trapping a continuous low T_g amorphous phase. This morphology has been accomplished by exploiting the significant difference in the crystallization temperatures of the neat PLLA versus its stereocomplex with the PDLA isomer. This morphology is formed by blending and co-crystallizing triblock copolymer with a configuration of the form PDLAn- Soft Blockm- PDLAn with PLLA. The type of morphology formed and the improvement in the sample toughness strongly depends on the miscibility of the midblock in the triblock copolymer with the matrix PLLA. This work explores the effect of the chemical nature of the midblock on the stereocomplex crystallization between the PDLA end-blocks and the PLLA matrix polymer and the blend morphology formed. It is found that miscible midblocks give rise to a soft continuous amorphous phase morphology while in case of immiscible midblocks a glassy phase separated amorphous phase morphology is formed. Dramatically different physical properties can be obtained for various PLLA/tri-block copolymer blends giving access to tough, semicrystalline PLLA blends.

12:39PM Q48.00008 ABSTRACT WITHDRAWN —

12:51PM Q48.00009 Molecular Dynamics Simulations of Polypropylene: Crystallization and Melting¹, MANISH AGARWAL, SHYNO MATHEW, SANAT KUMAR, Columbia University — The crystallization of polypropylene is studied using molecular dynamics (MD), using an all atom force field. Starting from basic ordered arrangements of oligomers, the α and β phases for isotactic polypropylene are recovered, with cell parameters in excellent agreement with crystallographic data. A high pressure phase similar to the smectic phase is also observed. The melting temperatures of these crystals, obtained by isobaric heating, match with the experiments. Oligomers of syndiotactic polypropylene mirror all structural features observed in experiments. The all-trans state is found to be the most stable. The characteristic 2/1 helical structure of syndiotactic polypropylene is also formed along with the all-trans “zigzag” conformation.

¹ Authors acknowledge support from ONR-MURI grant “Rational Design of Advanced Polymeric Capacitor Films.”

1:03PM Q48.00010 Molecular simulation of plastic deformation of semicrystalline polyethylene, JUNMO KIM, SANGHUN LEE, GREGORY RUTLEDGE, Massachusetts Institute of Technology — The detailed structure and the high anisotropy of semicrystalline polymer at the lamellar length scale play an important role in determining its mechanical response. In this study, we performed molecular dynamics simulation of semicrystalline polyethylene under various industrially important deformations, such as extension, compression, and shear, to characterize the plastic deformation response. The semicrystalline polyethylene model employed in this study consists of a 1-D alternating stack in the longitudinal z direction of crystalline lamellae and interlamellar noncrystalline domains, that are infinite in the lateral x and y directions. The molecular dynamics simulations are carried out at the temperature of 350K using united atom model and two deformation strain rates (fast and slow) are considered in each deformation. Stress-strain curves, elastic moduli, yield stresses and so on, are examined under each deformation and compared to each other. In addition, the entanglement statistics of semicrystalline polyethylene under various deformation modes are investigated using the Z-code.

1:15PM Q48.00011 ABSTRACT WITHDRAWN —

1:27PM Q48.00012 Digestive Ripening: A Quantitative Thermodynamic Analysis of Stable Nanocrystals, MICHAEL CLARK, SANAT KUMAR, Columbia University, IGAL SZLEIFER, RIKKERT NAP, Northwestern University — Previous studies have shown that stable, monodisperse nanocrystals (NCs) have been produced using strongly binding surfactants, e.g. Au NCs with alkylthiols or Co NCs with oleic acid, to name a few. Through a first-principles theoretical investigation, we develop the full quantitative thermodynamic expression for the state of these surfactant-coated NCs. The general free energy expression allows for the crystal free energy, the surfactant binding energy, surfactant conformational entropy, and the surfactant interactions with other surfactants through excluded volume, solvent depletion, and energetic interactions between surfactant molecules. The energetics of the surfactant chains are treated quantitatively through Single Chain Mean Field theory, which determines the optimal number of grafted surfactants on the surface of an R-sized NC. Then, the size distribution function $f(R)$ is calculated to determine the most favorable NC size and the equilibrium polydispersity. The theoretical conclusions will be compared quantitatively with experimental results. The full thermodynamic expression allows a parametric study of experimentally relevant conditions that govern whether Ostwald ripening vs. digestive ripening vs. dissolution will occur in a given nanocrystal-surfactant system.

1:39PM Q48.00013 Morphology and Shear Viscosity for a Phase-separating Polymer Blend of Polybutadiene and Polyisoprene under Simple Shear Flow¹, XIA DONG, FASHENG ZOU, CHARLES C. HAN, Institute of Chemistry Chinese Academy of Sciences — The domain structure and shear viscosity of a phase-separated polymer blend of polybutadiene /polyisoprene are investigated with optical microscopy, light scattering, and rheometry. At the steady shear state, the shear-induced structures can be the nearly spherical droplets, the partially interconnected domains, the typical string-like domains, or the string-like domains with blurred interface, depending on the shear rate. The steady shear viscosity displays a rather non-Newtonian fluid behavior. In the transient flow experiments, the time dependence of viscosity and morphology after a stepwise increase of shear rate is studied and found to mainly depend on the final shear rate. In particular, as long as the final structures are the partially interconnected domains, the morphology evolution proceeds in the same way and the behaviors of the corresponding shear viscosity are similar.

¹The funding support from NSFC No.50930002 and 51173195.

1:51PM Q48.00014 Dynamics of Polymer Blend Film Formation During Spin Coating¹, YOUNNA MOUHAMED, NIGEL CLARKE, RICHARD A.L. JONES, MARK GEOGHEGAN, University of Sheffield — Spin casting is a process broadly used to obtain a uniform film on a flat substrate. A homogeneous film results from the balance between centrifugal and viscous forces. Here we revisit the Meyerhofer model of the spin casting process by taking in account the centrifugal forces, a uniform time dependent evaporation rate, and account for the changes in viscosity using the Huggins intrinsic viscosity. Time resolved light reflectometry is used to monitor the thickness changes of a polystyrene-poly(methyl methacrylate) (which we denote as PS and PMMA) film initially dissolved in toluene and spin cast for ten seconds at 1000 rpm. The experimental data are in good agreement with the model. We also investigate how the volume fraction of PS and PMMA influences the thinning of the film during spin casting. A distinct change in the temporal evolution of thickness as a function of time delimits the first phase of the spin casting process where centrifugal forces are dominant from a second phase dominated by the solvent evaporation. This hypothesis is supported by in-situ off specular scattering data. The time at which this change from centrifugal to evaporation-dominated behaviour is delayed as the volume fraction of PMMA increases.

¹Engineering and Physical Sciences Research Council (EPSRC)

Wednesday, February 29, 2012 11:15AM - 2:15PM –
Session Q49 DMP DPOLY: Focus Session: Organic Electronics and Photonics - Photophysics and Excited State Dynamics 162A

11:15AM Q49.00001 Hybrid Phononiton in Organic-Semiconductor Materials¹, DAVID FACEMYER, QUE HUONG NGUYEN, Marshall University — In this work electronic structures and optical properties of organic-inorganic phononiton, a new elementary excitation existing in heterostructures combining both organic and semiconductor materials, are studied. In those systems, Wannier-Frenkel hybrid exciton has unique and interesting properties that can improve the efficiency of optical materials. When an organic-semiconductor combined heterostructure is illuminated by high-intensity electromagnetic radiation with the frequency of the photons at or near the resonance frequency of the Wannier-Frenkel exciton, we obtain a macroscopically occupied system of hybrid polaritons that further interacts with phonons which will in turn generate the hybrid phononiton. Electronic structure, energy and dispersion relation of phononitons are theoretically determined. By analyzing the interactions between the hybrid exciton, photons and phonons, the conditions for phononiton formation are discussed.

¹The support from NASA EPSCoR Seed Grant award 211012 is acknowledged.

11:27AM Q49.00002 Effect of structural distortion and polarization in localization of electronic excitations in organic semiconductor materials, IFFAT NAYYAR, Theoretical Div., Los Alamos National Lab, Los Alamos, NanoScience Technology Center and Dept. of Physics, University of Central Florida, Orlando, ENRIQUE BATISTA, Theoretical Div., Los Alamos National Lab, Los Alamos, SERGEI TRETIAK, Theoretical Div. and Center for Integrated Nanotechnologies, Los Alamos National Lab, Los Alamos, AVADH SAXENA, DARRYL SMITH, RICHARD MARTIN, Theoretical Div., Los Alamos National Lab, Los Alamos — Organic polymers find varied applications in optoelectronic devices such as solar cells, light emitting diodes and lasers. Detailed understanding of charge carrier transport by polarons and excitonic energy transfer producing singlet and triplet excitations is critical to improve their efficiency. We benchmarked the ability of current functional models to describe the spatial extent of self-trapped neutral and charged excitations for MEH-PPV owing to its superior luminescence and experimental evidence. Now we are interested in distinguishing between two distinct origins leading to localization; spatial localization of the wavefunction by itself on the undistorted geometry and localization of the wavefunction assured by distortion of the structure during its relaxation. We suggest localization is produced by electronic rearrangements and character of the functional. We also observe that different functionals place the highest occupied and lowest virtual orbitals at different positions in the energy band diagram based on their ability to predict the extent of localization of these states.

11:39AM Q49.00003 The Effect of LUMO Level Offset on the Electron Dissociation Rates in Low Bandgap Polymer Heterostructures, MATTHEW SFEIR, Brookhaven National Laboratory, DEANNA RODOVSKY, Konarka Technologies, Inc./National Institute of Standards and Technology, JASON AZOULAY, GUILLERMO BAZAN, University of California, Santa Barbara, JEFFREY PEET, Konarka Technologies, Inc. — In order to maximize the efficiency of polymer/fullerene bulk heterojunction solar cells, the voltage lost when the electron transfers from the polymer to the fullerene must be minimized. While the magnitude of this loss will significantly impact the maximum attainable efficiency of this technology, there have been relatively few attempts to quantify the dependence of the electron transfer rate and yield on the driving force for electron transfer. In order to isolate the effect of electrochemical potential difference on the exciton dissociation rate, we present results of photophysical measurements of a low bandgap copolymer mixed with a series of fullerene based acceptor materials in a bulk heterojunction geometry. The LUMO level of the acceptor material is varied relative to the polymer's so that the effect of the energy offset on the electron dissociation rate can be determined. Using photoluminescence and transient absorption measurements, we find that the exciton quenching rate varies systematically with increasing energy offset. We examine the mechanism of charge carrier generation by correlating the exciton quenching with charge carrier generation.

11:51AM Q49.00004 First principles study of optical and electronic properties of anthradithiophene based organic conductors, FAYE BARRAS, GUENTER SCHNEIDER, Oregon State University — Functionalized anthradithiophene (ADT) derivatives are high performance organic conductors where the addition of side groups such as triethylsilyl ethynyl (TES) to the ADT backbone induces a change in the morphology from a herringbone to a planar crystal structure in which improved intermolecular π -orbital overlap increases carrier mobility. Bulk type-II heterojunctions can be formed using matched pairs such as ADT-TES-F (donor) and ADT-TIPS-CN (acceptor). We report electronic and optical properties calculated from ab initio density functional theory (DFT) calculations for ADT derivatives. Exciton and exciplex formation and charge separation in ADT bulk heterojunctions is studied using 2 molecule model calculations for ADT-TES-F (donor) and ADT-TIPS-CN or C₆₀ (acceptor). We compare our results to available experimental results such as photo luminescence and photocurrent measurements.

12:03PM Q49.00005 Ultrafast exciton energy transfer from giant nanocrystals to layered J-aggregate films, ASJA RADJA, HUE NGUYEN, Department of Physics, The University of Texas at Dallas, Richardson, TX, 75080, JENNIFER HOLLINGSWORTH, Chemistry Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, L, ANTON MALKO, Department of Physics, The University of Texas at Dallas, Richardson, TX, 75080 — The integration of organic and inorganic materials at the nanoscale offers the possibility of developing new photonic devices that could combine the advantages of both classes of materials. Particularly interesting for such applications is a new class of core/shell CdSe/CdS nanocrystals (NQDs) with large number of shell monolayers (MLs) that are photostable, non-blinking and have an advantage of suppressed non-radiative Auger recombination leading to the existence of bright multiexcitonic (MX) states. However, due to large MLs thicknesses, the extraction of charge through such shells may pose considerable problems. In this work we studied hybrid structures composed of “giant”, ($\#ML > 10$) CdSe/CdS NQDs anchored on top of thin layers of strongly absorbing J-aggregates (JA) of cyanine dye (TDBC). We performed time-resolved and steady-state photoluminescence (PL) measurements to quantify the *excitonic energy transfer* (ET) rates from the gNQDs to JA layer. By varying temperature (from RT to 80K) we observed change in ET rates in accordance with the overlap integral between NQD PL emission and JA absorption. In all cases, ET transfer rates exceeded 99%. Hence, we foresee the utilization of gNQDs in applications in hybrid systems based on energy transfer.

12:15PM Q49.00006 ABSTRACT WITHDRAWN —

12:27PM Q49.00007 Ultrafast multidimensional spectroscopy of P3HT thin films, CONG MAI, NC State University, SINAN CAN, NC State University and Bogazici University, ANNE WATSON, HARALD ADE, KENAN GUNDOGDU¹, NC State University — We report on measurements of morphology dependence of exciton/polaron dynamics in P3HT thin films. Intrachain and interchain electronic coupling has a significant impact on optical and electronic properties of polymers. Due to flexibility of polymers, slight differences in processing results in a variation of morphologies and electronic coupling between the chains. We employ ultrafast multidimensional spectroscopy techniques to resolve the resulting polaron formation dynamics in different polymer thinfilms spin casted from different solvents. Our results suggest, depending on the average conjugation length and crystallinity of the thin film, polaron formation dynamics exhibit spectrally homogeneous or inhomogeneous behavior.

¹correspondent author

12:39PM Q49.00008 Charge transfer complex in diketopyrrolopyrrole polymers and fullerene blends: Implication for organic solar cell efficiency, D. MOGHE, P. YU, University of Missouri-Columbia, MO, C. KANIMAZHI, S. PATIL, Indian Institute of Science, Bangalore, India, S. GUHA, University of Missouri-Columbia, MO — Copolymers based on diketopyrrolopyrrole (DPP) have recently gained potential in organic photovoltaics. When blended with another acceptor such as PCBM, intermolecular charge transfer occurs which may result in the formation of charge transfer (CT) states. We present here the spectral photocurrent characteristics of two donor-acceptor DPP based copolymers, PDPP-BBT and TDPP-BBT, blended with PCBM to identify the CT states. The spectral photocurrent measured using Fourier-transform photocurrent spectroscopy (FTPS) and monochromatic photocurrent (PC) methods are compared with P3HT:PCBM, where the CT state is well known. PDPP-BBT:PCBM shows a stable CT state while TDPP-BBT does not. Our analysis shows that the larger singlet state energy difference between TDPP-BBT and PCBM along with the lower optical gap of TDPP-BBT obliterates the formation of a midgap CT state resulting in an enhanced photovoltaic efficiency over PDPP-BBT:PCBM.

12:51PM Q49.00009 Dynamic Monte Carlo Modeling of Exciton Dissociation in Organic Donor-Acceptor Solar Cells, MICHAEL HEIBER, ALI DHINOJWALA, University of Akron, Department of Polymer Science — A general dynamic Monte Carlo model for exciton dissociation at a donor-acceptor interface including exciton delocalization and hot geminate pair dissociation has been developed to model the experimental behavior observed for the P3HT:PCBM system and predict the theoretical performance of future materials systems. The presence of delocalized excitons and the direct formation of separated charge pairs has been recently measured by transient photo-induced absorption experiments, and has been proposed to facilitate charge separation efficiency. The excess energy of the exciton dissociation process has also been observed to have a strong correlation with the charge separation yield for a range of thiophene polymer:PCBM systems, suggesting that a hot charge separation process is also occurring. Hot geminate pair dissociation has been previously theorized as a cause for highly efficient charge separation, however a detailed model for this process has not been implemented and tested. Here, both conceptual models have been implemented into a dynamic Monte Carlo simulation and tested using a model bilayer donor-acceptor system.

1:03PM Q49.00010 Ultrafast Photo Physics of P3HT/PCBM blends for Organic Photovoltaic applications, BILL PANDIT, SANJEEV SINGH, ZEEV VALY VARDENY, Department of Physics and Astronomy, University of Utah, Salt Lake City, Utah, 84112 — We studied the ultrafast dynamics of photoexcitations in pristine polymer films of regio-regular polythiophene, regio-random polythiophene, and their blends with the fullerene derivative C₆₁-PCBM using the pump-probe photomodulation (PM) spectroscopy with ~150 fs time resolution. Our transient PM spectrum covers the broad spectral range of 0.25 – 2.4 eV using two different laser systems; which allows us to simultaneously monitor the dynamics of various photoinduced absorption bands such as intrachain excitons, charge transfer excitons, and polaron-pairs. Surprisingly, we have been able to monitor the decay of intrachain exciton on the polymer chains in films of polymer/fullerene blends, but unable to detect the subsequent generation of polarons in the donor (D) and acceptor (A) materials up to ~ 1 ns. We explain this finding considering that the excitons in the polymer chains form charge transfer excitons upon reaching the D-A interface, rather than undergo a more direct dissociation on the D-A materials. The understanding of charge separation at the D-A interface is crucial for improving the power conversion efficiency of organic solar cell devices. Supported in part by the DOE grant No. DE-FG02-04ER46109.

1:15PM Q49.00011 Can Singlet Fission Enhance the Performance of Organic Solar Cells?¹, J.A. MUNOZ, K. ARYANPOUR, S. MAZUMDAR, Dept of Physics, Univ of Arizona — The high efficiency of pentacene-fullerene (Pc-C₆₀) donor-acceptor solar cells has been ascribed to singlet fission, which generates two spin triplet excitons that each undergo ionization to give two pairs of electrons and holes [1,2]. For triplet ionization to give charge generation, the charge-transfer exciplex in the Pc-C₆₀ heterostructure should be energetically below the the molecular triplet state in Pc. Our initial calculations show that this is not a plausible scenario. We propose an alternate mechanism for the relatively high efficiencies of solar cells constructed from donors such as Pc, based on correlated-electron configuration interaction calculations [3] of ground state and photoinduced charge-transfer.

[1] Wilson M. W. B.; et al., J. Am. Chem. Soc, v133, 31, 11830-11833 (2011)

[2] Rao A.; et al., J. Am. Chem. Soc, v132, 36, 12698-12703 (2010)

[3] Yi Y.; Coropceanu V.; Brédas J. L.; J. Am. Chem. Soc, v131, 43, 15777-15783 (2009)

¹US NSF grant DMR-0705163 and the Univ of Arizona WEES program.

1:27PM Q49.00012 Exciton self-trapping and Stark effect in the optical response of pentacene crystals from first principles¹, DAVID A. STRUBBE, Department of Physics, University of California, Berkeley; Materials Sciences Division, Lawrence Berkeley National Laboratory, SAHAR SHARIFZADEH, JEFFREY B. NEATON, Molecular Foundry, LBNL, STEVEN G. LOUIE, Physics Dept., UC Berkeley; MSD and MF, LBNL — Pentacene is a prototypical organic semiconductor with optoelectronic and photovoltaic applications. It is known that the lowest-energy singlet excitation has a Stokes shift between absorption and emission of about 0.14 eV, but the deformation associated with this self-trapped exciton remains unknown. We begin with a calculation of the optical properties via the first-principles GW/Bethe-Salpeter (BSE) theory [ML Tiago, JE Northrup, and SG Louie, Phys. Rev. B 67, 115212 (2003); S Sharifzadeh, A Biller, L Kronik, and JB Neaton, arXiv:1110.4928 (2011)]. We then study the self-trapping phenomenon via our reformulation of the Bethe-Salpeter excited-state forces approximation of Ismail-Beigi and Louie [Phys. Rev. Lett. 90, 076401 (2003)], which can describe the structural relaxation after optical excitation. Whether excitons in pentacene have charge-transfer character has been controversial in electro-absorption experiments. We use the same BSE analytic derivatives approach to calculate the changes in excitation energies due to an applied electric field to understand this experimental controversy.

¹Support from DOE (DE-AC02-05CH11231) and NSF (DMR10-1006184). Computational resources from NERSC and TeraGrid.

1:39PM Q49.00013 Singlet Fission and Multi-Exciton Generation in Organic Systems, CHARLES MUSGRAVE, University of Colorado — Multi-exciton generation (MEG) has been observed in a variety of materials and might be exploited in solar-cells to dramatically increase efficiency. In tetracene and pentacene MEG has been attributed to singlet fission (SF), however a fundamental mechanism for SF has not been previously described. Here, we use sophisticated ab initio calculations to show that MEG in pentacene proceeds by transition of the lowest optically allowed excited state S1 to a dark state (D) of multi-exciton character, which subsequently undergoes SF to generate two triplets (2×T0). D satisfies the energy requirement for SF ($E_D > 2E_{T0}$) and lies just below S1 in pentacene, but above S1 in tetracene, consistent with the observed thermally activated SF process in tetracene, but no thermal activation in pentacene. While S1 exhibits single exciton character, D shows multi-exciton character comprising two separated electron-hole pairs. Dimer simulations predict S1 excimer formation and that fission of D into triplets proceeds through the excimer. The predicted energetics, wavefunctions and excimer interaction support the proposed mechanism, which accounts for the observed rapid, unactivated SF in pentacene. Results for SF in polyacenes, grapheme nanoribbons, rubrene and carbon nanotubes will be presented.

Wednesday, February 29, 2012 11:15AM - 2:15PM –

Session Q50 DPOLY: Focus Session: Dynamics of Polymers: Phenomena due to Confinement

II 162B

11:15AM Q50.00001 New insight into adsorption of polymer melts onto impenetrable surfaces¹, TAD KOGA, PETER GIN, NAISHENG JIANG, CHEN LIANG, ZEXI HAN, Stony Brook University, BULENT AKGUN, SUSHIL SATIJA, NIST, MAYA ENDOH, Stony Brook University — We report the novel structures of irreversibly adsorbed polystyrene (PS) layers composed of six different molecular weights ranging from 30k to 2,000k. Spin cast PS films (originally ~ 100 nm in thickness) prepared onto hydrogen-passivated silicon substrates were annealed at 170 °C for about 50h under vacuum and subsequently rinsed with toluene (a good solvent for PS) thoroughly. X-ray reflectivity results show that the adsorbed layers are well described by a two-layer model: the one is a higher density layer relative to the bulk adjacent to the substrate and the other is a nearly bulk density layer on top of the bottom layer. On the other hand, a single-layer model with the higher density layer is valid for the adsorbed layers composed of low molecular weights PS. We will reveal the origin of the difference, shedding light on a new pathway for the formation of the equilibrium adsorbed polymer layers at the impenetrable interfaces.

¹We acknowledge the financial support from NSF Grant No. CMMI-084626.

11:27AM Q50.00002 Effect of the interfacial interaction on the relaxation of polymer melts in nanofilms, LEI LI, YONGJIN WANG, Department of Chemical Engineering, University of Pittsburgh, JIANING SUN, J.A. Woollam Co. — The relaxation of polymer melts in nanofilms could be orders of magnitude slower than in bulk. To date, the governing mechanism remains unclear on the role of spatial confinement and interfacial interaction. Here we report the experimental results indicating that the polymer-substrate interfacial interaction plays a key role in the relaxation. Two perfluoropolyethers (PFPEs) with the same backbone and different endgroups, one polar and the other non-polar, have been studied. The relaxation of the nanofilms on silicon wafers was characterized by the contact angle measurement. For the PFPE with polar endgroups, the contact angle “relaxes” with time and the relaxation time constant, obtained from KWW model, is ten orders of magnitude higher than that of bulk polymer. However, for the PFPE with non-polar endgroups, the contact angle relaxation was not observed. The experimental results indicate that the relaxation is thermodynamically driven by the attractive interaction between the polar endgroups of the polymers and the polar sites on the solid substrate. The very slow kinetics of the relaxation has been attributed to the heterogeneity of the polymer-solid interfacial interaction and the cooperative nature of the molecular motions during the relaxation.

11:39AM Q50.00003 Differential AC chip calorimeter for in situ investigation of vapor deposited thin films, MATHIAS AHRENBERG, CHRISTOPH SCHICK, HEIKO HUTH, EVGENI SCHOIFET, University of Rostock, Germany, MARK EDIGER, KATIE WHITAKER, University of Wisconsin - Madison, Wisconsin, USA — Physical vapor deposition (PVD) can be used to produce thin films with particular material properties like extraordinarily stable glasses of organic molecules. We describe an AC chip calorimeter for in-situ heat capacity measurements of as-deposited nanometer thin films of organic glass formers. The calorimetric system is based on a differential AC chip calorimeter which is placed in the vacuum chamber for physical vapor deposition. The sample is directly deposited onto one calorimetric chip sensor while the other sensor is protected against deposition. The device and the temperature calibration procedure are described. The latter makes use of the phase transitions of cyclopentane and the frequency dependence of the dynamic glass transition of toluene and ethylbenzene. Sample thickness determination is based on a finite element modeling (FEM) of the sensor sample arrangement. A layer of toluene was added to the sample sensor and its thickness was varied in an iterative way until the model fits the experimental data.

11:51AM Q50.00004 Methyl Methacrylate Polymerization in Nanoporous Matrix: Reactivity and Resulting Properties¹ , HAOYU ZHAO, FATEMA BEGUM, SINDEE SIMON, Texas Tech University — Nanoconfinement is well known to affect the properties of polymers, including changes in the glass transition temperature (T_g). In this work, the focus is on the influence of nanoconfinement on free radical polymerization reaction kinetics and the properties of the polymer produced. Controlled pore glass (CPG) is used as a nanoconfining matrix for methyl methacrylate (MMA) polymerization with pore diameters of 13 nm, 50 nm, and 110 nm. The reaction is followed by measuring heat flow as a function of reaction time during isothermal polymerization at temperatures ranging from 60 °C to 95 °C using differential scanning calorimetry (DSC). After reaction, the properties of the polymer are measured, including T_g , molecular weight, and tacticity. Nanoconfinement is found to result in earlier onset of autoacceleration, presumably due to a decrease in the rate of termination arising from decreases in chain diffusivity in the confined state. In addition, T_g and molecular weight of the resulting PMMA are found to increase. A model of the nanoconfined reaction is able to quantitatively capture these effects by accounting for changes in chain diffusivity, and in native pores, also accounting for changes in intrinsic reaction rates.

¹Funding from the National Science Foundation CMMI 0826437 is gratefully acknowledged.

12:03PM Q50.00005 Polystyrene films confined between gold surfaces , KAREN JOHNSTON, Max Planck Institute for Polymer Research, VAGELIS HARMANDARIS, University of Crete, KURT KREMER, Max Planck Institute for Polymer Research — The properties of thin short-chain polystyrene films between two parallel Au(111) surfaces are studied using a combination of density functional theory (DFT) and classical molecular dynamics (MD) simulations. The chemical interaction with the surface is calculated with DFT and the results are used to develop accurate atomistic classical surface potentials. These potentials are used in the MD simulations to investigate several systems with various film thickness and the effect of increasing confinement on the structural and dynamical properties of the films will be presented. A coarse-grained model is developed and used to study longer-chain polystyrene films and larger systems.

12:15PM Q50.00006 Surface Mobility of Polymeric Systems of Varying Chain Lengths , ROHIT MALSHE, GREGORY TOEPPERWEIN, MARK EDIGER, LIAN YU, JUAN DE PABLO, University of Wisconsin — Thin films of polymeric material can exhibit drastically altered glass transition temperatures, mechanical responses, and overall dynamics as compared to the bulk. Differences in surface and bulk mobility are often cited as a primary explanation for such differences, but it has remained difficult to quantify local mobility as within the film. We have recently shown that decay constants from Mullins' surface diffusion model correspond directly to surface mobility for small-molecule glasses. In the current work, we examine long-chain polymers via two types of systems: polymeric pillars where the cross sections evolve from square to circular, and large particles which sink into polymeric thin films. For the pillars, we use Mullins' model to interpret changes in curvature. It is found that Mullins' decay constants correspond to relaxation times that can be identified with distinct segmental relaxation processes. Such decay constants exhibit a strong dependence on chain length and temperature. For the particle-thin film systems, we relate the rate of particle sinking to various measures of local mobility in the film. This setup is a direct analog to recent experimental work. The results presented here provide a connection between surface shape transformations, mobility, and diffusion.

12:27PM Q50.00007 Shear thinning near the rough boundary in a viscoelastic flow , SAYED HASAN, SERGEI OBUKHOV, Department of Physics, University of Florida — It was first noticed by de Gennes, that because of huge difference between viscosities of entangled polymeric liquid and monomeric liquid, the boundary conditions for a polymer flow near microscopically smooth boundary should be assumed as "slip". Nevertheless, in the presence of surface roughness, or undulations, the flow is characterized by mixed boundary conditions. We had shown that at certain slip velocities the deformation of the melt near the rough (undulated) boundary might become more elastic than viscous. This results in "shear thinning" of the roughness of boundary. At higher velocities, near the slip boundary, the chains can be considered simply trapped in an entangled mesh of other chains. They are subjected to oscillating strain rate, comparable to frequencies of internal Rouse modes of these chains. We calculate the total dissipation of energy due to oscillating strain and calculate the slippage of the polymer melt near the boundary as function of velocity, undulation wavelength and amplitude.

12:39PM Q50.00008 Relaxation of Capillary Wrinkles¹ , KAMIL TOGA, NARAYANAN MENON, THOMAS RUSSELL, University of Massachusetts, Amherst — We have investigated the relaxation of a wrinkle pattern on a thin viscoelastic film. The films are made from spin-coated PS (polystyrene) of thickness ranging from 40 to 240 nm that were floated on the surface of water. Viscoelastic behavior is introduced to the film by depressing the glass transition of PS with a soluble plasticizer, dioctyl phthalate. Wrinkle patterns are formed by placing a small droplet ($\sim 1\mu\text{L}$) at the center of the floating disc. Due to the differential tension generated across the film, radial wrinkles form around the drop where the compressive axial force buckles the membrane. Thereafter, length of the wrinkles decays, and so does their wavelength. We have studied the relaxation of wrinkles as a function of PS molecular weight and plasticizer content, in order to understand the relationship with the bulk glass transition temperature.

¹Supported by NSF-MRSEC

12:51PM Q50.00009 New insight into the melting behavior of nanoconfined semicrystalline polymers -The effect of an immobile interfacial layer at the substrate- , MITSUNORI ASADA, Kuraray Co., Ltd., NAISHENG JIANG, PETER GIN, LEVENT SENDOGDULAR, MAYA K. ENDOH, Department of Materials Science and Engineering, Stony Brook University, MORIYA KIKUCHI, Japan Science Technology Agency, ERATO, Takahara Soft Interfaces, ATSUSHI TAKAHARA, Japan Science Technology Agency, ERATO, Takahara Soft Interfaces, Graduate School of Engineering, Kyushu University, TADANORI KOGA, Department of Materials Science and Engineering, Stony Brook University, Chemical and Molecular Engineering Program, Stony Brook University — It is known that when semicrystalline polymer chains are confined on a nanometer length scale, the crystalline structures and dynamics differ from bulks, the so-called "nanoconfinement effects." In this talk, we will report the anomalous melting behavior of nano-confined polyethylene spin cast films prepared on Si substrates by integrating various in-situ grazing incidence scattering techniques. We found that a very thin adsorbed layer at the weakly interactive substrate interface plays a crucial role in the melting behavior.

1:03PM Q50.00010 Solvent Swelling as a Means to Modify the Properties of Polymer Thin Films , ANDREW CLOUGH, OPHELIA TSUI, Boston University, MITHUN CHOWDHURY, KAIWAN JAHANSAHI, GUENTER REITER, Albert-Ludwigs-Universitaet Physikalisches Institut, Freiburg, Germany — It has been observed that sample preparation can influence certain properties of polymer films. In particular, spin-coating from solutions of different solvent qualities result in films with different chain conformations. We surmise that upon formation by spin-coating, the chain conformation of a film is still adjustable by means of solvent swelling, resulting in modifications to the amount of entanglement and free volume. Initial measurements of thermal expansion upon heating after swelling suggest that there is a difference between polystyrene films swelled with a good solvent and a Θ solvent. We have begun a more detailed investigation by studying the effect of swelling on the dewetting behaviors. Preliminary data indicates that the quality of the solvent affects both the dewetting hole size and aging rate of the film.

1:15PM Q50.00011 Equilibration of Polymer Films Cast from Solutions with Different Solvent Qualities, RANXING NANCY LI, ANDREW CLOUGH, DONGDONG PENG, ZHAOHUI YANG, OPHELIA TSUI, Boston University — The preparation history can affect the physical properties of polymer thin films. In spin coating, films are made from a polymer solution. Due to rapid evaporation of solvent in this process, the polymer chains in the films cannot fully interpenetrate, resulting in a non-equilibrium conformation with reduced entanglement density. These in turn can affect the film's equilibration process and viscoelastic properties. On the basis that the chain conformation and entanglement density in a film depend on the conformation of the chains while in solution before spin-coating. We modify the structural properties of the films by adjusting the quality of the solvent used in spin-coating. We examine in detail how these adjustments affect the way polystyrene films approach equilibrium on annealing above the glass transition temperature. It is found that the equilibration time of the film is significantly increased as the solvent quality is decreased towards the Θ condition. We attribute this observation to reduced entanglement in the films with decreasing solvent quality.

1:27PM Q50.00012 Tuning confinement effects at constant film thickness, SIMONE NAPOLITANO, Universite Libre de Bruxelles — We show experimental evidence confuting the commonly accepted idea that the deviation from bulk behavior can be explained in terms of finite size effects and interfacial interactions. By reproducing Guiselin's experiment and upon variation of the molecular weight, we could prepare films of polystyrene spincoated on aluminum and annealed for the same time, having constant thickness but different glass transition temperature and tracer diffusivity. The results can be rationalized in terms of t^* , a dimensionless parameter obtained by the ratio of the annealing time and the adsorption time [1], quantifying the equilibrium character of the films. Further evidence on the relevance of t^* on understanding the behavior of polymers at the nanoscale is provided [2].

[1] Napolitano, S. and Wübbenhorst, M., Nature Communications, 2, 260 (2011).

[2] Rotella, C.; Wübbenhorst, M. and Napolitano, S., Soft Matter, 7, 5260 (2011).

1:39PM Q50.00013 Capillary levelling in thin polymer films as a nano-rheological tool to probe interface dynamics, JOSHUA MCGRAW, OLIVER BAEUMCHEN, MELISSA FERRARI, PAUL FOWLER, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1 — Entanglement of polymer chains in confinement is modified as a result of altered chain conformations. According to Silberberg's principle, chain segments are reflected at an interface causing a reduction of the inter-chain entanglement density. If the interface is transient, local polymer conformation changes can be inferred from a temporal change in flow properties: over time polymer chains become more entangled, thus there is more resistance to flow. Here, we measure the gradual disappearance of an entropic interface between two melts of identical polymer chains during the flow of stepped bilayer polymer films. Samples are prepared in the glassy state and, when in the melt, flow to relieve the Laplace pressure gradient induced by a step in the topography (McGraw *et al.*, Soft Matter, 2011). Our results reveal the dynamics of re-entanglement across the transient entropic interface.

1:51PM Q50.00014 Slow physical aging of thin polymer films of varying chain architecture¹, BRADLEY FRIEBERG, EMMANUIL GLYNOS, PETER GREEN, University of Michigan — The physical aging rate of supported polystyrene (PS) films is influenced by film thickness, H , and by macromolecular architecture. For linear PS films, in the thickness range 300 nm to 50 nm, supported by silicon oxide substrates, the aging rate decreased by 15 percent. On the other hand, star-shaped PS, with functionality $f=8$ and with an average molecular weight per arm of $M_{arm}=25$ kg/mol, exhibited a 25 percent decrease throughout the same thickness range. When M_{arm} was decreased to 10 kg/mol the depression in aging rate was 45 percent. We reconcile these changes in physical aging in terms of model that accounts for gradients in the local T_g of the film in the vicinity of interfaces. These findings have important implications for the processing and function of thin polymer films for different applications.

¹Support for this research from the National Science Foundation (NSF), Division of Material Research, Polymer Program No. 0906425 is gratefully acknowledged.

2:03PM Q50.00015 Diffusion of adsorbed theta-solvent polymers at a solid-liquid interface, CHANGQIAN YU, SUNG CHUL BAE, STEVE GRANICK, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN TEAM — We study how surface diffusion depends on temperature when this is varied below the theta temperature. In the polystyrene-cyclohexane system, we use FRAP (fluorescence recovery after photobleaching) to measure over times over 4 orders of magnitude, from 10 sec to 10^5 seconds. A fast component of motion is attributed to chains loosely bound to the surface. A slower component of motion is retained after rinsing; it is subdiffusive. At temperatures below the bulk coexistence temperature, the surface layer is thicker than a monolayer. We show that bulk phase separation of polymers in dilute solution produces a dense surface layer of emulsion and foamy near-surface structure.

Wednesday, February 29, 2012 11:15AM - 2:15PM —

Session Q51 DCMP DFD: Gels, Complex Fluids and Vesicles Boston Convention Center 154

11:15AM Q51.00001 Linear Viscoelasticity and Swelling of Polyelectrolyte Complex Coacervates, FAWZI HAMAD, RALPH COLBY, Pennsylvania State University — The addition of near equimolar amounts of poly(diallyldimethylammonium chloride) to poly(isobutylene-alt-maleate sodium), results in formation of a polyelectrolyte complex coacervate. Zeta-potential titrations conclude that these PE-complexes are nearly charge-neutral. Swelling and rheological properties are studied at different salt concentrations in the surrounding solution. The enhanced swelling observed at high salt concentration suggests the system behaves like a polyampholyte gel, and weaker swelling at very low salt concentrations implies polyelectrolyte gel behavior. Linear viscoelastic oscillatory shear measurements indicate that the coacervates are viscoelastic liquids and that increasing ionic strength of the medium weakens the electrostatic interactions between charged units, lowering the relaxation time and viscosity. We use the time-salt superposition idea recently proposed by Spruijt, et al., allowing us to construct master curves for these soft materials. Similar swelling properties observed when varying molecular weights. Rheological measurements reveal that PE-complexes with increasing molecular weight polyelectrolytes form a network with higher crosslink density, suggesting time-molecular weight superposition idea.

11:27AM Q51.00002 Multicomponent effects in diffusion within microemulsions, WYATT MUSNICKI, STEPHANIE DUNGAN, RONALD PHILLIPS, University of California Davis, CHEMICAL ENGINEERING AND MATERIAL SCIENCE DEPARTMENT TEAM — Holographic interferometry was used to monitor transport of hydrophobic solutes in systems containing nanometer-scale microemulsion droplets. In this technique, variations in the refractive index between a reference time and a later time are monitored via interference fringes that are formed with the help of a holographic plate. The refractive index change is driven by imposed concentration differences of either the solute (at constant surfactant concentration), or of the surfactant (at constant solute concentration). We find that, especially for hydrophobic solutes, the transport kinetics cannot be interpreted by using a pseudobinary approximation. Multicomponent interaction effects must be taken into account even at micelle concentrations as low as 6%. By performing multiple experiments with different initial concentration gradients, and extending earlier analyses of the experimental interference fringes, the multicomponent effects can be resolved, yielding results for all the relevant diffusion coefficients.

11:39AM Q51.00003 Determining the structure and properties of complex coacervate crosslinked triblock copolymer hydrogels, DANIEL KROGSTAD, SOO-HYUNG CHOI, JASON SPRUELL, NATHANIEL LYND, EDWARD KRAMER, Materials Research Laboratory, University of California at Santa Barbara, MATTHEW TIRRELL, Institute for Molecular Engineering, University of Chicago — The mechanical properties and structures of functionalized P(AGE-b-EO-b-AGE) hydrogels utilizing complex coacervation as a physical crosslink have been studied. The effects of variables such as polymer concentration, salt concentration, pH, stoichiometric ratios and temperature have been investigated by rheology and SAXS. It was found that the organization of the cores has a very strong effect on the mechanical properties. This can be observed as the storage modulus increases significantly between 15 and 16 wt% corresponding to a transition from a disordered gel to a BCC structure. Another dramatic change is observed when the storage modulus drops between 25 and 30 wt% as the hexagonal structure becomes predominant. Just as polymer concentration causes changes in structure and thus the properties, salt concentration has a similar effect due to the electrostatic nature of the hydrogels. As salt is added, the electrostatic interactions in the cores are screened until they are weak enough that the polymers are dissolved into the matrix. The mechanical properties and the physical nature of the crosslinks lead to the possibility of these gels being used as an injectable drug delivery system.

11:51AM Q51.00004 Density mode microrheology in polyacrylamide gels, BEATRIZ BURROLA GABILONDO, DANIEL SISAN, Georgetown University, JONATHAN LANDY, ALEX LEVINE, University of California, Los Angeles, JEFFREY URBACH, Georgetown University — In passive microrheology the viscoelastic properties of soft materials are deduced by observing thermal fluctuations of tracer particles embedded within the material, and the response function obtained from the spectrum of thermally excited modes is then related to the viscoelastic shear modulus. This approach is valid for single-component, isotropic, incompressible materials. However, for heterogeneous materials, such as hydrogels, a more comprehensive approach is needed. We measure the equilibrium density fluctuations of a cross-linked polymer gel swollen in a solvent and compare them to the predictions of the 'two-fluid' model of the dynamics of polymer gels. We will describe a direct method of extracting the longitudinal response function of a soft material based on the temporal and spatial correlations of density fluctuations of fluorescent markers, called density mode microrheology (DMM). We will also present results of applying DMM to fluorescent polyacrylamide gels in an aqueous solvent of varying viscosity and comparing them with parameters obtained from conventional microrheology.

12:03PM Q51.00005 Effect of Polymer Molecular Weight and Synthesis Temperature on Structure and Dynamics of Microgels¹, KRISTA G. FREEMAN, KIRIL A. STRELETZKY, Cleveland State University — Environmentally-sensitive microgels have been synthesized under varying conditions to study the dependences on polymer molecular weight (M_W) and synthesis temperature (T_{syn}). The dynamics and structure of the synthesized microgels below and above the LCST of the polymer ($T_c \sim 41^\circ\text{C}$) were studied using dynamic and static light scattering spectroscopy. All microgels exhibit a volume phase transition above the LCST of the polymer and undergo a reversible 15-50-fold volume shrinkage. The size distribution, structure, deswelling ability, and temperature response of microgels strongly depend on synthesis conditions. T_{syn} dependence was studied with 1000kDa polymer. Increasing $\Delta T = T_{syn} - T_c$ yields smaller microgels with a smaller swelling ratio up to $\Delta T = 8.5^\circ\text{C}$, after which the trend is reversed. The amphiphilic nature of the polymer may explain this trend. T_{syn} also affects the structure of microgels; low T_{syn} yields elongated particles, while high T_{syn} microgels are more spherical. Polymer M_W directly effects microgel polydispersity and temperature response. While microgels synthesized with 1000kDa polymer are relatively monodisperse, synthesis with low M_W polymers (80-370kDa) yields systems with a large population ($R_h \sim 1000\text{nm}$) precipitating out of solution and a smaller population ($R_h \sim 300\text{nm}$) staying in suspension. M_W also influences the temperature response of microgels; high M_W microgels show a gradual shrinkage with increasing temperature while low M_W microgels display a delayed and sudden shrinkage at high temperatures.

¹COTTRELL Science Award (CC6861) and CSU's FRD

12:15PM Q51.00006 Gelation and state diagram for a model nanoparticle system with adhesive hard sphere interactions, NORMAN WAGNER, University of Delaware, EBERLE AARON, NIST — We provide the first comprehensive state diagram of thermoreversible gelation in a model nanoparticle system from dilute concentrations to the attractive driven glass. We show the temperature dependence of the interparticle potential is related to a surface molecular phase transition of the brush layer using neutron reflectivity (NR) and small-angle neutron scattering (SANS) [1]. We establish the temperature dependence of the interparticle potential using SANS, dynamic light scattering (DLS), and rheology. The potential parameters extracted from SANS suggest that, for this system, gelation is an extension of the Mode Coupling Theory (MCT) attractive driven glass line (ADG) to lower volume fractions and follows the percolation transition. Below the critical concentration, gelation proceeds without competition for phase separation [2]. These results are used to develop a complete state diagram for the sticky hard sphere reference system.

[1] A.P.R. Eberle, N.J. Wagner, B. Akgun, S.K. Satija, Langmuir **26** 3003 (2010).

[2] A.P.R. Eberle, N.J. Wagner, R. Castaneda-Priego, Phys. Rev. Let. **105**704 (2011).

12:27PM Q51.00007 Hydrodynamics and Rheology of Active Liquid Crystals, ZHENLU CUI, Fayetteville State University — Active liquid crystals such as swimming bacteria, active gels and assemblies of motors and filaments are active complex fluids. Such systems differ from their passive counterparts in that particles absorb energy and generate motion. They are interesting from a more fundamental perspective as their dynamic phenomenons are both physically fascinating and potentially of great biological significance. In this talk, I will present a continuum model for active liquid crystals and analyze the behavior of a suspension subjected to a weak Poiseuille flow. Hydrodynamics, stability and rheology will also be discussed.

12:39PM Q51.00008 Electrostatics-driven assembly of uni-lamellar catanionic faceted vesicles, CHEUK-YUI LEUNG, LIAM PALMER, SUMIT KEWALRAMANI, RASTKO SKNEPNEK, GRAZIANO VERNIZZI, MEGAN GREENFIELD, SAMUEL STUPP, MICHAEL BEDZYK, MONICA OLVERA DE LA CRUZ, Northwestern University — Nature utilizes shape to generate function. Organelle and halophilic bacteria wall envelopes, for example, adopt various polyhedral shapes to compartmentalize matter. The origin of these shapes is unknown. A large variety of shell geometries, either fully faceted polyhedra or mixed Janus-like vesicles with faceted and curved domains that resemble cellular shells can be generated by coassembling water-insoluble anionic (−1) amphiphiles with high valence cationic (+2 and +3) amphiphiles. Electron microscopy, X-ray scattering, theory and simulations demonstrate that the resulting faceted ionic shells are crystalline, and stable at high salt concentrations. The crystallization of the co-assembled single tail amphiphiles is induced by ionic correlations, and modified by the solution pH. This work promotes the design of faceted shapes for various applications and improves our understanding of the origin of polyhedral shells in nature.

12:51PM Q51.00009 Modeling controlled release from responsive microgel capsules¹, ALEXANDER ALEXEEV, HASSAN MASOUD, Georgia Institute of Technology, George W. Woodruff School of Mechanical Engineering — We introduce a coarse-grained computational method that explicitly captures the release of nanoparticles and macromolecules from responsive microgel capsules. The model is based on the dissipative particle dynamics. Our simulations reveal that not only swelling, but also deswelling of hollow microcapsules can be harnessed for controlled release. We show that the release from swollen capsules is diffusion driven, whereas the release from deswelling gel capsules occurs due to the flow of encapsulated solvent that is expelled from the shrinking capsule interior. The latter hydrodynamic release is burst-like and continues only during capsule deswelling. We find that deformable polymer chains that can easily penetrate thorough membrane pores are released in larger amounts from deswelling capsules, than nanoparticles that are filtered out by shrinking membrane pores. Our simulations further demonstrate that the inclusion of rigid microrods inside deswelling capsules mitigates the membrane pore closing, and, in this fashion, provides an effective method for regulating the rate of hydrodynamic release of nanoparticles.

¹Financial supports from the Donors of the Petroleum Research Fund administered by the ACS and from the National Science Foundation (DMR-0844115) through ICAM-I2CAM (1 Shields Avenue, Davis, CA 95616) are gratefully acknowledged.

1:03PM Q51.00010 Thermoresponsive microcapsules for controlled release of hydrophilic cargo, ESTHER AMSTAD, DAVID WEITZ, Harvard University — Thermoresponsive microcapsules that collapse upon increasing the temperature above their lower critical solution temperature (LCST) such as poly(N-isopropyl acrylamide) (PNIPAM) capsules are well known. However, capsules consisting of thermoresponsive polymers that possess an upper critical solution temperature (UCST) and therefore swell upon increasing the temperature above their UCST are scarce. We will present a microfluidic method to assemble thermoresponsive poly([2-(methacryloyloxy)-ethyl]-dimethyl-[3-sulfopropyl-ammoniumhydroxide]) (PMEDSH) microcapsules that have UCST. These capsules are in a collapsed state at room temperature and become highly water permeable upon increasing the temperature above the UCST. To simultaneously allow for encapsulation of hydrophilic cargo and enable the water based polymerization reaction of the PMEDSH shell, these microcapsules are assembled as water/water/oil emulsions using capillary microfluidic devices. The resulting PMEDSH microcapsules are envisaged as delivery vehicles and microreactors that allow for temperature induced controlled release of hydrophilic cargo. .

1:15PM Q51.00011 A Nano Engineered Membrane for Oil-Water Separation, BRIAN SOLOMON, NASIM HYDER, KRIPA VARANASI, Massachusetts Institute of Technology, VARANASI RESEARCH GROUP TEAM — Oil and water separation is an extremely costly problem in the petroleum industry. Pumping the complete emulsion to the surface requires substantially more power than pumping the oil alone. A membrane that can efficiently separate oil from water at the source would revolutionize this process. To this end a novel, layered, hierarchical thermoplastic membrane was fabricated with both nanoscale and microscale features. Modifying the length scales involved in fabrication of the membrane yields interesting and non-obvious implications. Under certain regimes, the microscale features independently control the membrane's permeability, while the microscale features control only the membrane's breakthrough pressure. By operating in this regime, separation efficiencies can be realized that are otherwise unattainable by conventional membranes. Taking it a step further, chemical treatments have been used to achieve higher hydrophobicity for the membrane by lowering the surface energy of the membrane surface. Although this research focused on oil-water separation, the results have implications for other multiphase systems and hold for many other filtration and separation technologies including in lab-on-chip devices and micro/nanofluidic devices.

1:27PM Q51.00012 Tether formation on a settling vesicle, GWENN BOEDEC, M2P2 UMR 6181 CNRS Aix Marseille University, MARC JAEGER, M2P2 UMR 6181 CNRS Aix Marseille University - Centrale Marseille, MARC LEONETTI, IRPHE UMR 6594 CNRS Aix Marseille University — When submitted to a point-like force, a phospholipid vesicle (a lipid membrane enclosing a drop) is known to develop a narrow tether. This tether formation is reminiscent of drop pinch-off, but the peculiar properties of the vesicle interface prevents the apparition of a finite-time singularity. It is shown that a settling vesicle may develop such tethered shapes, with hydrodynamic stresses acting as the pulling force. These shapes are studied numerically and theoretically, and continuous families of stationary tethered shapes are found, depending on two control parameters. Dynamics of formation is studied and it is shown that changing the initial condition can lead to complex transients, with formation of pearls onto the tether.

1:39PM Q51.00013 Electrohydrodynamic instabilities of biomimetic bilayer membranes, JACOPO SEIWERT, PETIA VLAHOVSKA, Brown university — Living cells actively maintain electrochemical potentials across their membranes, which regulates cell migration, motility, and development. In this presentation, we focus on the effect of an external electric field on membrane dynamics. We present a physical model for the dynamic coupling between transmembrane potential and deformation of biomimetic membranes. We perform linear stability analysis to clarify and quantify the effects of the lipid bilayer properties (conductivity and capacitance), and asymmetry in the embedding electrolyte solutions, on membrane deformation.

1:51PM Q51.00014 Polyoxometalate (POM) Nanocluster-Induced Phase Transition and Structural Disruption in Lipid Bilayers., BENXIN JING, Y. ELAINE ZHU, Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, Indiana 46556, United States, MARIE HUTIN, LEROY CRONIN, School of Chemistry, University of Glasgow, Glasgow G12 8QQ, United Kingdom, CRONIN GROUP OF COMPLEX CHEMICAL SYSTEM COLLABORATION — Polyoxometalate (POM) nanoclusters that are transition metal oxygen clusters with well defined atomic coordination structures have recently emerged as new and functional nanocolloidal materials used as catalysts, anti-cancer medicines, and building blocks for novel functional materials. However, their implications to human health and environment remain poorly investigated. In this work, we examine the interaction of highly charged anionic POM nanoclusters with lipid bilayers as a model cell membrane system. It is observed that upon the adsorption of anionic POMs, lipid dynamics is significantly suppressed and lipid bilayers are disrupted with resultant pore and budding-like structural formation. Direct calorimetric experiment of POM interaction with lipid bilayers of varied lipid compositions confirms the POM-induced fluid-to-gel phase transition in lipid bilayers, due to strong electrostatic interaction between POM nanocluster and lipid head groups.

2:03PM Q51.00015 Liquid-to-solid transition in suspensions of swollen microgels, JUAN JOSE LIETOR-SANTOS, ALBERTO FERNANDEZ-NIEVES, BENJAMIN SIERRA-MARTIN, Georgia Tech — We investigate the phase and non-equilibrium behavior of suspensions comprised of swollen, ionic microgels as a function of particle stiffness. We find that stiff particles exhibit all three phases observed in hard sphere suspensions, liquid, crystal and glass. For particles with intermediate stiffness, the crystal phase disappears and the microgel suspension transitions from a liquid to a glassy state at certain particle concentration. For even softer particles, no glassy state is observed. Instead the system remains liquid within the experimentally accessed concentration range. Interestingly, for microgels with intermediate stiffness, we find that the bulk modulus of individual particles seems to control the mechanical properties of the microgel suspension in the overpacked regime, emphasizing the relevance of being compressible.

Wednesday, February 29, 2012 11:15AM - 2:15PM –
Session Q52 GSNP DFD: Focus Session: Extreme Mechanics - Shells & Snapping 153C

11:15AM Q52.00001 Mechanics and Dynamics of a Snapping Arch , DOUGLAS HOLMES, Virginia Tech, MATTHIEU ROCHÉ, TARUN SINHA, HOWARD STONE, Princeton University — Snap-buckling of geometric arches and thin spherical shells occur in a variety of different geometric situations, exhibiting a highly nonlinear response dictated by the geometry and material properties of the system. As this elastic instability often precedes the catastrophic failure of a mechanical system, significant work has focused on the stability criteria for such structures. In order to properly understand the biomechanics of plants that rely on this instability, and in addition use snap-buckling in the design of advanced materials, it is necessary to also develop a fundamental understanding of the timescale and post-buckling response of a snapping structure. Currently, a fundamental understanding of the osmotically-induced snap-buckling phenomena is lacking. In this presentation, we examine the osmotic swelling of a bistable arch to identify the stability criteria, relevant snap-through timescale, and the impact of geometric confinement on snap-through symmetry and damping.

11:27AM Q52.00002 Elastocapillary-driven snap-through instability , AURELIE FARGETTE, ARNAUD AN-TKOWIAK, SEBASTIEN NEUKIRCH, Institut Jean le Rond d'Alembert, UPMC — The snap-through instability, which is present in a wide range of systems ranging from carnivorous plants to MEMS, is a well-known phenomenon in solid mechanics : when a buckled elastic beam is subjected to a transverse force, above a critical load value the buckling mode is switched. Here, we revisit this phenomenon by studying snap-through under capillary forces. In our experiment, a droplet (which replaces the usual dry load) is deposited on a buckled thin strip, clamped horizontally at both ends. In this setup both the weight of the drop and capillary forces jointly act toward the instability. The possibility of reverse elastocapillary snap-through, where the droplet is put under the beam, is then tested and successfully observed, showing the predominance of capillary forces at small enough scales.

11:39AM Q52.00003 Fast Motion of Plants through mechanical instability: Mechanics without Muscles¹ , QIAOHANG GUO², College of Materials Science and Engineering, Fuzhou University; Fujian University of Technology, Fuzhou, China, ZI CHEN, Biomedical Engineering, Washington University in St. Louis, HUANG ZHENG, Fujian Radio and Television University, Fuzhou, China, WENZHE CHEN, Fuzhou University, Fujian University of Technology, Fuzhou, China — Plants are not well known for fast motions, yet some plants such as the Venus flytrap can move in a fraction of a second to capture insects, even though they do not have nerves or muscles. This type of rapid motion has intrigued scientists for centuries. Darwin did a first systematic study on the trap closure mechanism, and considered the plant as “one of the most wonderful in the world”. Thereafter, several physical mechanisms have been proposed, such as the rapid loss of turgor pressure, an irreversible acid-induced wall loosening mechanism, and the snap-through model by mechanical instability, but with no unanimous agreement among researchers. Here we propose a coupled mechanical bistable mechanism that explains the rapid closure of the Venus flytrap in a comprehensive manner, consistent with a series of experimental observations. Such bistable behaviors are theoretically modeled and validated with table-top experiments. Based on the principles learnt from the Venus flytrap, we are also able to manufacture a preliminary “flytrap robot”. Hence, it is promising to design smart bio-mimetic materials and devices with snapping mechanisms as sensors, actuators, artificial muscles and biomedical devices.

¹The authors acknowledge National Science Foundation of China (Grant No. 11102040) and Sigma Xi GIAR program.

²Qiaohang Guo and Zi Chen contributed equally to this work.

11:51AM Q52.00004 Strange instabilities of simple elastic structures , DAVIDE BIGONI, DIEGO MISSERONI, University of Trento, Trento, Italy, GIOVANNI NOSELLI, Cambridge University, UK, DANIELE ZACCARIA, University of Trieste, Trieste, Italy — A class of simple elastic structures is shown exhibiting bifurcation and instability under tensile dead loading, multiple bifurcations, and softening/hardening behaviour in the postcritical regime. These structures evidences new and unexpected behaviours which are theoretically predicted and experimentally verified. These nonlinear behaviours can be exploited in the design of flexible mechanics devices and open new perspective in the control of vibrations.

12:03PM Q52.00005 Materials with Tunable Behavior due to Constrained Instabilities: Performance and Stability Analysis , DENNIS KOCHMANN, California Institute of Technology, WALTER J. DRUGAN, University of Wisconsin-Madison — Combining several materials into a composite permits the creation of new materials with overall properties tunable via a careful choice of the constituent materials with favorable specifics. The probably simplest example is a particle-matrix system, in which particles of one material enhance the mechanical behavior of the matrix material. Recent advances have confirmed that the overall performance of such a composite (e.g., its viscoelastic properties) can be dramatically altered, and stiffness and damping can be tuned to an extreme if one allows for temporarily negative elastic moduli in the inclusion. Such incremental negative moduli imply instability; e.g. a free-standing body of negative stiffness is thermodynamically unstable. However, through its geometric constraint a matrix phase can stabilize the otherwise unstable state of the inclusion phase, thus rendering the overall composite stable. In this contribution, we show, based on dynamic stability analyses, that the matrix constraint does indeed allow for the existence and use of negative moduli, and that this effect can be utilized to design novel composites of superior performance. Approaches to stabilize the negative-stiffness effect will be discussed as well as the performance of such composites.

12:15PM Q52.00006 Snap-Through of Graphene: An Elasto-Capillary Perspective , TILL WAGNER, DAMTP, University of Cambridge, DOMINIC VELLA, OCCAM, University of Oxford — Understanding the interaction between graphene flakes and various substrates is of crucial importance for nanoelectromechanical systems (NEMS) applications, among others. The ‘snap-through’ instability of graphene flakes placed onto corrugated substrates has recently received much attention as a potential assay for the study of this interaction. A sharp transition has been found in the morphology of the graphene between a) closely adhering to the corrugations of the substrate and b) lying almost completely flat on top. Which of these morphologies is observed depends on the geometry of the substrate and the mechanical properties of the flake. In this talk we shall focus on understanding the nature of this transition and, in particular, the ‘sharpness’ of the transition. We investigate how the location of snap through and its sharpness might be used to yield estimates of adhesion strength and friction with the substrate.

12:27PM Q52.00007 Electromechanical phase transition in dielectric elastomers under uniaxial tension and electrical voltage , RUI HUANG, University of Texas at Austin, ZHIGANG SUO, Harvard University — Subject to forces and voltage, a dielectric elastomer may undergo electromechanical phase transition. A phase diagram is constructed for an ideal dielectric elastomer membrane under uniaxial force and voltage, reminiscent of the phase diagram for liquid-vapor transition of a pure substance. We identify a critical point for the electromechanical phase transition. Two states of deformation (thick and thin) may coexist during the phase transition, with the mismatch in lateral stretch accommodated by wrinkling of the membrane in the thin state. The processes of electromechanical phase transition under various conditions are discussed. A reversible cycle is suggested for electromechanical energy conversion using the dielectric elastomer membrane, analogous to the classical Carnot cycle for a heat engine. The amount of energy conversion, however, is limited by failure of the dielectric elastomer due to electrical breakdown. With a particular combination of material properties, the electromechanical energy conversion can be significantly extended by taking advantage of the phase transition without electrical breakdown.

12:39PM Q52.00008 Soft Dielectrics: Heterogeneity and Instabilities, STEPHAN RUDYKH, GAL DEBOTTON, Ben-Gurion University of the Negev, KAUSHIK BHATTACHARYA, California Institute of Technology — Dielectric Elastomers are capable of large deformations in response to electrical stimuli. Heterogeneous soft dielectrics with proper microstructures demonstrate much stronger electromechanical coupling than their homogeneous constituents. In turn, the heterogeneity is an origin for instability developments leading to drastic change in the composite microstructure. In this talk, the electromechanical instabilities are considered. Stability of anisotropic soft dielectrics is analyzed. Ways to achieve giant deformations and manipulating extreme material properties are discussed. 1. S. Rudykh and G. deBotton, "Instabilities of Hyperelastic Fiber Composites: Micromechanical Versus Numerical Analyses." *Journal of Elasticity*, 2011. <http://dx.doi.org/2010.1007/s10659-011-9313-x> 2. S. Rudykh, K. Bhattacharya and G. deBotton, "Snap-through actuation of thick-wall electroactive balloons." *International Journal of Non-Linear Mechanics*, 2011. <http://dx.doi.org/10.1016/j.ijnonlinmec.2011.05.006> 3. S. Rudykh and G. deBotton, "Stability of Anisotropic Electroactive Polymers with Application to Layered Media." *Zeitschrift für angewandte Mathematik und Physik*, 2011. <http://dx.doi.org/10.1007/s00033-011-0136-1> 4. S. Rudykh, A. Lewinstein, G. Uner and G. deBotton, "Giant Enhancement of the Electro-mechanical Coupling in Soft Heterogeneous Dielectrics." 2011 <http://arxiv.org/abs/1105.4217v1>

12:51PM Q52.00009 Modeling of dielectric elastomeric materials: theory, finite element simulation, and applications, DAVID HENANN, KATIA BERTOLDI, School of Engineering and Applied Science, Harvard University — Elastomeric materials that undergo large deformations in response to an electric field have garnered attention in recent years. Applications of these dielectric elastomeric materials include actuators capable of converting electrical energy to mechanical work and energy harvesting devices that convert mechanical energy into electrical energy. Furthermore, dielectric elastomers exhibit interesting instabilities, especially under constrained geometries, opening the door for possible applications in active surfaces. Interest has increased in the mechanics community concerning the formulation of a finite-deformation constitutive theory for an electro-mechanically-coupled material. While the details of the formulation of such a theory are beginning to come into focus in the literature, numerical techniques for solving these equations are in their infancy. In this work, we have developed a finite-element-based numerical simulation capability for dielectric elastomers. This talk will highlight the application of our numerical simulation capability to dielectric elastomeric actuators, energy harvesting devices, as well as instabilities of small dielectric elastomeric structures on a constraining substrate.

1:03PM Q52.00010 Giant linear voltage-induced deformation of a dielectric elastomer actuator, JIAN ZHU, School of Engineering and Applied Sciences, Harvard University, MATTHIAS KOLLOSCH, GUGGI KOFOD, University of Potsdam, Germany, ZHIGANG SUO, School of Engineering and Applied Sciences, Harvard University — For dielectric elastomers, one of the most conspicuous attributes is large deformation of actuation induced by voltage. However, electromechanical instability may limit their deformation. In this seminar, I will illustrate how dielectric elastomers survive or eliminate electromechanical instability, through mechanical designs. For example, I will analyze a dielectric elastomer with a "pure shear" boundary condition. The membrane is first prestretched along the transverse direction, and then fixed by a rigid bar. As a result, the stretch in transverse direction is fixed, and the membrane can only be actuated along the vertical direction. The theory shows that the actuator can avert electromechanical instability, and achieve a giant linear deformation of actuation. The experiments confirm the theoretical predictions. For SEBS material, the linear strain of actuation can be 80%. For VHB material, the linear strain of actuation can be 300%. The actuator shows advantages compared to the classic designs (say, tube and circular actuators), and can be used as artificial muscles in soft robots.

1:15PM Q52.00011 Geometry-induced rigidity in pressurized elastic shells, PEDRO REIS, Massachusetts Institute of Technology, BASTIAAN FLORIJN, MIT and Leiden University, ARNAUD LAZARUS, MIT — We study the indentation of pressurized thin elastic shells, with positive Gauss curvature. In our precision desktop-scale experiments, the geometry of the shells and their material properties are custom-controlled using rapid prototyping and digital fabrication techniques. The mechanical response is quantified through load-displacement compression tests and the differential pressure is set by a syringe-pump system under feedback control. Focus is given to the linear regime of the response towards quantifying the geometry-induced rigidity of pressurized shells with different shapes. We find that this effective stiffness is proportional to the local mean curvature in the neighborhood of the locus of indentation. Combining classic theory of shells with recent developments by D. Vella et al. (2011), we rationalize the dependence of the geometry-induced rigidity on: i) the mean curvature at the point of indentation, ii) the material properties of the shell and iii) the in-out differential pressure. The proposed predictive framework is in excellent agreement with our experiments, over a wide range of control parameters. The prominence of geometry in this class of problems points to the relevance and applicability of our results over a wide range of lengthscales.

1:27PM Q52.00012 S-cones in thin shells under indentation, ALICE NASTO, Massachusetts Institute of Technology, AMIN AJDARI, Northeastern University, ARNAUD LAZARUS, MIT, ASHKAN VAZIRI, Northeastern University, PEDRO REIS, MIT — We perform a hybrid experimental and numerical investigation of the localization of deformation in indented thin spherical elastic shells. Past the initial linear response, an inverted cap develops as a Pogorelov circular ridge. For further indentation, this ridge loses axis-symmetry and sharp points of localized curvature form. We refer to these localized objects as *s-cones* (for shell-cones), in contrast with their developable cousins in plates (*d-cones*). We quantify the effect of systematically varying the indenter's radius of curvature (from point to plate load) on the formation and evolution of *s-cones*. In our precision desktop-scale experiments we use rapid prototyped elastomeric shells and rigid indenters of various shape. The mechanical response is measured through load-displacement compression tests and the deformation process is further characterized through digital imaging. In parallel, the experimental results are contrasted against nonlinear Finite Element simulations. Merging these two complementary approaches allows us to gain further physical insight towards rationalizing this geometrically nonlinear process.

1:39PM Q52.00013 Folding and buckling pathways in spherical shells with soft spots, JAYSON PAULOSE, Harvard School of Engineering and Applied Sciences, Cambridge, MA 02138, DAVID NELSON, Department of Physics, Harvard University, Cambridge, MA 02138 — Thin elastic spherical shells subject to an external pressure undergo a buckling transition when the pressure reaches a critical value. Past the buckling instability, the shell typically takes on a shape with one or more inversions that focus the elastic deformation energy within narrow circular regions on the sphere. These inversions are associated with large volume changes and hysteresis, and their location is highly sensitive to very slight imperfections in the sphere. Recently, it has been demonstrated [1] that natural pollen grains have evolved soft sectors in their hard outer walls which guide them toward particular folding pathways when their internal volume is reduced due to desiccation, thus avoiding sudden and uncontrolled changes in shape. Motivated by these results, we study the effect of circular soft spots on the buckling of otherwise uniform spherical shells. Through a combination of scaling arguments and numerical simulations, we demonstrate that the shell can be tuned to follow distinct buckling pathways by varying the size and stiffness of the soft spot. [1] E. Katifori et al, *Proc. Natl. Acad. Sci. USA* **107**, 7635 (2010)

1:51PM Q52.00014 Buckliballs: Buckling-Induced Pattern Transformation of Structured Elastic Shells, KATIA BERTOLDI, JONGMIN SHIM, SEAS, Harvard Univ, CLAUDE J. PERDIGOU, MIT, ELIZABETH R. CHEN, University of Michigan at Ann Arbor, PEDRO M. REIS, MIT — We present a class of continuum shell structures, the buckliball, which, undergo a structural transformation induced by buckling under pressure loading. The geometry of the buckliball comprises a spherical shell patterned with a regular array of circular voids. Moreover, we show that the buckling-induced pattern transformation is possible only with five specific hole arrangements. These voids are covered with a thin membrane, thereby making the ball air tight. Beyond a critical internal pressure, the thin ligaments between the voids buckle leading to a cooperative buckling cascade of the skeleton of the ball. Both precision desktop-scale experiments and finite element simulations are used to explore the underlying mechanics in detail and proof of concept of the proposed structures. We find excellent qualitative and quantitative agreement between experiments and simulations. This pattern transformation induced by a mechanical instability opens the possibility for reversible encapsulation, over a wide range of length scales.

2:03PM Q52.00015 Wrinkling of a collapsing viscous bubble, JAMES BIRD, Boston University, HOWARD STONE, Princeton University, JOHN BUSH, Massachusetts Institute of Technology — Thin-sheets of sufficiently viscous liquid can behave similar to elastic sheets and buckle under certain external forces. A classic example is the “parachute instability” for which a ruptured viscous bubble wrinkles as it relaxes, with the explanation for the wrinkles being based on the liquid film falling under its own weight. In this talk we revisit the viscous bubble-bursting experiments and demonstrate that gravity is responsible for neither the collapse nor the resulting wrinkling instability. Using a combination of experiments and theory, we highlight the importance of capillary forces and elucidate their role in the wrinkling instability.

Wednesday, February 29, 2012 11:15AM - 2:15PM – Session Q53 DCMP: Packing, Self-Assembly, and Granular Memory 153B

11:15AM Q53.00001 Cooperative effects in DNA nanotile attachment, CORINNA MAASS, LANG FENG, TONG WANG, RUOJIE SHA, NADRIAN SEEMAN, PAUL CHAIKIN, NYU — In the context of realising a DNA nanotile system capable of exponentially replicating an information string encoded in a tile pattern with the aid of thermal and UV cycling [1], we encountered the problem of predicting the hybridisation transition temperatures of DNA tile pairs with multiple single strand connectors (sticky ends). For the common single-helix hybridisation transition, sufficiently accurate predictions can be derived from SantaLucia’s nearest-neighbour parameter analysis [2]. However, the case of several DNA strands hybridising cooperatively while attached to a rigid object is entropically different and we had to develop a method to factor in the resulting phase space restrictions (cf. a similar approach for DNA-covered colloids [3]). We were able to test our thermodynamic model by fluorescently labelling DNA tile pairs with variable numbers of sticky ends and recording the hybridisation transition using FRET. The data fit our prediction within an acceptable parameter range.

[1] T. Wang et al., *Nature*, 478(7368):225–228, 2011;

[2] J. SantaLucia, *PNAS*, 95(4):1460–1465, 1998

[3] R. Dreyfus et al.; *Phys. Rev. Lett.*, 102(4):048301, 2009.

11:27AM Q53.00002 Minimal energy packings of weakly semiflexible polymers: Application to targeted self-assembly of nanostructures¹, JARED HARWAYNE-GIDANSKY, Electrical Engineering and Integrated Graduate Program in Physical and Engineering Biology, Yale University, ROBERT S. HOY, COREY S. O’HERN, Mechanical Engineering & Materials Science, and Physics, Yale University — Using exact enumeration, we characterize how structure, mechanical and thermodynamic stability of minimal energy packings of short “sticky tangent sphere” (SHS) polymer chains vary with angular interaction strength k_b and equilibrium bond angle θ_0 . While flexible SHS polymers possess highly degenerate ground states (i. e. many differently ordered “macrostates” [1]), angular interactions dramatically break this degeneracy. The macrostate associated with the ground state semiflexible packing changes as k_b and θ_0 are varied. Further degeneracy breaking arises from angular interactions’ influence on packing size, asymmetry, and vibrational entropy. The strength of these effects increases with chain length N . Our exact analysis provides design principles for self-assembly of polymers into a variety of structures that can be tuned by varying N , k_b and θ_0 .

[1] R. S. Hoy and C. S. O’Hern, *Phys. Rev. Lett.* **105**, 068001 (2010).

¹Support from NSF Award No. DMR-1006537 is gratefully acknowledged.

11:39AM Q53.00003 Self-assembly of Low-coordinated Ground States via Monotonic Pair Potentials, ETIENNE MARCOTTE, FRANK H. STILLINGER, SALVATORE TORQUATO, Princeton University — Monotonically decreasing radially symmetric pair potentials can lead to the self assembly of unusual low-coordinated ground states. The states include, but are not limited to, the square, honeycomb, and simple cubic crystals in two and three-dimensional Euclidean spaces R^2 and R^3 . We can determine optimal potentials for targeted ground states using inverse statistical mechanical techniques. Using a linear programming method, we are able to search over a wide parameter space while still enforcing constraints such as monotonicity and convexity on optimized potentials. The features present in the classes of short-ranged potentials that conform to these constraints suggest sufficient requirements for colloids to self assemble into a desired ground state.

11:51AM Q53.00004 Dense packings of spheres in cylinders, ADIL MUGHAL, Aberystwyth University, HO-KEI CHAN, DENIS WEAIRE, STEFAN HUTZLER, AARON MEAGHER, Trinity College Dublin — We develop a simple analytical theory that relates dense hard sphere packings in a cylinder to corresponding disk packings on its surface. It applies for ratios $R=D/d$ (where d and D are the diameters of the hard spheres and the bounding cylinder, respectively) up to $R=2.738$. Within this range the densest packings are such that all spheres are in contact with the cylindrical boundary. The detailed results elucidate extensive numerical simulations by others and ourselves by identifying the nature of various competing phases. We also present results for the regime R greater than 2.738. These preliminary results explore packings that include internal spheres (i.e. spheres that do not contact the cylinder). This is done through a combination of experiments and numerical simulation (simulated annealing). Our experiments involve the packing of monodisperse bubbles in narrow micron-sized capillaries. Such “wet foams” are an excellent model of the hard sphere packing problem and are analyzed by X-ray tomography to provide structural information.

12:03PM Q53.00005 Novel structures from the densest binary sphere packings, ADAM HOPKINS, YANG JIAO, FRANK STILLINGER, SALVATORE TORQUATO, Princeton University — The densest binary sphere packings have historically been very difficult to determine. The only rigorously known packings in the α - x plane of small to large sphere radius ratio α and small sphere relative concentration x are at the Kepler limit $\alpha \rightarrow 1$, where packings are monodisperse. Utilizing an implementation of the Torquato-Jiao linear programming algorithm, we find many distinct families of novel densest binary packings and construct a phase diagram for all known densest packings over the α - x plane. In particular, these families of densest binary packings are examples of complicated, mechanically stable structures that can appear in colloidal systems without any anisotropic or attractive interactions.

12:15PM Q53.00006 Random and ordered phases of off-lattice rhombus tiles¹, STEPHEN WHITELAM, ISAAC TAMBLYN, Molecular Foundry, Lawrence Berkeley National Lab, PETER BETON, JUAN GARRAHAN, School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, UK — We study the covering of the plane by non-overlapping rhombus tiles, a problem well-studied only in the limiting case of dimer coverings of regular lattices. We go beyond this limit by allowing tiles to take any position and orientation on the plane, to be of irregular shape, and to possess different types of attractive interactions. Using extensive numerical simulations we show that at large tile densities there is a phase transition from a fluid of rhombus tiles to a solid packing with broken rotational symmetry. We observe self-assembly of broken-symmetry phases, even at low densities, in the presence of attractive tile-tile interactions. Depending on tile shape and interactions the solid phase can be random, possessing critical orientational fluctuations, or crystalline. Our results suggest strategies for controlling tiling order in experiments involving “molecular rhombi.”

¹This work was supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

12:27PM Q53.00007 Structure and stability of finite sphere packings via exact enumeration¹,

ROBERT S. HOY, Departments of Mechanical Engineering & Materials Science, and Physics, Yale University, JARED HARWAYNE-GIDANSKY, Department of Electrical Engineering and Integrated Graduate Program in Physical and Engineering Biology, Yale University, COREY S. O'HERN, Departments of Mechanical Engineering & Materials Science, and Physics, Yale University — We analyze the geometric structure and mechanical stability of complete sets of isostatic and hyperstatic sphere packings obtained via exact enumeration techniques. The number of nonisomorphic isostatic packings grows exponentially with the number of spheres N , and the fraction of packings possessing soft modes (for “sticky” spheres with contact attractions) grows faster. The diversity of structure and symmetry increases with N and decreases with the degree of hyperstaticity. We further show that maximally contacting packings are in general neither the densest nor the most symmetric. Our studies of the geometry of complete sets of sphere packings provide a basis for future work on ground and metastable states in systems with hard-core plus short-range attractive interactions including attractive colloids, collapsed proteins, and jammed particulate media.

¹Support from NSF Award No. DMR-1006537 is gratefully acknowledged.

12:39PM Q53.00008 Fabrication of sophisticated two-dimensional organic nanoarchitectures thought hydrogen bond mediated molecular self assembly¹,

FABIEN SILLY, CEA Saclay — Complex supramolecular two-dimensional (2D) networks are attracting considerable interest as highly ordered functional materials for applications in nanotechnology. The challenge consists in tailoring the ordering of one or more molecular species into specific architectures over an extended length scale with molecular precision. Highly organized supramolecular arrays can be obtained through self-assembly of complementary molecules which can interlock via intermolecular interactions. Molecules forming hydrogen bonds (H-bonds) are especially interesting building blocks for creating sophisticated organic architectures due to high selectivity and directionality of these bindings. We used scanning tunnelling microscopy to investigate at the atomic scale the formation of H-bonded 2D organic nanoarchitectures on surfaces. We mixed perylene derivatives having rectangular shape with melamine and DNA base having triangular and non symmetric shape respectively. We observe that molecule substituents play a key role in formation of the multicomponent H-bonded architectures. We show that the 2D self-assembly of these molecules can be tailored by adjusting the temperature and molecular ratio. We used these stimuli to successfully create numerous close-packed and porous 2D multicomponent structures.

¹The research leading to these results has received funding from the European Research Council under the European Union's Seventh Framework Programme (FP7/2007-2013) / ERC grant agreement no 259297.

12:51PM Q53.00009 Exploiting Mixed Self-Assembled Monolayers for Design and Fabrication of Patchy Particles¹,

INES PONS-SIEPERMANN, SHARON GLOTZER, Department of Chemical Engineering, University of Michigan — Previous computational studies [1,2] explained the formation of patterns (stripes and patches) in binary mixtures of immiscible surfactants adsorbed on gold nanoparticles [3]. These patterns can confer to the particles unexpected properties, including novel wetting behavior [4]. As an extension of those studies, we performed atomistic and mesoscale simulations of ternary and quaternary mixed self-assembled monolayers (SAMs) on nanosphere surfaces. Here we present predictions for new and unexpected patterns for patchy particles that could be synthesized through judicious choice of surfactant architecture, nanoparticle geometry, and SAM stoichiometry.

[1] C. Singh et al. Physical Review Letters 99, 226106 (2007)

[2] C. Singh et al. Nanoscale 3, 3244-3250 (2011)

[3] A.M. Jackson et al. Nature Materials, 3, 330-336 (2004)

[4] J.J. Kuna et al. Nature Materials, 8, 837-842 (2009)

¹Supported by Defense Threat Reduction Agency Grant HDTRAI-09-1-0012 and James S. McDonnell Foundation 21st Century Science Research Award/Studying Complex Systems.

1:03PM Q53.00010 Entropy density and Mutual Information measures to quantify the complexity of a nanoscale system ,

ILYA GRIGORENKO, VINCENT CRESPI, Penn State — Information-theoretic approach is the most general way to quantify complexity of nanoscale systems. In this study the entropy density and mutual information measures were used to identify the optimal interaction parameters between nanoparticles, which lead to the maximum geometric complexity of self-assembled nanostructures. A generalization of complexity measures at a finite temperature and for nonequilibrium systems is also presented. The developed theory can be used for efficient in silico design of new self-assembled nanostructures with a complex geometry not achievable before.

1:15PM Q53.00011 Road Usage Heterogeneity and Mitigation of Traffic Congestion ,

MARTA C. GOMZALEZ, PU WANG, MIT — Road networks form the backbone of the social and economic life of a city. Until recently, however, data have not been available to study the impact of trip selection on traffic congestion at an urban scale. To that end, we combined the most complete record of daily trips with the detailed road GIS data to analyze the road usage patterns in two US metropolitan areas. We classify the importance of road segments based on their ability to attract drivers from diverse sources and find that most of them are mainly used by drivers from very few sources. Thanks to this heterogeneity, we find that it is possible to design an efficient strategy to largely reduce the travel time in the road system.

1:27PM Q53.00012 Rippling “instability” in granular jet impact is a memory effect ,

NICHOLAS GUTTENBERG, WENDY ZHANG, JAKE ELLOWITZ, University of Chicago — Experiments and simulations of a dense granular jet impacting a target give rise to a collimated outflow despite the lack of cohesion in the system. This outflow eventually breaks up far away from the target. The breakup, however, is not a uniform dilution but rather takes the form of a series of wave-like undulations with a wavelength much larger than the grain scale. We investigate the possibility that this is another continuum hydrodynamic analog reproduced by bulk granular motion using 2D simulations. We find that these waves, unlike a Helmholtz instability, cannot readily be nucleated by perturbations of the granular flow surface. Instead, we find that they point to relics of the velocity fluctuations caused by the impact itself. We show that the ripples are an effect of the effectively ballistic flow far from the target remembering these original velocity fluctuations.

1:39PM Q53.00013 Transient Memories in Non-Equilibrium Disordered Systems ,

JOSEPH PAULSEN, SIDNEY NAGEL, University of Chicago — Some non-equilibrium systems can store information of their external driving in an unexpected manner. They “learn” multiple driving amplitudes that can subsequently be read out. Notably, only one memory is retained after many driving cycles, even if all of the amplitudes are continually fed in. This behavior has been observed in diverse scenarios such as traveling charge-density waves [1] and simulations of sheared suspensions [2]. Here we explore this latter system experimentally using a suspension of neutrally buoyant non-Brownian particles in a very viscous fluid that is sheared cyclically in a Couette cell geometry. Starting from a random configuration, the particle trajectories are irreversible at first but, as had been shown [3], eventually settle into a configuration where they retrace their paths exactly during each cycle. We show that the resulting configuration comprises a memory of the driving amplitude, which can be read out by measuring the degree of particle reversibility versus shear amplitude. We also discuss this system's capacity for storing multiple memories.

[1] S. N. Coppersmith et al., PRL 78, 3983 (1997).

[2] N. C. Keim, S. R. Nagel, PRL 107, 010603 (2011).

[3] L. Corté, P. M. Chaikin, J. P. Gollub, D. J. Pine, Nature Phys. 4, 420 (2008).

1:51PM Q53.00014 Role of interaction in the formation of memories in paste , AKIO NAKAHARA, YOUSUKE MATSUO, Nihon University — A densely packed colloidal suspension with plasticity, called paste, remembers the directions of vibration and flow. These memories in paste can be visualized by the morphology of desiccation crack patterns. We investigate the role of interaction in the formation of memories in paste. First, interparticle attractive forces, such as van der Waals interaction, are needed to construct a macroscopic network structure with plasticity. With the help of attractive interaction, a water-poor paste remembers the direction of vibration and a water-rich paste remembers the flow direction [1]. When particles are charged in water, however, Coulombic repulsive interaction prevents formation of dilute network structure under flow, which leads to the experimental result that a water-rich charged paste cannot remember flow direction. Addition of sodium chloride to such a paste gives the ability to remember flow direction due to the screening effect of Coulombic repulsive interaction between particles [2].

[1] A. Nakahara, Y. Shinohara and Y. Matsuo, J. Phys.: Conf. Ser. 319 (2011) 012014.

[2] Y. Matsuo and A. Nakahara, arXiv:1101.0953v1 [cond- mat.soft].

2:03PM Q53.00015 Resonances arising from hydrodynamic memory - The Color of Brownian motion , SYLVIA JENEY, MATTHIAS GRIMM, FLAVIO MOR, LASZLO FORRO, Ecole Polytech Fed de Lausanne, THOMAS FRANOSCH, Universitaet Erlangen-Nuernberg — Observation of the Brownian motion of a small probe interacting with its environment is one of the main strategies to characterize soft matter. Initially, the particle is driven by rapid collisions with the surrounding solvent molecules, referred to as thermal noise. Later, the friction between the particle and the viscous solvent damps its motion. Conventionally, thermal force is taken to be characterized by a Gaussian white noise spectrum. The friction is assumed to be given by the Stokes drag, suggesting that motion is overdamped at long times, when inertia becomes negligible. Here, we measured the noise spectrum of the thermal forces by tracking with high resolution a single micron-sized sphere suspended in a fluid, and confined by a stiff optical trap [1]. Coupling between sphere and fluid gives rise to hydrodynamic memory [2] and a resonance, equivalent to a colored peak in the power spectral density of the sphere's thermal fluctuations. Our results reveal that motion is not overdamped, even at long times. In view to exploit the particle-fluid-trap system as a nanomechanical resonator, we disentangle the two regimes in which the detected resonance is either sensitive to the fluid properties or to the particle's mass.

[1] Jeney et al. Nature 2011.

[2] Jeney et al. PRL 2008.

Wednesday, February 29, 2012 11:15AM - 2:15PM – Session Q54 DCMF: Superconductivity: Mesoscopic and Nanometer Scale 152

11:15AM Q54.00001 Designing high-impedance/low-noise superinductances for quantum electronics¹ , IOAN POP, ZLATKO MINEV, NICHOLAS MASLUK, ARCHANA KAMAL, MICHEL DEVORET, Yale University, Applied Physics — Superinductances are essential circuit elements which enable the suppression of charge fluctuations in superconducting fluxonium qubits [1] and in other Josephson junction devices [2]. Commonly implemented as an array of Josephson junctions, superinductances have two main limitations. Firstly, the spurious capacitive coupling of the chain islands to ground lowers the plasma frequency of the chain, and consequently limits the operational bandwidth. Secondly, coherent quantum phase-slips (CQPS) [3] in the Josephson junction chain induce time dependent inductance fluctuations via the Aharonov-Casher effect [4]. We present the application of a novel lithographic technique [5] which enables the fabrication of arrays with optimal junction-capacitance to ground-capacitance ratio. We also present new superinductance designs which topologically suppress the CQPS, allowing the implementation of practically phase-slip free high inductance Josephson junction.

[1] Manucharyan et al., Science, 326 (2009)

[2] Guichard and Hekking, PRB, 81 (2010)

[3] Matveev et al. PRL, 89 (2002)

[4] Pop et al., arXiv:1105.6204 and Manucharyan et al., arXiv:1012.1928

[5] Lecocq et al., Nanotechnology, 22 (2011)

¹Work supported by IARPA, ARO and NSF.

11:27AM Q54.00002 Powerful coherent terahertz emission from $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ mesa array¹ , TIMOTHY BENSEMAN, KEN GRAY, ALEXEI KOSHELEV, WAI-KWONG KWOK, ULRICH WELP, Materials Science Division, Argonne National Laboratory, HIDETOSHI MINAMI, KAZUO KADOWAKI, Institute for Materials Science, University of Tsukuba, Japan, TAKASHI YAMAMOTO, Quantum Beam Science Directorate, Japan Atomic Energy Agency — Stacks of intrinsic Josephson junctions (IJJs) in high-temperature superconductors enable the fabrication of compact sources of coherent THz-radiation. Here we demonstrate 150 microwatts of radiation power at 0.51 THz, using three synchronized stacks patterned on a single $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ crystal. The emitted power scales roughly as the square of the number of energized stacks, while the total power spectrum is monochromatic to within observational limits. These results imply that the stacks radiate coherently.

¹This research was funded by the Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

11:39AM Q54.00003 DC SQUID RF magnetometer with 200 MHz bandwidth¹ , VLADIMIR TALANOV, NESCO LETTSOME, ANTONIO OROZCO, Neocera, LLC, Beltsville, MD 20705, ALFRED CAWTHORNE, Trevecca Nazarene University, Nashville, TN 37210, VALERY BORZENETS, SLAC National Accelerator Laboratory, Menlo Park, CA 94025 — Because of periodic flux-to-voltage transfer function, Superconducting QUantum Interference Device (SQUID) magnetometers operate in a closed-loop regime [1], which linearizes the response, and increases the dynamic range and sensitivity. However, a transmission line delay between the SQUID and electronics fundamentally limits the closed-loop bandwidth at 20 MHz [1], although the intrinsic bandwidth of SQUIDS is in gigahertz range. We designed a DC SQUID based RF magnetometer capable of wideband sensing coherent magnetic fields up to 200 MHz. To overcome the closed-loop bandwidth limitation, we utilized a low-frequency flux-modulated closed-loop to simultaneously lock the quasi-static magnetic flux and provide AC bias for the RF flux. The SQUID RF voltage is processed by RF electronics based on a double lock-in technique. This yields a signal proportional to the amplitude and phase of the RF magnetic flux, with more than four decades of a linear response. For YBaCuO SQUID on bi-crystal SrTiO substrate at 77 K we achieved a flux noise density of $4 \mu\Phi_0/\sqrt{\text{Hz}}$ at 190 MHz, which is similar to that measured at kHz frequencies with conventional flux-locked loop. [1] D. Drung, *et al.*, Supercond. Sci. Technol. **19**, S235 (2006).

¹This work has been supported by NSF-SBIR IIP-0924610.

11:51AM Q54.00004 Wideband S-parameter characterization of DC-SQUID amplifiers at GHz frequencies, LEONARDO RANZANI, LAFE SPIETZ, JOSE AUMENTADO, NIST, Boulder — Superconducting quantum interference devices (SQUIDs) are widely used as gain elements to achieve ultra-low noise amplification from DC to microwave frequencies. SQUID amplifiers typically have high input and output stray reactance and therefore proper impedance matching is needed to couple enough power into the device. Broadband impedance matching could be obtained by measuring the microwave S-parameters of a SQUID amplifier and then treating it as an equivalent “black box” to which standard microwave design techniques can be applied. In this talk measurement results of the full 2-port S-parameter matrix of DC-SQUID amplifiers operating at 20mK will be presented. Accurate microwave calibration was performed with an automated Through-Reflect-Line (TRL) calibration system, operating at 20mK. Input and output reflection coefficients as well as forward and backward transmission were characterized in the 1 to 8GHz range. Implications for the design of wideband SQUID amplifiers and device stability will be discussed.

12:03PM Q54.00005 Characterization of Low Noise Superconducting Microwave Amplifiers, TED WHITE, University of California Santa Barbara, R. BAREND, J. BOCHMANN, B. CHIARO, Y. CHEN, J. KELLY, M. LENANDER, E. LUCERO, M. MARIANTONI, A. MEGRANT, C. NEILL, P. O'MALLEY, P. ROUSHAN, D. SANK, A. VAINSENER, J. WENNER, Y. YIN, ANDREW CLELAND, JOHN M. MARTINIS, UC Santa Barbara — We have developed an experimental setup to characterize low noise amplifier chains with a six port low temperature microwave switch controlled via room temperature electronics. This switch allows us to do a traditional Y-factor measurement, a reflection measurement with an open input, or a measurement using a Shot Noise Tunnel Junction (SNTJ) device developed by J. Aumentado and L. Spietz at NIST. The SNTJ allows one to measure system gain, system noise, and junction temperature as fit parameters. The SNTJ is sensitive enough to characterize amplifiers with noise due primarily to photon ground state fluctuations or quantum limited amplifiers. We first tested our setup using a HEMT and room temperature amplifier chain with calibrated noise and gain characteristics. We then characterized several iterations of the theoretically quantum limited SLUG amplifier developed by R. McDermott at U Wisconsin Madison.

12:15PM Q54.00006 Shot noise measurements in diffusive wire NSN structures¹, MARTIN STEHNO, D.J. VAN HARLINGEN, University of Illinois at Urbana-Champaign — Subgap transport across a normal metal/superconductor interface requires a conversion from normal to supercurrent. We study the conversion process in superconducting wire samples by attaching two short diffusive normal metal wires at a distance comparable to the coherence length in the superconductor. In addition to ordinary Andreev reflection, nonlocal processes involving electronic states in both contacts (Crossed Andreev reflection, and Elastic Co-tunneling) are expected to contribute and to give rise to a cross-conductance signal in transport measurements. As one of the wire contacts is biased into the shot noise regime, a significant increase of current fluctuations is observed in the other (unbiased) contact. Only a small fraction of the noise measured in the two contacts is correlated. The magnitude of the correlated signal scales with the observed cross-conductance. We will compare our results with theoretical predictions for nonlocal transport and previous experimental work.

¹Work supported by the National Science Foundation grant DMR 06-05813

12:27PM Q54.00007 Toward a Passive Lossless on-Chip Circulator in the 4-8 GHz Range, LAFE SPIETZ, JOSE AUMENTADO, NIST — We present further progress toward constructing a passive microwave circulator from Josephson junction circuits. We have designed, built and tested a circuit which demonstrates the basic properties required to construct a gyrator in the 4-8 GHz range. We describe the theory and present the data on this circuit and point to the path from these results to practical passive lossless on-chip circulators.

12:39PM Q54.00008 Calibration of a Microfabricated Phonon Spectrometer, JARED HERTZBERG, OBAFEMI OTELAJA, RICHARD ROBINSON, Cornell University, Department of Materials Science and Engineering — Non-thermal distributions of phonons may be locally excited and detected in silicon micro- and nanostructures by decay of quasiparticles injected into an adjacent superconducting tunnel junction [1]. Using this technique, narrow frequency bands of phonons may be isolated and applied to investigate phonon transport through nanostructures at sub-kelvin temperatures [2]. In our prototype phonon spectrometer we have demonstrated spatial resolution below 1 micron and frequency resolution of 10 GHz. We describe ways to control the spatial resolution, frequency resolution, frequency range, dynamic range and signal-to-noise ratio in this technique, by using different superconducting materials in the tunnel junctions and by inserting absorber materials into the phonon transmission path. This work is supported by DOE (DE-SC0001086).

[1] H. Kinder. Phys. Rev. Lett. 28, 1564 (1972)

[2] J. B. Hertzberg et al, Rev. Sci. Instr. 82, 104905 (2011).

12:51PM Q54.00009 Microwave Spectroscopy of a Cooper-Pair Transistor Coupled to a Lumped-Element Resonator, MATTHEW BELL, LEV IOFFE, MICHAEL GERSHENSON, Department of Physics and Astronomy, Rutgers, the State University of New Jersey — We have studied the microwave response of a single Cooper-pair transistor (CPT) coupled to a lumped-element microwave resonator. The resonance frequency of this circuit, f_r , was measured as a function of the charge n_g induced on the CPT island by the gate electrode, and the phase difference across the CPT, ϕ_B , which was controlled by the magnetic flux in the superconducting loop containing the CPT. The observed $f_r(n_g, \phi_B)$ dependences reflect the variations of the CPT Josephson inductance with n_g and ϕ_B as well as the CPT excitation when the microwaves induce transitions between different quantum states of the CPT. The results are in excellent agreement with our simulations based on the numerical diagonalization of the circuit Hamiltonian. This agreement over the whole range of n_g and ϕ_B is unexpected, because the relevant energies vary widely, from 0.1K to 3K. The observed strong dependence $f_r(n_g, \phi_B)$ near the resonance excitation of the CPT provides a tool for sensitive charge measurements.

1:03PM Q54.00010 Superconducting Low-Inductance Undulatory Galvanometer Microwave Amplifier: Theory, DAVID HOVER, GUILHEM RIBEILL, YUNG-FU CHEN, SHAOJIANG ZHU, ROBERT MCDERMOTT, University of Wisconsin-Madison — We present numerical studies of a phase-insensitive microwave linear amplifier based on the Superconducting Low-Inductance Undulatory Galvanometer (SLUG). Direct integration of the junction equations of motion provides access to the full scattering matrix of the SLUG element. We discuss the optimization of SLUG amplifiers and calculate amplifier gain and noise temperature in both the thermal and quantum regimes. The microwave SLUG amplifier is expected to achieve noise performance approaching the standard quantum limit in the frequency range from 5-10 GHz, with gain around 15 dB for a single-stage device and instantaneous bandwidth of order hundreds of MHz. We compare our numerical model with measured performance of state-of-the-art devices.

1:15PM Q54.00011 Superconducting Low-inductance Undulatory Galvanometer Microwave Amplifier, SHAOJIANG ZHU, DAVID HOVER, GUILHEM RIBEILL, YUNG-FU CHEN, ROBERT MCDERMOTT, University of Wisconsin — We describe a novel microwave linear amplifier based on the Superconducting Low-inductance Undulatory Galvanometer (SLUG). The compact SLUG element is straightforward to model at microwave frequencies, allowing separate optimization of the SLUG element and the resonant input matching network; we expect optimized devices based on high-Jc junctions to achieve gains around 15 dB in the range from 5-10 GHz, with instantaneous bandwidth of order hundreds of MHz and noise performance approaching the standard quantum limit. Using amplifiers based on low-Jc Al/AIO_x/Al junctions, we have achieved gain in excess of 20 dB at 3 GHz and greater than 15 dB at 9 GHz with bandwidth of several MHz. We discuss progress toward the incorporation of high-Jc Nb/AIO_x/Nb junctions in the SLUG amplifier, and describe strategies to promote the thermalization of the SLUG shunt resistors at dilution refrigerator temperatures by integrating large-volume normal metal cooling fins with the shunts.

1:27PM Q54.00012 Development and Implementation of a 1 GHz SQUID amplifier for the Axion Dark Matter Experiment, ANDREW WAGNER, University of Washington, AXION DARK MATTER EXPERIMENT COLLABORATION — The Axion Dark Matter eXperiment (ADMX) was designed to detect ultra-weakly interacting relic axion particles by searching for their conversion to microwave photons in a resonant cavity positioned in a strong magnetic field. Given the extremely low expected axion-photon conversion power we have designed, built and operated a microwave receiver based on a Superconducting QUantum Interference Device (SQUID). We describe the implementation of a SQUID amplifier in the ADMX microwave receiver chain and discuss progress made at the Washington Micro-Fabrication Facility toward the production of SQUID amplifiers from a Nb – Al_xO_y – Nb trilayer.

1:39PM Q54.00013 Quantum pumping of electrons at the Josephson frequency, FRANCESCO GIAZOTTO, PANAYOTIS SPATHIS, STEFANO RODDARO, SUBHAJIT BISWAS, FABIO TADDEI, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, Piazza S. Silvestro 12, I-56127 Pisa, Italy, MICHELE GOVERNALE, School of Chemical and Physical Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, P.O. B, LUCIA SORBA, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, Piazza S. Silvestro 12, I-56127 Pisa, Italy — A macroscopic fluid pump works according to the law of Newtonian mechanics and transfers a large number of molecules per cycle. By contrast, a nano-scale charge pump can be thought as the ultimate miniaturization of a pump, with its operation being subject to quantum mechanics and with only few electrons or even fractions of electrons transferred per cycle. It generates a direct current in the absence of an applied voltage exploiting the time-dependence of some properties of a nano-scale conductor. So far, nano-scale pumps have been realised only in system exhibiting strong Coulombic effects, whereas evidence for pumping in the absence of Coulomb-blockade has been elusive. Here we report the experimental detection of charge flow in an unbiased InAs nanowire embedded in a superconducting quantum interference device (SQUID). In this system, pumping occurs via the cyclic modulation of the phase of the order parameter of different superconductors. The symmetry of the current with respect to the enclosed flux and SQUID current is a discriminating signature of pumping. Currents exceeding 20 pA are measured at 250 mK, and exhibit symmetries compatible with a pumping mechanism.

1:51PM Q54.00014 NIS cooler platform: from 300 mK to 100 mK, THOMAS AREF, JUHA MUHONEN, HUNG NGUYEN, JOONAS PELTONEN, MATTHIAS MESCHKE, JUKKA PEKOLA, Low Temperature Laboratory, Aalto University, Finland — Normal-insulator-superconducting (NIS) tunnel junctions allow cooling of the normal metal by electrons tunneling across the insulating barrier. With proper biasing, hot electrons leave the normal metal and cold electrons enter from the superconductor, lowering the electronic temperature. The heat dissipation is determined primarily by the quasiparticle relaxation in the superconducting leads. We explore the effects of magnetic field, electrode geometry, direct quasiparticle traps and other fabrication modifications on cooler effectiveness. The overall aim is to produce a general electronic cooler for efficient, solid state, cooling of small devices from 300 to 100 mK.

2:03PM Q54.00015 Implementation and test of an Levitov's n-electron coherent source¹, JULIE DUBOIS, THIBAUT JULLIEN, PREDEN ROULLEAU, FABIEN PORTIER, PATRICE ROCHE, D. CHRISTIAN GLATTLI², Service de Physique de l'Etat Condensé, CEA Saclay — Injecting a controlled number of electrons in a quantum ballistic conductor opens the way to new kind of quantum experiments, yet never done. It is well known that a voltage biased contact applied on a single mode quantum conductor, such as a Quantum Point Contact, inject continuously single electrons at a rate eV/h , a remarkable property of the Fermi sea. Here we consider the injection of electrons during a very short time where is expected that a voltage pulse with $\int eV(t)dt = nh$ injects exactly n-electrons, n being integer. If in addition, if the voltage pulse has the form of a Lorentzian shape in time, Levitov has shown that the n-electron are not accompanied by neutral spurious electron-hole pair excitations and thus form a minimal excitation n-electron source. The electron being indistinguishable if the time-scale is shorter than the coherence time, the Levitov's source is coherent and new quantum experiments involving interference with several electrons become at reach. We present here experimental realization of the n-electron source using short sub-nanosecond pulses and tests of the minimal excitation number using the shot noise created by repeatedly sending n-electrons toward a quantum point realized in clean ballistic 2D electrons. The square-wave, sine-wave and Lorentzian shape pulses are compared. This is also accompanied by photon-assisted current measurements. J. Dubois, T. Jullien, P. Roulleau, F. Portier, P. Roche, and D.C. Glatthi, in preparation.

¹ERC Advanced grant 228273 MeQuaNo

²submitting author, Head of the Nanoelectronics Group.

1:00PM - 1:00PM –
Session S1 Poster Session III (1:00-4:00PM) Exhibit Hall C

S1.00001 APPLICATIONS (IT, Medical/Bio, Photonics, etc.) —

S1.00002 Charge Transport Anisotropy in n-Type Disk-Shaped Triphenylene-Tris(aryleneimidazole)s, STEVEN ALVAREZ, YUE ZHANG, DAVID HANIFI, FRANCISCO ANTONIO, ANDREW PUN, LIANA KLIVANSKY, ALEXANDER HEXEMER, BIWU MA, YI LIU, Lawrence Berkeley National Laboratory — Two novel n-type disk-shaped molecules containing a triphenylene core and three fused naphthaleneimide imidazole or peryleneimide imidazole “arms” are synthesized and characterized. Their optical and electronic properties are consistent with the pi-extended structural feature of the aromatic cores. The n-type charge carrier mobilities of these molecules are evaluated by both field effect transistors and space-charge limited-current measurements, which show drastically different mobility anisotropy. A strong correlation between film morphology and the charge transport behavior is established by X-ray scattering and atomic force microscopic analyses.

S1.00003 Identification of the Amorphous $\text{AlB}_4\text{H}_{11}$ Structure¹, YONGLI WANG, YONGSHENG ZHANG, Northwestern University, XUENIAN CHEN, JI-CHENG ZHAO, The Ohio State University, WEI ZHOU, TERRENCE UDOVIC, National Institute of Standards and Technology, C. WOLVERTON, Northwestern University — In recent experimental work, $\text{AlB}_4\text{H}_{11}$ has been identified as a potential hydrogen storage material with a good desorption temperature and partial reversibility. It is an amorphous, white solid at room temperature and its molecular structure is presently unknown. We combine experimental measurements (NMR, neutron vibrational spectra and IR) and a theoretical structure prediction method to identify the (local) structure of the amorphous $\text{AlB}_4\text{H}_{11}$ phase. The theoretical structure prediction method is a combination of the Monte-Carlo based prototype electrostatic ground state search (PEGS) method and first-principles calculation (DFT). The PEGS+DFT method has successfully predicted many crystalline solid structures, but has never been applied to the prediction of amorphous solid structures. The PEGS predictions of the $\text{AlB}_4\text{H}_{11}$ structure are quite successful: we find the calculated phonon density of states (pDOS) of our PEGS+DFT predicted structures is in close agreement with the experimental vibrational measurements. More broadly, our findings indicate that first-principles theoretical design of new amorphous materials for energy storage is now possible, paving a promising way for similar studies in the future.

¹NSF grant: CBET-0730929 DOE grant: DE-FG36-08GO08136/A003

S1.00004 Influence of xc functional on thermal-elastic properties of metal oxides: A DFT-based Debye-Grüneisen model approach, TAEHUN LEE, ALOYSIUS SOON, Yonsei University, Seoul, Korea — For high-temperature applications, the chemical stability, as well as the mechanical integrity of the oxide material used is of utmost importance. Solving these problems demands a thorough and fundamental understanding of their thermal-elastic properties. In this work, we report density-functional theory (DFT) calculations to investigate the influence of the xc functional on specific thermal-elastic properties of some common oxides CeO_2 , Cu_2O , and MgO . Namely, we consider the local-density approximation (LDA), the generalized gradient approximation due to Perdew, Burke, and Ernzerhof (GGA-PBE), as well as a recently popularized hybrid functional due to Heyd-Scuseria-Ernzerhof (HSE06). In addition, we will also report DFT+ U results where we introduce a Hubbard U term to the Cu $3d$ and the Ce $4f$ states. Upon obtaining the DFT total energies, we then couple this to a volume-dependent Debye-Grüneisen model [1] to determine the thermodynamic quantities of these oxides at arbitrary pressures and temperatures. We find an explicit description of the strong correlation (e.g. via the DFT+ U approach and using HSE06) is necessary to have a good agreement with experimental values. [1] A. Otero-de-la-Roza, D. Abbasi-Pérez et al. *Com. Phys. Com.* 182 (2011) 2232

S1.00005 Towards solar cells combining silicon nanopillars and various semiconductor nanoparticles¹, D. STIEVENARD, CNRS, Y. LAMBERT, ISEN, DI ZHOU, Univ de Lille, T. XU, ISEN, B. GRANDIDIER, N. RAMESH PRATIBHA, F. GOURBILLEAU, CNRS, S. TURRELL, C. KINOWSKI, O. ROBBE, Univ de Lille, G. PAN, R. BOUKHERROUB, CNRS, W. CHEN, R. LARDE, P. PAREIGE, Univ de Rouen, J. HABINSHUTTI, Univ de Lille, IEMN TEAM, CIMAP TEAM, LASIR TEAM, IRI TEAM, GPM TEAM — We have developed solar cells combining silicon nanopillars and various semiconductor nanoparticles-NPs- (silicon or CdSe ones obtained by chemical synthesis or silicon ones obtained by thermal annealing of multilayer structure $\text{Si-SiO}_2(2)/\text{SiN}(x)$ fabricated by reactive magnetron sputtering.). Nanopillars are obtained by standard RIE process using silica spheres as active mask for the etching. NPs are chemically grafted or deposited by Langmuir Blodgett technique on the p-type pillars and therefore covered by a thin polysilicon n type layer. The doping level and of the different interfaces are monitored by 3D Atom Probe Tomography. Photocurrents curve without and with NPs will be presented, evidencing the NPs active role.

¹Work partly supported by DGA contract REI 2008 34 0031.

S1.00006 An Antireflective Top Contact for Optoelectronic Devices Using Niobium Doped Titanium Dioxide, JOHN CHIVERS, THOMAS VANDERVELDE, Tufts University, REAP LABS TEAM — We present an investigation of an integrated top contact system for optoelectronic semiconductor devices (e.g. solar cells, photo-detectors, etc.). Niobium-doped titanium dioxide (TNO) is used as a transparent conductor and a graded $\text{TiO}_2/\text{SiO}_2$ layer with a nanostructured SiO_2 surface is added to suppress reflection and improve durability. TNO was chosen to replace indium tin oxide (ITO), the industry standard transparent conductor, in an effort to reduce dependence on increasingly scarce resources (i.e. indium). TNO offers other potential benefits over ITO, including superior durability, higher index of refraction, and superior transparency in the infrared. The graded antireflective layer takes advantage of the common crystalline structure of TiO_2 and SiO_2 , making fabrication simpler and more reliable than would be possible if the materials had differing structures. The nanostructured SiO_2 surface uses a “moth’s eye” pattern of sub-wavelength-scale cones to create a gradual optical transition from ambient air to the SiO_2 . All materials are deposited using RF magnetron sputtering. Results are compared to current standards and the strengths and weaknesses of the TNO system are discussed.

S1.00007 Thermal Properties of Polarization Switching in Vertical-Cavity Surface-Emitting Lasers, YU-HENG WU, YUEH-CHEN LI, WANG-CHUANG KUO, TSU-CHIANG YEN, Department of Physics, National Sun Yat sen University — This investigation studied the thermal properties of the polarization switching (PS) in vertical-cavity surface-emitting lasers (VCSELs). The studies were performed by experiments. In experiments, the current modulation frequency and ambient temperature of VCSELs were varied to study their thermal effects on PS. The hysteresis loop of polarization switching broadens as the modulation frequency increased and narrows as the modulation frequency decreased. We assumed that PS is activated as the temperature in the active region reaches a certain temperature. The PS of the VCSEL controlled by continuously varied ambient temperature is also studied. The experiments results show that the thermal effect plays a major role in PS and the hysteresis of PS. These results contribute to the understanding of the mechanism of VCSEL’s polarization switching.

S1.00008 Temperature dependence of the null hysteresis loop in polarization switching of vertical-cavity surface-emitting lasers, YUEH-CHEN LI, YU-HENG WU, WANG-CHUANG KUO, TSU-CHIANG YEN, Department of Physics, National Sun Yat sen University — This research investigated the frequency-dependent polarization switching hysteresis loop (PSHL) of vertical-cavity surface-emitting lasers (VCSELs) in constant ambient temperature. The special feature of VCSELs is the polarization switching (PS). In most case, the switching current in the rise and decline bias are not the same, and shows hysteresis. The ambient temperature was controlled in this experiment. The hysteresis loop width of polarization switching disappears as the modulation frequency is lower than a critical frequency. Experimental results show that the critical frequency depends on the ambient temperature. Experimental data presents that the thermal effect plays a major role in the hysteresis of PS. These results greatly contribute to the understanding of the VCSEL’s PSHL.

S1.00009 Linear and nonlinear properties in soft glass optical fibers for device applications, LEILY KIANI, Physics and Chemistry, School of Natural Sciences, University of California, Merced, TILANKA MUNASINGHE, WEN QI ZHANG, SHAHRAAM AFSHAR, Institute for Photonics and Advanced Sensing (IPAS), School of Chemistry and Physics, University of Adelaide, Australia, JAY SHARPING, Physics and Chemistry, School of Natural Sciences, University of California, Merced, APPLIED PHOTONICS GROUP AND INSTITUTE FOR PHOTONICS AND ADVANCED SENSING (IPAS) COLLABORATION — Optical fiber technology is predominantly based on silica glass fibers. Non-silica soft glass fibers exhibit substantially different optical properties such as higher refractive index, larger nonlinear coefficient and structural fabrication flexibility. We aim to exploit these novel properties for device applications such as sensing and light generation. We report measurement of linear dispersion and nonlinear coefficient in the range of $1.5\ \mu\text{m}$ in two custom designed soft glass microstructure optical fibers. The fibers are composed of SF57 (Schott) and Bismuth-doped silica (Asahi Glass Co.) respectively with Hexagonal Wagonwheel microstructure design. These fibers are designed to allow phase matching of nonlinear optical processes near $1.6\ \mu\text{m}$. Our measurements indicate nonlinear coefficients 1000 times that of standard silica fiber. Transverse modes in these fibers are difficult to separate leading to a complicated dispersion results. Next steps include observation of parametric generation and Brillouin gain.

S1.00010 Observation of New Photoluminescence Emission in the YAG Structure and Its significant Effects on the Material Optical Properties¹, FARIDA SELIM, CHRISTOPHER VARNEY, SHERIF REDA, DAVID MACKAY, Washington State University — Yttrium Aluminum Garnets, $\text{Y}_3\text{Al}_5\text{O}_{12}$ (YAG) are widely used as host materials for transition and rare earth elements in laser, optoelectronic and scintillation applications. They are the most important solid state laser host materials and the most promising scintillation materials. New photoluminescence peaks were observed at 700 and 800 nm in undoped yttrium aluminum garnet (YAG) single crystals. This luminescence has great effects on the optical properties of rare-earth doped YAG crystals and their performance in laser and scintillation applications. Photoluminescence measurements revealed a number of luminescence peaks in all YAG crystals regardless of the growth conditions due to native defects and low-level impurities. The strong 700 and 800 nm emissions were attributed to low level of iron impurities as confirmed by Glow Discharge Mass Spectrometry analysis. This study reveals that iron is a native impurity in all YAG crystals that plays a significant role on modifying the optical and scintillation properties of this important class of photonic materials.

¹This work was funded by NSF (DMR 1006772)

S1.00011 Development of new semi-rigid coaxial cables for low temperature experiments, AKIHIRO KUSHINO, Asahikawa National College of Technology, SOICHI KASAI, COAX CO., LTD. — Coaxial cables with seamless outer electrical conductors are promising for low-noise readout from novel cryogenic devices such as superconducting radiation or particle detectors, operating below helium temperature. Low thermal conductance as well as small signal attenuation is essential in wiring with coaxial cables for array detectors consisting of hundreds of pixels. We developed thin semi-rigid coaxial cables employing normal alloys (CuNi, SUS and beryllium copper) and superconducting alloys (NbTi and Nb). Superconducting coaxial cables with outer diameters from 0.86 mm to 2.19 mm showed good superconducting transitions at 9–10 K, and flat attenuation properties up to above 5 GHz.

S1.00012 Investigation of 1/f flux noise in superconducting circuits, A. PUGLIELLI, S. SENDELBACH, Department of Physics, University of Wisconsin-Madison, C.B. EOM, J. PODKAMINER, K.H. CHO, Department of Materials Science and Engineering, University of Wisconsin-Madison, R. MCDERMOTT, Department of Physics, University of Wisconsin-Madison — Low-frequency 1/f flux noise is a dominant source of dephasing in the Josephson phase and flux qubits. Recent work has revealed the presence of a high density of unpaired spins at the surfaces of superconducting thin films; it is now believed that these spins are the source of the noise, although the microscopic noise mechanism is not understood. Here we describe experiments on SQUIDS and Josephson phase qubits designed to shed light on the underlying noise mechanism, and we describe efforts to develop novel materials with reduced levels of noise.

S1.00013 Biompatible gold nanorods conjugated with photosensitizers assisted for photostability and photodestructive ability, WEN-SHUO KUO¹, SHEAN-JEN CHEN², National Cheng Kung University — Light-exposure-mediated higher temperatures that markedly accelerate the degradation of indocyanine green (ICG) in aqueous solutions by thermal decomposition have been a serious medical problem. In this work, we present the example of using gold nanorods (Au NRs) simultaneously serving as photodynamic and photothermal agents to destroy malignant cells. Au NRs were successfully conjugated with hydrophilic photosensitizer, indocyanine green (ICG), to achieve photodynamic therapy (PDT) and photothermal therapy (PTT). We also demonstrated that Au NRs conjugated with ICG displayed high chemical stability and acted as a promising diagnostic probe. Due to its stability even via higher temperatures mediated by laser irradiation, the combination of PDT and PTT proved to be efficiently killing cancer cells as compared to PDT or PTT treatment alone and enhanced the effectiveness of photodestruction and was demonstrated to enhance its photostability.

¹Advanced Optoelectronic Technology Center, Department of Engineering Science, Department of Chemistry

²Advanced Optoelectronic Technology Center, Department of Engineering Science

S1.00014 Encapsulation of Protoporphyrin IX in PGLA for Biological Applications, BRIAN BUI, UT Arlington, NANOBIO-PHYSICS GROUP TEAM — In biological studies, Protoporphyrin IX has been utilized in researching with photodynamic therapy. With different situations that arise, it is beneficial to have products tailored to the given investigation. Here we propose encapsulating Protoporphyrin IX into poly(lactic-co-glycolic acid) (PLGA) with different parameters in hopes of obtaining products with necessary properties, including photoluminescent intensity, size and loading levels. We hypothesize the intensity of Protoporphyrin IX can be tuned, and this study will help to find the conditions for intensity change. We use chloroform and PVA solutions in the emulsion extraction/evaporation. The extraction and evaporation phases are different such that we can get particles sooner or later, respectively, which can lead to differences in loading levels. We vary diverse parameters, including volumes of the organic solvent, the aqueous solution, the drug volume (consisting of Protoporphyrin IX in a solvent). The products PLGA-Protoporphyrin IX (Pppix) were obtained, characterized and optical properties were observed.

S1.00015 Hydrothermal Solution-Processed Reduced Nano-Graphene Oxide as Blue Photoluminescence Quantum Dots, JIGANG WANG, University of Texas Arlington, YONGSHENG WANG, DAWEI HE, Beijing Jiao Tong University, KE JIANG, WEI CHEN, University of Texas Arlington — Chemical derived graphene oxide, an atomically thin sheet of graphite with 2-D construction, offers interesting electronic, chemical and mechanical properties that are currently being explored for advanced electronics, membranes and composites. Herein, we synthesize and explore the blue photoluminescence (PL) nano-graphene quantum dots (QD) through hydrothermal-solution-processed reduced graphene oxide. The PL investigation indicated that graphene oxide solution showed weak fluorescence. However, when the nano-graphene oxide solution samples were heated at different temperatures, from 200–300 °C, the blue PL intensity of the solution improved radically as heating temperature increased. We also investigated time dependence at a certain heating temperature and the PL Intensity and peak based on graphene QDs under different pH values by adding NaOH. The FT-IR measurements showed that the functional groups of the graphene oxide had been altered due to the hydrothermal routes. In addition, we also investigated the absorption spectrum of the graphene QDs under different conditions, XRD and XPS images of the graphene oxide, TEM and SEM images based on graphene QDs under different conditions.

S1.00016 Nanocomposite for radiation detection, SUNIL SAHI, University of Texas at Arlington — Cerium fluoride is among the widely studied inorganic scintillators for radiation detection, because of its high light output and high stopping power. Herein, platelets shape CeF_3 nanoparticles for radiation detection was synthesis by bisolvent solvothermal method. The characterization of nanoparticles was done by photoluminescence, XRD and SEM measurement. The synthesized CeF_3 nanoparticles have broad emission peak around 330 nm. ZnO is a semiconductor scintillator, having fast decay time. ZnO nanoparticles were synthesized using solvothermal method and UV-Vis, photoluminescence and SEM measurement were done for their characterization. The absorption spectrum of the ZnO nanoparticles is dependent on the size of the nanoparticles. By changing the temperature and the concentration of zinc salt and surfactant, ZnO with absorption spectra overlapping with the emission spectra of CeF_3 were made for the purpose of creating nanocomposites, with improved scintillation properties. The energy transfer between two nanoparticles was also studied and the changes in Photoluminescence intensity of the nanocomposites were described.

S1.00017 METALS —

S1.00018 Simulating slow strain-rate processes in disordered solids , PENGHUI CAO, HAROLD S. PARK, XI LIN, Department of Mechanical Engineering, Boston University — A generic computational scheme is developed in this work to investigate extremely slow strain rate processes, including the experimentally accessible strain rates and even lower ones, for disordered materials systems. We use a self-learning metabain escape algorithm to capture the strain-rate and temperature dependent stress relaxation events for a binary Lennard-Jones alloy. It is found that the yield stress decreases when the strain rate decreases and when the temperature increases.

S1.00019 Plasmon Resonance Energy of Nickel Manganese Films , JAMIE SMITH, KEN PODOLAK, SUNY Plattsburgh — Plasmonics studies how light interacts with conductors at the nanoscale level. Plasmons result from a collective oscillation of charges. Surface plasmonics has become of interest due to the ability to confine optical energy into subwavelength volumes, however the ability to control and manipulate them has yet to be developed. In the future, plasmonics can revolutionize optical devices with increased performance speed and functionality. To alter the properties of a surface plasmon wave, an active layer is grown beneath a metal surface. Since, part of the plasmon's electromagnetic field resides in this layer, the layer couples to the surface plasmons. Thus, each sample studied was composed of an amorphous nickel manganese film grown on top of silicon with a capping copper layer. Optical absorption measurements were made with these films using a Cary-OLIS spectrophotometer from 190 – 450 nm. Two peaks in the absorption of each sample were found: one around 3.30 eV which is the surface plasmon peak as seen in previous literature and a bound electron peak at 4.45 eV. The full width half maximum of the surface plasmon peak is observed to increase when increasing the manganese concentration in each sample. A discussion as to possible reasons why will be presented.

S1.00020 Electronic States of Nickel Effected By Magnetic Doping , KEN PODOLAK, JAMIE SMITH, SUNY Plattsburgh — Spin currents have a great potential to replace charge currents. This would revolutionize how we read/write information. The generation and switching of spin currents however must be well understood. Transport measurements suggest that magnetic impurities can alter the mean free path of carriers and thereby create spin currents. Angle-resolved photoemission is used to determine the change in the electronic states of Ni induced by doping with iron, chromium, and manganese near the Fermi Energy. The samples were single crystals of nickel(110) with variable amounts of dopant diffused into it. Alloy single crystals were used over epitaxial thin films due to the sharper features at the Fermi Energy that they produced. The mean free path, magnetic splitting, and carrier density are affected by a few percent of each of the dopants. Iron suppresses the mean free path of minority spins only, while chromium and manganese suppresses both spins and decreases the magnetic splitting. The strong variation of these affects from one impurity to the other supports the concept of tailoring spin transport by magnetic doping. [1] K. N. Altmann et al., Phys. Rev. Lett. **87**, 137201 (2001) [2] K.R. Podolak, Ph.D. Thesis, Penn. State (2008)

S1.00021 COMPLEX STRUCTURED MATERIALS, INCLUDING GRAPHENE —

S1.00022 Fabrication of graphene device from graphite intercalation compound , RYUTA YAGI, HIROAKI KOBARA, MIDORI SHIMOMURA, FUMIYA TAHARA, SEIYA FUKADA, AdSM, Hiroshima University — The mechanical exfoliation of graphite is possibly the simplest and practical method in laboratories to obtain graphene flakes for scientific research. However efficiency for obtaining graphene, with desired layer-number and size, depends largely on crystal specific characters, eg., dislocations. To improve the issue, we have adopted graphite intercalation compound (GIC) instead of graphite for a starting material. Generally, GIC is chemically active. We used SbCl_5 -GIC, which is stable in the atmosphere. Stage structure of SbCl_5 -GIC could be tuned by temperature of intercalation. We found that considerable number of undoped graphene flakes coexisted with thin SbCl_5 -GIC flakes, on a substrate where flakes were transferred. Statistical inspection of number of graphene layer indicated that it is significantly dependent on the stage number of GIC.

S1.00023 Graphene synthesis by calcination of ethylene-glycol intercalated layered silicates: x-ray and Raman scattering studies , NOBORU WADA, TOMOYA SUSA, Toyo University — Excellent electrical, mechanical and chemical properties of graphene make it fascinating for various applications including high-speed and high-performance electric devices. Although there have been many synthesis methods innovated to obtain graphene in the past, a simple and controllable synthesis method of graphene mass production is still being pursued for such applications. Here, layered silicates are chosen as a host material to intercalate ethylene glycol (EG). EG-intercalated layered silicates are then calcinated in air or vacuum to synthesize graphene between the silicate layers. Layered silicates used are taeniolite, fluorinated mica and vermiculite. Our Raman scattering and x-ray diffraction experiments suggest that graphene may be made between the silicate layers after calcination. In particular, second-order Raman peaks found in vermiculite samples indicate that vermiculite may be most suited to synthesize well-crystallized graphene among the layered silicates used.

S1.00024 AFM and SThM Characterization of Graphene , CHRISTOPHER FOY, ANTON SIDOROV, XUNCHI CHEN, MING RUAN, CLAIRE BERGER, WALTER DE HEER, ZHIGANG JIANG, Georgia Inst of Tech — We report on detailed characterization of epitaxial grown graphene on SiC and chemical vapor deposition grown graphene on Cu foil using atomic force microscopy (AFM) and scanning thermal microscopy (SThM). We focus on the electronic and thermal properties of graphene grain boundaries, and thus providing valuable feedback to materials growth. Specifically, we perform thermal conductivity contrast mapping and surface potential mapping of graphene, and compare with that obtained on the Au electrodes and the substrate.

S1.00025 Wafer-scale synthesis of defect-negligible monolayer graphene at reduced temperature on hydrogen-rich evaporated (111) copper films¹ , LI TAO, MILO HOLT, HARRY CHOU, JONGHO LEE, RODNEY S. RUOFF, DEJI AKINWANDE, The University of Texas at Austin — In contrast to commercially available copper foils, evaporated copper film on wafer scale supporting substrates holds great promise in chemical vapor deposition (CVD) of graphene for direct integration into device manufacturing processes. Monolayer graphene with negligible defects (<5%) was synthesized on evaporated copper films at temperatures < 900 °C using hydrogen-free methane precursor that has not been previously reported. In this work, high-quality monolayer graphene obtained on evaporated copper film was likely enabled by the distinct properties of hydrogen-rich (111) preferred crystal orientation as indicated by X-ray diffraction (XRD) and electron back scattering diffraction (EBSD). The distinct difference in the crystal orientation of copper films versus foils resulted in dissimilar interplay with the precursor gas, as confirmed by time-of-flight secondary ion mass spectroscopy (TOF-SIMS). This study demonstrates experimental evidence for differences in the growth dynamics of CVD graphene on copper film versus conventional foils.

¹Support of our work from ONR is appreciated.

S1.00026 Anisotropic Hydrogen Etching of Chemical Vapor Deposited Graphene, YI ZHANG, ZHEN LI, LUYAO ZHANG, PYOJAE KIM, CHONGWU ZHOU, University of Southern California — In terms of the preparation of graphene, chemical vapor deposition (CVD) has raised its popularity as a scalable and cost effective approach for graphene synthesis. While the formation of graphene on copper foil has been intensively studied, the reverse reaction of graphene reacts with hydrogen has not been systematically studied. In this talk we will present a simple, clean, and highly anisotropic hydrogen etching method for CVD graphene catalyzed by the copper substrate. By exposing CVD graphene on copper foil to hydrogen flow around 800 °C, we observed that the initially continuous graphene can be etched to have many hexagonal openings. In addition, we found that the etching is temperature dependent and the etching of graphene at 800 °C is most efficient and anisotropic. 80% of the angles of graphene edges after etching are 120°, indicating the etching is highly anisotropic. No increase of D band along the etched edges indicates that the crystallographic orientation of etching is zigzag direction. Furthermore, we observed that copper played an important role in catalyzing the etching reaction, as no etching was observed for graphene transferred to Si/SiO₂ under similar conditions. This highly anisotropic hydrogen etching technology may work as a simple and convenient way to determine graphene crystal orientation and grain size, and may enable the etching of graphene into nanoribbons for electronic applications.

S1.00027 Density functional theory calculations on the effects of oxygen adsorption on graphene in the presence of defects, FAISAL MEHMOOD, WEIJIE LU, JOHN J. BOECKL, RUTH PACTHER, Air Force Research Laboratory, Materials & Manufacturing Directorate, Wright-Patterson Air Force Base, Ohio 45433 — Density functional theory calculations were carried out to investigate effects of oxygen adsorption on the electronic and optical properties of single layer graphene (SLG) in the presence of defects. Stone-Wales and single and double vacancy defects, also including the 555-777 and 5555-6-7777, were considered. Analysis of changes upon oxygen adsorption will be reported in detail, regarding morphology, binding energies and electronic structure, as compared to pristine SLGs, for pure GGA, hybrid and van der Waals corrected functionals. Nudged elastic band calculations of various pathways were investigated in order to understand the diffusion and dissociation of oxygen on SLGs in the presence of defects. Calculation of the optical response carried out at different levels of theory will be discussed, using both hybrid and long-range corrected hybrid functionals, with consideration of comparison to experimental characterization. Finally, implications of the effects of oxygen adsorption on graphene in the presence of defects for aspects of catalyst-free growth or electron transport will be suggested.

S1.00028 Using the G' Raman cross-section to understand the phonon dynamics in bilayer graphene systems, DANIELA MAFRA, Universidade Federal de Minas Gerais, PAULO ARAUJO, Massachusetts Institute of Technology, KENTARO SATO, RIICHIRO SAITO, Tohoku University, MILDRED DRESSELHAUS, JING KONG, Massachusetts Institute of Technology — The integrated area (IA) of the four peaks (P₁₁, P₁₂, P₂₁ and P₂₂) of the G' Raman band of AB stacked bilayer graphene are analyzed as a function of the laser power for different laser lines. We show that the IA of each peak depends on temperature and also depends on the laser excitation energy. This special dependence is explained in terms of the electron-phonon coupling and the relaxation time of the photon-excited electron. Due to the short relaxation time of the photo-excited electron by emitting phonons, the relative intensities of the four peaks are determined by a different combination of relaxation processes that give rise to some G' peaks increasing in IA at the expense of others, thereby making the IA of the peaks different from each other and dependent on laser excitation energy and power level. Also, we report an anomalous behavior of the G' IA for the 532 nm laser energy, that shows a resonance regime in which a saturation of what we call the P₁₂ process occurs. This effect is a relevant phenomenon that gives important information about the electron and phonon dynamics and needs to be taken into account for certain applications of bilayer graphene in the field of nanotechnology.

S1.00029 Adhesive interaction between graphene membranes and amorphous substrates, RUI HUANG, WEI GAO, University of Texas at Austin — To integrate graphene in functional devices, it is essential to understand interfacial adhesion between graphene and surrounding materials for mechanical support and encapsulation. In complement with recent efforts aiming to measure the adhesion energy experimentally, we present a theoretical model for adhesive interaction between a graphene monolayer and an amorphous substrate. The model is extended to analyze the morphological stability of a graphene membrane on an oxide substrate. It is found that the bending modulus, which increases drastically from monolayer to multilayered graphene, plays an important role in the transition from conformal to non-conformal morphology of the graphene membranes on a corrugated surface. Furthermore, the work of adhesion is predicted to drop considerably from monolayer to bilayer graphene, in good agreement with recent measurements. The theoretical results suggest that tunable adhesion of graphene can be achieved by controlling the surface roughness of the substrate.

S1.00030 Structural Properties of Epitaxial Graphenes on 4H-SiC(0001): A Theoretical Study¹, MING YU, PAUL DAVIS, MICHAEL WOODCOX, C.S. JAYANTHI, S.Y. WU, University of Louisville — The structural properties of the epitaxial graphene including the buffer layer on 4H-SiC(0001) are studied using the recently developed SCED-LCAO molecular dynamics scheme [PRB 74, 15540 (2006)]. Both Si-terminated and C-terminated SiC substrates are considered. In a previous work [BAPS, Vol. 56, 463 (2011)], we had shown that 10x10 monolayers of carbon on 8x8 4H-SiC(0001) substrate as well as 13x13 monolayers of carbon on 6√3x6√3 4H-SiC(0001) substrate are minimum in strain between the buffer layer and the substrate and that they are nearly commensurate. In this work, we have added an epitaxial layer of graphene to the above geometries and both C-terminated and Si-terminated SiC surfaces will be considered. We will highlight the roles played by the buffer layer, the epitaxial layer, and the substrate on the structural properties of this system. Analysis of the structure in terms of local bonding arrangements and charge distributions will also be provided.

¹Acknowledgment: This work is supported by the Research Corporation (RC19902).

S1.00031 Intercalation of metal islands and films at the interface of epitaxially grown graphene and Ru(0001) surfaces¹, LI HUANG, YI PAN, LIDA PAN, MIN GAO, WENYAN XU, YANDE QUE, HAITAO ZHOU, YELIANG WANG, SHIXUAN DU, HONGJUN GAO, Institute of Physics, Chinese Academy of Sciences, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES TEAM — Epitaxial graphene on Ru(0001) provides a high quality adlayer, but has a strong interaction with the substrate. This interaction can be effectively weakened via intercalating a layer of other element between epitaxial graphene and its substrate. In this work, we intercalated seven kinds of metals including noble metals Pt, Pd and Au, magnetic metals Ni and Co, a IIIA group metal In and a rare earth metal Ce, at the interface of epitaxially grown graphene and Ru(0001), to show the universality of metal intercalations in this system. These metals form different intercalated structures that have different impacts on the corrugation of graphene. Atomic resolution images of a perfect graphene lattice on the intercalated structures can always be obtained, which confirms that the intercalation of these metals is a non-damaging process. Additionally, based on primary DFT calculations, we propose a model involving metal-atom-aided-defect and self-healing of C-C bonds at high temperature, which can well explain the intercalation process of some metals and provide the potential to better understand the intercalation mechanism.

¹The authors gratefully acknowledge financial support from CAS, NSFC (10834011, 60976089) and National “863” and “973” projects of China (2009CB929103, 2010CB923004, 2011CB932700).

S1.00032 Superconductivity in Graphene-Lithium Systems¹ , DAVID GUZMAN, RADI AL-JISHI, Department of Physics and Astronomy, California State University - Los Angeles, HAMAD ALYAHYAEI, Department of Physics and Astronomy, University of California - Riverside — We present first-principles calculations on systems consisting of a few layers of graphene and lithium. In particular, we investigate the evolution of the electron-phonon coupling strength with an increasing number of layers. We find that for intercalated systems such as C₆-Li-C₆ or C₆-Li-C₆-Li-C₆ the electron-phonon coupling is weak. However, for systems of equal number of graphene and lithium layers, such as C₆-Li or C₆-Li-C₆-Li, the electron-phonon coupling is strong. We investigate the optimal configuration that yields the highest superconducting transition temperature.

¹Supported by the NSF under grant No. HRD-0932421 and CSU-LSAMP under grant No. HRD-1026102-518741.

S1.00033 ABSTRACT WITHDRAWN —

S1.00034 ABSTRACT WITHDRAWN —

S1.00035 Impermeable “single-monolayer” Graphenic encasement of bacteria for high vacuum Transmission electron microscopy¹ , BALABALAJI PADAVALA, PHONG NGUYEN, JOSHUA PODREBARAC, JENAE TATE, VIKAS BERRY, Kansas State University — Biological cells are hygroscopic, permeable, and electron-absorbing, and imaging them *via* electron microscopes has been an important challenge due to the volumetric-shrinkage and structural degradation of cells under high vacuum and fixed electron beam. In this talk, we will show that “single-monolayer” graphenic encasement of individual whole “wet” bacterial cells can enable wet-phase TEM imaging by preserving their dimensional, topological characteristics and cellular water under high vacuum (10⁻⁵ Torr) and beam current (150 A/cm²). Ultrathin and impermeable “single monolayer” graphene microsheet was wrapped around or laid on bacteria. The combination of strongly-packed honeycomb-lattice, high Young’s modulus, high electrical and thermal conductivity, and mesoscale flexibility of the single graphene monolayer reduced the permeability of cells under TEM conditions, significantly abated electron beam damage and cell-delamination from substrate.

¹KSU-Startup

S1.00036 η^6 Chemical Modification of Epitaxial Graphene: An Avenue for Non Destructive Surface Functionalization and Atomic Layer Deposition , PHONG NGUYEN, VIKAS BERRY, KABEER JASUJA, Kansas State University — Graphene’s superior properties are expected to develop next generation electronic applications. However, a major challenge which still remains is to incorporate it into different systems via its functionalization. Moreover, such functionalization must not alter graphene’s superior properties. In most cases, functionalization leads to conversion of the planar sp² hybridized state of carbon into the tetrahedral sp³ states. This conversion leads to an increase in carrier-scattering and a reduction in carrier-density. In this talk, we demonstrate a novel η^6 functionalization route, where the d-orbital of a transition metal binds with the pi-cloud at the center of graphene’s aromatic rings resulting in a unique grafting of a monolayer of metal atoms. As a result, the sp² state of the carbon atoms is preserved and its superior properties (high carrier density and low carrier scattering) are maintained. We envision that this functionalization route will allow graphene to be interfaced with several systems, thus significantly broadening the scope of its applications.

S1.00037 A three-dimensional architecture of vertically aligned multilayer graphene facilitates heat dissipation across joint solid surfaces , QIZHEN LIANG, XUXIA YAO, WEI WANG, C.P. WONG, Georgia Institute of Technology — Low operation temperature and efficient heat dissipation are important for device life and speed in current electronic and photonic technologies. Being ultra-high thermally conductive, graphene is a promising material candidate for heat dissipation improvement in devices. In the application, graphene is expected to be vertically stacked between contact solid surfaces in order to facilitate efficient heat dissipation and reduced interfacial thermal resistance across contact solid surfaces. However, as an ultra-thin membrane-like material, graphene is susceptible to Van der Waals forces and usually tends to be recumbent on substrates. Thereby, direct growth of vertically aligned free-standing graphene on solid substrates in large scale is difficult and rarely available in current studies, bringing significant barriers in graphene’s application as thermal conductive media between joint solid surfaces. In this work, a three-dimensional vertically aligned multilayer graphene architecture is constructed between contacted Silicon/Silicon surfaces with pure Indium as a metallic medium. Significantly higher equivalent thermal conductivity and lower contact thermal resistance of vertically aligned multilayer graphene are obtained, compared with those of their recumbent counterpart. This finding provides knowledge of vertically aligned graphene architectures, which may not only facilitate current demanding thermal management but also promote graphene’s widespread applications such as electrodes for energy storage devices, polymeric anisotropic conductive adhesives, etc.

S1.00038 Ballistic Transport in Graphene pnp Junctions Formed by Embedded Local Gates , SEUNG-GEOL NAM, DONG-KEUN KI, Department of Physics, Pohang University of Science and Technology, Pohang, Korea, JONG-WAN PARK, Technology Development Team, National NanoFab Center, Korea, YOUNGWOOK KIM, JUN-SUNG KIM, HU-JONG LEE, Department of Physics, Pohang University of Science and Technology, Pohang, Korea — Due to its gapless energy spectrum, one enables to tune the carrier type and density in graphene and realize pnp-type potential barriers in situ by using electrostatic gating. Such potential barriers provide opportunities to investigate novel phenomena such as Klein tunneling and quantum-Hall edge-state equilibration. In this study, we obtained high-quality graphene pnp junctions by embedding pre-patterned local gates in a substrate without dielectric-layer deposition or electron-beam exposure of the graphene sheet. We achieved ballistic and phase-coherent carrier transport in a graphene pnp device with a 130-nm-wide local gate, which is almost an order magnitude wider than reported previously[1]. In a high magnetic field, device with a 1-micro meter-wide local gate exhibited the $2e^2/h$ quantum-Hall plateau, indicating no backscattering in the local gate region. The conductance across our pnp junctions shows a gate-voltage dependence that is very distinctive from that of top-gated junctions, indicating a strong screening of the electric field by the embedded local gate. [1] A. F. Young and P. Kim, Nature Physics **5**, 222 (2009)

S1.00039 Carbon Nucleation from ring seeds on Icosahedral Fe₁₃¹ , ANTENEH TEFERA, MOGUS MOCHENA, Florida A&M University — Using ab initio molecular dynamics calculation, we computed the initial stages of carbon nanotube growth from ten – atom carbon rings on icosahedral Fe₁₃. The carbon ring interacts with Fe₁₃ to form a zigzag structure due to a mismatch between the number of atoms on the ring and the atoms on the pentagonal ring of Fe₁₃, with formation energy of 2.2 eV. A mixture of carbon dimers and carbon atoms interact with the Fe₁₃ + C₁₀ structure to yield a tubular structure with the lowest energy. Another configuration of carbon atoms distributed in the vicinity hexagonal lattice sites interacts with Fe₁₃ + C₁₀ structure to form also a tubular structure that is almost degenerate in energy to the ground state. The results indicate that the icosahedral symmetry of the Fe₁₃ with its magnetic moment almost intact is retained whenever the tubular structure is formed.

¹This research was supported by NSF grant: DMR-0804805. This research was supported in part by the NSF through TeraGrid resources provided by NCSA under grant number TG-DMR100055.

S1.00040 Anomalous dependence of band gaps of binary nanotubes on diameters¹, KAPIL ADHIKARI, MUHAMMAD HUDA, ASOK RAY, Department of Physics, University of Texas at Arlington — Using cluster approximation, AlN, BN, GaN, SiGe, SiC, and GeC armchair type 1 nanotubes have been spin optimized using the hybrid functional B3LYP, a double ζ basis set and the GAUSSIAN 03 software. The electronic structures of group III nitride and group IV-IV nanotubes indicate that the band gap increases with tube diameter contrary to behavior expected from quantum size effects. A detailed study indicates that, in a class of binary nanotubes with partial ionic contributions in the bonds, for example, AlN, BN, GaN, GeC, and SiC, ionicity of the bonds decreases as diameter decreases due to increased sp^3 contribution. This causes the band gap to increase with diameter. But in nanotubes with covalent bonding, for example SiGe, the gap decreases with diameter. A general trend for a class of binary nanotubes is established.

¹This work is supported by the Welch Foundation (Grant No. Y-1525) and the National Renewable Energy sub-contract XEJ-9-99042-01.

S1.00041 Ultra high Transparent and Conductive Electrodes Based on As-Grown SWNT with Metallic Conductivity, TEREZA PARONYAN, ELENA PIGOS, GUGANG CHEN, AVETIK HARUTYUNYAN, Honda Research Institute USA Inc., Columbus, OH, 43212, USA, HONDA RESEARCH INSTITUTE USA INC. TEAM — Carbon based materials have been proven to be a unique material for transparent conducting films, with potential for application on liquid crystal displays, touch screens and solar cells. We successfully grew SWNT films by Chemical Vapor Deposition method using Fe nanocatalysts on quartz substrates. The ratio of semiconductor/metallic nanotubes varied depending on the treatment conditions of the catalyst nanoparticles, according to Raman analysis. SEM analysis of the samples revealed homogeneous coverage of the quartz substrates by SWNTs, which exhibit transparencies higher than 98%. Sheet resistance measurements of these SWNT films, by Van der Pauw method, demonstrated the correlation between the conductivity and the abundance of semiconductor and metallic nanotubes in the films. Increasing the content of metallic SWNTs in the film up to 90% decreased the sheet resistance down to 4-5 K Ω /, while maintaining a high transparency of over 98%. For comparison, transparent electrodes based on high quality monolayer graphene sheets were also fabricated. The conductivity and transparency of the electrodes of as grown SWNTs were comparable to the electrodes based on monolayer graphene.

S1.00042 Determination of the vibration frequencies of Carbon Nanotubes and Carbon Nanoribbons¹, M. PACHECO, Universidad Federico Santa Maria, A. LEON, Universidad Diego Portales — The optical properties of organic materials are similar to the properties of the molecules that constitute it. This motivates the study of molecular complexes that would form new materials. Interesting optical properties are observed in conjugated polymers due to delocalized π electrons, which allow transitions in the visible spectrum. In this work we present results of the vibration spectrum for pristine and functionalized carbon nanoclusters. The electronic properties are obtained by first principles calculations, based on the Becke-Perdew GGA approximation. The frequencies are computed numerically by differentiation of the energy gradients in slightly displaced geometries. The three stages of calculations will be performed using the ADF code. The geometric optimization protocols for pristine and functionalized structures are made adopting the “quasi Newton approach.” The vibration spectra show interesting properties when the structures are functionalized with organic molecules.

¹Financial support of FONDECYT grants 1100672 and 11100045

S1.00043 High surface area electrode for high efficient microbial electrosynthesis, HUARONG NIE, Department of Polymer Science & Engineering, University of Massachusetts, Amherst, MENG MENG CUI, HAIYUN LU, Department of Polymer Science & Engineering, University of Massachusetts, Amherst, TIAN ZHANG, Department of Microbiology, University of Massachusetts, Amherst, THOMAS RUSSELL, Department of Polymer Science & Engineering, University of Massachusetts, Amherst, DEREK LOVLEY, Department of Microbiology, University of Massachusetts, Amherst — Microbial electrosynthesis, a process in which microorganisms directly accept electrons from an electrode to convert carbon dioxide and water into multi carbon organic compounds, affords a novel route for the generation of valuable products from electricity or even wastewater. The surface area of the electrode is critical for high production. A biocompatible, highly conductive, three-dimensional cathode was fabricated from a carbon nanotube textile composite to support the microorganism to produce acetate from carbon dioxide. The high surface area and macroscale porous structure of the intertwined CNT coated textile ?bers provides easy microbe access. The production of acetate using this cathode is 5 fold larger than that using a planar graphite electrode with the same volume. Nickel-nanowire-modified carbon electrodes, fabricated by microwave welding, increased the surface area greatly, were able to absorb more bacteria and showed a 1.5 fold increase in performance

S1.00044 In-Air Growth of Carbon Nanoflowers¹, CHRISTOPHER HUYNH, RYAN LU, KIMI CSANADI, AYAX RAMIREZ, SPAWAR SYS CEN PAC, DEBJYOTI BANERJEE, Texas AM University — A new class of carbon nanostructures was fabricated under rapid heating in air. Solid carbon sources and metal catalysts were used to facilitate growth. Their microstructures were characterized using scanning electron microscopy and micro Raman spectroscopy. The results indicate patches of graphene and carbon tapered tubules. Two methods of fabrication are presented.

¹Supported by ONR

S1.00045 A Molecular Dynamics Study on the Confinement of Carbon Dioxide Molecules in Carbon Nanotubes¹, MEAGAN LAZOR, DENIZ RENDE, NIHAT BAYSAL, RAHMI OZISIK, Rensselaer Polytechnic Institute — The influence of atmospheric carbon dioxide (CO₂) concentration on global warming is considered as one of the primary environmental issues of the past two decades. The main source of CO₂ emission is human activity, such as the use of fossil fuels in transportation and industrial plants. Following the release of Kyoto Protocol in 1997, effective ways of controlling CO₂ emissions received much attention. As a result, various materials such as activated carbon, zeolites, and carbon nanotubes (CNTs) were investigated for their CO₂ adsorbing properties. CNTs were reported to have CO₂ adsorption capability twice that of activated carbon, hence they received the most attention. In the current study, single walled carbon nanotubes (SWNTs) were used as one dimensional nanoporous materials and their CO₂ adsorption capacity was analyzed with Molecular Dynamics simulations. Results indicated that SWNTs are excellent CO₂ adsorbers and their effectiveness increase at low CO₂ concentrations. In addition, we showed that by varying temperature, CO₂ can be removed from the SWNTs, providing a simple method to reuse SWNTs.

¹Partial support was provided by NSF Grant No. 1003574 and RPI. DR is also supported by TUBITAK 2219 program.

S1.00046 A Molecular Dynamics Study on the Exfoliation of Single Walled Carbon Nanotubes in Supercritical Carbon Dioxide¹, SEMRA SENTURK-OZER, Stevens Institute of Technology, DENIZ RENDE, NIHAT BAYSAL, RAHMI OZISIK, Rensselaer Polytechnic Institute — Carbon nanotubes (CNTs) could be used in various technological applications due to their structural, electrical and mechanical properties. However, in order to get the theoretically predicted benefits, nanotubes have to be successfully dispersed in the polymer matrix. Supercritical fluids were previously shown to result in good dispersion of nanofillers (in the case of clays and spherical nanofillers). In the current study, we investigated the potential use of supercritical carbon dioxide to unbundle single walled carbon nanotubes via molecular dynamics simulations. Various carbon nanotube systems were simulated with XenoView simulation software, and the effect of surface modification of nanotube with CO₂-philic chemicals was investigated on nanotube dispersion. Results showed that surface modification of nanotubes improves their dispersion in supercritical carbon dioxide.

¹Partial support was provided by NSF Grant No. 1003574 and RPI. DR is also supported by TUBITAK 2219 program.

S1.00047 Interplay of Wetting and Elasticity in the Nucleation of Carbon Nanotubes , DMITRI SCHEBARCHOV, SHAUN C. HENDY, Industrial Research Ltd., ELIF ERTEKIN, University of Illinois, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology — Controlling the structure of single-walled carbon nanotubes during synthesis is one of the outstanding challenges of nanoscale science. Some degree of control has been demonstrated through catalytic synthesis, where the interaction with the catalyst is believed to play a key role, but the exact mechanisms leading to preferential growth remain unclear. Here we report on the development of a model that focuses on the lift-off of carbon nanotube caps after nucleation. We test the model using atomistic molecular dynamics simulations and discuss the implications of the model for understanding growth processes that may control chirality. We illustrate the role of the competition between cap strain energy and adhesive forces in the lifting of these caps from the catalyst surface prior to elongation. We show that, given a particular cap structure, there is a lower bound on the catalyst size from which the cap can lift. This lower bound explains the mismatch between nanotube and catalyst diameters observed in experiment. These findings offer new insight into the nucleation of single-walled carbon nanotubes, and they may lead to the design of catalysts that can better control nanotube structure.

S1.00048 Electronic properties of carbon nanodisks and nanocones , ANDREA LATGE, Instituto de Física, UFF, Niterói-RJ, Brazil, PABLO ULLOA, MONICA PACHECO, Departamento de Física, UTFSM, Valparaíso, Chile, LUIZ EDUARDO OLIVEIRA, Instituto de Física, UNICAMP, Campinas-SP, Brazil — The electronic properties of graphene nanodisks and nanocones are calculated following a tight-binding approach. The total density of states of both structures are found to be quite similar when a large number of atoms is considered, including the peak at the Fermi energy associated with the contribution of the border atoms. We have also calculated, for both systems, the local density of states which highlight the differences of the electronic structures due to the particularities of the spatial symmetry of the nanodisks and nanocones. Moreover, the electronic properties are thoroughly discussed via the analysis of the joint density of states and absorption spectra of the nanostructures.

S1.00049 Synthesis and field emission properties of periodic arrays of vertically aligned carbon nanotubes on copper¹ , SUMAN NEUPANE, WENZHI LI, Florida International University — Periodic arrays of carbon nanotubes (CNTs) with different densities were synthesized on copper substrate by employing nanosphere lithography (NSL) and plasma enhanced chemical vapor deposition. Vertically aligned CNTs were formed using Ni as catalyst at a growth pressure of 8 torr of C₂H₂/NH₃ mixture and a temperature of 520 °C. Electron emissions of the CNTs with different densities were investigated to reveal the dependence of the electron emission properties of the CNTs on their densities. Experimental results showed that low-density CNTs exhibited better field emission properties as compared to the high-density CNTs. Low-density CNTs exhibited lower turn-on and threshold electric fields, and a higher field enhancement factor. The high density of CNTs resulted in the deterioration of the FE properties due to the screening of the electric field by the adjoining CNTs.

¹This work is supported by the National Science Foundation under the grant DMR-0548061

S1.00050 Fabrication of Micro-Electromagnetic Devices for the Manipulation of Carbon Nanotubes , JOHN BRIDSTRUP, ANTHONY SPEZIALE, SCOTT PAULSON, James Madison University — With advances in microscopy techniques, such as transmission electron and scanning transmission electron microscopy, it has become increasingly more interesting to study and manipulate the structures of solid state materials at the atomic scale. One of the issues with the study of these properties is that these advanced microscopes require that the sample be confined to a space not very conducive to traditional methods of actuation, such as atomic force microscopy and electrostatic methods. In our research, we are primarily focused on building tiny “electro-magneto-mechanical” devices on carbon nanotubes in order to manipulate them without breaking vacuum or removing them from the microscope. Our current project is focused on putting small, magnetizable paddles on to the carbon nanotubes, using an SEM for electron beam lithography and a metal evaporation deposition system, then running current to induce a magnetic field with which the paddles, which can have any magnetic dipole we want, will align. In order to create these devices we must first choose a type of material and a method for creating the magnetic paddles, in our work we use iron. The main problem with iron is the rate at which it oxidizes at the nanoscale, it is practically instantaneous. Because of this we have developed a method, using what basically amounts to simple geometry, for encasing our iron paddles with gold and thus preventing the oxidation. It is our hope that this research opens the doors for many new opportunities in nanoscale materials science, and at the least greatly reduce the time required for many current experiments.

S1.00051 2D Fluidization of Nanomaterials by Biomimetic Membranes , KATHLEEN KELLY, MARTIN FORSTNER¹, Physics Department, Syracuse University, Syracuse, NY, 13244 — The last decade has seen much progress in the synthesis and manufacturing of a large variety of nanometer sized particles of different materials, geometries and properties. If they can be assembled into larger structures, these manmade nano-objects are posed to be the “atoms” and “molecules” of new materials. In order to facilitate their dynamic rearrangements we have developed a method that uses material specific binding peptides to anchor nano-objects to lipids in supported bilayers (SLB). In this study we use single walled carbon nanotubes (CNT) with a mean length of 1 micrometer as model of a potential nano-building block. By fluorescently labeling CNTs we are able to use video-microscopy to investigate the dynamic behavior of membrane anchored CNTs. We show that the 2D fluidity of the lipid membrane can be successfully templated on the CNTs and that they stay laterally mobile while being confined to a plane. Furthermore, the dependence of CNT mobility on specific binding stoichiometries is discussed.

¹Syracuse Biomaterials Institute, Syracuse University, Syracuse, NY, 13244

S1.00052 SWNT Imaging Using Multispectral Image Processing , MICHAEL BLADES, MASSOOMA PIRBHAI, SLAVA V. ROTKIN, Lehigh University — A flexible optical system was developed to image carbon single-wall nanotube (SWNT) photoluminescence using the multispectral capabilities of a typical CCD camcorder. The built in Bayer filter of the CCD camera was utilized, using OpenCV C++ libraries for image processing, to decompose the image generated in a high magnification epifluorescence microscope setup into three pseudo-color channels. By carefully calibrating the filter beforehand, it was possible to extract spectral data from these channels, and effectively isolate the SWNT signals from the background.

S1.00053 Absorption of Carbon Monoxide Molecules On Carbon Nanotubes¹ , LIANGBO LIANG, VINCENT MEUNIER, Rensselaer Polytechnic Institute — Carbon nanotubes (CNTs) have been demonstrated to be promising nanoscale molecular sensors for detecting gas molecules such as NH₃, NO₂ and O₂. But pristine CNTs show limitations in detection of highly toxic gases such as carbon monoxide (CO). In our work, interaction of CO molecules with both armchair and zigzag single-walled CNTs (SWCNTs) has been investigated through Density Functional Theory (DFT) simulations using the software VASP. SWCNTs with structural deformation, Stones-Wales (SW) defects or single vacancy (SV) defects are considered. It has been found that structural deformation, resulting in the significant change of local physical properties, enables strong chemical absorption of CO molecules on the surface of CNTs. In addition, a SV defect also brings about dramatic change in the local geometrical structure and higher chemical reactivity, facilitating strong binding of one and two CO molecules on CNTs. Compared to pristine and SW-defect CNTs, deformed and SV-defect CNTs are more promising as gas sensors to detect toxic carbon monoxide molecules.

¹Liangbo Liang acknowledges Computational Center for Nanotechnology Innovation at RPI to provide computation resources.

S1.00054 Van der Waals Interactions of Organic Molecules on Semiconductor and Metal Surfaces: a Comparative Study¹, GUO LI, Institute of Physics, CAS, China; ICQD/HFNL, USTC, China, VALENTINO COOPER, Oak Ridge National Lab, JUN-HYUNG CHO, Hanyang University, Korea, ISAAC TAMBLYN, Lawrence Berkeley National Lab, SHIXUAN DU, Institute of Physics, CAS, China, JEFFREY NEATON, Lawrence Berkeley National Lab, HONG-JUN GAO, Institute of Physics, CAS, China, ZHENYU ZHANG, ICQD/HFNL, USTC, China; Harvard University — We present a comparative investigation of vdW interactions of the organic molecules on semiconductor and metal surfaces using the DFT method implemented with vdW-DF. For styrene/H-Si(100), the vdW interactions reverse the effective intermolecular interaction from repulsive to attractive, ensuring preferred growth of long wires as observed experimentally. We further propose that an external E field and the selective creation of Si dangling bonds can drastically improve the ordered arrangement of the molecular nanowires [1]. For BDA/Au(111), the vdW interactions not only dramatically enhances the adsorption energies, but also significantly changes the molecular configurations. In the azobenzene/Ag(111) system, vdW-DF produces superior predictions for the adsorption energy than those obtained with other vdW corrected DFT approaches, providing evidence for the applicability of the vdW-DF method [2].

¹Supported by NNSF, “973” programs of China; DOE, OBES, MSED, USNSF; and NRF of Korea.

S1.00055 Analyzing the frequency shift of physi-adsorbed CO₂ in metal organic framework materials¹, YANPENG YAO, Rutgers, The state university of New Jersey, NOUR NIJEM, University of Texas at Dallas, JING LI, Rutgers, The state university of New Jersey, YVES CHABAL, University of Texas at Dallas, DAVID LANGRETH, Rutgers, The state university of New Jersey, TIMO THONHAUSER, Wake Forest University — Combining first-principles density functional theory simulations with IR and Raman experiments, we determine the frequency shift of vibrational modes of CO₂ when physi-adsorbed in the iso-structural metal organic framework materials Mg-MOF74 and Zn-MOF74. Surprisingly, we find that the resulting change in shift is rather different for these two systems and we elucidate possible reasons. We explicitly consider three factors responsible for the frequency shift through physi-absorption, namely (i) the change in the molecule length, (ii) the asymmetric distortion of the CO₂ molecule, and (iii) the direct influence of the metal center. The influence of each factor is evaluated separately through different geometry considerations, providing a fundamental understanding of the frequency shifts observed experimentally.

¹This work is support by DoE.

S1.00056 Zinc in +III oxidation state, DEVLEENA SAMANTA, PURU JENA, Virginia Commonwealth University — The possibility of Group 12 elements, such as Zn, Cd, and Hg existing in an oxidation state of +III or higher has fascinated chemists for decades. Significant efforts have been made in the past to achieve higher oxidation states for the heavier congener mercury (since the 3rd ionization potential of the elements decrease as we go down the periodic table). It took nearly 20 years before experiment could confirm the theoretical prediction that Hg indeed can exist in an oxidation state of +IV. While this unusual property of Hg is attributed to the relativistic effects, Zn being much lighter than Hg has not been expected to have an oxidation state higher than +II. Using density functional theory we show that an oxidation state of +III for Zn can be realized by choosing specific ligands with large electron affinities i.e. superhalogens. We demonstrate this by a systematic study of the interaction of Zn with F, BO₂, and AuF₆ ligands whose electron affinities are progressively higher, namely, 3.4 eV, 4.4 eV, and 8.4 eV, respectively. Discovery of higher oxidation states of elements can help in the formulation of new reactions and hence in the development of new chemistry.

S1.00057 A multi-scale model using single ion impacts predicts large-scale pattern formation in irradiated solids, SCOTT NORRIS, Southern Methodist University — Energetic particle irradiation of solids can lead to highly regular nanoscale pattern formation under the right environmental conditions. The widespread use of this technology in current industrial settings for doping and hardening suggests the promise of harnessing spontaneous pattern formation to create novel devices. However, existing theoretical models of ion irradiation fail to agree broadly with experiment even in the linear regime of small-amplitude patterns. A central challenge in modeling this system is to rigorously connect the pico-second effect of single ion impacts, spanning mere nanometers of material, to the long-time evolution of surface structures spanning tens to hundreds of nanometers. Here, we present a multi-scale framework that achieves this end. We start with molecular dynamics simulations of single ion impacts, and upscale this data into a continuum PDE for the surface topography. Stability analysis of the PDE predicts the characteristic pattern wavelength as the incidence angle is varied. The predictions agree remarkably well with experiment, and overturn the long-held assumption that pattern formation is due to the removal of target atoms by sputter erosion.

S1.00058 Multiscale atomistic and coarse-grained-particle analysis of fracture of graphene sheet, RYO KOBAYASHI, TAKAHIDE NAKAMURA, SHUJI OGATA, Nagoya Institute of Technology — The problems related to material strength such as crack propagation, dislocation motion, and response to nano-indentation involve multiscale phenomena which atomistic or non-linear events occur at a certain confined region and elastic or linear deformation takes place at surrounding wide-spread region. In order to tackle these multiscale problems, we have developed the hybrid molecular-dynamics/coarse-grained-particle (MD-CGP) method which eliminates the artificial effects often occurred at the interface of atomistic and coarse regions by using extra atoms and particles at the interface and applying the Langevin thermostat for the extra atoms and particles. The method allows us to perform multiscale simulations of any materials such as metals, semiconductors, and insulators and of dynamic phenomena at finite-temperatures. We have performed the multiscale simulation of fracture of defect-free graphene membrane by nano-indentation and clarified that decrease of the fracture strength with respect to temperature is almost same as that by existence of a vacancy. We will discuss detail about the computational efficiency of this method and simulation results.

S1.00059 Interface magnetism in LSMO-BiFeO₃ heterostructures, DIPANJAN MAZUMDAR, Center for Materials for Information Technology, University of Alabama, CECILIA SANCHEZ HANKE, Advanced Light Source, Lawrence Berkeley National Lab, ARUNAVA GUPTA, Center for Materials for Information Technology, University of Alabama, SUJOY ROY, Advanced Light Source, Lawrence Berkeley National Lab, U ALABAMA TEAM, LBNL TEAM — The interplay of the magnetic and ferroelectric order parameter is currently a topic of intense research. This magnetoelectric coupling can potentially be enhanced at the interface of a FM-FE heterostructure and, therefore, study of such prototype interfaces could provide fundamental insight to design of multiferroic materials. In this work interface magnetism investigations of multiferroic BFO (3-5nm) with a high-spin polarization ferromagnet (LSMO, 10nm) is presented. We have performed detailed resonant reflectivity studies at the Mn (for LSMO) and Fe (for BFO) L₃ edges in LSMO/BFO as a function of temperature. Analysis of the data using rigorous scattering theory employing the tensor nature of the refractive index has elucidated the charge and magnetic density depth profiles along the depth of the film. Investigations at room temperature do not show magnetism at the Fe-edge which imply that the antiferromagnetic order in BFO persists both in bulk and interface. A comprehensive interface characterization as a function of temperature will be presented.

S1.00060 Designing Smart Surfaces to Segregate Cells , GERMAN KOLMAKOV, SAMDEN LAMA, FERNANDO HERNANDEZ, ERVIN IBRAGIMOV, New York City College of Technology CUNY, COLLIN EDINGTON, RICHARD KOEPEL, JILL ANDERSEN, DANIEL MCKEEL, McGowan Institute for Regenerative Medicine, University of Pittsburgh, SUNGEUN EOM, TAKEO KANADE, CARSEN KLINE, Carnegie Mellon University, ZVI LIRON, Israel Institute for Biological Research, HIRONOBU MURATA, ALAN RUSSELL, McGowan Institute for Regenerative Medicine, University of Pittsburgh, ANNA BALAZS, Chemical Engineering Department, University of Pittsburgh — Our aim is to utilize smart surfaces to separate specific populations of cells from a heterogeneous sample. There are a number of diseases (e.g., malaria and various cancers) that alter the elasticity of biological cells. In this work, we use the mechanical stiffness of the cells as a key parameter since it can reveal the presence of disease. By integrating mesoscale models for hydrodynamics of surrounding fluids and for micromechanics of cells, and the Hierarchical Bell Model for specific cell-substrate interactions, we examine the fluid-driven motion of cells in a microchannel over a hard, weakly adhesive surface that contains “sticky” diagonal stripes. We show that as cells roll along the surface, they obtain a net displacement perpendicular to the direction of the fluid flow. This displacement is a function of the cell’s stiffness, meaning that two cells with different compliances or adhesive properties exhibit different amounts of displacement, and in this manner are effectively sorted. We compare the results of the simulations with the data obtained in the experiments with HL-60 cells.

S1.00061 Biocompatibility of Carbon Nanotubes in Mammalian Cells: An Imaging Based Approach , HOWARD CHEN, Massachusetts General Hospital, Harvard Medical School, JESSICA LUCAS, Simmons College, HANNAH PONEK, CHRISTOPHER EVANS, BRADLY BAER, SARA CHOUNG, MICHELLE CHEN, Point Loma Nazarene University — Carbon nanotubes have been widely researched for ultrasensitive biomolecule detection and drug delivery. However, its impact on cells is yet to be fully characterized, mainly due to the complex biological in vivo environment. We report here a mammalian cell-imaging paradigm to study the cellular response to single-walled carbon nanotubes (SWNTs) at the single-cell level. Chinese Hamster Ovarian cells were exposed to SWNTs resuspended in phosphate buffered saline (PBS) at various concentrations. Upon exposure, we optically imaged the cells (1) to visually quantify the SWNTs’ crossing of the cell membrane in real-time; (2) to both qualitatively and quantitatively assess the morphological changes associated with cellular stress in the presence of SWNTs; and (3) to serially quantify cell survival with highly sensitive bioluminescence-based imaging. Consistent with literature reports, high concentration of SWNTs acutely compromised cell division and decreased cell survival. Low concentrations were well tolerated by the cells initially but had similar effects after prolonged exposure. We discuss the inter-relationships among the cell morphology, viability, and intracellular SWNT uptake parameters, as a function of nanotube concentration and exposure time.

S1.00062 Radial Distribution Function of Silicene¹ , MA. RAYO CHAVEZ-CASTILLO, Instituto de Fisica BUAP, MARIO ALBERTO RODRIGUEZ-MEZA, Depto. de Fisica, ININ, LILIA MEZA-MONTES, Instituto de Fisica BUAP — Silicene is the counterpart of graphene and its potential applications as a part of the current electronics, based in silicon, make it a very important system to study. We perform molecular dynamics simulations and analyze the structure of two and three dimensional arrays of Si atoms by means of the radial distribution function at different temperatures and densities. As a first approach, for the 2D case, the Lennard-Jones potential is used and two sets of parameters are tested. We found that the radial distribution function does not change with the parameters and resembles the corresponding to the (111) surface of the FCC structure, which is similar to that of the honeycomb lattice although with different peak heights. The liquid phase appears at very high temperatures, suggesting a very stable system in the solid phase. In 3D, a comparison with potentials developed specifically for silicon, as suggested by Stillinger and Weber[F. H. Stillinger and T. A. Weber, Phys. Rev. B 31, 5262 (1985)] will be presented.

¹Partially supported by CONACYT CB-133516 and VIEP-BUAP.

S1.00063 Electronic and transport properties of metallic hexaboride nanorods , LU WANG, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68132, DANIEL VALENCIA, JUN-QIANG LU, Department of Physics, University of Puerto Rico at Mayagüez, PR 00681, RENAT SABIRIANOV, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68132, CHIN LI CHEUNG, Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588 — In this work, we performed electronic structure calculations of quasi one-dimensional metallic hexaboride XB₆ nanorods, where X are mostly rare-earth metals with 4f levels such as La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, and Lu, which usually regarded as good thermoelectric materials because of their low work functions and transport properties. Our purpose is to facilitate the research and manufacture of metal boride probes, thus we study extensively the size-dependence and element-specificity of the electronic properties. In these nanorods, we uncovered few general features that elucidate their excellent thermionic and field emission property. To further investigate the transport properties, we adopted the combined Landauer-Buttiker formalism and non-equilibrium Green’s function technique to compute the transmission coefficients near the Fermi level and found that hexaboride nanorods can be converted from metallic to semiconducting by applying a gate voltage larger than 10 V.

S1.00064 Electronic transport in aperiodic nanosheets, nanotubes and nanowires¹ , VICENTA SANCHEZ, Departamento de Fisica, Facultad de Ciencias, Universidad Nacional Autonoma de Mexico., CHUMIN WANG, Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico. — Based on the Kubo-Greenwood formula, we study the electronic transport in cubically-structured quasiperiodic nanosheets, nanotubes and nanowires, where the nanotubes are made by connecting one of the boundaries of a square-lattice sheet and the nanowires have a cross section of 90×90 atoms. Calculations of electrical conductivity were performed by using a tight-binding Hamiltonian and by combining the convolution theorem with the real-space renormalization method [1]. The *dc* conductance shows quantized spectra, where nanotubes have steps with a double height in comparison with those of a nanosheet, both in contrast to an inhomogeneous step structure derived from nanowires. The *ac* conductivity shows a Drude and an oscillating behavior, when the electric field is along a periodic or quasiperiodic direction, respectively. Finally, the theoretical results are compared with experimental data.

[1] V. Sanchez and C. Wang, *Phys. Rev. B* **70**, 144207 (2004).

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S1.00065 Trainable solar cell effect in TPPS4 nanowires.¹ , KATHERINE L. VAN AKEN, MARJON ZAMANI, IAN W. HALVIC, Haverford College, ZHENGQING J. QI, A.T. JOHNSON, University of Pennsylvania, WALTER F. SMITH, Haverford College — We have measured photovoltaic currents for self-assembled *meso*-tetra(4-sulfonato-phenyl)porphine (TPPS4) nanowires. This is surprising, given that our devices are symmetrical. However, by “training” the nanowires with a bias voltage, we can break this symmetry. After training, when the nanowires are illuminated with a 488 nm laser under zero bias voltage, a solar cell current is observed, with polarity opposite to the training voltage. The magnitude of solar cell current depends on both the time of training and the magnitude of the training voltage. After the training voltage is removed, the solar cell current decays very quickly initially and then transitions to a much slower decay. This suggests that there are different populations of trapped charges that are repositioned by the electric field of the training voltage, and that are responsible for the solar cell current. We present a qualitative model in which the Schottky barriers at the interfaces with electrodes are affected by these trapped charges, leading to asymmetrical charge transport and thus to the observed current.

¹This work was supported by NSF grant CHE-0616615.

S1.00066 Structural Properties and Stability of Double Walled Armchair Silicon Nanotubes¹

HAOLIANG CHEN, ASOK RAY, Physics Department, University of Texas at Arlington, Arlington, Texas 76019 — A systematic study of armchair double-walled Si nanotubes (DWNT) $(n,n)@(m,m)$ ($3 \leq n \leq 6$; $7 \leq m \leq 12$) using the finite cluster approximation is presented. The geometries of the tubes have been spin optimized with an all electron 3-21G* basis set and the B3LYP functional. The study indicates that the stabilities of the double-walled Si nanotubes are of the same order as those of single-walled Si nanotubes suggesting the possibilities of experimental synthesis of both single-walled and double-walled Si nanotubes. The binding energy per atom or the cohesive energy of the double-walled nanotubes depends not only on the number of atoms but also on the coupling of the constituent single-walled nanotubes. Some nanotubes with small interlayer separations do not hold the coaxial cylindrical structure after optimization. The NTS $(n, n)@(n+3, n+3)$ are found to have large formation energies and binding energies per atom. For example, $(3,3)@(6,6)$, $(4,4)@(7,7)$, $(5,5)@(8,8)$, and $(6,6)@(9,9)$ all have large binding energies per atom, around 3.7eV/atom. All double-walled Si nanotubes are found to be semiconductors. However, the band gap, in general, is observed to decrease from single walled nanotubes to double walled nanotubes.

¹Work partially supported by the Welch Foundation. (Grant No. Y-1525)

S1.00067 Hierarchically driven nanostructure electrocatalysts for direct sensing of biomolecules

YUMIN LEE, JUN HO SHIM, MINKYUNG KANG, HYE SU JANG, Department of Chemistry & Nano Science, Ewha Womans University, JEONG MIN BAIK, School of Mechanical and Advanced Materials Engineering, Ulsan National Institute of Science and Technology, YOUNGMI LEE, CHONGMOK LEE, MYUNG HWA KIM, Department of Chemistry & Nano Science, Ewha Womans University — Applying nanoscale device fabrications toward biomolecules, ultra sensitive, selective, robust, and reliable chemical or biological microsenors have been one of the most fascinating research directions in our life science. It is still challenging to make miniaturized sensors having the sensitive detectability to biologically relevant species due to limitations in terms of catalytic efficiency and sustainability. We introduce hierarchically driven iridium dioxide nanowires (IrO_2 NWs) directly on a platinum (Pt) microwire, which allows a simple fabrication of the amperometric sensor and shows a favorable electronic property desired for sensing of H_2O_2 and NADH without aid of enzymes. We have prepared highly crystalline IrO_2 needlelike-NWs by an atmospheric pressure chemical vapor deposition of IrO_2 powder without catalyst on a Pt wire surface, IrO_2 NWs-Pt, which was tested as an amperometric microsensor. The structures and morphologies of the IrO_2 NWs were characterized using FE-SEM, HRTEM and Raman spectroscopy. This rational engineering of a nanoscale architecture based on the direct formation of the 1-D nanostructures on an electrode can offer a useful platform for high performance electrochemical biosensors efficiently, sensitive detection of biologically important molecules.

S1.00068 Hierachically grown RuO_2 nanowires on electrospun IrO_2 nanofiber

JAEEYON LEE, Department of Chemistry & Nano Science, Ewha Womans University, HEE-SUNG YANG, Department of Nano Science & Technology, Sejong University, YUKYUNG CHO, Department of Chemistry & Nano Science, Ewha Womans University, HAE-YOUNG SHIN, SEOKHYUN YOON, Department of Physics, Ewha Womans University, JEONG MIN BAIK, School of Mechanical and Advanced Materials Engineering, Ulsan National Institute of Science and Technology, YOUNG-SOO SEO, Department of Nano Science & Technology, Sejong University, MYUNG HWA KIM, Department of Chemistry & Nano Science, Ewha Womans University — Electrospinning is a well known tool to synthesize nanofibers with the various diameters. Iridium oxide(IrO_2) and Ruthenium oxide(RuO_2) have a great potential as materials for electrodes in electrochemical devices due to their high electrical conductivity, chemical stability, and characteristics. So when they are mixed, we expect superior electrochemical properties and stability. We synthesize IrO_2 nanofibers from mixture of Iridium precursor and polymer. At certain condition, we were able to obtain uniform and continuous fibers that the average diameter of nanofibers is approximately 150 nm. After calcination, RuO_2 nanowires were then hierarchically grown on IrO_2 nanofibers by APCVD at about 650 ° without any catalyst. The diameters of nanowires are about 50 nm and the length is $\sim 1.5 \mu\text{m}$. The structures and morphologies were examined using scanning electron microscopy (FE-SEM), high resolution electron microscopy (HRTEM), X-ray diffraction (XRD) spectrum and Raman spectroscopy.

S1.00069 Synthesis of metallic ReO_3 nanowires

DONGSHIN MYUNG, Department of Chemistry & Nano Science, Ewha Womans University, JEONG MIN BAIK, School of Mechanical and Advanced Materials Engineering, Ulsan National Institute of Science and Technology, MYUNG HWA KIM, Department of Chemistry & Nano Science, Ewha Womans University — Rhenium trioxide (ReO_3) is well known as an unusual transition metal oxide with unexpectedly high electrical conductivity close to that of copper. We present the synthesis of highly crystalline metallic rhenium trioxide (ReO_3) nanowires. ReO_3 nanowires were grown on a 200 nm silica-covered Si (001) wafer by atmospheric-pressure chemical vapor deposition (APCVD) at about 300 ° without any catalyst. The wafer was placed in the quartz boat approximately 15 cm downstream from the fine mashed ReO_3 powder and heated at 320 ° with flowing of high purity Ar (500 sccm) for 2 h and then kept at 450 ° for an additional 3 h. The two-step heating enhanced the growth of ReO_3 nanowires. The structures and morphologies were examined using scanning electron microscopy (FE-SEM) and high-resolution electron microscopy (HRTEM). Based on HRTEM, the ReO_3 nanowires exhibit a core of perfect cubic perovskite type single crystal structure with a shell of thin amorphous and disordered structures of less than 2 nm in the near surface layers. Possibly this is due to proton intercalation induced by the surface reaction of single crystal ReO_3 with water.

S1.00070 The effect of frequency noise on the spectral response of nanomechanical oscillators

FENGPEI SUN, Department of Physics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, JIE ZOU, Department of Physics, University of Florida, Gainesville, Florida 32611, USA, HO BUN CHAN, Department of Physics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong — We study the spectral response of an underdamped nanomechanical oscillator in the presence of frequency noise. Motion of a nanobeam is excited and measured using the magnetomotive technique. Telegraph noise is applied on nearby side gates, so that the eigenfrequency of the nanobeam randomly jumps back and forth between two values due to electrostatic coupling. This arrangement is analogous to a mechanical oscillator dispersively coupled to a classical or quantum two-level system. The spectrum displays two distinct peaks when the two eigenfrequencies are separated by a distance larger than the damping constant λ of the oscillator. As the switching rate $\dot{W}$ of the telegraph noise increases, we observe that the two peaks merge into one. The width of the single spectral peak decreases with increasing $\dot{W}$. At $\dot{W} \gg \lambda$, the spectral width approaches its intrinsic value as if frequency noise is absent. The results are in agreement with theoretical predictions.

S1.00071 Self-standing Hybrid Nanofibers of TiO_2 and TiO_2 /Hydroxyapatite: Application in

Photocatalytic and Photovoltaic Systems, PARVANEH ROUHANI, Physic Department, Sharif University of Technology, Tehran, Iran, NIMA TAGHAVINIA TEAM, MASOUD RAHMAN TEAM, LEYLA SHOOSHTARI TEAM — A Hybrid fibers of Hydroxyapatite TiO_2 , HAP/ TiO_2 with modified photocatalytic properties were synthesized using a template method. Liquid phase deposition (LPD) technique was employed to grow TiO_2 layers on cellulose fibers, followed by deposition of HAP from a pseudo body solution, and finally heat removing the cellulose template. The resulting material has a fibrous structure, mimicking the cellulose fibers shape, and have a typical surface area of 114 m^2/g , compared to 74 m^2/g for pure TiO_2 fibers. Adsorption and photocatalytic degradation tests showed that addition of HAP to TiO_2 fibers increased the adsorptive from 17% to 35%. Nano particulated TiO_2 fibers as one-dimensional long structures were introduced into TiO_2 P25 nano particle films using co-electrophoretic deposition. This resulted in less porosity and higher roughness factor of the films that provided more favorable conditions for electron transport. The films used as the photoanode of a dye solar cell (DSC) produced 65% higher photovoltaic efficiency. TiO_2 fibers can be excellent binders in single-step, organic-free electrophoretic deposition of TiO_2 for DSC photoanode.

S1.00072 Family-Dependent Rectification Characteristics in Ultra-Short Graphene Nanoribbon p-n Junctions, JIAXIN ZHENG, XIN YAN, LILI YU, HONG LI, RUI QIN, State Key Laboratory of Mesoscopic Physics, Department of Physics, Peking University, Beijing 100871, P. R. China, GUANGFU LUO, Department of Theoretical and Computational Molecular Science, Institute for Molecular Science, Okazaki 444-8585, Japan, ZHENGXIANG GAO, DAPENG YU, JING LU, State Key Laboratory of Mesoscopic Physics, Department of Physics, Peking University, Beijing 100871, P. R. China — We present the first transport property investigation of a-few-nm-long armchair graphene nanoribbon (AGNR) p-n junctions by using first-principles method. Intriguingly, family-dependent rectification is observed. To be specific, traditional rectification effect in the forward direction is observed in the AGNR p-n junctions with $3n$ and $3n+2$ widths whereas reverse rectification effect is observed in the AGNR p-n junctions with $3n+1$ width. The analysis of the spatial distribution of molecular projected self-consistent Hamiltonian eigenstates and the projected density of states give an insight of the observed results.

S1.00073 Chirality Distribution Measurements of the NIST Single-Wall Carbon Nanotube Reference Material Using Resonance Raman Spectroscopy¹, L.F. SCHEEL², J.R. SIMPSON³, Towson University, J.A. FAGAN, A.R. HIGHT WALKER, National Institute of Standards and Technology (NIST) — The ability to rapidly and easily determine the chiral vector distribution within a nanotube population remains a key measurement need for carbon nanotube processing and applications. We report Resonance Raman Spectroscopy (RRS) measurements of a SWCNT reference material from NIST. The SWCNT samples were synthesized using the CoMoCat method, dispersed in aqueous solutions by wrapping in deoxycholate surfactant, and separated by length using ultracentrifugation. We measure Raman spectra over a wide range of excitation wavelengths from 457 nm to 850 nm using a series of discrete and continuously tunable laser sources coupled to a triple-grating spectrometer with a liquid-nitrogen-cooled detector. The spectra reveal Raman-active vibrational modes including the low-frequency radial breathing mode and higher-order modes. Chirality distributions are determined from the Raman spectra, specifically the RBM frequency and energy excitation profiles, together with input from theoretical models. RRS is sensitive to both major and minor chiral species in the sample. We will compare the resulting chirality distribution obtained from RRS with those obtained from other orthogonal measurement techniques.

¹JRS acknowledges support from the Research Corporation's CCSA.

²Presently at Oak Ridge National Laboratory.

³Towson University and NIST.

S1.00074 A study of 3-dimensionally periodic carbon nanostructures, MING YIN, Benedict College Columbia, SC 29204, MICHAEL BLEIWEISS, JAFAR AMIRZADEH, TIMIR DATTA, University of South Carolina Columbia, SC 29208, FOUZI ARAMMASH, Benedict College, Columbia, SC 29204 — Electronic structures with intricate periodic 3-dimensional arrangements at the submicron scale were investigated. These may be fabricated using artificial porous opal substrates as the templates in which the targeted conducting medium is introduced. In the past these materials were reported to show interesting electronic behaviors. [Michael Bleiweiss, et al "Localization and Related Phenomena in Multiply Connected Nanostructured," BAPS, Z30.011, Nanostructured Materials Session, March 2001, Seattle]. Several materials were studied in particular disordered carbon which has been reported to show quantum transport including fractional hall steps. The results of these measurements, including the observation of localization phenomena, will be discussed. Comparisons will be made with literature data.

S1.00075 Charge redistribution and interlayer coupling in twisted bilayer graphene under electric fields, PATRICIO VARGAS, ERIC SUAREZ MORELL, Physics Department, Universidad Tecnica Federico Santa Maria, Casilla 110-V, Valparaiso, Chile, LEONOR CHICO, LUIS BREY, Departamento de Teoria y Simulacion de Materiales, Instituto de Ciencia de Materiales de Madrid, CSIC, E-28049 Cantoblanco, Spain — There is an ongoing controversy on the electronic characteristics of rotated bilayer graphene. Several experiments on rotated few-layer graphene grown on SiC show an electronic behavior similar to that of single-layer graphene, with the same carriers' velocity as that of an isolated graphene monolayer; for this reason, these systems have been considered as composed of uncoupled graphene sheets. We investigate the electronic density redistribution of rotated bilayer graphene under a perpendicular electric field, showing that the layers are actually coupled even for large angles. This layer-layer coupling is evidenced by the charge transfer on these structures as a function of the external voltage. We find an inhomogeneous excess charge distribution that is related to the moiré patterns for small angles, but that persists for larger angles where the carriers' velocity is equal to that of single layer graphene. Our results show that rotated bilayer systems are coupled for all rotation angles.

S1.00076 Spin-density-wave instability in graphene doped near the van Hove singularity, RALPH VAN GELDEREN, DMYTRO MAKOGON, Utrecht University, RAFAEL ROLDÁN, Instituto de Ciencia de Materiales de Madrid, CRISTIANE MORAIS SMITH, Utrecht University — We study the instability of the metallic state towards the formation of a new ground state in graphene doped near the van Hove singularity. The system is described by the Hubbard model and a field theoretical approach is used to calculate the charge and spin susceptibility. We find that for repulsive interactions, within the random phase approximation, there is a competition between ferromagnetism and spin-density wave (SDW). It turns out that a SDW with a triangular geometry is more favorable when the Hubbard parameter is above the critical value $U_c(T)$, which depends on the temperature T , even if there are small variations in the doping. Our results can be verified by ARPES or neutron scattering experiments in highly doped graphene.

S1.00077 Effects of static charging and exfoliation of layered crystals, MEHMET TOPSAKAL, SALIM CIRACI, UNAM-Institute of Materials Science and Nanotechnology — Using first-principle plane wave method we investigate the effects of static charging on structural, electronic and magnetic properties of suspended, single layer graphene, graphane, fluorographene, BN and MoS(2) in honeycomb structure. The limitations of periodic boundary conditions in the treatment of charged layers are clarified. Upon positive charging the band gaps between the conduction and valence bands increase, but the single layer nanostructures become metallic owing to the Fermi level dipping below the maximum of valence band. Moreover, their bond lengths increase leading to phonon softening. As a result, the frequencies of Raman active modes are lowered. High level of positive charging leads to structural instabilities in single layer nanostructures, since their specific phonon modes attain imaginary frequencies. Similarly, excess positive charge is accumulated at the outermost layers of metallized BN and MoS(2) sheets comprising a few layers. Once the charging exceeds a threshold value the outermost layers are exfoliated. Charge relocation and repulsive force generation are in compliance with classical theories.

S1.00078 Effects of Peptide Adsorption on the Electronic Properties of Graphene, BRAHIM AKDIM, ZHIFENG KUANG, SANG KIM, RAJESH NAIK, BARRY FARMER, AFRL, TIFFANY WALSH, University of Warwick, RUTH PACTHER, AFRL — In this work we aim to explain the increase in the electrical conductance in a single-layer graphene (SLG) field-effect transistor (FET) upon binding the peptide HSSYWYAFNNKT, which we previously demonstrated. The adsorption of the peptide onto the SLG has been carefully modeled by applying empirical molecular dynamics simulations with the AMOEBA force-field. The peptide adsorbed SLG structure demonstrates $\pi - \pi$ stacking with aromatic amino acids, namely His, Tyr, Thr and Ph. Based on this large-scale peptide-SLG system, calculations on the electron transport using the nonequilibrium Green's function formalism at the extended Huckel level were carried out. Transmission eigenchannels and spectra, projected density of states, effects of modeling realistic leads (gold vs. graphene) and $I - V$ characteristics will be discussed in detail. In this context, suppositions as to the mechanism of increased conductance for the peptide-SLG FET will be proposed.

S1.00079 Heat transfer at interfaces with graphene, ZHIPING XU, Tsinghua University — Graphene has an ultrahigh in-plane thermal conductivity (5500 W/mK), but simultaneously a much lower conductivity along the c-axis in graphite or at the interfaces with other materials. As graphene finds more and more applications in nanoelectronics and high-performance composites, these interfaces become critically important in defining their heat dissipation and conduction performance. Unlike conventional interfaces in materials such as grain boundaries, the interfaces with graphene can be tuned by chemically modifying the graphene monolayer or intercalating the interfaces. These nano-engineering proposals require fundamental understanding of the heat transfer mechanisms. In order to obtain some insights on the transfer processes of mechanical and thermal energy across these interfaces, we perform series of molecular dynamics simulations, in combination with theoretical analysis by considering the quasi-ballistic nature of phonon transport at nanoscale. The result shows that heat dissipation or transport can be divided into two stages, beginning with an interface-controlled process. The effects of interface structures and binding properties on the whole process will be covered in this talk, with several examples showing how the interfacial thermal transfer can be engineered.

S1.00080 Nonlocal resistance in a bilayer graphene under a magnetic field¹, CHANG-RAN WANG, TSUNG-YEH YANG, CHIA-TSO HSIEH, YUNG-YU CHIEN, WEI-LI LEE, Institute of Physics, Academia Sinica — We have performed nonlocal resistance measurement in bilayer graphene with Hall-bar geometry under high magnetic fields. We observed large nonlocal resistance near the charge neutral point (CNP) which grows rapidly with field intensity. At 15 Tesla, the relative increase of nonlocal resistance near CNP is an order of magnitude larger than the local resistance at the same condition. This behavior is similar to the recent nonlocal measurement result in a single layer graphene. The detailed field and temperature dependences will be presented.

¹National Science Council in Taiwan

S1.00081 Edge currents and an array of nanopores in zigzag and chiral graphene nanoribbons as a route toward high-ZT thermoelectrics, PO-HAO CHANG, Department of Physics and Astronomy, University of Delaware, Newark, DE 19716-2570, USA — We exploit peculiar transport properties of graphene nanoribbons (GNRs) with zigzag or chiral edges where local current density of quasiparticles close to the Dirac point is largely confined around their edges. Thus, drilling an array of nanopores in the interior of such nanoribbons will not affect much the electronic transport while substantially suppressing the phonon transport in sufficiently long wires. For nanoribbons of length $\sim 1 \mu\text{m}$ and width 4.1 nm and nanopores of diameter 2 nm, the ZT for both zigzag GNRs and chiral GNRs is $\simeq 4$ at $T = 77 \text{ K}$ and $\simeq 1.5$ at $T = 300 \text{ K}$. With slightly asymmetric arrangement of nanopores, the ZT of zigzag GNRs can be further enhanced to reach $\simeq 13$ at $T=77 \text{ K}$ and $\simeq 5$ at $T=300 \text{ K}$.

S1.00082 Low-frequency noise in graphene FETs, NAN SUN, GERALD ARNOLD, KRISTOF TAHY, JIANCHUN ZENG, DEBDEEP JENA, HUILI XING, STEVEN RUGGIERO, University of Notre Dame, UNIVERSITY OF NOTRE DAME TEAM — We report on the low-frequency electronic noise in graphene-based FET structures. Samples were created using standard e-beam lithography and exfoliated, epitaxially-grown, and CVD-grown single-layer graphene films. The lowest overall noise was observed in epitaxially-grown films on SiC. We also investigated the gate dependence of the noise amplitude. Previous studies have suggested that the noise dependence should be either Λ -shaped in keeping with the Hooge model, or M-shaped as described by the charge-noise model. We here propose a new noise model based upon resonant scattering theory, which not only explains both types of gate dependence on noise, but also models the general noise behavior in graphene.

S1.00083 Magnetic Properties of Graphene Superlattices, SI WU, University of Waterloo, MATTHEW KILLI, ARUN PARAMAKANTI, University of Toronto — We studied graphene superlattices (SL) in the presence of magnetic fields. We found magnetic properties of single layer and bilayer graphene SLs in a weak magnetic field are strongly determined by emergent Dirac physics. Moreover, the spatial anisotropy of diagonal conductivities can be reversed when magnetic field is tuned from weak to intermediate strength. In a strong magnetic field, all anisotropies disappear and results from pristine graphene are restored.

S1.00084 ABSTRACT WITHDRAWN —

S1.00085 Co-adsorption of n Monomer Species on Terraces and Nanotubes¹, ALAIN PHARES, Villanova University — We consider the partition function, Z , of the system of n monomer species adsorbed on a terrace or a nanotube of arbitrary periodic lattice geometry, L atomic sites in length, and M' sites in the width of the terrace or in the normal cross-section of the nanotube. Z is related to the eigenvalues of a real and non-negative matrix (**T** matrix) of rank $(n+1)^M$, where M is an integer multiple of M' . In the infinite- L limit, we also prove that Z is the largest eigenvalue of the **T**-matrix, raised to the power $1/M$. Because the rank of this matrix increases exponentially with M , we develop a technique for its recursive construction applicable to any lattice geometry, which is easily programmed and efficiently adaptable for supercomputing and multiparallel processing. As examples, we consider the co-adsorption on square, equilateral triangular, and honeycomb surfaces. This general formulation can now be applied to model a whole new set of experiments involving the coadsorption of two or more monomer species, on terrace or nanotube surfaces with various periodic lattice structures.

¹This work is supported in part by the National Institute for Computational Sciences grant # CHE040001.

S1.00086 SEMICONDUCTORS —

S1.00087 Temperature dependence of optoelectronic properties of $\text{CdS}_x\text{Se}_{1-x}$, $\text{CdS}_x\text{Te}_{1-x}$, $\text{CdSe}_x\text{Te}_{1-x}$, DONGGUO CHEN, NUGGEHALI RAVINDRA, New Jersey Institute of Technology — Temperature dependence of the optoelectronic properties of ternary compounds, $\text{CdS}_x\text{Se}_{1-x}$, $\text{CdS}_x\text{Te}_{1-x}$ and $\text{CdSe}_x\text{Te}_{1-x}$, are presented. The analysis of the temperature dependence of the energy gap of these compounds, for various compositions, is discussed in light of the Varshni formula. Extension of this study is then made to include the contributions of the temperature dependence of the gap of the component binary semiconductors. The model takes into account the implications of the above results on the refractive indices of these ternary compound semiconductors.

S1.00088 Modeling Random Dopant Fluctuation Effects in Nanoscale Tri-Gate MOSFETs, JOSHUA OGDEN, ABDUSSAMAD MUNTAHI, KRISHNA YALAVARTHI, SHAIKH AHMED, Southern Illinois University — The tri-gate FET has been hailed as the biggest breakthrough in transistor technology in the last 20 years. The increase in device performance (faster switching, low power, improved short channel effects, etc.), coupled with the reduction in device size, would allow for huge gains in the electronics industry. In this work, an atomistic quantum-corrected Monte Carlo 3-D device simulator was used to not only investigate the validity of these claims, but also how quantum size quantization and random dopant fluctuation (RDF) affect the tri-gate FET performance and how to curb these issues. The main findings are as follow: 1) carrier scattering leads to ON current degradation of $\sim 30\%$ and hence cannot be ignored; 2) deviations in threshold voltage due to random channel doping are smaller in the tri-gate FET; 3) RDF due to the source/drain discreteness can be engineered by adjusting the source/drain junction depth. With randomness reduced, the overall performance should increase when used in ICs, where consistency in device characteristics is essential.

S1.00089 ABSTRACT WITHDRAWN —

S1.00090 Spin Torque and Its Efficiency in 3D Rashba Models with Localized Spins, KAZUHIRO TSUTSUI, SHUICHI MURAKAMI, Tokyo Institute of Technology — In addition to the magnetization reversal by the spin-transfer torque, the magnetization reversal driven by a strong spin-orbit coupling has been intensely investigated experimentally and theoretically. In this presentation, we focus on 3D Rashba models coupled with localized spins, and study the spin torque theoretically. This is motivated by the recent discovery of BiTeI as 3D Rashba systems. As a result, we find that the spin torque in 3D Rashba models is largely enhanced in the high-carrier-density regime compared with 2D Rashba models. We also find that the spin-torque efficiency defined as the ratio between the spin torque and the electric current is enhanced when the Fermi energy lies on only lower band, both in 3D and 2D. As we change the Rashba spin-orbit coupling, the spin-torque efficiency becomes maximum when the Rashba spin-orbit coupling is comparable to the exchange coupling to the localized spins. The optimum spin-torque efficiency becomes large when the Rashba spin-orbit coupling is large, and it is preferable for the magnetization reversal with smaller amount of current injection.

S1.00091 All-optical patterning of Nuclear Polarization in Gallium Arsenide¹, YUNPU LI, JONATHAN P. KING, JEFFREY A. REIMER, CARLOS A. MERILES, None — We employ Stray-Field NMR Imaging for ⁶⁹Ga and ⁷¹Ga to monitor the spatially-dependent polarization of nuclear spins in semi-insulating bulk GaAs at 9.4 T. By exploiting two competing mechanism as hyperfine and quadrupolar interaction for optical nuclear polarization at different illumination intensities and wavelengths, we demonstrate all-optical creation of three-dimensional patterns of positive and negative nuclear polarization. We also observe the isotope dependence of the patterning process, where different isotopes (⁶⁹Ga and ⁷¹Ga) have opposite polarization at the same location in the sample. By combining the optical pumping with varied NMR pulse sequences, we demonstrate the control of nuclear polarization.

¹The authors acknowledge support from NSF under Project ECS0608763.

S1.00092 Dynamical simulation of a two-electron spin qubit based on hyperfine interaction¹, MIGUEL ANGEL RODRIGUEZ-MORENO, Centro de Investigaciones en Semiconductores ICUAP, LILIA MEZA-MONTES, Instituto de Física BUAP, DAVID HERNANDEZ DE LA LUZ, Centro de Investigaciones en Semiconductores ICUAP — The interaction with the nuclear field is one of the main sources of decoherence in solid state quantum bits. However, recently it has been shown that hyperfine interaction can also be used to manipulate the spin state of electrons in double quantum dots. In this work, we simulate numerically the dynamics of a spin-based quantum bit consisting of two electrons confined in a double quantum dot, including the interaction with a random nuclear field. The two electron wavefunction is built using an antisymmetric function expansion and the total hamiltonian is discretized spatially using finite differences. For the dynamic simulation, an exponential approximation of the time propagator is used. In order to model the hyperfine interaction, a normally-distributed random magnetic field is assigned to each simulation grid point. The dynamics of the system is calculated by averaging over an ensemble of quantum dots. It is shown how the hyperfine field can be used to drive transitions between singlet and triplet states, an effect that has already been found experimentally. Particularly, it is shown how these transitions can be controlled using an applied electric field, thus allowing for the realization of a two-electron quantum gate.

¹Partially supported by CONACYT CB-133516 and VIEP-BUAP.

S1.00093 ABSTRACT WITHDRAWN —

S1.00094 The interaction of hydrogen donors with compensating acceptors in semiconducting oxides, JOEL VARLEY¹, HARTWIN PEELAERS, ANDERSON JANOTTI, CHRIS VAN DE WALLE, University of California, Santa Barbara — Hydrogen is a common impurity that can act as a donor and an acceptor in a semiconductor, leading to a variety of behavior that may impact the desired performance. In one class of materials, wide-band-gap semiconducting oxides, the role of H has been strongly linked to n-type conductivity. In these systems H acts predominantly or exclusively as a shallow donor as an interstitial or while substituting on an O site. In addition to the resulting n-type conductivity, the incorporation of H or other donor dopants also leads to an increase in compensating acceptor defects. The interaction of H with cation vacancies, the dominant acceptor impurity involved in compensation, has yet to be fully explored. Using first-principles calculations employing hybrid functionals, we investigate the complexes formed between cation vacancies and interstitial H donors. We report on the formation energies, binding energies, and vibrational frequencies of the hydrogenated cation vacancies in the transparent semiconducting oxides SnO₂, In₂O₃ and Ga₂O₃ [1]. We find that H can interact strongly with vacancies in both atomic and molecular form, and can have a significant impact on the electrical properties of devices employing these oxides.

[1] J.B.Varley et al., J.Phys. Cond. Matter 23, 334212 (2011).

¹Stanford University

S1.00095 Electronic properties of doped cesium niobate, LU WANG, RENAT SABIRIANOV, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68132, ROBERT SMITH, Department of Chemistry, University of Nebraska at Omaha, Omaha, NE 68132, CHIN LI CHEUNG, Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588 — Antiferroelectric cesium niobate Cs₂Nb₄O₁₁ (CNO) is known to have novel water splitting capability. It was reported that the broad blue photoluminescence was observed at 77 K. Particularly when treated with NiO₂, the water-splitting activity under UV-light irradiation increased five times. In this work we present systematic studies of the electronic properties of doped CNO by using density functional theory calculations. We first obtain direct band gap of 3.12 eV for the pure sample that agrees well with experimental value of 3.55 ± 0.05 eV. Then we notice, at both the high and low-density regions, the band gap effectively reduced after oxygen atoms substituted by sulfur and nitrogen, and niobium by vanadium. As a final point, we present and discuss relations between impurity concentration and band gap reduction.

S1.00096 Inspecting the microstructure of electrically active defects at the Ge/GeO_x interface, MARCO FANCIULLI, Department of Material Science, University of Milano Bicocca, Italy and MDM Laboratory, IMM-CNR, Agrate Brianza, Italy, SILVIA BALDOVINO, ALESSANDRO MOLLE, MDM Laboratory, IMM-CNR, Agrate Brianza, Italy — High mobility substrates are important key elements in the development of advanced devices targeting a vast range of functionalities. Among them, Ge showed promising properties promoting it as valid candidate to replace Si in CMOS technology. However, the electrical quality of the Ge/oxide interface is still a problematic issue, in particular for the observed inversion of the n-type Ge surface, attributed to the presence of dangling bonds inducing a severe band bending [1]. In this scenario, the identification of electrically active defects present at the Ge/oxide interface and the capability to passivate or anneal them becomes a mandatory issue aiming at an electrically optimized interface. We report on the application of highly sensitive electrically detected magnetic resonance (EDMR) techniques in the investigation of defects at the interface between Ge and GeO₂ (or GeO_x), including Ge dangling bonds and defects in the oxide [2]. In particular we will investigate how different surface orientations, e.g. the (001) against the (111) Ge surface, impacts the microstructure of the interface defects. [1] P. Tsipas and A. Dimoulas, Appl. Phys. Lett. 94, 012114 (2009) [2] S. Baldovino, A. Molle, and M. Fanciulli, Appl. Phys. Lett. 96, 222110 (2010)

S1.00097 Quantum Transport in Ultra-scaled Junctionless Transistors¹, SUNGGEUN KIM, Purdue University, MATHIEU LUISIER, ETH Zurich, GERHARD KLIMECK, Purdue University, NCN COLLABORATION² — As the dimensions of metal-oxide-semiconductor field-effect transistors have been scaled down to a few nano-meters, short channel effects have started to significantly degrade their performance. The junctionless transistor is an alternative device structure which is expected to reduce short channel effects. However, an extreme device scaling raises another issue, namely, source-to-drain tunneling. Junctionless transistors contain several doping atoms in the channel which can enhance tunneling processes and cause electrons to scatter with them. Through self-consistent quantum transport simulations based on the tight-binding model with electron-phonon scattering included, it is found that junctionless nanowire transistors with a gate length of 5 nm do not outperform conventional inversion-mode transistors with the same dimension in terms of their on-state characteristics, mainly due to impurity scattering in the channel. The advantage of the junctionless transistor in the subthreshold region vanishes due to large tunneling currents through doping impurities.

¹We acknowledge MSD for funding, RCAC, NCCS, NICS, and TACC for supercomputing resources, and nanoHUB for computational resources

²Network for Computational Nanotechnology

S1.00098 Band crossing in isovalent semiconductor alloys with large size mismatch, HUI-XIONG DENG, SU-HUAI WEI, National Renewable Energy Laboratory — Mixing isovalent compounds AC with BC to form alloys $A_{1-x}B_xC$ has been an effective way in band structure engineering to enhance the availability of material properties. In most cases, the mixed isovalent atoms A and B, such as Al and Ga in $Al_{1-x}Ga_xAs$ or As and Sb in $GaAs_{1-x}Sb_x$ are similar in their atomic sizes and chemical potentials; therefore, the physical properties of $A_{1-x}B_xC$ change smoothly from AC to BC. However, in some cases when the chemical and size differences between the isovalent atoms A and B are large, adding a small amount of B to AC or vice versa can lead to a discontinuous change in the electronic band structure. These large size- and chemicalmismatched (LSCM) systems often show unusual and abrupt changes in the alloys' material properties, which provide great potential in material design for novel device applications. In this report, based on first-principles band-structure calculations we show that for LSCM $GaAs_{1-x}N_x$ and $GaAs_{1-x}Bi_x$ alloys at the impurity limit the N (Bi)-induced impurity level is above (below) the conduction-(valence-) band edge of GaAs. These trends reverse at high concentration, i.e., the conduction-band edge of $GaAs_{1-x}N_x$ becomes an N-derived state and the valence-band edge of $GaAs_{1-x}Bi_x$ becomes a Bi-derived state, as expected from their band characters. We show that this band crossing phenomenon cannot be described by the popular BAC model but can be naturally explained by a simple band broadening picture.

S1.00099 Engineering Efficiency Droop in InGaN/GaN Multiple Quantum Well LEDs, YASH-VANTH PUTTASWAMY, SASI SUNDARESAN, KRISHNA YALAVARTHI, SHAIKH AHMED, Southern Illinois University — In this work, we address the technologically important issue of efficiency droop pronounced in InGaN/GaN multiple quantum well (QW) LEDs. A two-fold modeling approach is employed where: 1) the NEMO 3-D tool is used to compute the atomistic strain fields and associated polarization potentials in the active region, and 2) the outputs from NEMO 3-D are then coupled to the Synopsys TCAD tool to determine the terminal electrical and optical properties of the device. Next, a series of numerical experiments are performed that mainly aims to improve the efficiency droop without compromising the internal quantum efficiency (IQE) of the device. These include: 1) varying the QW thickness, 2) employing different configurations of tri-material barriers, 3) varying the molar concentration of the barrier materials, and 4) varying the doping density in the barrier region.

S1.00100 Using Polarization Effects in Deep UV Nitride Emitters, G. BRUMMER, H. SUN, A. NIKIFOROV, T. MOUSTAKAS, Boston University — We numerically and experimentally investigate the effects of compositional grading in high Al content AlGaN, with applications to deep UV emitters. The large polarization fields create a fixed charge density in the graded regions, which by necessity, are screened by mobile electrons and holes. The net effect is a pn junction band structure in which bound polarization charge assumes the role of immobile ionized dopants, and the screening charge assumes the role of mobile carriers released from the dopants. Using this phenomenon it should be possible to overcome the difficulties in doping high Al content AlGaN, and make efficient deep UV light emitting diodes, and lasers.

S1.00101 Improvement of M-plane GaN thin film grown on pre-annealing β -LiGaO₂ (100) substrate¹, CHIA-HSUAN HU, CHENG-HUNG SHIH, IKAI LO, YING-CHIEH WANG, CHEN-CHI YANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan, MITCH CHOU, Department of Materials and Optoelectronic Science, National Sun Yat-Sen University, Kaohsiung, Taiwan — M-plane GaN thin films have been grown on β -LiGaO₂ (100) substrates by plasma-assisted molecular-beam epitaxy. In order to improve the quality, we tried to grow M-plane GaN thin films on pre-annealed in vacuum and in air ambient LiGaO₂ (100) substrates. X-ray diffraction data indicated that the M-plane GaN thin film grown on the LiGaO₂ (100) substrate pre-annealed in air ambient has better crystal quality than that grown on the LiGaO₂ (100) substrate pre-annealed in vacuum. In addition, we found that the strain between GaN and LiGaO₂ substrate can be relaxed by growing GaN thin film on pre-annealed LiGaO₂ substrate in air. It reveals that LiGaO₂ substrate annealing in air ambient can suppress the formation of lithium-rich surface effectively to grow a high quality M-plane GaN thin film on the LiGaO₂ substrate.

¹The project was supported by the National Research Council of Taiwan(NRC 98-2112-M-110-003-MY3)

S1.00102 The Growth of InGaN on Single Crystal ZnO (000-1) Substrate by Metal Modulation Epitaxy Method¹, YING-CHIEH WANG, C.H. SHIH, IKAI LO, C.C. YANG, C.D. TSAI, Department of Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan — The growth of InGaN film on single crystal ZnO (000-1) substrate by plasma assisted-molecular beam epitaxy has been investigated. The metal modulation epitaxy (MME) technique was applied in this experiment. The growth mechanism of InGaN thin film on ZnO (000-1) was in the form of 2D growth model by *in-situ* observation of reflection high-energy electron diffraction (RHEED). From the observation of atomic force microscope (AFM), we found that surface roughness of InGaN thin film can be improved using MME technique. The crystal quality and the indium content of InGaN thin film was determined by the X-ray diffraction method. The full width at half-maximum (FWHM) and the indium content of InGaN thin film is 298.64 arc-sec and 17 %, respectively. According to the calculation of bowing parameters, the 17 % indium content of InGaN thin film closed to $In_{0.18}Ga_{0.82}N$ which is perfect lattice-matching to ZnO (000-1). The micro-structure analysis of InGaN grown on ZnO by high-resolution transmission electron microscope (HR-TEM) was performed, which shows that the interface between the substrate and the film is clearly indicating $In_{0.17}Ga_{0.83}N$ to be lattice-matching with ZnO (000-1).

¹The project is supported by National Reaserch Council of Taiwan (NRC 98-2112-M-110-003-MY3).

S1.00103 Studies on the Growth and Characterization of hexagonal boron nitride thin films, M.L. NAKARMI, B. CAI, Department of Physics, Brooklyn College and Graduate Center of the CUNY, Brooklyn, NY 11210, A. DELMONT, A. SPROW, R.C. RAI, Department of Physics, SUNY College at Buffalo, Buffalo, NY 14222 — Hexagonal Boron Nitride (h-BN) with a direct band gap of ~ 5.9 eV has emerged as a promising deep ultraviolet photonic material. We will present the studies on the growth and characterization of h-BN thin films grown on different substrates such as sapphire, YSZ, quartz, and metal substrates. The samples were grown by electron beam evaporation technique. Atomic force microscopy, x-ray diffraction, optical spectroscopy, and Hall effect measurement were employed to characterize surface morphology, structural, optical and electronic, and electrical properties, respectively. We will also present the results of Mg-doped h-BN thin films in an effort to make p-type BN. Implementation of our findings on the development of deep ultraviolet photonic devices will also be discussed.

S1.00104 Electrical characterization of homoepitaxially deposited boron-doped diamond¹, SUNIL KARNA, YOGESH VOHRA, GOPI SAMUDRALA, GEORGI TSOI, None — Homoepitaxial boron doped single crystal diamond films were deposited on 100 oriented lb type synthetic diamond substrates via microwave plasma chemical vapor deposition. The gas phase chemistry of 6% methane/ hydrogen ratio and 5000 ppm of (B/C)_{gas} was used for all samples deposited at different temperature from 900 to 1200°C. The deposited films were characterized by FTIR, AFM, Raman spectroscopy and XRD Rocking curve measurement to assess doping level, surface morphology and crystalline quality. The high growth rate 16 micron per hour has been obtained by optimizing growth parameters such as microwave power, chamber pressure, and gas flow rate. The four-probe electrical resistance measurements on boron-doped samples were conducted between 14 K and 350 K and show competing effects of intrinsic and hoping conductivity.

¹GAFFP

S1.00105 ABSTRACT WITHDRAWN —

S1.00106 A simple approach to the polytypism in boron nitride, TOMONORI ITO, TORU AKIYAMA, KOHJI NAKAMURA, Department of Physics Engineering, Mie University — Boron nitride (BN) is well known as having a polytype including cubic (c-BN) with zinc blende structure (3C) and hexagonal BN (h-BN) phases similarly to C. From the experimental viewpoints, it is found that h-BN appears at ambient temperature and pressure whereas c-BN is preferable at high temperature and high pressure. In order to clarify its polytypism, there have been some ab initio calculations mainly focusing on four-fold coordinated structures such as 3C-, 6H-, 4H-, and 2H-BN. Although the ab initio calculations predict the polytypes for bulk BN, the physical interpretation of the polytypism is still unclear because of the complexity of identifying individual contribution in the ab initio calculations. In order to make up this deficiency, we investigate the polytypism for BN in bulk form using a simple approach on the basis of empirical interatomic potentials. The calculated respective energy differences between 6H and 3C, between 4H and 3C, and between 2H and 3C are 5.0 meV, 7.5 meV, and 17.1 meV when the ionicity $\epsilon_i=0.143$ for BN is employed. These results are consistent with previously reported ab initio calculations. Furthermore, we also discuss the relative stability between h-BN and c-BN using this simple approach.

S1.00107 Morphological Studies on GaN Nanowire Growth Modes¹, ZHENG MA, XIAOHONG AN, SWASTIK KAR, MONEESH UPMANYU, EUGEN PANAITESCU, LATIKA MENON, Northeastern University — We describe our results on growth of single crystal GaN nanowires in three different growth modes (straight, serrated and epitaxial) on catalyst-patterned substrates by means of chemical vapor deposition. The growth is carried out in a tube furnace wherein gallium oxide is used as reactor source and a mixture of ammonia and hydrogen gas is used as precursor. Growth of GaN nanowires are demonstrated on both Au and Ni-catalyst patterned substrates. We show that by controlling the deposition parameters, specifically the size of the catalyst and amount of gallium oxide, we can control the growth morphology. While straight GaN nanowires typically grow on substrates patterned with catalyst particles with dimensions of the order of 100nm, the epitaxial nanowires grow on substrates with much smaller dimensions of catalyst particles 50nm. The newly demonstrated GaN wire growth mode with periodic serrations, typically grow under conditions involving large catalyst size ~ 300 nm and excess gallium oxide. In this work, a detailed investigation is carried out on the structural properties of the three different growth modes by means of high resolution transmission microscopy, x-ray diffraction and Raman spectroscopy studies in order to obtain a better understanding of their growth mechanism.

¹NSF ECCS Grant # 0925285 is acknowledged.

S1.00108 Pulse-duration dependent structural change mechanism in Ge₂Sb₂Te₅, DONG HAK KIM, DAEYOUNG LIM, Kyung Hee University — The mechanism of ultrafast structural change in Ge₂Sb₂Te₅ (GST) induced by optical excitation was studied by using pump-probe coherent optical phonon (COP) spectroscopy. The structural change mechanism showed strong dependency on the duration of the pump pulse. While the frequency of displacively generated A₁ COP was observed to red-shift (by more than $\sim 5\%$) in the 2-3 ps time-scale for a long pulse excitation (~ 100 fs), it was instantaneous in the case of short pulse excitation. Furthermore, the shifted COP frequency in the intermediate, transient state was almost independent of the pulse duration or the fluence of the optical pump, which, along with the pulse duration dependency, cannot be explained by photoexcited high-density carriers or thermal effect. The strong dependency of the observed time-scale on the pulse duration and the fluence-independent COP frequency in the transient state indicate that coherent atomic motion due to ultrafast COP generation plays a dominant role in the transition to intermediate, transient state.

S1.00109 The Calculation for the Microscopic Capacitance of Gate Electrode in High Electron Mobility Transistors, CHIN-SHENG WU, Yuan Ze University — Novel nanodevices have developed below 60 nm. Accurate characterization requires detailed electronic structure. In field effect transistor, a dielectric layer isolates the channel from the gate electrode. The model is based on the nanoscale MOSFET with gate length 60 nm, channel length 25 nm and insulator thickness 10 nm. The capacitance of the gate is the series combination of the geometric capacitance. Its dielectric constant is associated with the local electron density. The carrier density decreases from the source to drain in the channel. The capacitance is assumed in parallel connection along this direction.

S1.00110 ABSTRACT WITHDRAWN —

S1.00111 ABSTRACT WITHDRAWN —

S1.00112 ABSTRACT WITHDRAWN —

S1.00113 Characterizing Heat Spreading and Performance Degradation in Organic Light-Emitting Diodes, AMELIA PLUNK, Mount Holyoke College, ANDREW DAVIS, University of Massachusetts Amherst, KADHAIR AL-HEMYARI, ALEXI ARANGO, Mount Holyoke College, KENNETH CARTER, University of Massachusetts Amherst, JANICE HUDGINGS, Mount Holyoke College — In this work, we present for the first time high resolution thermal images of operating organic light-emitting diodes (OLEDs) and show that the surface temperature of these devices can be used to map current density and identify the origin of localized defects and performance degradation. Both luminance and lifetime of OLEDs decrease dramatically with increased operating temperature due to self-heating. Furthermore, localized Joule heating at defects results in local hot spots, thus degrading the brightness homogeneity, altering the electro-optical characteristics of the OLED, and leading to electrode delamination and black spots. Increasing the lifetime of OLEDs clearly relies at least in part on improved thermal management. Using thermoreflectance microscopy, we observed evidence of the correlation between structural defects and areas of low current density by examining areas of operating devices which showed visual damage and had a low relative surface temperature. We also show the validity of using thermoreflectance microscopy to perform basic characterization of operating OLEDs, such as examining diode behavior, extrapolating material qualities such as diffusivity and conductivity, and quantifying the heat flow through working devices.

S1.00114 Spatially Resolved Thermal Analysis of High Power LEDs Using Thermoreflectance Microscopy, HEXUAN WANG, KADHAIR AL-HEMYARI, SUSU YAN, JOSEPH SUMMERS, JANICE HUDGINGS, Mount Holyoke College — The efficiency, reliability, and lifetime of high power light emitting diodes (LEDs) depend critically on their operating temperature. The lateral temperature distribution is of particular importance with large area, high power LEDs as defects related to overheating in high power LEDs usually occur at a high rate at the surface. In this work, we present the use of lock-in thermoreflectance imaging to measure the spatially resolved surface thermal distribution of operating LEDs. This non-invasive thermography technique offers high spatial and thermal resolutions. We show that results of thermoreflectance surface temperature are quantitatively consistent with temperature measurements obtained using forward voltage bias and wavelength shift techniques. We demonstrate the power of spatially resolved thermoreflectance by imaging the highly non-uniform surface temperature distribution of an operating LED at high electrical bias power. We conclude that the non-uniform surface temperature distribution is resulted from non-uniformly distributed inject current and overheating at the contacts. We also investigate the thermal impact of encapsulating commercial LEDs with a plastic lens and silicone epoxy.

S1.00115 Optical Properties of PbTe and PbSe¹, CHINEDU EKUMA, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA, DAVID SINGH, Material Science and Technology Division, Oak Ridge National Laboratory, TN, USA, JUANA MORENO, MARK JARRELL, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA — We report optical properties of PbTe and PbSe as obtained from first principles calculations with the Tran-Blaha modified Becke-Johnson potential. The results are discussed in relation to existing experimental data, particularly in relation to the temperature dependence of the band gap.

¹Work at ORNL was supported by the Department of Energy, Basic Energy Sciences through the S3TEC Energy Frontier Research Center. Work at LSU was funded in part by the National Science Foundation Award Number: EPS 1003897.

S1.00116 Strained layer relaxation effect on current crowding and efficiency improvement of GaN based LED, DEEDER AURONGZEB, Arizona State University, Department of Electrical Engineering, Tempe, Arizona 85287 — Efficiency droop effect of GaN based LED at high power and high temperature is addressed by several groups based on carrier delocalization and photon recycling effect (radiative recombination). We extend the previous droop models to optical loss parameters. We correlate strained layer relaxation at high temperature and high current density to carrier delocalization. We propose a third order model and show that Shockley-Hall-Read and Auger recombination effect is not enough to account for the efficiency loss. Several strained layer modification scheme is proposed based on the model.

S1.00117 Wigner-crystallization of Rydberg-Polaritons in the lowest Landau level, FABIAN GRUSDIT, MICHAEL FLEISCHHAUER, Department of Physics and Research Center OPTIMAS, TU Kaiserslautern — For electrons and dipolar fermions in the lowest Landau level the critical filling for Wigner-crystallization was shown to be $\nu_c \approx 1/7$ [Baranov et. al., Phys. Rev. Lett. 100 (2008)]. We investigate the fractional quantum Hall effect for Van-der-Waals interacting bosons as realized e.g. by stationary-light polaritons in a Rydberg gas and find no transition to the Wigner crystal (WC). Our numerical studies suggest a crystalline groundstate below $\nu = 1/6$ which is expected to be described by a correlated WC of composite quasiparticles. Taking into account a cut-off in the Van-der-Waals interaction we find the WC to be favorable for large cut-offs. Numerical results for different geometries are presented and realistic implementations are discussed.

S1.00118 INSTRUMENTATION AND MEASUREMENTS —

S1.00119 Kelvin Probe Microscopy and Electrostatic Force Microscopy of reduced graphene oxide platelets, JOSEPH RAHAMIM, CHRISTOPHER KEHAYIAS, Physics and Astronomy, Tufts University, SAMUEL MACNAUGHTON, SAMEER SONKUSALE, Electrical and Computer Engineering, Tufts University, CRISTIAN STAIL, Physics and Astronomy, Tufts University — We present combined Scanning Kelvin Probe Microscopy (SKPM) and Electrostatic Force Microscopy (EFM) measurements on reduced graphene oxide (rGO). Although the as-synthesized graphene oxide is insulating, controlled reduction chemistry can render this material semiconducting or even semi-metallic. The availability of several types of oxygen functional groups allows rGO to interact with a wide range of organic and inorganic compounds. We perform sensitive SKPM and EFM measurements on patterned rGO electronic circuits and show that the electrical potential and charge distribution are significantly changed when the device is exposed to various organic dopants. We also demonstrate that these experiments allow a systematic study of the conducting channels through rGO as a function of the chemical dopant.

S1.00120 Length, Radius, and Tilt Angle Control of Carbon Nanotube Probes for High Resolution Atomic Force Microscopy, BENJAMIN ALEMAN, BIBIANA ONOA, University of California, Berkeley, CLAUDIO RIVETTI, Università degli Studi di Parma, MARTA KOPACZYŃSKA, CARLOS BUSTAMANTE, ALEX ZETTL, University of California, Berkeley — The lateral spatial resolution of modern atomic force microscopy (AFM) is largely limited by the radius of curvature of the probe. Owing to their extraordinary mechanical strength, large aspect-ratio, and sub-nanometer radius, carbon nanotubes (CNTs) have emerged as the ideal AFM probe tip material, yet existing methods for CNT-AFM probe fabrication have not been optimized. In this work, we present a fabrication method that yields direct control over the CNT's length, radius, and tilt angle by using a positioning stage operated in a transmission electron microscope (TEM) to directly attach a single-walled CNT to the apex of an AFM probe tip. The CNT probes are then utilized to image gold nanoparticles and DNA with tapping-mode AFM in ambient conditions. While imaging gold nanoparticles, we report a full-width radius dilation of 5.5 Å and nearly 8 nm resolution enhancement compared to commercially available super sharp Si AFM probes. We also measure a DNA fullwidth of less than 5.0 nm and observe, in some cases, the fine structure associated with the DNA double-helix with a pitch of 3.32 nm, which agrees well with the theoretical value of 3.4 nm.

S1.00121 Experiments in NMR Force Microscopy¹, ISAAC MANZANERA, University of Texas at Austin. Department of Physics, ROSA CARDENAS, Sandia National Laboratories at Livermor, JEREMY PASTER, AMANDA TURBYFILL, JOHN MARKERT, University of Texas at Austin. Department of Physics — We report details of the construction and use of three nuclear magnetic resonance force microscopy (NMRFM) probes, as well as the development of control systems for three-dimensional nanoscale imaging and spectroscopy. Our variable temperature probe performed position-dependent ¹H NMR force measurements on a 25x15x7 μm^3 single crystal of ammonium sulfate $(\text{NH}_4)_2\text{SO}_4$ at room temperature in a sample-on-oscillator geometry. Force signals were detected with a signal-to-noise ratio of 6, and 12 μm resolution, in a one-dimensional scan. Measurements of NMR relaxation times $T_2^* = 1.5 \pm 0.2 \mu\text{s}$, $T_2 = 44 \pm 2 \mu\text{s}$, and $T_1 = 5.6 \pm 0.7 \text{ s}$ were obtained. We describe the upgrade of our ³He NMRFM probe for measurements towards the base temperature of 0.3K for investigation of nanoscale structures and metal oxide interfaces using the iOSCAR technique and perpendicular-cantilever geometry. Force-detected ¹¹B NMR signals in a 30 μm crystal of superconductor MgB_2 have also been achieved using this probe. Efforts in the development of our NMRFM probe for the study of biological samples in liquid media are reported. Magnetic field effects on micromagnet films on cantilevers are being studied for the characterization of the mechanical sensors to be used in these liquid experiments.

¹This work was supported by NSF Grant No. DMR-0605828 and Welch Grant No. F-1191

S1.00122 A Technique for In Situ Ballistic Electron Emission Microscopy, ROBERT BALSANO, College of Nanoscale Science and Engineering, University at Albany, SUNY, Albany, New York 12203, USA, JOHN GARRAMONE, Dept of Materials Science & Engineering, McCormick School of Engineering & Applied Science, Northwestern University, Evanston, IL 60208-3108, USA, VINCENT LABELLA, College of Nanoscale Science and Engineering, University at Albany, SUNY, Albany, New York 12203, USA — Ballistic electron emission microscopy (BEEM) is a scanning tunneling microscopy (STM) technique that can measure transport of hot electrons through materials and interfaces with high spatial and energetic resolution. BEEM requires an additional contact to ground the metal base layer of a metal semiconductor junction. Performing BEEM *in situ* with the sample fabrication requires a custom built STM or modifying a commercial one to facilitate the extra contact, which leaves the technique to highly trained experts. This poster will describe our work to develop a special silicon substrate that has the extra contact built in to enable *in situ* BEEM without modifications to the STM. Electrically isolated contact traces are lithographically patterned *ex situ* onto the silicon substrate and connected to the BEEM sample plate which is then inserted into the ultra-high vacuum chamber. The metal is then deposited through a shadow mask and then mounted *in situ* onto the STM for BEEM measurements. BEEM measurements comparing both *in situ* and *ex situ* deposited films will be presented.

S1.00123 Nano and Micro Structures Image Based on Lens-Crystal System For Hard X-Ray Radiation, DAVID KUYUMCHYAN, California State University, Northridge, CA 91330, USA, ARMEN KUYUMCHYAN, American NanoScience and Advanced Medical Equipment, INC, CA 91204, USA, VICTOR KOHN, National Research Center "Kurchatov Institute", 123182, Moscow, Russia, ANATOLY SNIGIREV, IRINA SNIGIREVA, European Synchrotron Radiation Facility, B.P. 202, F - 38043 Grenoble, France, EVGENY SHULAKOV, Institute of Microelectronics Technology, RAS, 142432, Chernogolovka, Russia, CALIFORNIA STATE UNIVERSITY, NORTHRIDGE COLLABORATION, AMERICAN NANOSCIENCE AND ADVANCED MEDICAL EQUIPMENT, INC, CA 91204, USA COLLABORATION, NATIONAL RESEARCH CENTER "KURCHATOV INSTITUTE" COLLABORATION, EUROPEAN SYNCHROTRON RADIATION FACILITY, B.P. 202, F - 38043 TEAM, INSTITUTE OF MICROELECTRONICS TECHNOLOGY, RAS, 142432, CHERNOGOLOVKA, RUSSIA COLLABORATION — We present results of imaging properties of the lens-crystal system for hard x-ray radiation. The system is based on a beryllium parabolic refractive lens placed in front of the sample, and an asymmetric silicon single crystal placed behind the sample. We record the magnified x-ray phase contrast image at the x-ray energy 15 keV. The peculiarities of image transformation are investigated both experimentally and theoretically when the focus of refractive lens is moved across and along the optical axis. The computer program was elaborated for a simulation of image formation in the system based on the refractive lens and the crystal with asymmetric Bragg diffraction. The algorithm is based on the FFT procedure.

S1.00124 High Throughput Tomography at the Advanced Photon Source 2BM Beamline enabling the Study of the Morphological Changes in MgH₂ Destabilized LiBH₄ Systems¹, TABBETHA DOBBINS, Rowan University, SHATHABISH NARASEGOWDA, Louisiana Tech University — Understanding morphologies in two phase hydride systems, such as MgH₂ and LiBH₄ mixtures, will permit the study of mass transport (i.e. diffusion), interface reaction (i.e. H₂ desorption reactions) and ultimately models for H₂ desorption and uptake rates. Many hydride systems are prepared by high energy ball milling which delivers stochastic microstructures from which many images are needed in order to collect reliable particle size and interfacial area data. The high throughput tomographic imaging system at 2BM of the Advanced Photon Source permitted data collection from a series of mixed hydrides—with the goal of optimizing energy for absorption contrast from a two phase system and determining relative amounts of hydride phase as well as interfacial area between the hydrides. Two-phase mixtures at LiBH₄:MgH₂ ratios of 1:3, 1:1, and 2:1 were imaged. The optimal energy for measurement was determined to be 15 keV (having 18% transmission for the MgH₂ phase and above 90% transmission for the LiBH₄ phase). Results showed that the % of interfacial area for the mixed composite system was always higher in the catalyzed system—increasing from 15% to 34% in the 1:3 system, from 27% to 60% in the 1:1 system, and 22% to 37% in the 2:1 system.

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S1.00125 A study of biofunctionalized silica nanospring surface for immunosensor applications, YUKTA P. TIMALSINA, DAVID N. MCILROY, University of Idaho — A study of biofunctionalized VANS (vertically aligned (silica) nanospring) surface for immunosensor applications is presented. VANS surface treated with 3-aminopropyltriethoxysilane (APTES) leaves a primary amine groups on the VANS surface. Glutaraldehyde (GA) reacts with APTES modified VANS surface forming imine bonds at one end of glutaraldehyde, leaving aldehyde groups at the other end to react with the antibody. X-ray photoelectron study verifies each step of VANS surface functionalization. A goat anti mouse antibody (GαM IgG I) is immobilized as a biorecognition layer on the APTES-GA modified surface and targeted to mouse IgG. It is investigated that mouse IgG captured from the solution phase specifically binds to goat anti mouse IgG on APTES-GA- GαM IgG I. Then layer of GαM IgG II attached to the APTES-GA- GαM IgG I-mouse IgG surface reacts only when there is mouse IgG instead of rabbit IgG. A modeling of a resistor-inductor-capacitor (RLC) circuit of impedance spectra measured after the addition of successive layer indicates the these biological layers behave as insulating layers. It is explored that there is a greater magnitude of change between successive bio-layers below 10 kHz. Changes in the magnitudes of the elements of the RLC equivalent circuit indicate that the addition of biological layers impedes ionic motion thereby changing the effective dielectric response by the biomolecule polarization.

S1.00126 Terahertz detection of nanorectifiers, SHAHRIR R. KASJOO, CLAUDIO BALOCCO, XIAOFENG F. LU, LINQING Q. ZHANG, YASAMAN ALIMI, School of Electrical and Electronic Engineering, University of Manchester, Manchester M13 9PL, U.K, STEPHAN WINNERL, Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany, AIMIN M. SONG, School of Electrical and Electronic Engineering, University of Manchester, Manchester M13 9PL, U.K — Despite of a broad range of applications in the terahertz (THz) region, there is still a lack of compact, low-cost, solid-state devices that can function at room temperature. Here we report on THz detection by a novel type of unipolar nanodiode, known as self-switching diode (SSD), which is realized by breaking the symmetry of a nanochannel. The SSD has a completely different working principle from conventional diodes since it does not rely on any doping junction or Schottky barrier. Its intrinsically low parasitic capacitance enables electrical rectification at ultrahigh speed. In this report, the SSDs are coupled with standard bow-tie antennas. The THz signals are generated by means of a free-electron laser, at several THz frequencies ranging from 1.3 THz to 2 THz. The THz detection measurements were carried out at room temperature and 20 K. We find that the highest estimated voltage sensitivity achieved at room temperature and 20 K operations are around 390 mV/mW and 46 V/mW, respectively. For detection at room temperature, this is the highest speed reported in nanorectifiers to date. Furthermore, we also observe evidence of THz detection enhancement by localised plasma oscillation before the cut-off frequency as reported in the Monte-Carlo simulations.

S1.00127 Characterization of Solar Cells via LED Spectrophotometer with Consideration of Spatial and Spectral Distributions of the LED Light Sources, JAEHYEONG LEE, NCSSM, ROB GOURLEY, SIIB, SANGMIN LEE, LSL — Fast and cheap spectral response measurement systems are required in solar cell manufacturing lines in order to produce high quality solar cells. Using LEDs as light sources is the most promising technique. However, since LEDs inherently have 10 - 15 nm spreads in wavelength, the resolution for the wavelength is about 10 times worse than conventional spectrophotometers. In this report, a method to compensate for the wavelength spread of LEDs

has been developed. The output power from a solar cell can be expressed as, $P_{out} = \int P_{in}(\lambda) \times \varepsilon(\lambda) d\lambda \cong \int P_{in}(\lambda) \times \sum_{i=0}^n a_i \times \lambda^i d\lambda$, where $P_{in}(\lambda)$ is the

distribution function of LED light power, $\varepsilon(\lambda)$ is the efficiency of a solar cell, λ is the wavelength and a_i is the coefficient of an n^{th} order polynomial approximation of $\varepsilon(\lambda)$. Since 8 different wavelength LEDs were used, the maximum value of n is 7. With the same method, quantum efficiency was also approximated. Two different sizes of Si single crystal solar cells were examined with this method. For the larger solar cell, the effect of spatial distribution of LED light intensity was also calibrated. By comparing the data from larger solar cell with existing data sheet, it was confirmed that the solar cell efficiency can be accurately measured by an LED spectrophotometer without assuming monochromatic light sources.

S1.00128 Simulation and Modeling of charge particles transport using SIMION for our Time of Flight Positron Annihilation Induce Auger Electron Spectroscopy systems¹, PRASAD JOGLEKAR, K. SHASTRY, SUMAN SATYAL, ALEXANDER WEISS², University of Texas at Arlington — Time of flight Positron Annihilation Induced Auger Electron Spectroscopy system, a highly surface selective analytical technique using time of flight of auger electron resulting from the annihilation of core electrons by trapped incident positron in image potential well. We simulated and modeled the trajectories of the charge particles in TOF-PAES using SIMION for the development of new high resolution system at U T Arlington and current TOFPAES system. This poster presents the SIMION simulations results, Time of flight calculations and larmor radius calculations for current system as well as new system.

¹NSF DMR 0907679 Welch Foundation Y1100

²Advisor

S1.00129 Solar cell evaluation using electron beam induced current with the large chamber scanning electron microscope, TARA WINK, EDWARD KINTZEL, Western Kentucky University, PETER MARIENHOFF, MARTIN KLEIN, Ellcie Maintenance GmbH — An initial study using electron beam induced current (EBIC) to evaluate solar cells has been carried out with the large chamber scanning electron microscope (LC-SEM) at the Western Kentucky University Nondestructive Analysis Center. EBIC is a scanning electron microscope technique used for the characterization of semiconductors. To facilitate our studies, we developed a Solar Amplification System (SASY) for analyzing current distribution and defects within a solar cell module. Preliminary qualitative results will be shown for a solar cell module that demonstrates the viability of the technique using the LC-SEM. Quantitative EBIC experiments will be carried out to analyze defects and minority carrier properties. Additionally, a well-focused spot of light from an LED mounted at the side of the SEM column will scan the same area of the solar cell using the LC-SEM positioning system. SASY will then output the solar efficiency to be compared with the minority carrier properties found using EBIC.

S1.00130 SUPERLATTICES, NANOSTRUCTURES, AND OTHER ARTIFICIALLY STRUCTURED MATERIALS —

S1.00131 Circular dichroism in double layer metallic crossed-gratings, WENSHENG GAO, HO MING LEUNG, Physics Department, HKUST, YUNHUI LI, HONG CHEN, Pohl Institute of Solid State Physics, Tongji University, Shanghai, WINGYIM TAM, Physics Department, HKUST — We report on the fabrication of double layer gold crossed-gratings consisting of a top convoluted layer of gold grating over a bottom gold grating using an e-beam direct write technique together with a lift-off process. The crossed-gratings exhibit, in the visible range, strong circular dichroism which is dependent upon the incident direction due to the convoluted top gold grating and also the conducting substrate. Resonance dips in the transmittance of circularly polarized light are also observed. The experimental results are explained qualitatively by simulations using a finite-integration technique. The simulations confirm that the dips in the transmittance are electromagnetic resonances corresponding to parallel and anti-parallel current flows in the crossed-gratings. (Accepted by J.Opt)

S1.00132 Enhancement of magnetic moment in powder Mn₁₁Si₁₉, KIYOTAKA HAMMURA, Hitachi Cambridge Laboratory, University of Cambridge, HARUHIKO UDONO, TOMOSUKE AONO, Ibaraki University — Higher-manganese silicides (HMSs), having a formula of MnSi_{1.75-x}, have drawn much attention in terms of future spintronics materials, following provisional findings of ferromagnetism in them. However, their magnetic properties have still been controversial. In this paper, magnetic moment in Mn₁₁Si₁₉ was measured at temperatures 5K to 290K, both in bulky and in powdery state. The bulk specimen was carefully prepared using a temperature gradient solution growth (TGSG) method and confirmed to be of single crystal by x-ray characterisation. It was found that Mn₁₁Si₁₉ had paramagnetism. Moreover, its magnetic moment was enhanced from 0.16 Wb m/ μ_B to 0.22 Wb m/ μ_B by changing its structure from bulky and powdery, respectively.

S1.00133 Blue Afterglow from ZnS:Ag,Co Water Soluble Nanoparticles, LUN MA, XIAOJU ZOU, MARIUS HOSSU, WEI CHEN, UT Arlington — Blue afterglow has been obtained from water soluble ZnS:Ag,Co nanoparticles by using a simple wet chemistry synthesis. The nanoparticles have a cubic zinc blende structure with average sizes of about 4 nm as determined by high-resolution transmission electron microscopy (HRTEM) and X-ray diffraction (XRD). The blue emission peaked at 441 nm is due to the transition from surface defects to Ag⁺ luminescent centers. However, the afterglow from ZnS:Ag,Co nanoparticles is centered at 475 nm. The presence of Co²⁺ is necessary to obtain the afterglow. The X-ray photoelectron spectroscopy (XPS) measurement indicates that oxidation occurred on the particle surfaces is also important. The blue afterglow ZnS:Ag,Co nanoparticles may open new applications in biological imaging, detection and treatment.

S1.00134 Magnetic and structural properties of ferrofluids based on Cobalt-Zinc ferrite nanoparticles¹, P. PRIETO, J. LOPEZ, M.E. GOMEZ, J. PRADO, J. CAICEDO, G. ZAMBRANO, CENM Universidad del Valle, L. GONZALEZ, Depto Química Universidad del Valle, J. ESTEVE, Universitat de Barcelona, Catalunya, Spain — Ferrofluids are colloidal systems composed of a single domain of magnetic nanoparticles with a mean diameter around 10 nm, dispersed in a liquid carrier. Magnetic Co_(1-x)Zn_xFe₂O₄ ferrite nanoparticles were prepared via co-precipitation method from aqueous salt solutions in an alkaline medium. The composition and structure of the samples were characterized through EDX and XRD, respectively. Transmission Electron Microscopy studies permitted determining nanoparticle size. Grain size of nanoparticle conglomerates was established via Atomic Force Microscopy. The magnetic behavior of ferrofluids was characterized by Vibrating Sample Magnetometer; and finally, a Magnetic Force Microscope was used to visualize the magnetic domains of nanoparticles. The mean size of the crystallite of nanoparticles determined by using the Scherrer approximation diminished when the Zn concentration increases. The size of the nanoparticles obtained by TEM is in good agreement with the crystallite size calculated from XRD measures. The magnetic properties investigated at room temperature presented super-paramagnetic behavior, determined by the shape of the hysteresis loop. Finally, our magnetic nanoparticles are considered a soft magnetic material.

¹Work supported by “El Patrimonio Autónomo Fondo Nacional de Financiamiento para la Ciencia, la Tecnología y la Innovación Francisco José de Caldas” Contract RC-No. 275-2011.

S1.00135 Magnetic Quenching of Plasmon-photonic Activities in Fe₃O₄-Elastomer Composite¹, DUSTIN HESS, DANHAO MA, DEREK CAPLINGER, KOFI ADU, Department of Physics, The Pennsylvania State University, Altoona College, Altoona, PA 16601, USA, RICHARD BELL, Department of Chemistry, The Pennsylvania State University, Altoona College, Altoona, PA 16601, USA — We present preliminary results on the effect of particle size on the optical response of Fe₃O₄-silicone elastomer composite in the presence of external static magnetic field. The optical response of composites containing 2wt% of Fe₃O₄ particles of diameter range 20-30nm, 40-60 nm and d<500nm in silicone elastomer were measured using a PerkinElmer lambda 950 UV/vis/NIR spectrometer. We observed a systematic redshift in the optical response of composites containing nanoparticles (20nm-30nm and 40-60nm) with increasing static magnetic field strength, which saturates near 600 Gauss. However, we observed a dramatic suppression to near quenching of the plasmonic activities in the micron size particle (d < 500nm) elastomer composites. This occurred even at very low applied static magnetic fields, suggesting particle size limitations in modulation of plasmon-photonics by external magnetic field.

¹This Work is Funded by Penn State Altoona Undergraduate Research Grant.

S1.00136 Photo-Switching of Magnetization in Iron Nanoparticles, NABIL AL-AQTASH, ALEXANDER HOSTETTER, RENAT SABIRIANOV, University of Nebraska at Omaha — We report the theoretical studies of light induced switching in core-shell nanoparticles. The core of the nanoparticle is made of Fe coated with the shell of azobenzene. The latter is a photochromic material with the reversible *trans-cis* photoisomerization upon irradiation by UV and visible light. The magnetization of nanoparticles can be reversibly switched by using specific wavelengths of light. *trans-cis* photoisomerization of azobenzene induces both the change in surface local magnetic moments and alters the exchange interactions on the surfaces of the nanoparticles. These two mechanisms can lead to induced magnetization switchable by light pulse. We study the effects of photoisomerization of azobenzene on iron (Fe) nanoparticle. Ab initio calculations using SIESTA code show that the ferromagnetic (FM) and antiferromagnetic (AFM) exchange interaction in Fe dimer increase by 40% due to photoisomerization of azobenzene. While an infinite flat Fe monolayer shows variation on the exchange interactions on the surfaces as result of photoisomerization. The local magnetic moments of Fe sheet increase by 6% due to photoisomerization. Using an *ab initio* parameterization of magnetic interactions, we propose statistical model based on competing exchange interactions for the investigation of Fe nanoparticle magnetization. We performed Monte Carlo simulations of magnetization of the core-shell nanoparticle as a function of temperature. The results show that Fe nanoparticles magnetization at room temperature can change by at least 40% due to photoisomerization of azobenzene.

S1.00137 On the scattering of polarized neutrons by solitons in low dimensional magnetic systems, IRINA BARIAKHTAR, Boston College, VICTOR BARIAKHTAR, Institute of Magnetism, Kyiv, Ukraine, ALEXANDER NAZARENKO, Acceletech, Framingham, MA — The cross section of the scattering of polarized neutrons by solitons in low dimensional systems with the magnetic structure is calculated. The authors consider solitons corresponding to the formation of a kink in a system of adatoms on the surface of a substrate or a crowdion in a chain of atoms in crystals described by the sine-Gordon equation, a breather with zero topological charge, and also solitons in a bound electron-phonon quasi-one-dimensional molecular chain. It is shown that study of the polarized neutrons scattering provides the possibility to investigate the static and dynamic properties of the solitons. In addition, the information obtained from the neutron scattering allows for experimental reconstruction of the magnetic momentum distribution in these structures. We suggest that prospective experiments on observing and studying the solitons can deepen the insight into the physics of the strongly correlated systems.

S1.00138 Theory of electrically-tunable coupling between magnetic nanoparticles on graphene, HUA CHEN, University of Tennessee at Knoxville, University of Texas at Austin, QIAN NIU, University of Texas at Austin, ZHENYU ZHANG, University of Science and Technology of China, Harvard University, University of Texas at Austin, ALLAN H. MACDONALD, University of Texas at Austin — We will present a study of the dependence on graphene carrier density of the coupling between magnetic nanoparticles adsorbed on a graphene sheet. Small system *ab initio* coupling strength results will be compared with semi-analytic results based on a phenomenological Dirac-band model for graphene's π -bands. The model calculation uses kinetic exchange coupling parameters for the interaction between a magnetic nanoparticle and the graphene π -bands that are extracted from *ab initio* results for graphene/ferromagnetic metal interfaces.

S1.00139 Synthesis and thermoelectric properties of PbTe nanostructures¹, KAMAL KADEL, LATHA KUMARI, WENZHI LI, Florida International University — Lead Telluride (PbTe) nanostructures were synthesized via the solvothermal/hydrothermal route. X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission emission microscopy (TEM) were used to characterize the as-prepared samples and indicated that the PbTe nanoparticles were cubical in shape and had face centered cubic structure. The effects of the addition of surfactants on the shapes and sizes of the nanocubes were investigated. PbTe nanocubes synthesized with the addition of surfactants showed uniform well-defined shapes. The effect of the synthesis temperature on the structure and morphology was also investigated; it was found that the particle size increased with the synthesis temperature. Thermoelectric property of the as-synthesized PbTe nanostructures was also investigated.

¹This work is supported by the National Science Foundation under the grant DMR-0548061.

S1.00140 Ab-initio Calculation of the Magnetic Properties of BN Nanoribbon¹, JEFF RUFINUS, Widener University, Science Division, Chester, PA 19013 — Recently, the search for new spintronics materials has also included graphene-based materials due to the theoretical prediction that this type of material may show the half-metallic property. Here, we present the results of a density functional theory within a generalized gradient approximation study of narrow Boron Nitride nanoribbon (BNNR). The objective of this study is to determine whether this type of material will be ferromagnetic (FM), antiferromagnetic (AFM), or ferrimagnetic. Our results show that the narrow zigzag shaped BNNR prefers antiferromagnetic state. The energy difference among the three states (FM, AFM, ferrimagnetic), however, is very small. Increasing the width of BNNR, was predicted to cause the stabilization of FM state instead of the AFM state.

¹Work supported by Widener University grants. Computational time from PSC and OSCER-OU is acknowledged.

S1.00141 Ab initio nonadiabatic molecular dynamics of the ultrafast excitation energy transfer in small semiconducting carbon nanotube aggregates, OLENA POSTUPNA, RUN LONG, OLEG PREZHDO, University of Rochester, Rochester, NY — Outstanding physical properties of carbon nanotubes (CNTs), such as well-defined optical resonance and ultrafast nonlinear response, result in CNTs gaining popularity in academic and industrial endeavors as potential effective energy generating devices. Following recent experiments on ultrafast excitation energy transfer in small semiconducting carbon nanotube aggregates [1], we report results of ab initio nonadiabatic molecular dynamics simulation of the energy transfer taking place in two carbon nanotube systems. We investigate the energy transfer between (8,4) and (10,0) CNTs, as well as (8,4) and (13,0) CNTs. In both cases, the CNTs are orthogonal to each other. Luer et al. in [1] elucidate the second excitonic transitions followed by fast intratube relaxation and energy transfer from the (8,4) CNT toward other acceptor tubes. Our project aims to provide a better understanding of the energy transfer mechanism in the given systems, which should foster development of a theory for the electronic structure and dynamics of CNT networks, hence enhancing their tailoring and application in the future. References 1. Larry Luer, Jared Crochet, Tobias Hertel, Giulio Cerullo, Guglielmo Lanzani. ACSNano. Vol.4, No. 7, 4265-4273

S1.00142 Transport Imaging in the Near-Field Regime for the Determination of Carrier Diffusion Behavior in ZnO and GaN Nanostructures¹, NANCY HAEGEL, Physics Department, Naval Postgraduate School, DANIEL CHISHOLM, Mechanical Engineering Dept., Naval Postgraduate School, LEE BAIRD, R. ADAM COLE, Physics Department, Naval Postgraduate School — Optical imaging of the spatial dependence of recombination luminescence generated at a point source is used to determine minority carrier diffusion lengths in GaN and ZnO nanostructures. By combining the resolution of near-field optics with the localized carrier generation capability of the scanning electron microscope, both diffusion and waveguiding behavior can be directly imaged in a contact-free manner for any luminescent material. This approach has been used to investigate the effect of different shell materials on GaN core/shell nanowires on surface recombination and carrier transport [Baird et. al. Appl. Phys. Lett. 98, 132104(2011)]. In ZnO, transport imaging shows variations in transport behavior depending on growth technique and morphology. Diffusion lengths in excess of 1 μm have been observed in ZnO nanobelts, consistent with reports of low concentrations of point and extended defects in these materials.

¹This work was supported in part by National Science Foundation Grant DMR0804527.

S1.00143 Effect of Magnetic-Dielectric Interface on Capacitor Functions of Fe-Doped Barium Titanate Nanocomposites at Low Frequency (< 1 MHz), ATAUR CHOWDHURY, University of Alaska Fairbanks, KAPIL KULKARNI, NanoLab, Inc., Newton, MA, GAUTAM SARKAR, US Department of Defense — Metal-dielectric interfaces have been shown to greatly influence the capacitor functions of nanodielectric composites. However, the effect of magnetic metal impurities in nanocomposites on dielectric properties is not well understood. Nanodielectric composites of iron in off stoichiometric barium titanate were fabricated by sol-gel process with varying pH concentrations. The fabricated samples containing 1-2% iron reveal unique interfacial structure as studied by X-ray and atomic force microscopy. The capacitance of the as prepared samples was measured with an Agilent LCR meter at frequencies ranging from 20 Hz to 1 MHz. All nanodielectric composites show similar capacitor characteristic and reveal continuous decrease in capacitor density with increasing frequency. For a particular sample, this continuous decrease is a direct result of the porous interface between the iron granules and the dielectric material. This behavior, however, is not measurably influenced by an applied magnetic field in all samples.

S1.00144 Spin dependent thermoelectric effect in magnetic tunnel junctions, LAURENT CHAPUT, Institut Jean Lamour, WEIWEI LIN, universite paris sud, MICHEL HEHN, Institut Jean Lamour, BEATRICE NEGULESCU, CNRS-CEA, STEPHANE ANDRIEU, FRANCOIS MONTAIGNE, STEPHANE MANGIN, Institut Jean Lamour — Thermoelectric effects in magnetic nanostructures and the so-called spin caloritronics are attracting much interests. Indeed it provides a new way to control and manipulate spin currents which are key elements of spin-based electronics. Here we report on the magneto thermoelectric effect in a magnetic tunnel junction. The thermovoltage in this geometry can reach 1 mV. Moreover a magneto-thermoelectric effect could be measured with ratio similar to the tunnel magnetoresistance ratio. The Seebeck coefficient can then be tuned by changing the relative magnetization orientation of the two magnetic layers in the tunnel junction. Therefore our experiments extend the range of spintronic devices application to thermoelectricity and provide a crucial piece of information for understanding the physics of thermal spin transport.

S1.00145 Enhanced thermoelectric properties using modulation-doping strategy in nanocomposites¹, MONA ZEBARJADI, MIT, BO YU, ZHIFENG REN, Boston College, MILDRED DRESSELHAUS, GANG CHEN, MIT, S3TEC TEAM — We introduce the modulation-doping strategy in bulk SiGe nanostructures to improve the thermoelectric power factor. By separating carriers from their parent atoms via embedding heavily doped nanoparticles inside a host matrix, the ionized impurity scattering rate could be largely reduced, resulting in enhanced mobility. By band engineering, the carriers can spill over from nanoparticles into the host matrix, resulting in similar carrier concentrations, Fermi levels and consequently Seebeck coefficients as those of the uniform nanocomposites. In addition, nanoparticles with low thermal conductivities can further reduce the overall thermal conductivity of the sample. Combining the enhanced electrical conductivity, the reduced thermal conductivity and the unaffected Seebeck coefficient, we were able to enhance the thermoelectric properties of Ge-dilute Si95Ge5. And therefore were able to fabricate a low-cost sample with a competitive performance as those of the state of the art Si80Ge20. The fabricated modulation-doped sample has a higher figure of merit, compare to its equivalent uniform nanocomposite sample and compare to ionized impurity-doped host matrix.

¹This presentation is based upon work supported as part of the MIT S3TEC, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science.

S1.00146 Ternary p-type half-Heuslers: another perspective bulk thermoelectrics, XIAO YAN, WEISHU LIU, HUI WANG, DEZHI WANG, Boston College, GANG CHEN, MIT, ZHIFENG REN, Boston College, BOSTON COLLEGE TEAM, MIT COLLABORATION — By employing the nanocomposite approach, we have achieved peak ZT of 0.8 at 700 °C for p-type $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{CoSb}_{0.8}\text{Sn}_{0.2}$. A larger difference in atomic mass and size of Hf and Ti than Hf and Zr in the crystal structure has produced a peak ZT of ~ 1.1 at 800 °C for p-type $\text{Hf}_{0.8}\text{Ti}_{0.2}\text{CoSb}_{0.8}\text{Sn}_{0.2}$. However the ZT peak is on the high temperature side. A ternary combination of Ti, Zr, and Hf at M site (MCoSb) has given rise to higher ZT in n-type MnInSn system. Will ternary on the M site yield better ZT for p-type? In this report, we will present our recent achievement of 10-25% ZT improvement for temperature range 25-700 °C without sacrificing the peak ZT value of 1.1 at 800 °C.

S1.00147 Potassium resonant doping in $\text{Bi}_{92.5}\text{Sb}_{7.5}$ material, HUAIZHOU ZHAO, MANI POKHAREL, CYRIL OPEIL, Department of Physics, Boston College, GANG CHEN, Department of Mechanical Engineering, Massachusetts Institute of Technology, ZHIFENG REN, Department of Physics, Boston College, REN'S LAB AT BOSTON COLLEGE COLLABORATION, GANG CHEN'S LAB AT MIT COLLABORATION — $\text{Bi}_{1-x}\text{Sb}_x$ alloy material is a narrow band semiconductor when x is in the range of 0.07 – 0.4. The energy gap reaches a maximum value of 0.014 eV in the composition range of $x = 0.15$ to 0.2. Thermoelectric properties on this material have been investigated for half a century due to the promising cooling applications. However, the low efficiency originating from the medium thermoelectric Power Factor (PF) prohibited this material from real applications. Here, we demonstrated that by potassium doping, both the Seebeck Coefficient and electrical conductivity can be enhanced by 25% for the ingot samples for a broad temperature range. Further more, by combining with our nano grain size approach, thermal conductivity of ingot sample was reduced by 20%, this lead to the figure of merit ZT increase of 50% comparing to ingot counterpart. The potassium resonant doping was accounted for the PF enhancement for ingot $\text{Bi}_{92.5}\text{Sb}_{7.5}$ sample. We also find that the resonant doping can be realized for nano composite samples through parameters optimization.

S1.00148 Simple solvothermal synthesis of large scale single crystal PbS nanorods and their properties, SYAMANTA KUMAR GOSWAMI, EUNSOON OH, Chungnam National University — PbS nanorods and quantum dots have lots of applications such as in solar cells, gas sensors, infra-red detectors etc. PbS nanorods were synthesized via a very simple and inexpensive solvothermal method. Two reagents viz. Ethylenediaminetetraacetic acid (EDTA) and PEG-PPG-PEG triblock copolymer (P123) were employed in this growth for two special purposes. EDTA helps in slowing down the reaction and P123 plays the role of 1D structure directing agent. Comparison of the X-ray diffraction patterns of the nanowires synthesized using EDTA and without using EDTA clearly shows that the crystalline quality is significantly improved with EDTA. Transmission Electron Microscopy images and Selected Area Electron Diffraction patterns demonstrate that the nanorods are single crystalline. The average diameter of the nanorods was found to be about 18 – 20 nm. Thus, the nanorods are within the quantum regime as the exciton Bohr radius of PbS is 18 nm. Raman spectra of these samples are compared.

S1.00149 Superlattice formed by quantum dot sheets: density of states and IR absorption¹, VLADIMIR MITIN, FEDIR VASKO, Electrical Engineering Department, University at Buffalo, SUNY — Low-energy electronic states in heterostructures formed by periodically placed quantum dot (QD) sheets are studied taking into account (i) ultranarrow (single or several monolayers thickness) wetting layers and (ii) scattering by randomly-placed QDs. The host material is described within the effective mass approximation, scattering by the QD sheets is governed by the periodical Dyson equation, and effect of wetting layers is taken into account within the transfer matrix approach. Using the current conservation and inversion symmetry requirements, the transfer matrix is evaluated beyond effective mass approximation. The binding energy of localized state, the reflection (transmission) coefficient for the single QD sheet case, and the energy spectrum of superlattice are determined for the case of GaAs host matrix with InAs QD sheets. Spectral dependency of mid-IR absorption in superlattice due to photoexcitation of electrons from localized states into minibands is determined by the QD's concentration, period of sheets, and wetting layer characteristics. Such a dependency modifies the characteristics of optoelectronic devices based on heterostructures with QD sheets.

¹This work is supported by AFOSR.

S1.00150 Voltage-tunable IR photodetector based on asymmetrically doped coupled quantum wells¹, JAE KYU CHOI, NIZAMI VAGIDOV, ANDREI SERGEEV, GOTTFRIED STRASSER, FEDIR VASKO, VLADIMIR MITIN, Electrical Engineering Department, University at Buffalo, SUNY — We report on the mid-IR two-color photodetector with spectral photoresponse tunable by biased voltage. The device is based on GaAs/AlGaAs asymmetrically doped coupled quantum well structures grown by molecular beam epitaxy. A single unit of the detector is composed of 6.5 nm-thick GaAs layer doped with Si up to $5 \times 10^{11} \text{ cm}^{-2}$ and 6.5 nm-thick undoped GaAs separated by 3.1 nm-thick $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$. Units are separated by 50 nm-thick $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$ barriers. Our devices consist of 25 identical units. We demonstrated that in temperature range 20 - 70 K the peak detection wavelengths can be switched from $7.5 \mu\text{m}$ to $11.1 \mu\text{m}$ by varying bias from -5 V to +5 V. Our modeling shows that spectral tunability is basically determined by three factors. First, electron energy levels are shifted due to Stark effect. Second, electric field leads to the charge redistribution in the coupled wells and electron energy levels are shifted by electron-electron interaction. Third, tunneling processes from photoexcited quasi-localized electron states in wells to conducting states are enhanced in the electric field due to Fowler-Nordheim effect. The modeling results are in very good agreement with the experimental data. The proposed detectors are promising candidates for adaptive tunable sensing in the IR range.

¹This work is supported by AFOSR.

S1.00151 Analytical minimization of total spread of generalized Wannier functions in one-dimensional crystals¹, DENIS R. NACBAR, ALEXYS BRUNO-ALFONSO, Universidade Estadual Paulista, Brazil — Since their introduction in 1937, Wannier functions have become key theoretical and computational tools in Solid State Physics. In this work, generalized Wannier functions of several bands in a one-dimensional crystal are investigated. For the case of two bands, necessary condition for minimum of total variance leads to a non-linear set of four second-order differential equations having a simple analytical solution. This is a new alternative to current iterative numerical procedures. Results are displayed for diatomic crystals with inversion symmetry. The relation between generalized Wannier functions and orthogonalized atomic orbitals is discussed. It is shown that such functions may present increased exponential localization when compared with Wannier functions of separate bands. Our findings should be relevant in studies of layered semiconductor and photonic structures and linear atomic chains. Hopefully, it will speed progress both in understanding and applications of Wannier functions.

¹We thank Brazilian Agencies CNPq and FAPESP for financial support.

S1.00152 Capacitively coupled double quantum dot system in the Kondo regime¹, EDSON VERNEK, IRISNEI FERREIRA, Universidade Federal de Uberlândia - Brazil, PEDRO ORELLANA, Universidad Catolica del Norte - Chile, GEORGE MARTINS, Oakland University - USA, FABRICIO SOUZA, Universidade Federal de Uberlândia - Brazil — We present a detailed study of the low-temperature physics of an interacting double quantum dot system in a T-shape configuration is presented. Each quantum dot is modeled by a single Anderson impurity and we include an inter-dot electron-electron interaction to account for capacitive coupling that may arise due to the proximity of the quantum dots. By employing a numerical renormalization group approach to a multi-impurity Anderson model, we study the thermodynamical and transport properties of the system in and out of the Kondo regime. We find that the two-stage-Kondo effect reported in previous works is drastically affected by the inter-dot Coulomb repulsion. In particular, we find that the Kondo temperature for the second stage of the two-stage-Kondo effect increases exponentially with the inter-dot Coulomb repulsion, providing a possible path for its experimental observation.

¹We would like to thank FAPEMIG and CNPq for financial support.

S1.00153 Electrical Characterization of a Hybrid 1D-0D System of Quantum Dot Chains¹, THOMAS REMBERT, VASYL KUNETS, GREGORY SALAMO, Institute for Nanoscience & Engineering, University of Arkansas — Recent developments in the area of material science and nanotechnology open new horizons to fabricate novel artificial materials with the possibility to engineer the electron and phonon material properties. Our objective is to create structures with high electrical conductivity and low thermal conductivity. The outcome will allow efficient transfer of thermal energy into the electrical output. Early theoretical and experimental research indicates that one-dimensional (1D) quantum wires and zero-dimensional (0D) quantum dots can be used to fabricate very efficient thermoelectric devices. This project focuses on the development of artificial material systems, called quantum dot chains, where 1D states, which are important for high electrical conductivity, coexist with 0D states, causing efficient acoustic phonon scattering, reducing the thermal conductivity. The samples are InGaAs/GaAs grown using an MBE technique of strain-induced self-assembly. Current analysis of our results shows anisotropies of temperature-dependent measurements of sheet resistance and electron mobility, along with physical characterization via AFM scans. Continued studies of electron and phonon physics in this system will help determine the potential for chains of quantum dots in thermoelectric applications.

¹Supported by the Arkansas Department of Higher Education and NSF EPSCoR, VICTER Project (No. EPS1003970).

S1.00154 Tunable Quantum Phase Transition in a Dissipative Resonant Level¹, D.E. LIU, H. ZHENG, H.T. MEBRAHTU, G. FINKELSTEIN, H.U. BARANGER, Duke University — We show that quantum phase transitions (QPT) exist in a simple dissipative resonant level system. The electromagnetic environment couples both to tunneling processes (characterized by lead resistance R_e) and to voltage fluctuations of the gate (characterized by gate resistance R_g). We bosonize this model and map it to a Tomonaga-Luttinger type model. Using a “Coulomb-gas” RG analysis, we relate our dissipative resonant level model to the double barrier problem in a Luttinger liquid. For the symmetric case and $R_e + R_g > 2h/e^2$, a Kosterlitz-Thouless QPT separates strong-coupling and weak-coupling phases. Interestingly, in the symmetric case, all relevant couplings between tunneling processes and the environment disappear, leading to perfect transmission at $T=0$. A second order QPT is also induced by coupling asymmetry for $R_e + R_g < 2h/e^2$. The two phases correspond to the resonant level merging with the right lead while the left lead decouples, and vice versa.

¹Supported by the U.S. Dept. of Energy (Materials Sciences and Engineering, awards DE-SC0005237 and DE-SC0002765).

S1.00155 Effects of intrasubband coupling on the scattering phases and density of states in a quantum wire, VASSILIOS VARGIAMIDIS, Aristotle University, Thessaloniki, Greece, VASSILIOS FESSATIDIS, Fordham University, Bronx, USA, PH. KOMNINOU, Aristotle University, Thessaloniki, Greece — The properties of scattering phases and density of states in a quantum wire with an attractive scatterer are analyzed. We consider two bound states, belonging to different subbands, which couple to a scattering channel and give rise to two Fano resonances. It is shown that varying the parameters of the scatterer (such as its strength and position) produces significantly different effects on the phase behavior and density of states, depending on the subband they occur. These effects stem mainly from the difference between the coupling matrix elements of the two resonant levels with the propagating channel mode. As a consequence, the phase evolution in one subband may exhibit opposite behavior from the phase evolution in another subband. These findings may prove experimentally useful in ballistic transport through narrow channels.

S1.00156 Porous silicon nanowire arrays decorated by Ag nanoparticles for surface enhanced Raman scattering study¹, L. SU, H.J. XU, Y.F. CHAN, X.M. SUN, Beijing University of Chemical Technology, STATE KEY LABORATORY OF CHEMICAL RESOURCE ENGINEERING TEAM — A large scale and highly ordered Ag nanoparticle-decorated porous silicon nanowire array was fabricated for a uniform and reproducible surface-enhanced Raman scattering (SERS) substrate. The overall process for the proposed structure is simple and reliable with the use of only chemical etching and metal reduction processes. The SERS sensitivity of the novel substrate as low as 10^{-16} M for rhodamine 6G (R6G) and the Raman enhancement factor as high as 10^{14} were obtained. The excellent SERS performances were mainly attributed to the strong local electromagnetic effect which is associated with the formation of large-quantity Ag nanoparticles on porous silicon nanowire array and the existence of semiconductor silicon nanowires. Significantly, the quadratic relation between the logarithmic concentrations and the logarithmic integrated Raman peak intensities provided quantitative detection of R6G. Our results open new possibilities for applying SERS to trace detection of low-concentration biomolecules.

¹This work was supported by the National Natural Science Foundation of China (Grant No. 11104008), Doctoral Fund of Ministry of Education of China (Grant No. 20090010120014) and the Beijing Natural Science Foundation (Grant No. 1103033).

S1.00157 Atomistic Modeling of Degradation Mechanisms in Nanoscale HEMT Devices, VAMSI GADDIPATI, SASI SUNDARESAN, KRISHNA YALAVARTHI, SHAIKH AHMED, Southern Illinois University — In this work, through atomistic numerical simulations, we investigate how performance degradation of state-of-the-art AlGaIn HEMTs is governed by an intricate coupling of the underlying thermo-electro-mechanical processes while operating at high power and/or high-temperature. The polarization induced charge density is shown to be strongly dependent on the thickness of the AlN barrier layer. This further demonstrates that the degradation in these HEMT devices is related to the reduction of the effective thickness of the AlN barrier layer, which, during operation at high device temperature, could arise from the diffusion of gate metal into the barrier material matrix. This finding has been validated using the massively parallel LAMMPS molecular dynamics tool and available experimental data. We have also demonstrated that the polarization fields alone can induce channel carriers at zero external bias and lead to a significant increase in the ON current.

S1.00158 Electron transport properties in self switching nano-diodes, TATSUYA KISO, KAZUICHI NISHISAKA, TOSHIHIKO MAEMOTO, SHIGEHICO SASA, Osaka Institute of Technology, SEIYA KASAI, Hokkaido University, MASATAKA INOUE, Osaka Institute of Technology — Ultra-fast novel nanodevices, namely the self-switching diode (SSD) were fabricated from the InAs/AlGaSb heterostructures grown by solid-source molecular beam epitaxy on a semi-insulating GaAs (100) substrate. The two lines were etched thorough the 2DEG layer and become insulating. The effective channel width was actually smaller because of the depletion layer at the etched boundaries. Depending on the sign of the applied voltage the effective channel width will increase or reduce, giving rise to the diode-like characteristics. The diode-like characteristics were clearly observed for the InAs SSDs at 300K, and turn on voltage is strongly dependent on the channel width of the SSDs. In the SSD with $W = 460$ nm, the InAs channel of was fully pinched of under the equilibrium condition, and positive voltage of 1.46 V was needed to drive a current thorough the InAs channel. On the other hand, the positive voltage of 2.32 V was needed to drive a current in the SSD with $W = 230$ nm. We found to need the higher the turn-on voltage in the SSD of the narrower channel width. Furthermore, multi-channel SSDs were fabricated. $I - V$ characteristics and the AFM images of the SSD array of the symmetric nanowires, which are $1.5 \mu\text{m}$ long and approximately $W = 170$ nm. The current densities were clearly increased with increasing the number of the nano-wires. The clear diode-like nonlinear behavior and rectification reflected ballistic nature of electrons in InAs-based SSD were observed.

S1.00159 Modeling NIR-to-Visible Upconversion Kinetics in Er^{3+} , Yb^{3+} : NaYF_4 Nanocrystals and Finite-difference Time-domain Simulations of Noble-metal Enhancement Substrates, ROBERT ANDERSON, South Dakota School of Mines and Technology, GE YAO, QUOCANH LUU, University of South Dakota, HARI PAUDEL, KHADIJEH BAYAT, MAHDI BAROUGH, South Dakota State University, CUIKUN LIN, MARY BERRY, STANLEY MAY, University of South Dakota, STEVE SMITH, South Dakota School of Mines and Technology — Upconversion (UC) phosphors are able convert infra-red light to visible wavelengths. The (erbium) Er^{3+} , (ytterbium) Yb^{3+} : NaYF_4 system is the most efficient upconversion phosphor known, and yet the quantitative aspects of the mechanism responsible for upconversion, such as the values of key microscopic rate constants, have not been determined. In this work, the dynamics of the photo-physical processes leading to near-infrared (NIR) to visible upconversion in Er^{3+} , Yb^{3+} : NaYF_4 nanocrystals are investigated using a nonlinear rate-equation model. In tandem with this effort, we use finite difference time domain (FDTD) simulations to analyze noble-metal nanostructures designed to enhance the absorption and emission of the upconverting phosphor. Simulation results are compared with time-resolved luminescence and reflectivity of the plasmonic substrates, which show systematic improvement in fluorescence yield and good agreement with simulated kinetics.

S1.00160 Optical properties of Benzylpiperazine/CuI (111) system¹, TAKAT RAWAL, VOLODYMYR TURKOWSKI, Physics Department and NSTC, University of Central Florida, RICHARD BLAIR, Department of Chemistry and Forensic Science Center, University of Central Florida, TALAT S. RAHMAN, Physics Department and NSTC, University of Central Florida — We are interested in understanding the mechanism responsible for the recently observed [1] strong orange fluorescence in systems that contain Benzylpiperazine (BZP) molecules adsorbed on CuI film. To study possible optical transitions we use ab-initio electronic structure calculations based on density functional theory with the generalized-gradient (PBE) approximation for the exchange-correlation functional. In particular, we examine in detail the band structure including defect states of the CuI film with the lowest energy (111) surface and the excited states of the BZP molecule. It is shown that while optically non-active in the corresponding energy window, the two parts of the system, CuI slab and BZP, produce strong visible light emission when coupled together. Our numerical analysis demonstrates that the reason for such emission is the optical transitions between the excited molecule and the iodine vapor atom states on the CuI (111) surface. We discuss possible applications of the effect and that of defect vapor atom states on other optical properties of the system, including excitonic effects in the ultrafast response. [1] R. Blair, unpublished.

¹Work supported in part by DOE-BES grant DE-FG02-07ER46354.

S1.00161 Room temperature sub-diffraction-limited plasmon laser by total internal reflection, RENMIN MA, RUPERT OULTON, VOLKER SORGER, GUY BARTAL, XIANG ZHANG, UC Berkeley — Plasmon lasers are a new class of coherent optical amplifiers that generate and sustain light well below its diffraction limit. Their intense, coherent and confined optical fields can enhance significantly light-matter interactions and bring fundamentally new capabilities to bio-sensing, data storage, photolithography and optical communications. However, metallic plasmon laser cavities generally exhibit both high metal and radiation losses, limiting the operation of plasmon lasers to cryogenic temperatures, where sufficient gain can be attained. Here, we present room temperature semiconductor sub-diffraction limited laser by adopting total internal reflection of surface plasmons to mitigate the radiation loss, while utilizing hybrid semiconductor-insulator-metal nano-squares for strong confinement with low metal loss. High cavity quality factors, approaching 100, along with strong $\lambda/20$ mode confinement lead to enhancements of spontaneous emission rate by up to 18 times. By controlling the structural geometry we reduce the number of cavity modes to achieve single mode lasing.

S1.00162 Probing semiconductor band structures and heterojunction interface properties with ballistic carrier emission: GaAs/Al_xGa_{1-x}As as a model system, WEI YI, VENKATESH NARAYANAMURTI, School of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts 02138, USA, HONG LU, MICHAEL A. SCARPULLA, ARTHUR C. GOSSARD, Materials Department, University of California, Santa Barbara, California 93106, USA, HARVARD TEAM, UCSB TEAM — Utilizing tunnel emission of ballistic electrons and holes in a tunnel transistor with a Mott-barrier collector, we have developed a method to self-consistently determine the energy gap of a semiconductor and band offsets at a semiconductor heterojunction without using a priori material parameters. As a model system, electronic band gaps of the AlGaAs alloys together with conduction and valence band offsets at the GaAs/AlGaAs (100) interfaces are measured with a resolution of several meV at 4.2 K. The direct-gap band offset ratio for the GaAs/AlGaAs (100) interface is found to be 59:41. In the indirect-gap regime, ballistic electrons from direct tunnel emissions probe the X valley in the conduction band, while those from Auger-like scattering processes in the metal base film probe the higher-lying L valley. Such selective electron collection may be explained by their different momentum distributions and parallel momentum conservation at the quasiepitaxial Al/GaAs (100) interface. We argue that the present method is in principle applicable to arbitrary type-I semiconductor heterostructures. [W. Yi. at al. Phys. Rev. B 81, 235325 (2010)]

S1.00163 Chaotic dynamics of electron resonant tunneling in a quasi-one-dimensional super-lattice, PAULA FEKETE, US Military Academy, West Point, NY 10966, GODFREY GUMBS, Hunter College at the City University of New York, NY 10065, DANHONG HUANG, Air Force Research Laboratory, Kirtland Air Force Base, NM 87117, OLEKSIY ROSLYAK, Hunter College at the City University of New York, NY 10065 — A novel approach is employed for studying the dynamics of electron resonant tunneling in a quasi-one-dimensional superlattice. The semiclassical force-balance transport equation is used to describe the time-dependence of the dynamical equation for the electron center-of-mass velocity in the presence of an applied DC electric field and two external AC fields. Evolution of phase space trajectories from initial non-equilibrium states is obtained. The attractors of this dynamical system are determined and their stability for different sets of system parameters is obtained. Coupling between the electron's velocity and the external fields gives rise to rich spatiotemporal behavior including chaos.

S1.00164 Cloaking Effect of Superlens in Time Domain, MENG XIAO, The Hong Kong University of Science and Technology, JIAN WEN DONG, Sun Yat-Sen (Zhongshan) University, XUEQIN HUANG, CHE TING CHAN, The Hong Kong University of Science and Technology — A “perfect lens” (ideal absorption-less slab with $\mu = -1$) or “superlens” (a perfect lens with small absorption) can cloak a small object located in its vicinity such that no far field observer can detect the small particle, i.e., being invisible. While the problem is well understood in the steady state by solving the Maxwell equation in frequency domain, its time domain properties, such as how the cloaking effect started, remained unknown. In this paper, by using the time-dependent Green's function approach, we present a time domain study of the cloaking properties of the “superlens” As a current source is turned “on,” the system's response will be consisted of a transient response in the beginning and a steady state response in the long run. It turns out that it takes a long time (tens of thousands of cycle) for the “perfect lens” to build up the cloaking effect, and this required period depends on a number of factors, such as the separation between the lens and the particle, the absorption of the slab, and the dispersion of the slab. Moreover, along with many other interesting effects, we also find that, the dipole moment, on its way to be invisible, it oscillates with a decreasing amplitude.

S1.00165 Quantum mechanical investigation of CO, NO and HCN adsorption on Ag₈ nanoclusters; (structural, electronic and topological properties), HADI AKBARZADEH, ZAHRA TORBATIAN, S. JAVAD HASHEMIFAR, Isfahan University of Technology — We used DFT-GW method to study pure Ag₈ nanocluster and CO, NO, HCN adsorption on it. The pure Ag₈ stabilizes in Td structure and the behavior of binding energy is consistent with the total charge density at bond points while bond length exhibits a behavior similar to the mean bond charge. Adsorption of CO, NO and HCN molecules on different atomic sites of Ag₈ were studied and it was found that all these molecules, mainly due to electron donation, prefer to be adsorbed by LUMO orbital. This finding is in qualitative agreement with the experimental observation of the enhanced binding of CO molecule on positively charged silver atoms, compared with the neutral and negatively charged samples [J. Phys. Chem. A 2006, 110, 7167-7172]. Our calculation shows no significant charge transfer during NO adsorption on Ag₈. The CO, NO and HCN adsorbed nanoclusters as well as cationic and anionic samples do not stabilize in Td structure. This charge induced geometry transition is related to the high (low) value of LUMO (HOMO) state in Td structure which indicates high energy cost of electron donation (acceptation) in this isomer. The topological analysis of electron density clarify that the adsorption energy of molecules on Ag₈ is consistent with the value of the charge density at the topological bond point between molecule and nanocluster.

S1.00166 SURFACES, INTERFACES AND THIN FILMS —

S1.00167 Electronic transport and scanning tunneling microscopy study of bismuth quantum films, SHENGYONG QIN, TAE-HWAN KIM, THOMAS Z. WARD, AN-PING LI, Oak Ridge National Laboratory — Semimetal films, such as bismuth films, have attracted great interest due to their unique electronic properties around the Fermi level. Bulk Bi has three conduction band minima at L points about 40mV lower than the single valance band maximum at T point. However, with decreasing Bi layer thickness, an energy gap is expected to open when the size confinement becomes sufficient to raise the lowest electron subband above the highest hole subband. We have utilized quantum growth method to fabricate atomically flat Bi thin films with thickness controllable down to single atomic layer. The quantum films are then studied in situ with a cryogenic four-probe STM to examine the correlation of the electronic and transport properties. An oscillatory resistivity change is observed as function of film thickness, which is discussed in comparison with the local density of states.

S1.00168 First-order phase transition in In/Si(111)-4×1, JONGHOON YEO, HYUNGJOON SHIM, GEUNSEOP LEE, Department of Physics, Inha University — In/Si(111)-4×1 surface is known to undergo a temperature-induced structural phase transition between a high-temperature (HT) 4×1 phase and a low-temperature (LT) 8×2 phase. The issues on the nature of this temperature-dependent phase transition, whether it is of order-order (displacive) or order-disorder type and first-order or second-order, are unsettled. We investigated the 4×1-to-8×2 phase transition by using LEED and STM. We observed a hysteresis of the LEED beam intensities as the temperature changes during cooling and heating. This hysteresis indicates that the structural phase transition is of first order. STM images revealing the coexistence of the 4×1-HT and 8×2-LT phase domains during the transition are consistent with the first-order transition. An influence of the defects on the phase transition of this In/Si(111) surface will be discussed.

S1.00169 Glancing Angle Deposition of Ag on Si(111)7x7, A.N. COBBLAH, S.T. HAYDEN, YIYAO CHEN, J. KREMENAK, M.W. GRAMLICH, P.F. MICELI, U. Missouri — Ag(111) films were vapor-deposited in ultra-high vacuum on Si(111)7x7 substrates. The angle of deposition was varied from normal incidence to 80 degrees and the films were studied by x-ray reflectivity. It is found that, even for very thin films, the film roughness increased dramatically with the angle of deposition. This poster will highlight experimental results as well as the development of a UHV chamber that enables a laboratory x-ray source to monitor low angle reflectivity during film growth. Funding is acknowledged from the Ronald E. McNair Post-baccalaureate Achievement Program and NSF DMR-0706278. Some measurements were performed on the 6IDC beam line, supported by the US-DOE (through Ames Lab, W-7405-Eng-82), at the Advanced Photon Source (US-DOE, W-31-109-Eng-38) located at Argonne National Laboratory.

S1.00170 Photoluminescence characterization of Cl – doped Cu₂O thin film photoelectrodes¹, WAQQAS KHAN, ROHANA GARUTHARA, Hofstra University — Electrodeposition was used to deposit Cl-doped Cu₂O thin films on ITO substrates. Photocurrent and the Photoluminescence (PL) measurements were done on prepared electrodes. CuCl₂ and different pH values of the solution bath were used to control the doping level in Cu₂O. Photocurrent responses in photoelectrochemical cells clearly showed improved performance over the un-doped Cu₂O thin films as seen by the difference in the light and the dark current. A deconvoluted PL spectra assuming Gaussian spectral profile showed three underlying peaks. The temperature dependence of the peak energy position and intensity was analyzed. Furthermore, the electrodeposition and the nature of the conductivity of the films were also analyzed. These results of the Cl-doped Cu₂O films will be compared with those for the Cu₂O un-doped films and presented.

¹Research supported by Department of Energy DEFG02-08ER64623–Hofstra University Center for Condensed Matter

S1.00171 High transconductance zinc oxide thin-film transistors on flexible plastic substrates, YUTA KIMURA, TOMOHIRO HIGAKI, TOSHIHIKO MAEMOTO, SHIGEHICO SASA, MASATAKA INOUE, Osaka Institute of Technology — We report the fabrication and characterization on high-performance ZnO based TFTs on unheated plastic substrate. ZnO films were grown by pulsed laser deposition (PLD) on polyethylene naphthalate (PEN) substrates. Top-gate ZnO-TFTs were fabricated by photolithography and wet chemical etching. The source and drain contacts were formed by lift-off of e-beam deposited Ti(20 nm)/Au(200 nm). An HfO₂ with thickness 100 nm was selected as the gate insulator, and top gate electrode Ti(20 nm)/Au(200 nm) was deposited by e-beam evaporation. We prepared a set of the structure with SiO₂/TiO₂ to investigate the characteristic changes that appear in the film characteristics in response to bending. From the $I_D - V_{DS}$ and the transfer characteristics which are affected by bending and return for the ZnO-TFT with SiO₂/TiO₂ buffers, the TFTs were bent to a curvature radius of 8.5 mm. The transconductance, g_m is obtained 1.7 mS/mm on flat, 1.4 mS/mm on bending and 1.3 mS/mm on returning the film, respectively. The $I_D - V_{DS}$ characteristics were therefore not changed by bending. All of the devices exhibited a clear pinch-off behavior and a high on/off current ratio of $\sim 10^6$. The threshold voltages, V_{th} were not changed drastically. Furthermore, TFT structures were changed from a conventional top-gate type to a bottom-gate type. A high transconductance of 95.8 mS/mm was achieved in the bottom-gate type TFT by using Al₂O₃ oxide buffer.

S1.00172 Transition Metal Disulfide Films by Reactive Sputtering: Structure, Magnetism, and Electronic Transport, A. BARUTH, M. MANNO, D. NARASIMHAN, A. SHANKAR, X. ZHANG, E. S. AYDIL, C. LEIGHTON, University of Minnesota - Twin Cities — Transition metal disulfides (*i.e.*, TMS_2 , where $TM = Cu, Co, Fe, Ni$, etc.) are a unique class of materials displaying diverse functional properties such as highly spin-polarized ferromagnetism ($Co_{1-x}Fe_xS_2$), superconductivity (CuS_2), a Mott insulating ground state (NiS_2), and unusually high potential for solar absorber applications (FeS_2). Significant research has been performed on bulk crystals of these materials but little has been done on thin films, despite the obvious potential for heterostructured systems due to their diverse functionality and intrinsic epitaxial compatibility. In this work we report on the wide applicability of reactive sputtering from metallic targets in an Ar/H₂S gas environment as a reliable deposition method. Via detailed characterization of crystal structure, microstructure, and electronic, magnetic, and optical properties, we demonstrate successful deposition of a wide variety of single phase polycrystalline thin films with bulk-like properties. A brief survey of optimized growth conditions, resulting physical properties, and general trends based on metal reactivity, will be presented. We argue that this method holds great promise for the synthesis of a novel family of all-sulfide-based heterostructured devices. Work funded by NSF MRSEC and UMN IREE.

S1.00173 Titanium Isopropoxide Precursor Volume Consumption as a Function of Temperature for Titanium Dioxide Thin Films Grown by Atomic Layer Deposition¹, COSTEL CONSTANTIN, James Madison University — Atomic layer deposition (ALD) offers tremendous opportunities for controlling material synthesis on an atomic level and for creating nanolayers with unique new functionalities. ALD is a chemical gas phase thin film deposition method based on alternating surface reactions that employs two or more precursors. ALD is often used for growth of high k dielectric constant oxide films. Titanium dioxide material have a k value of 80, and a band gap of ~ 3 eV, and due to strong oxidizing properties thin films coated on construction materials and glass have fog proof, and self cleaning properties. Our ALD reactor employs liquid Titanium Isopropoxide $[Ti\{OCH(CH_3)_2\}_4]$ as a metal precursor and distilled H₂O as an oxygen source to grow thin films of titanium dioxide $[TiO_2]$ on silicon [Si], gallium nitride [GaN], and Aluminium foil [Al-foil] substrates. Titanium Isopropoxide exhibit a vapor pressure surge above 40° C and we report the volume precursor consumption as a function of precursor temperature and thin film thickness for ALD grown TiO₂ on Si, GaN, and Al-foil substrates. We will also present dielectric constants of the TiO₂ thin films measured with a variable angle spectroscopic ellipsometer.

¹DOD-ASSURE/NSF-REU grant # DMR-0851367

S1.00174 Epitaxial growth of BiFeO₃ thin films on SrTiO₃/Si substrates¹, RYAN LAUGHLIN, DANIEL CURRIE, GOKUL RADHAKRISHNAN, WEERASINGHE PRIYANTHA, ROCIO CONTRERAS-GUERERRO, RAVINDRANATH DROOPAD, NIKOLETA THEODOROPOULOU, Texas State University - San Marcos — We are using molecular beam epitaxy (MBE) to grow BiFeO₃ (BFO) thin films. SrTiO₃ (STO) on Si is used as a virtual substrate to enable the growth of BFO. Commensurate growth of STO on Si using MBE has been achieved by using co-deposition with the fluxes adjusted for stoichiometric growth and the growth rate is determined using RHEED intensity oscillations. The native oxide of the Si substrates is removed in-situ by deoxidation at around 750 °C using a flux of Sr. The substrate is cooled to 500 °C and additional Sr is added to form template with a (2x1) surface structure. BFO is then deposited on well-characterized STO (2-20nm thick) on Si using Fe and oxygen plasma with an overpressure of Bi flux- the growth rate being controlled by the incoming Fe flux. The RHEED pattern taken during deposition of BFO shows 2-D growth front with a 6-fold surface reconstruction. The structural and magnetic properties of the BFO samples have also been measured.

¹This work was supported by AFOSR under grant FA 9550-10-0133

S1.00175 Disorder trapping during crystallization of the B2 ordered NiAl system, DEYAN SUN, XIAOQING ZHENG, YANG YANG, YUFENG GAO, Department of Physics, East China Normal University, Shanghai 200062, China, JEFF J. HOYT, Department of Materials Science and Engineering, McMaster University, Hamilton, ON, Canada, MARK ASTA, Department of Materials Science and Engineering, University of California, Berkeley, CA 94720 — Using molecular dynamics (MD) simulations, disorder trapping associated with solidification is studied for the (100), (110) and (111) growth directions in the B2 NiAl ordered alloy compound. At the high interface velocities studied we observe pronounced disorder trapping, i.e., the formation of antisite defects and vacancies in the crystal at higher than equilibrium concentrations upon rapid solidification. The vacancies are located primarily on the Ni sublattice and the majority of antisite defects are Ni atoms on the Al sublattice, while the concentration of Al on the Ni sublattice is negligibly small. The defect concentration is found to increase in an approximately linear relationship with an increase of the interface velocity or undercooling. Further there is no significant anisotropy in the defect concentrations for different interface orientations.

S1.00176 ABSTRACT WITHDRAWN —

S1.00177 Strain Engineering in Self-Assembled Vertically Aligned Nanocomposite Thin Films, ZHENXING BI, MPA-CINT, MS K771, Los Alamos National Laboratory, NM 87545, USA, AIPING CHEN, Texas A&M University, SOPHIE HARRINGTON, University of Cambridge, HAIYAN WANG, Texas A&M University, JUDITH DRISCOLL, University of Cambridge, QUANXI JIA, MPA-CINT, MS K771, Los Alamos National Laboratory — Self-assembled vertically aligned nanocomposite (VAN) thin films hold great promises in engineering material functionalities including ferroelectric, ferromagnetic, and multiferroics by tunable intrinsic strains. The VAN exhibits a well ordered vertically columnar structure with highly epitaxial quality in thin film. In this work, we describe the approach of strain tuning in $(\text{BiFeO}_3)_x:(\text{Sm}_2\text{O}_3)_{1-x}$, $(\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3)_{0.7}:(\text{Mn}_3\text{O}_4)_{0.3}$ and $(\text{BaTiO}_3)_x:(\text{Sm}_2\text{O}_3)_{1-x}$ VAN thin films grown by pulsed laser deposition (PLD). We investigate the intrinsic strain mechanism in VAN thin films as well as the effects of film growth kinetics and thermodynamic stability to the final VAN architecture. We also demonstrate the tunable “microstructure - strain - physical properties” relationships in VAN thin films. Experiment results reveal that: 1) Enhanced vertical strain can cause systematic reduction of dielectric loss of VAN thin films; 2) Strain tuning in ferromagnetic VAN thin films can lead to tunable T_c and magneto resistance; and 3) RT ferroelectric can be achieved by strain tuning of BTO and results the highest T_c in VAN thin film. Furthermore, geometrically controlled nanoporous structure can also be processed by thermal treatment on VAN thin films.

S1.00178 STM Examination of Trithiapentacene on Vicinal Gold (788), AMANDA BROWN, JEREMIAH VAN BAREN, University of New Hampshire, Department of Physics, JEREMY KINTIGH, University of New Hampshire, Department of Chemistry, JUN WANG, University of New Hampshire, Department of Physics, GLEN MILLER, University of New Hampshire, Department of Chemistry, KARSTEN POHL, University of New Hampshire, Department of Physics — Trithiapentacene (TTPO) is a member of a group of promising novel pentacene derivatives of interest in organic electronics for their excellent resistance to photooxidation and a range of band gaps. TTPO is a robust molecule with a HOMO-LUMO gap of 1.95 eV that can be thermally evaporated onto an electrode. TTPO is a polar species of pentacene with centered oxygen and sulfur bridge substituents. The vicinal gold (788) surface is a well studied surface on which pentacene molecules and other pentacene derivatives such as 6,13-dichloropentacene self assemble in long range order. We will present a STM study of TTPO on Au (788) addressing the possibility of self-assembly for organic semiconductor applications.

S1.00179 High resolution STM imaging of a unit cell of $\text{SrTiO}_3(100)-\sqrt{5} \times \sqrt{5} - R26.6^\circ$ surface superstructures, ICHIRO SHIRAKI, University of Yamanashi, KAZUSHI MIKI, National Institute for Materials Science (NIMS), SHUHENG PAN, University of Houston — $\text{SrTiO}_3(100)-\sqrt{5} \times \sqrt{5} - R26.6^\circ$ surfaces were studied by scanning tunneling microscope (STM) in ultra-high vacuum conditions at room temperatures. In the our previous report, we showed the arrangement of titanium and oxygen atoms in the unit cells of a $(\sqrt{5} \times \sqrt{5})$ surface superstructure with scanning tunneling microscope and concluded the TiO_2 layer is the terminating plane of the $(\sqrt{5} \times \sqrt{5})$ surface [1]. Recently, we succeeded in imaging the surfaces in filled states with much higher spatial resolution. Oxygen atomic orbitals are individually recognized and the local structures at the center of the O fourfold hollow site with $(\sqrt{5} \times \sqrt{5})$ periodicity are more clearly seen. Comparing our experimental results with the previous works, especially a theoretical study of O-vacancy model [2] and an experimental and theoretical study of Sr adatom model [3], detailed discussion on $\sqrt{5} \times \sqrt{5}$ surfaces became possible.

- [1] I. Shiraki and K. Miki, Surf. Sci. 605, 1304(2011)
- [2] Z. Fang and K Terakura, Surf. Sci. 470, L75(2000)
- [3] T. Kubo and H. Nozoye, Phys. Rev. Lett. 86, 1801(2001)

S1.00180 Real-Time Grazing Incidence Small Angle X-Ray Scattering Studies of the Growth Kinetics of Sputter-Deposited Silicon Thin Films, ALEXANDER DEMASI, Department of Physics, Boston University, Boston MA, GOZDE ERDEM, Division of Materials Science and Engineering, Boston University, Boston MA, PRIYA CHINTA, Department of Physics, University of Vermont, Burlington VT, RANDALL HEADRICK, Department of Physics and Materials Science Program, University of Vermont, Burlington VT, KARL LUDWIG, Department of Physics, Boston University, Boston MA — The fundamental kinetics of thin film growth remains an active area of investigation. In this study, silicon thin films were grown at room temperature on silicon substrates via both on-axis and off-axis plasma sputter deposition, while the evolution of surface morphology was measured in real time with *in-situ* grazing incidence small angle x-ray scattering (GISAXS) at the National Synchrotron Light Source. GISAXS is a surface-sensitive, non-destructive technique, and is therefore ideally suited to a study of this nature. In addition to investigating the effect of on-axis versus off-axis bombardment, the effect of sputter gas partial pressure was examined. *Post-facto*, *ex-situ* atomic force microscopy (AFM) was used to measure the final surface morphology of the films, which could subsequently be compared with the surface morphology determined by GISAXS. Comparisons are made between the observed surface evolution during growth and theoretical predictions. This work was supported by the Department of Energy, Office of Basic Energy Sciences.

S1.00181 Structure of electrolyte decomposition products on high voltage spinel cathode materials determined by in situ neutron reflectometry, JIM BROWNING, GABRIEL VEITH, LOIC BAGGETTO, NANCY DUDNEY, WYATT TENHAEFF, Oak Ridge National Laboratory — Interfacial reactions on electrical energy storage (EES) materials mediate their stability, durability, and cycleability. Understanding these reactions in situ is difficult since they occur at the liquid-solid interface of an optically absorbing material that hinders the use of techniques such as infra-red spectroscopy. Furthermore, since the interfaces involve liquids classic vacuum-based analytical methods can only probe reaction products, which are stable under vacuum. Here, we present the results of an in situ neutron reflectometry study detailing the formation of a thick solid-electrolyte interphase (SEI) on a high voltage spinel cathode material. The cathode/electrolyte system used in this study is a $\text{LiMn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ thin film subjected to a 1.2 molar LiPF_6 in 1:1 ethylene carbonate - dimethyl carbonate electrolyte solution.

S1.00182 Dependence of optical absorption of thin nanocomposite films on inclusions distribution, IRINA BARIAKHARTAR, Boston College, VALERI LOZOVSKI, OLGA OBRAZUMOVA, GALINA STRILCHUK, KNU, Ukraine — It is well known, that one of the ways to widen the spectral range of the elements of photovoltaic systems is using the nanocomposite films as part of its active element. The problem of characterization of the optical properties of nanocomposite thin films, especially with inhomogeneous distribution of inclusions, arises. In this work, we propose an approach which allows us to determine the parameters of the nanocomposite film which cannot be measured directly. The approach is based on the previous works where the ultrathin films electrostatics was studied earlier. The absorption spectrum sensibly depends on the film parameters. They are the inclusions' concentration in the film, the presence of a shell of the inclusion particles and the size of this shell, the spatial orientation of particles in a layer and the presence of different types of particles and their relative spatial distribution in the film. The strong dependence of the absorption profiles on the type of distribution of particles along the film, *ceteris paribus*, is demonstrated in this report.

S1.00183 Precise Control of Areal Density of 'Click' Functional Groups on Nanoparticle Surfaces, YANIR MAIDENBERG, JEFFREY KOBERSTEIN, Columbia University — Tremendous effort has been invested into devising methods that enable full control of surface functionalities by use of a mixture of two self-assembled monolayers (SAM). By assuming control of the relative amounts of SAM moieties on a surface it is possible to fabricate materials with well-known molecular compositions and, thus, well-characterized properties. This could be achieved by mixing one reactive and another inert modifying agent or by utilizing two agents with complementary properties. These surfaces have shown benefits in various applications ranging from sensing to DNA sequencing. Two methods are performed to control the exact amount of 'click' functionalities on the curved surfaces of silica and iron oxide. The density of alkyne is controlled by mixing two silanes, of which one bears the alkyne functionality, and the other does not. Azide density, however, is controlled in a novel method using the kinetic control of the substitution reaction of bromide to azide on a bromide-terminated silanized surface. We report herein a novel method to quantitatively ascertain no phase separation of the silanes occurred on the curved surface, and that true mixing was achieved. We also show that true mixing of silanes occurs regardless of surface geometry or identity for both systems

S1.00184 First-principles study of adsorption and dissociation of CO₂ on α -Pu (020) surface¹, JIANGUANG WANG, ASOK K. RAY, Department of Physics, University of Texas at Arlington, Arlington, Texas 76019, USA — The adsorption and dissociation of CO₂ on the α -Pu (020) surface has been investigated using density functional theory (DFT) within generalized gradient approximation (GGA). The full-potential FP/LAPW+lo method has been used to calculate the adsorption energies at the scalar relativistic with no spin-orbit coupling (NSOC) and fully relativistic with spin-orbit coupling (SOC) theoretical levels. The completely dissociated configurations (C+O+O) exhibit the strongest binding with the surface, followed by the partially dissociated configurations (CO+O), with the molecular CO₂ adsorption having the weakest binding with the Pu surface. It is found that the SOC effect increases the adsorption energies for all considered adsorptions. For all initial vertically upright orientations, the geometry and orientation of the CO₂ molecule do not change after optimization. For all initial flat lying orientations, the final state of the CO₂ molecule corresponds to a bent geometry with a bond angle of $\sim 130^\circ$. For CO+O co-adsorption, the stable configurations corresponded to CO dipole moment orientations of $105^\circ - 167^\circ$ with respect to the normal surface. The local density of states and difference charge densities are also discussed.

¹This work is partially supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525) and by the Department of Energy.

S1.00185 GENERAL THEORY/COMPUTATIONAL PHYSICS —

S1.00186 Calculating thermodynamics properties of quantum systems by a non-Markovian Monte Carlo procedure¹, YANIER CRESPO HERNANDEZ, International Centre for Theoretical Physics (ICTP), ALESSANDRO LAIO, GIUSEPPE SANTORO, ERIO TOSATTI, Scuola Internazionale Superiore di Studi Avanzati (SISSA), CONDENSED MATTER TEAM — We present a history-dependent Monte Carlo scheme for the efficient calculation of the free energy of quantum systems inspired by Wang-Landau and metadynamics. In the two-dimensional quantum Ising model, chosen here for illustration, the accuracy of free energy, critical temperature, and specific heat is demonstrated as a function of simulation time and successfully compared with the best available approaches. The approach is based on a path integral formulation of the quantum problem and can be applied without modifications to quantum Hamiltonians of any level of complexity. The combination of high accuracy and performance with a much broader applicability is a major advance with respect to other available methods.

¹Supported by a MIUR/PRIN contract and benefited from the environment provided by the CNR/ESF/EUROCORES/FANAS/AFRI project.

S1.00187 Application of Group Representation Theory to Derive Hermite Interpolation Polynomials on a Triangle¹, P.G. KASSEBAUM, C.R. BOUCHER, L.R. RAM-MOHAN, Worcester Polytechnic Institute — Current methods used to devise sets of Hermite interpolation polynomials of minimal order that ensure $C^{(n)}$ continuity across triangular element boundaries in two dimensions are not readily extensible to higher dimensions. The extension of such methods is especially difficult when the number of degrees of freedom afforded by data at points is different from the number of degrees of freedom determined by the coefficients of a complete polynomial basis to a particular order. This work introduces a formalism based on group representation theory that can accomplish this task in general. The method is introduced through the derivation of $C^{(1)}$ continuous Hermite polynomials that interpolate data at the three vertices of an equilateral triangular element. These interpolation polynomials are reported here for the first time. The polynomials derived here are compared to the standard polynomials defined in a right triangle by using the two sets of polynomials to solve the Laplace equation over finite elements, and also by interpolating example functions over a single triangle element.

¹NSF grant ECS-0725427 and DARPA grant FA8650-10-1-7046

S1.00188 Finite Temperature Properties of Clusters by Replica Exchange Metadynamics: The Water Nonamer, YINGTENG ZHAI, Key Laboratory for Computational Physical Sciences (MOE) and Surface Physics, Fudan University, Shanghai 200433, China, ALESSANDRO LAIO, ERIO TOSATTI, International School for Advanced Studies (SISSA), via Bonomea 265, 34136 Trieste, Italy, XINGAO GONG, Key Laboratory for Computational Physical Sciences (MOE) and Surface Physics, Fudan University, Shanghai 200433, China — We introduce an approach for the accurate calculation of thermal properties of classical nanoclusters. Based on a recently developed enhanced sampling technique, replica exchange metadynamics, the method yields the true free energy of each relevant cluster structure, directly sampling its basin and measuring its occupancy in full equilibrium. All entropy sources, whether vibrational, rotational anharmonic and especially configurational – the latter often forgotten in many cluster studies – are automatically included. For the present demonstration we choose the water nonamer (H₂O)₉, an extremely simple cluster which nonetheless displays a sufficient complexity and interesting physics in its relevant structure spectrum. Within a standard TIP4P potential description of water, we find that the nonamer second relevant structure possesses a higher configurational entropy than the first, so that the two free energies surprisingly cross for increasing temperature.

S1.00189 The predictive integration method for dynamics of infrequent events, EKIN CUBUK, AMOS WATERLAND, EFTHIMIOS KAXIRAS, Harvard University — With the increasing prominence and availability of multi-processor computers, recasting problems in a form amenable to parallel solution is becoming a critical step in effective scientific computation. We present a method for parallelizing molecular dynamics simulations in time scale, by using predictive integration. Our method is closely related to Voter's parallel replica method, but goes beyond that approach in that it involves speculatively initializing processors in more than one basin. Our predictive integration method requires predicting possible future configurations while it does not suffer from restrictions due to correlation time after transitions between basins.

S1.00190 Coarse graining approach to First principles modeling of radiation cascade in large Fe super-cells, KHORGOLKHUU ODBADRAKH, DON NICHOLSON, AURELIAN RUSANU, Oak Ridge National Laboratory, YANG WANG, Pittsburgh Supercomputing Center, ROGER STOLLER, XIAO GUANG ZHANG, GEORGE STOCKS, Oak Ridge National Laboratory — First principles techniques employed to understand systems at an atomistic level are not practical for large systems consisting of millions of atoms. We present an efficient coarse graining approach to bridge the first principles calculations of local electronic properties to classical Molecular Dynamics (MD) simulations of large structures. Local atomic magnetic moments in crystalline Fe are perturbed by radiation generated defects. The effects are most pronounced near the defect core and decay with distance. We develop a coarse grained technique based on the Locally Self-consistent Multiple Scattering (LSMS) method that exploits the near-sightedness of the electron Green function. The atomic positions were determined by MD with an embedded atom force field. The local moments in the neighborhood of the defect cores are calculated with first-principles based on full local structure information. Atoms in the rest of the system are modeled by representative atoms with approximated properties. This work was supported by the Center for Defect Physics, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences.

S1.00191 Modeling Nonlinear Non-Stationary Self-Organized Asymptotic States in High Energy Density Plasmas Driven by Intense Crossing Laser Beams¹, BEDROS AFEYAN, Polymath Research Inc., Pleasanton, CA — The multiscale dynamics of Vlasov-Maxwell and Vlasov-Poisson systems where non-stationary self-organized states can be formed is a grand challenge. From chaotic particle orbits there arise collective self-consistent fields which are highly coherent. We will explain the novel aspects of these states and contrast them with electron plasma waves which are small amplitude disturbances that are naturally resonant. We will also point out connections between these systems and the high Reynolds number limit of 2D incompressible (Euler) turbulence, galaxy formation models and applications in the nonlinear optics of laser-matter interactions. Techniques will be given of capturing the multiscale dynamics and the conformal invariance hypothesis in the fine scale structures beneath the large scale order found in such systems.

¹Work supported by a grant from the DOE NNSA SSAA program

S1.00192 Multiscale modeling of nanofoams under irradiation¹, E.M. BRINGA, CONICET & Instituto de Ciencias Basicas, Universidad Nacional de Cuyo, Argentina, J. RODRIGUEZ-NIEVA, Instituto Balseiro, Universidad Nacional de Cuyo, Argentina, J.D. MONK, Cain Department of Chemical Engineering, Louisiana State University, J.A. CARO, Los Alamos National Laboratory, M.J. LOEFFLER, NASA Goddard Space Flight Center, Astrochemistry Branch, Code 691, T.A. CASSIDY, CalTech/JPL, R.E. JOHNSON, R.A. BARAGIOLA, Laboratory for Atomic and Surface Physics, University of Virginia, D. FARKAS, Department of Materials Sciences, Virginia Tech — Nanoscale porosity appears in solids under a number of conditions: radiation damage in nuclear reactors, initial stages of ductile failure, in astro-materials, etc. Using molecular dynamics (MD) simulations, we analyze the radiation damage and surface modification of materials with various nanoscale porosities, where experimental techniques can be difficult to use and interpret. We consider (a) irradiation with ions with energies in the range 1-25 keV, of interest for fusion and fission energy applications; (b) swift heavy ion irradiation, with energies up to few GeV, relevant for track formation and interstellar grain evolution. We find that irradiation effects have larger spatial extent than for full-density solids and include the production of point-defects and twins which change the mechanical properties of the samples. We use our MD results as input for a Monte Carlo (MC) code to calculate sputtering yields from nanofoams of different geometries under different irradiation conditions. We also use our MD results to build models which predict possible radiation endurance under intense irradiation.

¹E.M. Bringa thanks support from PICT2009-0092

S1.00193 Application of Gaussian Approximation Potentials to Barium Titanate, JASON VIELMA, GUENTER SCHNEIDER, Oregon State University — The computational study of complex phenomena over long time and distance scales not accessible to first principles calculations requires empirical potentials usually derived by integrating out the electronic degree of freedoms. Recently, a parameter free approach called Gaussian Approximation Potentials (GAP) has been shown that it can duplicate first principles density functional theory (DFT) total energies and atomic forces accurately [1]. In a GAP the atomic neighborhood of an atom is projected onto the angular momentum channels of Wigner-D functions, yielding a bispectrum of the expansion coefficients of the atomic density. A non-parametric Gaussian Process regression is used to fit a database of total energies and forces to the combination of angular momentum channels constituting the bispectrum. We report initial results of using a GAP to describe the ferroelectric perovskite Barium Titanate (BaTiO_3).

[1] A. P. Bartok, M. C. Payne, R. Kondor, and G. Csanyi, Phys. Rev. Lett. **104** 136403 (2010).

S1.00194 Ab initio simulation of radiation damage in nuclear reactor pressure vessel materials, DANIEL WATTS, DANIEL FINKENSTADT, U.S. Naval Academy — Using Kinetic Monte Carlo we developed a code to study point defect hopping in BCC metallic alloys using energetics and attempt frequencies calculated using VASP, an electronic structure software package. Our code provides a way of simulating the effects of neutron radiation on potential reactor materials. Specifically we will compare the Molybdenum-Chromium alloy system to steel alloys for use in nuclear reactor pressure vessels.

S1.00195 Influence of Nutation of the Projectile on Fracture of the Anisotropic Target, ANDREY RADCHENKO, Tomsk State University of Architecture and Building, Russia, PAVEL RADCHENKO, Institute of Strength Physics and Materials Science SB RAS, Russia — In actual practice the direction of the vector of velocity, as a rule, doesn't coincide with the direction of a longitudinal axis of a moving body, and makes with it some angle named the angle of nutation. The nutation influence on process of interaction of the projectile and a target is defined not only by its size, but also geometrical and kinematic parameters of the process. It is obvious that for a case of the prolonged projectile the angle of nutation influence is more considerable, than for the compact projectile because in this case the nutation angle presence changes not only a picture of strain-stress state of interaction bodies, but also leads to loss of stability in the projectile. The three-dimensional problem of oblique high-velocity interaction of the prolonged cylindrical projectile from steel with an anisotropic target from organoplastic is considered. Lengthening of the projectile makes from 15 to 30 calibers, the range of initial velocities of the projectile from 700 to 3000 m/sec is researched. Modeling is carried out numerically by a method of finite elements. Influence of nutation angle and rotation of the projectile on fracture of target and stability of the projectile is analyzed.

S1.00196 Mechanical Behavior of Ceramic Composites under Pulse Loadings¹, EVGENIYA SKRIPNYAK, VLADIMIR A. SKRIPNYAK, VLADIMIR V. SKRIPNYAK, National Research Tomsk State University, TOMSK STATE UNIVERSITY TEAM — The prediction of mechanical behavior ceramic composites under pulse loadings is the complicated problem owing to insufficient knowledge about laws of structure evolution and nucleation and accumulation of damages. Computer simulation of mechanical behavior of ceramic composites at single and repeated pulse influences of submicrosecond duration are presented in the given work. The model of the structured representative volume of ultrafine-grained ceramics composites was developed using the data of microscopic researches. Deformation and damage of structured representative volumes of some ceramic composites on meso-scale level were simulated under pulse loadings having amplitudes near several GPa. The critical fracture stress on meso-scale level depends not only on relative volumes of voids and strengthened phases, but also sizes of corresponding structure elements. It was shown that the isolated micro- and meso-scale cracks can be generated in ceramic composites at pulse amplitude less than the Hugoniot elastic limit. In the studied ceramic composites the critical failure stress in spall zone is changed nonmonotonically with growth of the volume concentration of strengthened phases.

¹The authors wish to gratefully acknowledge that this research was partially supported by Russian Ministry of Sciences and Education (Grant P1247 06/07/2010).

S1.00197 Interaction of free boundary of fluid layer with Taylor wave created by laser pulse, ALEXEY SYUNDYUKOV, MIPT, MICHAEL ASTASHKIN, VICTOR BARANOV, ALLA GEORGIEVSKAYA, ANATOLY GOLUBINSKY, RFNC-VNIIEF, EVGENIY MESHKOV, SarFTI NRNU MEPhI, DMITRIY IRINICHEV, VITALIY KHATUNKIN, RFNC-VNIIEF — In the hydrodynamic laboratory of SarFTI NRNU MEPhI experiments carry out to study the instability of the free surface of a thin (about 2 mm) layer of fluid, developing after the going to surface nonsteady decaying shock wave (Taylor wave) with amplitude of about 1 kbar. The Taylor wave was produced by evaporating a thin (about 1 mm) target located on the surface layer under the influence of the laser pulse duration of 10 ns. The results of the experiments and discussion are presented.

S1.00198 Superconductivity and Magnetism in isovalent substituted Europium Iron-Arsenide Superconductor $\text{EuFe}_2\text{As}_{2-x}\text{P}_x$, TAKUYA ISHIKAWA, YOHEI JONO, KASUMI TASHIMA, KAZUO KADOWAKI, TAKANARI KASHIWAGI, University of Tsukuba — The $\text{EuFe}_2\text{As}_{2-x}\text{P}_x$ system is known as a coexisting system of superconductivity and magnetism with varying isovalent substitution concentration of P in place of As. Magnetism seems to originate from localized Eu^{2+} moments around 19 K, whereas Superconductivity occurs at 28 K in $x = 0.4$. We have studied magnetic and transport properties in various single crystals grown by the self-flux method in a vertical Bridgman furnace, whose compositions are characterized by EPMA and ICP-AES. From temperature dependence of magnetic susceptibility Eu has a magnetic moment of $7.9\mu_B$ indicating Eu^{2+} obtained previously, and did not depend on x upto $x = 0.3$, then coexists with superconductivity above $x = 0.4$. At the coexisting region we showed a reentrant behavior of the superconductivity in resistivity and it shows a peculiar magnetic field dependence. We show the precise phase diagram and superconductivity as a function of x .

S1.00199 Four Types of Single-Walled SiGe Nanotubes: Existence and Stability¹, PRABATH WANAGURU, ASOK K. RAY, The University of Texas at Arlington — Four types of SiGe armchair nanotubes from (3, 3) to (12, 12) have been studied using the cluster approximation and the dangling bonds saturated by H atoms. The tubes have been spin- and geometry optimized using the hybrid functional B3LYP, the all electron 6-31G**//3-21G* basis set and the GAUSSIAN 03/09 suite of software. Cohesive energies, band gaps, bond lengths, hybridization of Ge and Si atoms, among others will be presented in details. In general, cohesive energy of type I tubes decrease and saturate around 3.389eV and that of, type IV tubes increase and saturate around 3.411eV. The cohesive energy of both type II and type III tubes indicates oscillatory behavior eventually reaching saturation as the tube diameter increases. Band gaps, in general for all four types decrease as the tube diameter increases. The band gap of type I tubes saturate at around 1.0eV and type IV tubes indicate the lowest saturation gap of about 0.3eV. While most types I-III tubes show sp^2 or a mixture of sp^2 and sp^3 bonding, some type IV tubes show predominantly p bonding. Results of types I-III will be compared with previous results using the cluster approximation and the B3LYP/LANL2DZ level of theory.²

¹This work is supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525).

²S. Rath and A. K. Ray, Chem. Phys. Lett. 466, 79 (2008).

S1.00200 Rational computational design of high energy density capacitor dielectrics through navigation of the polymer chemical space¹, GHANSHYAM PILANIA, CHENCHEN WANG, CHUN-SHENG LIU, R. RAMPRASAD, University of Connecticut — Next generation capacitor dielectrics should provide an attractive combination of high dielectric constant, fast response, low dielectric loss, high breakdown field and high temperature stability. With these objectives in mind, we adopt a research strategy in which newly developed high throughput first principles computational techniques are used to rapidly, and accurately, navigate the polymer chemical space to identify promising candidates. After validating our high throughput approach against computationally expensive dispersion corrected density functional theory calculations, we systematically study a number of C, Si and Ge backbone containing polymers with various side chain functional groups. Our initial accomplishment is the identification of new class of polymer systems with a large dielectric constant, and band gap large enough to provide reasonable insulating properties. These predictions are currently being validated by parallel experimental work, and are being further refined.

¹This research is based upon work supported by the Office of Naval Research. Computational support was provided through a National Science Foundation Teragrid Resource Allocation.

S1.00201 Constraint density functional calculations for multiplets in ligand-fields: Applications to Fe-phthalocyanine and $\text{Al}_2\text{O}_3:\text{Cr}^{3+}$, Y. KITAOKA, K. NAKAMURA, T. AKIYAMA, T. ITO, Mie University, M. WEINERT, University of Wisconsin-Milwaukee, A.J. FREEMAN, Northwestern University — In transition-metal-based complexes and molecules, multiplet structures are essential in understanding the electronic structure. However, it is often difficult to evaluate a *true* ground state or the *lowest* state within a given ligand (or crystal) symmetry from first principles calculations based on density-functional theory (DFT). Here, we propose a simple DFT approach, implemented into the FLAPW method², to treat multiplets in ligand-fields, by imposing a density matrix constraint on the *d*-orbital occupation numbers. We demonstrate the utility of this approach for the case of an isolated single Fe phthalocyanine (FePc) and a Cr impurity in a corundum Al_2O_3 . For the FePc, results predict that there are three stationary states of ^3E_g , $^3B_2$, and $^3A_2$ in the Fe^{2+} ion, and our total energy calculations clearly demonstrate that the ground state is $^3A_{2g}$. In the case of the $\text{Al}_2\text{O}_3:\text{Cr}^{3+}$, where an on-site Coulomb correlation correction ($+U$) is incorporated, the ground state is $^4A_2$ and the total energy difference between the ground state and the excited state $^4T_2$, 2.9 eV, roughly agrees with an experimental value of 2.23 eV.

¹Work at Northwestern University was supported by the U.S. Department of Energy (DE-FG02-88ER45372).

²Wimmer, Krakauer, Weinert, Freeman, PRB²⁴, 864; Weinert, Wimmer, Freeman, PRB²⁶, 4571

S1.00202 The effects of micro-alloying elements on a BCC iron grain boundaries, SUNGHO KIM, SEONG-GON KIM, HONGJOO RHEE, MARK HORSTEMEYER, Mississippi State University — The effects of micro-alloying elements, vanadium and niobium, on a few of BCC Fe grain boundaries are studied using Density Functional Theory calculations to develop an advanced high-strength steel alloy material. The lowest energy configuration of the grain boundaries structures are obtained from the first-principles calculations. The substitutional and interstitial point defect formation energies of micro-alloying elements in the grain boundaries are compared. The segregation energies of micro-alloying elements onto the grain boundaries and its fractured surfaces are computed. The cohesive energy calculations of the grain boundaries with and without micro-alloying elements are performed to investigate the effects of micro-alloying elements on the cohesive strength of the grain boundaries. The tensile and shear tests on the grain boundaries with and without the segregants are carried out to study the effect on the grain boundaries.

S1.00203 Diamond-like carbon-metal nanocomposites for solar thermal energy, GEORGIOS TRITSARIS, EFTHIMIOS KAXIRAS, Harvard University, KAXIRAS RESEARCH GROUP TEAM — Solar thermal energy systems are a possible technology for clean energy production. Carbon-based materials, including diamond-like carbon (DLC), have been suggested as promising for solar energy harvesting [1]. A strategy for tuning the properties of DLC is the incorporation of transition metal nanoparticles in the material [2]. Using density functional theory calculations, we study the structural, mechanical, and optical properties of DLC with transition metal nanoinclusions such as silver and copper. Key properties of the nanocomposites, such as the sp^2/sp^3 bonding ratio, elastic properties, and optical band gaps are reported. Such carbon-metal alloys are calculated to show enhanced performance over DLC.

[1] P. Patsalas, Thin Solid Films 519, 3990-3996 (2011).

[2] P. Oelhafen and A. Schler, Solar Energy 79, 110-121 (2005).

S1.00204 ABSTRACT WITHDRAWN —

S1.00205 The effects of 5-7 defects on the mechanical characteristics of carbon nanotubes intramolecular junctions and their influences on electronic properties, WEN-JAY LEE, JEE-GONG CHANG, YENG-TSENG WANG, WAN-SHENG SU, National Center for High-Performance Computing, Tainan 741 — This study utilizes molecular dynamics simulations and first-principles techniques to investigate mechanical and electronic properties of the single-walled carbon nanotube (SWCNT) intramolecular junctions (IMJs). Results show that the mechanical behaviors are mainly affected by the diameter of thinner segment of two composed tubes, whereas are barely able to be influenced by the number of 5-7 defects in the interface region. With applied compression, the yielding stress and Young's modulus of the SWCNT IMJs are found to be strongly associated with the orientation of two contacted heptagon rings where their ordering values are vertical > tilted > parallel to the axial direction. Under applied tensile, a lowest value in the yielding stress and Young's modulus is found on the parallel status, but the other two reveal alternating relations. Moreover, the magnitude of the stress amplitude is proportional to the Young's modulus and yielding stress and the buckling location is shown to be dependence on different orientations of two contacted heptagon rings. Finally, our first-principles calculations indicated that the considered SWCNT (5,0)/(8,0) IMJs at a certain length with different distributions of 5-7 defects on the tube wall exhibit diverse electronic properties, such as the changes of the density of states and modulation of energy gap. With increasing length, the numbers of states near the Fermi level region increase significantly and the energy gap tends to shrink as well.

S1.00206 Optical absorption in degenerately doped semiconductors: Mott transition or Mahan excitons?, ANDRÉ SCHLEIFE, Lawrence Livermore National Laboratory, CLAUDIA RÖDL, KARSTEN HANNEWALD, FRIEDHELM BECHSTEDT, Institut fuer Festkoerpertheorie und -optik, Friedrich-Schiller-Universitaet Jena — In the exploration of material properties, parameter-free calculations are a modern, sophisticated complement to cutting-edge experimental techniques. *Ab-initio* calculations are now capable of providing a deep understanding of the interesting physics underlying the electronic structure and optical absorption, e.g., of the transparent conductive oxides. Due to electron doping, these materials are conductive even though they have wide fundamental band gaps. The degenerate electron gas in the lowest conduction-band states drastically modifies the Coulomb interaction between the electrons and, hence, the optical properties close to the absorption edge. We describe these effects by developing an *ab-initio* technique which captures also the Pauli blocking and the Fermi-edge singularity at the optical absorption onset, that occur in addition to quasiparticle and excitonic effects. We answer the question whether free carriers induce an excitonic Mott transition or trigger the evolution of Wannier-Mott excitons into Mahan excitons. The prototypical *n*-type zinc oxide is studied as an example.

S1.00207 Fast and Accurate Modeling of Molecular Energies with Machine Learning, ANATOLE VON LILIENFELD, Argonne National Laboratory, MATTHIAS RUPP, Technical University Berlin, ALEXANDRE TKATCHENKO, Fritz-Haber Institute Berlin, KLAUS-ROBERT MUELLER, Technical University Berlin — A machine learning model for the prediction of atomization energies of a diverse set of organic molecules, based on nuclear charges and atomic positions only, will be discussed. The problem of obtaining molecular energies across chemical compound space, aka. as solving Schrodinger's equation, is mapped onto a non-linear statistical regression problem of reduced complexity. We use eigenvalues of a "Coulomb"-matrix to encode all Cartesian and atomic number variables of a molecule. Regression models are trained on, and compared to, atomization energies computed with hybrid density-functional theory for a sub-set of the GDB-13 database consisting of more than seven thousand molecules. Cross-validation yields a mean absolute error of less roughly 10 kcal/mol. Applicability and transferability is demonstrated for the prediction of potential energy curves of unseen molecules.

S1.00208 Development of a relativistic impurity embedding code based on the KKR Green function method, DAVID BAUER, PASCAL KORDT, PHIVOS MAVROPOULOS, RUDOLF ZELLER, STEFAN BLÜGEL, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — We present a new implementation of the KKR Green function method for electronic structure calculations of impurity atoms embedded in a crystalline host. Our code is able to treat impurity atoms not necessarily positioned at host sites. This became possible by a two step approach: For large deviations of the impurity from the host position a virtual atom method is used where the host Green function is expanded around the new impurity position. Then, small displacements are treated by an expansion of the Green function. In addition, we include in our code a newly developed accurate method to directly solve the coupled Lippmann-Schwinger equations for non-spherical potentials via a system of algebraic equations. When spin-orbit effects are included in the presence of spin polarization, this is especially important for the irregular solutions because of the coupling of different angular momenta up to the origin. We apply the method to solve the Schrödinger, the scalar-relativistic as well as the Dirac equation by using appropriate source terms.

S1.00209 A constraint method for variational total energy calculations of electronic excitations within the Kohn-Sham scheme¹, BABAK SADIGH, Lawrence Livermore National Laboratory — We propose a general constraint on the occupations of single-particle orbitals within (hybrid) density-functional theory that allows a variational total energy formulation for extended systems containing arbitrary electronic excitations. This method is simple to implement and is ideal for studying structural relaxations and molecular-dynamics simulations in the presence of excitations since accurate forces can be calculated via the Hellman-Feynman theorem.

¹This work performed under the auspices of the U.S. Department of Energy by LLNL under Contract DE-AC52-07NA27344 with support from the National Nuclear Security Administration (NNSA) office of Non-proliferation Research and Development (NA-22)

S1.00210 Quantum phase transitions of 2-d dimerized spin-1/2 Heisenberg models with spatial anisotropy , MING-TSO KAO, DENG-RUEI TAN, FU-JIUN JIANG, National Taiwan Normal University, FU-JIUN JIANG TEAM — Motivated by the unexpected Monte Carlo results as well as the theoretical proposal of a large correction to scaling regarding the critical theory for the staggered-dimer spin-1/2 Heisenberg model on the square lattice, we study the phase transitions induced by dimerization of several dimerized quantum Heisenberg models with spatial anisotropy using first principles Monte Carlo method. We focus on investigating the finite-size scaling of the observables $\rho_{s1}2L$ and $\rho_{s2}2L$ since such strategy might reveal the subtlety of determining the corresponding critical theory as suggest in [1]. Here ρ_{si} with $i \in \{1, 2\}$ and L refer to the spin stiffness in the i -direction and the spatial box size, respectively. Surprisingly, similar to the results found in [1], while we do observe a large correction to scaling for $\rho_{s1}2L$ of the staggered-dimer model on the honeycomb lattice, the observable $\rho_{s2}2L$ of the same model receives a negligible correction to its scaling. Further, our simulation data for all the models considered here including the herringbone- and ladder-dimer models are compatible with the established numerical values for $\nu, \beta/\nu$ and ω in the $O(3)$ universality class. To explain the results presented in this study, a deepened theoretical understanding for the critical theories of the models considered here is required.

S1.00211 Local-TQO and Stability of Frustration-Free Hamiltonians , JUSTYNA PYTEL, Oregon State University, SPYRIDON MICHALAKIS, California Institute of Technology — The attention of the condensed matter and mathematical physics communities has recently focused on Hamiltonians with low-energy sectors exhibiting some form of topological order. In our work [1], we present a generalization of the result of Bravyi et al. [2,3] on the stability of topological quantum order for Hamiltonians composed of commuting projections with a common zero-energy subspace. In particular, the commutativity condition can be removed: We prove stability of the spectral gap for gapped, frustration-free Hamiltonians under general, quasi-local perturbations. Also, we will discuss the “Local Topological Quantum Order” and “Local-Gap” conditions sufficient for proving stability.

[1] S. Michalakis and J. Pytel, *Stability of Frustration-Free Hamiltonians*. arXiv:1109.1588 (2011).

[2] S. Bravyi and M.B. Hastings, *A short proof of stability of topological order under local perturbations*. arXiv:1001.4363.

[3] S. Bravyi, M.B. Hastings, and S. Michalakis, *Topological quantum order: stability under local perturbations*. J. Math. Phys. **51**, 093512 (2010).

S1.00212 New limits on violations of the equivalence principle from solar system observations , JACK MITCHAM, JAMES OVERDUIN, Towson University — The equivalence principle is the foundation of general relativity theory, but violations of this principle are generically predicted by theories that attempt to unify gravity with the other fundamental interactions of nature. Violations of equivalence could lead to measurable deviations of solar system bodies from their expected positions near stable or semi-stable Lagrange points. We extend earlier constraints using new observational data on Trojan and artificial satellites near Jupiter, Neptune, Mars and Earth.

S1.00213 Is Dark Energy Composed of Photons with Negative Mass (Dark Photons)? , DOUGLAS SNYDER, None — Dark energy may be composed of photons with negative inertial and gravitational mass. Since the photons comprising dark energy would have negative mass, they could not be observed even though they exert a repulsive gravitational force on photons that have positive mass. Furthermore, dark photons possess little mass which is a feature of dark energy. Dark photons are small enough to comprise the needed density to support a universe that is close to flat. They also may allow for repelling entities with positive mass while they are attracted to particles with positive mass, a possible requirement of dark energy. First presented at Space Telescope Science Institute Spring Symposium: A Decade of Dark Energy, May 5-8, 2008, Baltimore, MD.

S1.00214 Visualization and Analysis of Synthetic Observations of Star Forming Regions , MICHELLE BORKIN, Harvard University, CHRISTOPHER BEAUMONT, Institute for Astronomy, University of Hawaii, THOMAS ROBITAILLE, Max Planck Institute for Astronomy, STELLA OFFNER, ALYSSA GOODMAN, Harvard-Smithsonian Center for Astrophysics — We present multidimensional visualizations used for the exploration, analysis, and comparison of simulated synthetic observations and real astronomical observational data cubes. By comparing synthetic observations of simulated star forming regions to real observational radio data cubes utilizing 2D and 3D visualization techniques we are able to more effectively and efficiently compare these types of data, in particular their hierarchical structure and kinematic features such as outflows or expanding shells. For our synthetic data we use simulations performed with the ORION adaptive mesh refinement (AMR) three-dimensional gravito-radiation-hydrodynamics code which follow the collapse and evolution of protostars down to AU size scales. The synthetic observations are produced using MOLLIE, a molecular line radiative transfer code. Through comparisons of 2D dendrogram representations of the star forming region’s hierarchical structure, 2D column maps, and 3D data visualizations we are able to gain a better understanding of the physical structures and kinematic features, and enhance the interpretation of astronomical data cubes.

S1.00215 Implementation of cryptographic hash function SHA256 in C++ , AKASH SHRIVASTAVA, Manipal Institute of Technology, Udipi, Karnataka, India — This abstract explains the implementation of SHA Secure hash algorithm 256 using C++. The SHA-2 is a strong hashing algorithm used in almost all kinds of security applications. The algorithm consists of 2 phases: Preprocessing and hash computation. Preprocessing involves padding a message, parsing the padded message into m-bits blocks, and setting initialization values to be used in the hash computation. It generates a message schedule from padded message and uses that schedule, along with functions, constants, and word operations to iteratively generate a series of hash values. The final hash value generated by the computation is used to determine the message digest. SHA-2 includes a significant number of changes from its predecessor, SHA-1. SHA-2 consists of a set of four hash functions with digests that are 224, 256, 384 or 512 bits. The algorithm outputs a 256 bits message block with an internal state block of 256 bits and initial block size of 512 bits. Maximum message length in bit is generated is $2^{64}-1$, over all computed over a series of 64 rounds consisting of several operations such as and, or, Xor, Shr, Rot. The code will provide clear understanding of the hash algorithm and generates hash values to retrieve message digest.

S1.00216 HIGH PRESSURE PHYSICS —

S1.00217 Pressure-Induced Structural, Magnetic and Transport Transitions in the Two-Legged Ladder $\text{Sr}_3\text{Fe}_2\text{O}_5$, TAKAFUMI YAMAMOTO, CEDRIC TASSEL, YOJI KOBAYASHI, Kyoto University, TAKATERU KAWAKAMI, Nihon University, TAKU OKADA, TAKÉHIKO YAGI, University of Tokyo, HIDE TO YOSHIDA, TAKANORI KAMATANI, YOSHITAKA WATANABE, Nihon University, TAKUMI KIKEGAWA, High Energy Acceleration Research Organization (KEK), MIKIO TAKANO, KAZUYOSHI YOSHIMURA, HIROSHI KAGEYAMA, Kyoto University — The layered compound SrFeO_2 with an FeO_4 square-planar motif exhibits an unprecedented pressure-induced spin state transition ($S = 2$ to 1), together with an insulator-to-metal (I-M) and an antiferromagnetic-to-ferromagnetic (AFM-FM) transition. In this study, we have studied the pressure effect on the structural, magnetic and transport properties of the structurally related two-legged spin ladder $\text{Sr}_3\text{Fe}_2\text{O}_5$. When pressure was applied, this material first exhibited a structural transition from $Immm$ to $Ammm$ at $P_s = 30 \pm 2$ GPa. This transition involves a phase shift of the ladder blocks from $(1/2, 1/2, 1/2)$ to $(0, 1/2, 1/2)$, by which a rock-salt type SrO block with a seven-fold coordination around Sr changes into a CsCl -type block with eight-fold coordination, allowing a significant reduction of volume. However, the $S = 2$ antiferromagnetic state stays the same. Next, a spin state transition from $S = 2$ to $S = 1$, along with an AFM-FM transition was observed at $P_c = 34 \pm 2$ GPa, similar to that of SrFeO_2 . A sign of an I-M transition was also observed at pressure around P_c .

S1.00218 Uncover the nature of cubic-rhombohedral transition in Fe_{1-x}O, QINGYANG HU, George Mason University, YANG DING, HPSynC, Carnegie Institute Washington, HONGWEI SHENG, George Mason University — Transition metal monoxide Fe_{1-x}O is an archetypal Mott insulator and an important geological compound. Despite considerable study during the past few decades, the origin of the high-pressure cubic-rhombohedral transition in this fundamental material is still not fully understood. Combining high-pressure nanoscale x-ray diffraction imaging techniques, we conducted density-functional theory (DFT) based first-principles calculations to reveal the nature of the transition. Our theoretical calculations confirm the conclusions drawn from our imaging experiments that the pressure-induced rhombohedral distortion of Fe_{1-x}O is associated with <111> stacking defects cluster and is ferroelectric in nature.

S1.00219 MAGNETISM —

S1.00220 Structural, magnetic, electronic properties of the filled skutterudite EuFe₄As₁₂, HELGE ROSNER, ANDREAS LEITHE-JASPER, WALTER SCHNELLE, MIRIAM SCHMITT, YURI PROTS, MPI CPfS Dresden, ANGELA TRAPANANTI, CORNELIUS STROM, ESRF Grenoble, YURI GRIN, MPI CPfS Dresden — The filled skutterudite EuFe₄As₁₂ has been synthesized and its structural, electronic, magnetic and thermodynamic properties have been carefully investigated. In this compound, the Fe and Eu moments order ferrimagnetically at $T_C = 151$ K, the highest magnetic ordering temperature among filled skutterudite compounds. LDA+*U* band structure calculations confirm the observed magnetic polarizations and suggest that the conduction electrons in EuFe₄As₁₂ have a large spin polarization, although slightly smaller than in the isostructural EuFe₄Sb₁₂. We present a joint experimental and theoretical study of the electronic and magnetic properties for both compounds, including the isostructural EuFe₄P₁₂, where the exchange of the pnictide can be considered as chemical pressure. To separate the influence of mere volume effects and a change of the pnictide we also studied the behaviour under hydrostatic pressure for EuFe₄As₁₂, both experimentally and theoretically.

S1.00221 Bi_{3-x}M₃O₁₁+? (M=Cr, Rh, Ir, Pt, Pd): A series of new KSbO₃-type structural magnetic materials, WEI YI, National Institute for Materials Science — KSbO₃-type family is interesting because it can adopt three interpenetrating networks with the composition changing from ABO₃ (KSbO₃ and KIrO₃) to ABO_{3.667} (Bi₃Ru₃O₁₁, La₃Ru₃O₁₁, and Bi₃Ga₃Sb₂O₁₁). Recently Belik et. al reported a new KSbO₃-type random ferrimagnet Bi₃Mn₃O₁₁ with high T_C . Here we reported a series of new KSbO₃-type structural materials Bi_{3-x}M₃O₁₁+? (M=Cr, Rh, Ir, Pt, Pd) synthesized by high pressure and high temperature (HPHT). We investigated the effects of oxygen content on the structural, physical, and chemical properties of these materials, because a wide variation of ? value (changed from -0.5 to 0.6) in this system keeps the same cubic structure. In addition, we also studied the effects of Bi content on the structure, physical, and chemical properties. The value of x was changed from 0 to 0.4 in Bi_{3-x}Cr₃O₁₁+?.

S1.00222 ABSTRACT WITHDRAWN —

S1.00223 ABSTRACT WITHDRAWN —

S1.00224 Electronic and Magnetic Structures in 2D Graphene and BN Nanoflakes¹, WEI-MING SHI, MING JIANG², Department of Physics, Yantai University — The two-dimensional nanomaterials have been attracting great attention for potential applications. Using first-principles calculations, we have studied the geometric and electronic properties of zigzag graphene nanoflake(ZGNF)and single-layer BN nanoflake (ZBNF)before and after hydrogen and oxygen adsorption. The interplay between atomic adsorption, crumpling structures, zigzag edges and magnetic structures has been investigated systematically. Our calculated results show that the total magnetic moments of the ZGNF with the adsorbed atoms increase significantly. The adsorbed atoms induce the crumpling structures and central spin polarization, while the magnetic orders of zigzag borders are controlled. A detailed electronic structure analysis is given. The single-layer BN nanoflake has a special crumpling struture different from the ZGNF. The left-right symmetry of atomic height displacements is broken. This study demonstrates a new approach to manipulate the properties of 2D nanomaterials. This work was supported by the SRFROCS,SEM and Shandong OYS Foundation.

¹This work was supported by the SRFROCS,SEM and Shandong OYS Foundation.

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S1.00225 Non-destructive generation of nano-scale periodic pinning potentials for magnetic domain walls: a way to bias domain wall propagation, PETER METAXAS, School of Physics, University of Western Australia, PIERRE-JEAN ZERMATTEN, Spintec, Grenoble, France, RAFAEL NOVAK, JEAN-PIERRE JAMET, RAPHAEL WEIL, STANISLAS ROHART, JACQUES FERRE, ALEXANDRA MOUGIN, Labo. de Phys. des Solides, CNRS/Universite Paris-Sud 11, France, ROBERT STAMPS, School of Physics, University of Western Australia and SUPA - School of Physics and Astronomy, Uni. Glasgow, UK., VINCENT BALTZ, BERNARD RODMACQ, GILLES GAUDIN, Spintec, Grenoble, France — The stray magnetic field of an array of ferromagnetic nanodots is used to generate a spatially periodic pinning potential for domain walls moving through a physically separate, weakly disordered, magnetic layer lying beneath the array. This technique represents a non-destructive method to create tunable and localised pinning sites for domain walls which are consequently subject to co-existing (but independent) periodic and disordered pinning potentials. Beyond the fundamentally attractive application of creating a model experimental system to study interface motion through multiple co-existing pinning potentials, our system interestingly exhibits many characteristics that are normally associated with exchange bias. This is a direct result of the fact that pinning effects induced by the periodic pinning potential depend upon the polarity of the applied magnetic field which drives the domain wall motion, a phenomenon which manifests itself in field-polarity-dependent domain wall mobilities and profiles.

S1.00226 Probing antiferromagnetism in NiMn/Ni/(Co)/Cu₃Au(001) single-crystalline epitaxial thin films, M. YAQOUB KHAN, CHII-BIN WU, WOLFGANG KUCH, Freie Universität, Institut für Experimentalphysik, D-14195 Berlin, Germany — Antiferromagnetism of equi-atomic single-crystalline NiMn thin film alloys grown on Ni/Cu₃Au(001) is probed by means of magneto-optical Kerr effect (MOKE). Thickness-dependent coercivity enhancement of NiMn/Ni/Cu₃Au(001) showed that 7 atomic monolayers (ML) NiMn order antiferromagnetically at room temperature. It is found that NiMn can couple to out-of-plane (OoP) as well as in-plane (IP) magnetized Ni, the latter stabilized by Co under-layer deposition. The antiferromagnetic (AFM) ordering temperature (T_{AFM}) of NiMn coupled to OoP Ni is found to be much higher (up to 110 K) than in the IP case, for otherwise identical interfacial conditions. This is attributed to the 'magnetic proximity effect' in which the ferromagnetic (FM) layer substantially influences the T_{AFM} of the adjacent AFM layer and can be explained by either (i) a higher interfacial coupling strength or/and (ii) more thermally stable NiMn distorted spin structure when coupled to Ni magnetized in OoP direction than in IP. An exchange-bias effect could only be observed for the thickest NiMn film studied (35.7 ML); the exchange-bias field is higher in the OoP exchange-coupled system than in the IP one due to the same reason/s.

S1.00227 Tunable carrier spin polarization in PbMnS through quantum confinement¹, GEN LONG, HONGWANG ZHANG, HUI XING, BIPLOB BARMAN, YUTSUNG TSAI, ATHOS PETROU, HAO ZENG, Department of Physics, University at Buffalo-SUNY — We report magneto-photoluminescence studies on manganese-doped lead sulfide ($\text{Pb}_{1-x}\text{Mn}_x\text{S}$, $x = 0$ to 5%) quantum dot system synthesized by solution-phase chemical method. The size (3 to 15nm), temperature (7K to 100K), magnetic field (0 to 7T), and laser power dependence (1mW to 20mW) of photoluminescence were systematically investigated, with a focus on carrier spin polarization. Depending on the sizes and growth conditions, the spin polarization can be tuned from being positive to negative. Core/shell structured quantum dots with Mn^{2+} ions doped in the core or shell were also studied. The sign change in the spin polarization suggests tunable exchange interactions caused by quantum confinement effect and wave function engineering through heterostructure design.

¹Research supported by NSF.

S1.00228 Spin Dynamics in Recombinant H-chain Ferritin Reconstituted with 500Fe/Protein¹, GEORGIA PAPAETHYMIU, Villanova University — Ferrihydrite mineral cores averaging 500 Fe/protein shell were grown within recombinant human H-chain ferritin and characterized by Mössbauer spectroscopy. At 4.2 K, two magnetic phases ascribed to iron at surface and interior sites of the antiferromagnetic nanolattice of the mineral core were identified, registering hyperfine fields of 445 kOe and 486 kOe, respectively. With increasing temperature, from 4.2 K to 20 K, their values decrease at widely different rates; at a rate of 3.52 kOe/K for interior and 19.33 kOe/K for surface sites, before spectral lines collapse to quadrupolar doublets at a blocking temperature of $T_B = 22$ K. Below T_B , spin relaxation at interior sites is consistent with the theory of collective magnetic excitations of a superparamagnetic particle, whereas spin dynamics at surface sites are more consistent with theories of many-spin nano-magnet systems with greater complexity in the potential energy landscape that supports low energy spin-wave excitations. The entire Mössbauer temperature spectral profile will be presented and discussed in the light of the above observations.

¹Supported by NSF-DMR Nanomaterials Grant # 0604049.

S1.00229 Magnetic Anisotropy of GaAs/Fe/Au Core-Shell Nanowires Grown by MBE, KRITSANU TIVAKORNASATHORN, RICHARD PIMPINELLA, VU NGUYEN, XINYU LIU, MALGORZATA DOBROWOLSKA, JACEK FURDYNA, Department of Physics, University of Notre Dame — In order to increase the storage density of magnetic memories while maintaining thermal stability, new types of recording media and technologies need to be explored. In this context, perpendicular recording geometry is among the most attractive ideas. In this work we demonstrate a novel method of fabricating such perpendicular media, in the form of GaAs/Fe/Au core-shell nanowires (NWs) grown by molecular beam epitaxy on GaAs(111)B substrates. Scanning electron microscopy images show that the Fe shell has successfully coated the sidewalls of GaAs nanowires. Magnetic anisotropy of GaAs/Fe core-shell NWs was studied by ferromagnetic resonance and by superconducting quantum interference device (SQUID) magnetometry. Our results show that the magnetic anisotropy of this novel core-shell NW system cannot be simply described by any known theory, as revealed by our attempts to perform micromagnetic simulation using the object oriented micromagnetic framework (OOMMF). The observed features thus suggest the existence of a domain structure that is specific to this new system. We will now attempt to identify the domain structure of this complex system by magnetic force microscopy.

S1.00230 Anomalous field dependence of magnetoresistance in magnetic multilayers based on the Fibonacci sequence¹, LEONARDO DANTAS MACHADO, CLAUDIONOR GOMES BEZERRA, MARCIO ASSOLIN CORREA, CARLOS CHESMAN, Departamento de Física Teórica e Experimental - UFRN, Brazil, JOHN E. PEARSON, AXEL HOFFMANN, Materials Science Division, Argonne National Laboratory, USA — The discovery of giant magnetoresistance and concomitant effects such as oscillatory exchange coupling in magnetic multilayers was the starting point of the spintronics era. In the present study, a multilayer of Fe and Cr was designed, using the Fibonacci sequence for the growth of the non-magnetic spacers. Using the gradient method we simulated the magnetic field dependence of these nanostructures for in-plane magnetic fields. The simulations included magnetocrystalline anisotropy for the [100] and [110] directions, as well as bilinear and biquadratic exchange coupling. The resultant magnetization and magnetoresistance behavior shows unusual behavior, such as a Devil's staircase for the magnetization and increasing magnetoresistance with increasing applied magnetic fields. When the ratio of the biquadratic to bilinear coupling exceeds 30% the magnetic field response is expected to show even fractal behavior. These numerical simulations will also be compared to experimental measurements on samples prepared with nominally the same thicknesses.

¹Work supported by the CNPq (Brazilian Agency) and U.S. Department of Energy, Office of Science, Basic Energy Sciences, under contract No. DE-AC02-06CH11357.

S1.00231 Large exchange anisotropy in nanostructured $\text{Cu}_{30}\text{Mn}_{70}$ ribbons¹, J. MARION, F. JIMÉNEZ-VILLACORTA, L.H. LEWIS, Northeastern University Department of Chemical Engineering — Exchange bias (H_{ex}), arising from coupling between antiferromagnetic (AFM) and ferromagnetic (FM) materials, is a diagnostic metric of magnetic interactions in inhomogeneous systems. An extremely large H_{ex} of 10 kOe is found in the rapidly-solidified alloy $\text{Cu}_{30}\text{Mn}_{70}$ at 10 K [1-2], but disappears at temperatures above the system blocking temperature of 123 K. X-ray diffraction reveals the presence of two well-crystallized FCC γ -phases with cubic a-parameters 3.744 and 3.750 Å, unit cell volumes of 52.5 and 52.7 Å³, respectively, and a crystallite size of ~30 nm. We hypothesize that the γ -phase with larger a-parameter is Mn-rich while the other is Mn-poor. The observed magnetic behavior is attributed to exchange interactions between Mn-rich regions where AFM coupling between nearest-neighbor Mn atoms dominates, and Mn-poor regions where FM coupling between next-nearest-neighbors dominates [1]. Compositional fluctuations result in an additional cluster-glass-like freezing behavior due to magnetically frustrated interactions between Mn atoms [2].

[1] Kouvel, J.S., J. Appl. Phys. S31 (1961) 5, S142-147.

[2] Mydosh, J. A. (1995), Spin Glasses, Taylor & Francis.

¹This research was conducted under ONR grant # N000141010533. The author would also like to acknowledge Drs. Matthew Willard and Maria Daniil at NRL.

S1.00232 Spin polarized surface states on stepped magnetic surfaces: ab-initio approach, OLEG STEPANYUK, OLEG POLYAKOV, ALEXANDER SALETSKY, Moscow State University, WOLFRAM HERGERT, Martin-Luther-Universität Halle-Wittenberg — It was shown that surface state electrons become spin polarized above magnetic layers and nanoislands [1]. In the present work we perform the state of the art ab-initio studies of surface state electrons at steps of magnetic metals. We focus on steps of 3d metals on Cu(111) surface. We have revealed a spin-dependent charge transfer at step edges which is explained by Smoluchowski effect. Strongly inhomogeneous spin polarization of surface states [1] at steps is revealed. Our results indicate that tunneling magnetoresistance at steps can exhibit very strong changes at the atomic scale.

[1] L. Diekhoner et. al. Phys. Rev. Lett. 90, 236801

S1.00233 Core/Shell and High Aspect Ratio Magnetic Oxide Nanoparticles for Antenna Applications, THOMAS F. EKIERT, JR., Air Force Research Lab - WPAFB, Universal Technology Corporation, MATTHEW O'MALLEY, Air Force Research Lab - WPAFB, BRANDON YOCUM, JENNIFER LIPPOLD, MALLORY LYLE, ANGELA GRINER, CORY FLYNN, ANNA NICKEL, Air Force Research Lab - WPAFB, Southwestern Ohio Council for Higher Education, MAX D. ALEXANDER, JR., Air Force Research Lab - WPAFB — Improved antenna gain, reduced antenna aperture size, and improved bandwidth are of interest to an increasingly mobile world. To obtain these improvements our efforts are directed at developing new magnetic oxide nanoparticle/polymer composites with modifiable permeability and permittivity and low electrical losses. Our approach consists of producing core/shell and shape controlled magnetic nanoparticles. Methods of synthesis utilize microwave and traditional heating to perform hydrothermal and solvothermal reactions. Decomposition of metal acetylacetonates is performed using various alcohols resulting in spherical nanoparticles with diameters of ≈ 8 -16 nm and 3-7 nm for Fe_3O_4 and CoFe_2O_4 , respectively. Microwave methods result in similar particles, but are produced in an hour or less as compared to 48 hrs via the traditional solvothermal method. Successive growths are used to produce larger monolithic particles as well as core/shell systems where exchange coupling between the core and shell is observed. Hexaferrite particles have been produced via hydrothermal synthesis, while high aspect ratio Fe_3O_4 nanoparticles (≈ 10 -100 nm) produced via hydrothermal synthesis result in nanoneedles with high μ_r .

S1.00234 Magnetism and structure of amorphous Co-W alloyed nanoparticles, ADRIANA FIGUEROA, JUAN BARTOLOME, ICMA - CSIC, Spain, LUIS M. GARCIA, ICMA - Universidad de Zaragoza, Spain, FERNANDO BARTOLOME, ICMA - CSIC, Spain, CESAR MAGEN, ALFONSO IBARRA, INA - Universidad de Zaragoza, Spain, LUISA RUIZ, JOSE M. GONZALEZ-CALBET, Universidad Complutense, Spain, FREDERIC PETROFF, C. DERANLOT, CNRS - Thales, France, SAKURA PASCARELLI, ESRF, France, PETER BENCOK, Diamond Synchrotron, UK, NICHOLAS B. BROOKES, FABRICE WILHELM, ANDREI ROGALEV, ESRF, France — W-capped Co nanoparticles dispersed in an alumina matrix are studied by means of high-resolution transmission electron microscopy, extended x-ray absorption fine structure, SQUID-based magnetic measurements, ac magnetic susceptibility, and x-ray magnetic circular dichroism. Results show the formation of amorphous Co-W alloy nanoparticles, the magnetic properties of which are modified by the amount of W or Co present in the samples. The average Co magnetic moment depends on the number of W atoms surrounding it. Co-W particles show superparamagnetic behavior and are described as an array of noninteracting particles with random anisotropy axes and an average moment per particle proportional to the particle volume and to the average Co moment for each alloy composition. Values of the magnetic anisotropy constant of the particles are on the order of 10^6 erg/cm³, higher than that of bulk Co. Evidence of short-range ordering within each amorphous particle is found that provides insight of the origin of their magnetic anisotropy.

S1.00235 Competition between quantum criticality and Fermi liquid behavior revealed by transport measurements in ultrapure $\text{Sr}_3\text{Ru}_2\text{O}_7$, JAN BRUIN, HIDEAKI SAKAI, University of St Andrews, ROBIN S. PERRY, University of Edinburgh, ANDREW P. MACKENZIE, University of St Andrews — The layered perovskite metal $\text{Sr}_3\text{Ru}_2\text{O}_7$ has gained considerable interest since the discovery of its field-tuned quantum criticality [1] and the subsequent discovery of a new electronic phase with a high magnetoresistive anisotropy, consistent with the existence of an electronic nematic fluid [2]. Further studies have explored the properties of the “normal state” from which the anisotropic phase emerges in terms of thermodynamics [3] and quantum oscillations [4], but a comprehensive study of the transport properties of the purest samples has so far been lacking. Here, we present the first study of the normal state resistivity of ultrapure $\text{Sr}_3\text{Ru}_2\text{O}_7$, involving temperature control over more than two orders of magnitude and a 15T magnet system. The high signal to noise of this measurement allows for precise extraction of the temperature dependence exponent and provides detailed understanding of the transport signatures of field-tuned quantum criticality.

[1] S. A. Grigera *et al.*, Science **294**, 329 (2001).
 [2] R. A. Borzi *et al.*, Science **315**, 214 (2007).
 [3] A. W. Rost *et al.*, Science **325**, 5946 (2009).
 [4] J.-F. Mercure *et al.*, Phys. Rev. B **81**, 235103 (2010).

S1.00236 The Influence of Layer Thickness-Ratio on Magnetoresistance in $\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3/\text{La}_{1/3}\text{Ca}_{2/3}\text{MnO}_3$ Exchange Biased System, MARIA ELENA GOMEZ, SANDRA MILENA DIEZ, LINA MARIA CUARTAS, Universidad del Valle, LORENA MARIN, Ina Universidad de Zaragoza, PEDRO PRIETO, CENM Excellence Center for Novel Materials — Isothermal magnetic field dependence of the resistance in $\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3$ (F-LCMO)/ $\text{La}_{1/3}\text{Ca}_{2/3}\text{MnO}_3$ (AF-LCMO) bilayer and AF-LCMO/F-LCMO/AF-LCMO trilayer at temperatures below Néel temperature of the antiferromagnetic layer were carried out to study the thickness layers influence on magneto transport properties. We grew multilayers using a high oxygen pressure sputtering technique. We systematically varied the thickness of the F-LCMO layer, t_F , maintaining constant the thickness of the AF-LCMO layer, t_{AF} . We studied the influence of the thickness ratio t_F/t_{AF} on the ZFC and FC magnetoresistance (MR) loops. H_{FC} was varied from 100 Oe to 400 Oe. We found that MR has hysteretic behavior as observed in $[\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3/\text{La}_{1/3}\text{Ca}_{2/3}\text{MnO}_3]_N$ superlattices, where MR increases with the increasing field from $H=0$ to a maximum and then it decreases continuously. The position and magnitude of the maximum is not symmetric with respect to the axis $H=0$ for both FC and ZFC loops. We found that magnetoresistance behavior of the bilayer and trilayer is thickness-ratio dependent for both ZFC and FC loops.

S1.00237 Micromagnetic simulations and experimental calibration of magnetic behavior in multiferroic BiFeO_3 , DIANA QIU, KHALID ASHRAF, SAYEED SALAHUDDIN, University of California, Berkeley — BiFeO_3 (BFO) is a magneto-electric multiferroic that exhibits ferroelectric and antiferromagnetic (AFM) ordering at room temperature. BFO films are frequently coupled to a ferromagnet (FM) layer grown on the BFO surface, but the behavior of the magnetization in BFO films and at the BFO/FM interface is not understood. We propose a micromagnetic model for the magnetization in BFO in which spin canting throughout the film, induced by the Dzyaloshinskii-Moriya (DM) effect, creates weak ferromagnetism on the BFO surface. This surface ferromagnetism is significantly enhanced by an exchange interaction with the FM at the BFO/FM interface. We perform OOMMF micromagnetic simulations of BFO/CoFe bilayers and reproduce experimentally reported one-to-one mapping between BFO and CoFe domains as well as enhanced magnetic moment on the BFO surface, on the order of $0.5 \mu_B$ per unit cell. From this model, we can extract AFM/FM exchange energies and DM energies by fitting experimentally reported values for BFO surface magnetic moment and hysteresis. We also demonstrate that magnetization switching of the BFO domains can induce switching in the FM. We reproduce experimentally observed 180° total magnetization switching through 90° switching in stripe-like domains.

S1.00238 Growth of ferromagnetic $\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3$ / ferroelectric BaTiO_3 heterostructures¹,

MARIA ELENA GOMEZ, JOHN EDWARD ORDOÑEZ, WILSON LOPERA, Department of Physics, Universidad del Valle, Cali, Colombia, PEDRO PRIETO, CENM Excellence Center for Novel Materials, Colombia, LORENA MARIN, J.A. PARDO, L. MORELLON, P. ALGARABEL, Instituto de Nanociencia de Aragón, Universidad de Zaragoza, Spain — Multiferroic materials exhibiting simultaneous ferroelectricity and ferromagnetism have potential applications in information storage and in the emerging field of spintronics. Ferromagnetic / ferroelectric multilayers could be a way to obtain a multiferroic heterostructure. We addressed to deposit the ferromagnetic phase of the $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ and the ferroelectric BaTiO_3 seeking a multiferroic properties in these hetero structures. We have optimized the growth parameters for depositing $\text{BaTiO}_3(\text{BTO})$ / $\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3(\text{LCMO})$ / $(001)\text{SrTiO}_3$ by pulsed laser deposition (PLD) at pure oxygen atmosphere and a substrate temperature of 820 °C. The bilayer structure and microstructure were studied by x-ray diffraction (XRD) and atomic force microscopy (AFM). For individual layers, lattice parameter is $a_{\text{BTO}}=4.068$ Å, and $a_{\text{LCMO}}=3.804$ Å, whereas in the bilayer, Bragg peaks for LCMO maintain its position but BTO peak shift to lower Bragg angle indicating a strained BTO film. Magnetization and polarization measurements indicate a possible multiferroic heterostructures

¹Support by INA, Spain; “El Patrimonio Autón. Fondo Nal. de F/miento CT&I. FJC,” Contract RC 275-2011; 1106-48-925531 Colciencias project

S1.00239 Characterization of Nano-oxidation Lithography on $\text{La}_{0.7}\text{Ba}_{0.3}\text{MnO}_3$ Thin Films Grown by Pulse-Laser-Deposition

EKEMBU KEVIN TANYI, DAVID SCHAEFER, RAJESWARI KOLAGANI, PARUL SRIVASTAVA, Towson University — Nano-oxidation using Atomic Force Microscopy has been used to produce nano-scale patterns on a variety of materials, including semiconductors, insulators, metals and superconductors. Perovskite Oxide thin films have demonstrated unique material characteristics. The ability to make localized modifications on these films would allow nanofabrication of devices utilizing these unique properties. In this study, the atomic force microscope was used to modify the surface of $\text{La}_{0.7}\text{Ba}_{0.3}\text{MnO}_3$ thin films grown using Pulsed Laser Deposition Techniques. Surface patterns were produced and studied as a function of humidity, applied tip voltage, temperature, and growth conditions. Reproducible patterns were produced using both positive and negative tip voltages. Two growth modes were observed. A moderate growth rate was common for positive tip voltages up to 15 V (at $T=75.1\pm1$; $H=78\pm2\%$) which allowed the controlled formation of features considerably larger than those produced on materials like silicon. Additionally, a significantly larger growth rate was observed for negative tip voltages exceeding -12V. This growth mode provides the potential to produce structures at significantly higher write speeds, making these manganese films candidates for data storage devices.

S1.00240 Finite-Size Scaling Effects in Chromia thin films¹, WILL ECHTENKAMP, XI HE, CHRISTIAN BINEK, Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln — Controlling magnetism by electrical means remains a key challenge in the area of spintronics. The use of magnetoelectrically active materials is one of the most promising approaches to this problem. Utilizing Cr_2O_3 as the magnetoelectric pinning layer in a magnetic heterostructure both temperature assisted and isothermal electrical control of exchange bias have been achieved [1,2]. Interestingly, this ME switching of exchange bias has only been achieved using bulk Cr_2O_3 crystals, isothermal switching of exchange bias using thin film chromia remains elusive. We investigate the origin of unusually pronounced finite-size scaling effects on the properties of Cr_2O_3 grown by Molecular Beam Epitaxy; in particular we focus on the different temperature dependencies of the magnetic susceptibility of bulk vs. thin film chromia, the change in Neel temperatures, and the implications for the magneto electric properties of chromia thin films.

[1] P. Borisov et al., Phys. Rev. Lett. 94, 117203 (2005).

[2] X. He et al., Nature Mater. 9, 579 (2010).

¹This project is supported by NSF through Career DMR-0547887, MRSEC DMR 0213808, and by the NRC/NRI supplement to MRSEC.

S1.00241 ABSTRACT MOVED TO A13.00014 —

S1.00242 Control of noise in magnetic multilayers by spin torque, ADNAN REBEI, King Abdullah Institute for Nanotechnology — In this work we show that the stability of magnetic nanostructures can be enhanced by time-dependent spin momentum transfer. Building reliable magnetic devices at smaller scales need to address the issue of thermal noise. Using two commonly studied magnetic systems with multiple stable states at zero temperature as examples, we show that periodic spin torques can enhance the stability of the system and hence suppress the noise due to interwell transitions. In the case of weak periodic spin torques, stochastic resonance which is usually associated with ac magnetic fields is also manifested for non-conservative torques. In more complex systems with a relatively low energy barrier, it is shown that high frequency spin torques can inhibit interwell transitions and in effect suppress the telegraph noise due to the switching between neighboring states.

S1.00243 Full Field-Frequency Study of Standing Spin Wave Modes in FM / NM / FM

Trilayers¹, PETER WARNICKE, JAVIER PULECIO, SHAWN POLLARD, YIMEI ZHU, DARIO ARENA, Brookhaven National Laboratory — Spin waves constitute an attractive avenue for spintronic devices as they can be used to carry information through magnetic media as well as to store information in form of localized modes. As a way of manipulating these entities, external microwave fields can be employed. For a given precession frequency, the amplitude of the localized spin wave mode in a single ferromagnetic layer is determined by the confining geometry and applied magnetic field strength. By introducing a non-magnetic spacer layer into the layer, the development of spin waves can be modified in a frequency range by varying the spacer layer thickness [1,2]. Here we investigate the role of the spacer layer thickness in a Permalloy/Copper/Permalloy trilayer by means of full field-frequency ferromagnetic resonance (FMR) spectroscopy.

[1] H. Bosse and H. Gärtner, JMMM 80 339 (1989).

[2] M. Belmeguenai, T. Martin, G. Woltersdorf, M. Maier, and G. Bayreuther, PRB 76 104414 (2007).

¹This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

S1.00244 Electronic and Optical properties of Mn δ -doping InGaAs/GaAs Quantum Wells¹,

UDSON MENDES, JOSÉ BRUM, Department of Condensed Matter Physics, Institute of Physics Gleb Wataghin, State University of Campinas, Campinas - São Paulo, Brazil — Recent magneto-optical measurements in InGaAs quantum wells (QWs) with GaAs barriers with δ -doped layers of Mn and C, show a strong oscillations of circularly polarized QW emission as a function of the magnetic field. The oscillations amplitude increases with the Mn content and they persist up to 25 K [Appl. Phys. Lett. 98, 251901 (2011)]. In order to understand these magneto-oscillations we studied the electronic and optical properties of the two-dimensional hole gas (2DHG) formed in the QW. The holes are provided by both Mn and C doping. We used the spin-density functional theory within the $\mathbf{k}\cdot\mathbf{p}$, the envelope function and the virtual crystal approximations to describe the electronic states of the system. The $sp-d$ interaction was described by the Zener kinetic-exchange model. Our results show that when an external magnetic field is applied a spin-polarized 2DHG is formed at the Mn δ -doped layer, inducing an effective magnetic field. This field affects the charge redistribution of the system inducing oscillations in the Fermi and energy levels, and consequently in the QW emission. The strength of these oscillations is strongly dependent on the nature of the Mn doping, in particular the distance between the QW and the Mn layers.

¹This work is supported by FAPESP and CAPES.

S1.00245 Structural and magnetic properties of GaAs-MnAs nanowires grown by MBE¹, A. SIUSYS, A. RESZKA, P. DZIAWA, B.J. KOWALSKI, P. DLUZEWSKI, H. PRZYBYLINSKA, M. SAWICKI, Institute of Physics, Polish Academy of Sciences, Warsaw, Poland, J. SADOWSKI, MAX-Lab, Lund University, Lund, Sweden, Institute of Physics, Polish Academy of Sciences — Ferromagnetic (FM) Nanowires (NWs) have been proposed recently as a base of a new type of nano-magnetic memory structures. In this context, the investigations of NWs combining FM materials with commercially used semiconductors (SCs) like Si or GaAs are desirable. NW structures of GaAs combined with (Ga,Mn)As FM SC and MnAs FM metal were grown by MBE. Primary core GaAs NWs growth was induced by different nanocatalysts on two substrates for comparison reasons: by the autocatalytic growth mode on Si(100), Si(111) and by Au nanodroplets induced catalytic growth on GaAs(111)B. In both cases NW cores of GaAs were grown at high temperature (550 C for GaAs(111)B and 600 C for Si). The (Ga,Mn)As and MnAs shells were grown on both types of primary GaAs NW cores at low temperature (250 C). Structural properties of the core-shell GaAs-(Ga,Mn)As NWs were investigated by electron microscopy (SEM, TEM) and magnetic properties were studied by SQUID magnetometry and FM resonance. The NWs grown on GaAs(111)B are thinner (50 nm), shorter (3 microns) and denser than the NWs grown on Si (typical diameters of 100 nm, lengths up to 15 microns). The FM behavior observed in these NW structures up to room temperature is related rather to MnAs nanoclusters than to individual NW.

¹This work has been supported by the EC Network SemiSpinNet

S1.00246 Electrical spin injection and detection in Si nanowires¹, SHIXIONG ZHANG, YAN LI, SHADI A. DAYEH, DARRYL L. SMITH, SCOTT A. CROOKER, S. TOM PICRAUX, Los Alamos National Laboratory — While electrical spin injection and detection in bulk Si has now been established, the availability of high quality single crystalline silicon nanowires has stimulated considerable interest in demonstrating spin-polarized transport in these 1-dimensional structures. Here, we report our efforts to electrically inject spin-polarized electrons from cobalt contacts into n-type silicon nanowires through Al_2O_3 tunnel barriers. The electrically doped nanowires were synthesized by the vapor-liquid-solid process with a cold wall chemical vapor deposition system using silane and phosphine precursors. Low temperature magneto-transport studies have shown spin-valve like behavior in both two-terminal and four-terminal lateral devices. The spin-valve signal as functions of temperature and bias voltage will be discussed. We will also show the influence of defects and trap states on the stability of nanowire devices.

¹Supported by the Los Alamos LDRD program

S1.00247 Bond operator theory for the frustrated anisotropic Heisenberg antiferromagnet on a square lattice¹, ANTONIO PIRES, Universidade Federal de Minas Gerais — In this work we use the bond operator formalism in a mean field approximation to study quantum phase transitions in the $S = 1$ Heisenberg antiferromagnet with single ion anisotropy up to the next-nearest neighbor coupling (the J1-J2-J3 model) on a square lattice. The model features a complex $T = 0$ phase diagram, whose ordering vector is subject to quantum corrections with respect to the classical limit. The phase diagram shows a quantum paramagnetic phase situated among Néel, spiral and collinear states.

¹This work was partially supported by CNPQ.

S1.00248 Behavior of the overlap distribution of various spin glasses at low temperature, JULIO F. FERNÁNDEZ, Universidad de Zaragoza, JUAN J. ALONSO, Universidad de Malaga — Numerical results for the probability distribution, $P(q, T)$, of the spin-overlap q as a function of temperature T , is reported for several randomly frustrated systems. These include (i) random bond Ising systems, such as the Edwards-Anderson spin-glass model, (ii) site diluted systems which are geometrically frustrated, such as FCC lattices with 40% of their sites occupied with up-down spins, and (iii) random-field systems. $P(q, T)$ stands for an average of $P_{\mathcal{J}}(q, T)$ over many system samples with different realizations of quenched randomness $\mathcal{J}$. We also report statistical fluctuations of $P_{\mathcal{J}}(q, T)$ which are relevant to the issue of self-averaging.

S1.00249 Second Frustration for Artificial Spin Ice, CRISTIANO NISOLI, TAMMIE NELSON, Theoretical Division, Los Alamos National Laboratory — Since its introduction six years ago, artificial spin ice has been employed to successfully study frustration and disorder, to explore extensions of thermodynamics to granular systems, to investigate topological defects and information encoding, and has become ground for direct imaging of “magnetic monopoles.” The research has concentrated so far on a few basic geometries (square, ladder, honeycomb, triangular) in which the frustration of the magnetic interaction at the vertices could (or not) bring about a degeneracy. Here we propose new topologically non-trivial geometries, which we call “of second frustration.” In these arrays each vertex, while frustrated, has a unique low energy configuration, and is therefore non degenerate; yet a second frustration is regained globally and vertex excitations are topologically protected on loops inside the array. These topological excitations, which control the entropy, cannot be suppressed, can move, merge and exchange topological charge. As novel, more dynamical artificial spin ice is being developed by many, these new lattices could provide an interesting playground for driving and controlling topological excitations, and for tailor-design of probe-response properties.

S1.00250 Low temperature spin glass transition in Gallium ferrite single crystals, SOMDUTTA MUKHERJEE, RAJEEV GUPTA, Department of Physics, Indian Institute of Technology Kanpur, ASHISH GARG, Materials Science and Engineering, Indian Institute of Technology Kanpur — Magnetoelectric gallium ferrite (GaFeO_3 or GFO) manifests close to room temperature ferrimagnetism owing to inherent cationic site disorder in an otherwise antiferromagnetic ground state structure. In GFO, Fe ions at Fe1 and Fe2 sites are antiferromagnetically coupled while Fe and Ga at Fe2 and Ga2 sites respectively are ferromagnetically coupled. Ga1 site is magnetically inactive. Here, we present a detailed study to probe phase transitions in GFO using ac and dc magnetic characterization methods to demonstrate spin glass behavior in GFO below 200 K. Our dc magnetization measurement exhibits that while GFO undergoes standard para (PM) to ferromagnetic (fM) transition at $T_c \sim 290$ K, splitting between field cooled and zero-field cooled plots is observed at low temperatures hinting at the spin-glass like behavior. Further, temperature dependent ac susceptibility measurements at different frequencies and at different dc fields demonstrate that the system exhibits a non-equilibrium canonical spin glass (SG) state below the spin glass transition temperature ~ 210 K. The spin glass state has been further characterized by memory effect and aging measurements. The origin of such a spin-glass phase is proposed to arise from a network of geometrically frustrated spin system attributed to combination of antiferromagnetic interaction among the Fe ions in the two Fe sites and Ga2 site as well as inherent cation site disorder.

S1.00251 Spin $S = 1$ “Quantum spin liquid”: quantum criticality in $6\text{H-B-Ba}_3\text{NiSb}_2\text{O}_9$, GANG CHEN, MICHAEL HERMELE, LEO RADZIHOVSKY, CU Boulder — We present a minimal model for a recently discovered material $6\text{H-B-Ba}_3\text{NiSb}_2\text{O}_9$ which was proposed as a candidate for $S = 1$ quantum spin liquid on a triangular lattice. Our spin-1 model lies on a stacked multilayer triangular lattice. In our minimal model, we point out the competition between Heisenberg exchange interactions, which favor magnetic ordering, and the easy-plane single-ion anisotropy, which favors a uniform quantum paramagnetic state with $S^z = 0$ state at each site. We argue that the system is close to the quantum critical point separating these two phases and on the quantum paramagnetic phase side. Viewing the system as a three dimensional multilayer structure, we find that the frustrated interlayer and intralayer exchange interaction induces nodal lines of low energy spin excitations at the quantum critical point. Moreover, due to the quasi-2D nature of the system and proximity to the quantum critical point, we show there exists a broad intermediate temperature regime with linear temperature dependence of specific heat. Various other predictions and suggestions for experiments are discussed.

S1.00252 Order by disorder in kagome-type magnets¹, GIA-WEI CHERN, University of Wisconsin at Madison and Los Alamos National Lab, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems — Magnets on kagome lattice have been and continue to be the archetypical setting in which to study exotic order induced by geometrical frustration in theory and experiment. Approximate realizations of kagome magnet has been observed in compounds such as SCGO and herbertsmithite. Artificial kagome spin ice has also been created using lithographically fabricated arrays of nanoscale magnets. The frustration comes from the fact that nearest-neighbor spin interactions on a network of corner-sharing triangles cannot be satisfied simultaneously, leading to a huge degeneracy in its classical ground state, for both discrete and continuous spins. Here, we present some recent progress in simulating numerically, and analysing field-theoretically, kagome magnets with differing sets of interactions.

¹GWC acknowledges the support of ICAM and NSF Grant DMR-0844115.

S1.00253 Exact Diagonalization of the Kondo Necklace Model on a Triangular Lattice, ARA GO, Department of Physics and Astronomy and Center for Theoretical Physics, Seoul National University, GUN SANG JEON, Department of Physics, Ewha Womans University, MOO YOUNG CHOI, Department of Physics and Astronomy and Center for Theoretical Physics, Seoul National University — We consider the Kondo necklace model on a triangular lattice. The interplay of magnetic ordering and Kondo screening is investigated through the use of exact diagonalization of finite clusters with periodic boundary conditions. In the absence of Kondo screening, the system is in the magnetically ordered phase whereas the magnetic moments reduce monotonically as the screening strength is increased. It is found that the system has a unique ground state in the entire range of the parameters studied, which excludes the possibility of partially ordered degenerate ground states. We also discuss the effects of quantum fluctuations in the model, with emphasis on the lifted degeneracy of partially ordered states.

S1.00254 Tensor network simulation of phase diagram of frustrated J1-J2 Heisenberg model on a checkerboard lattice, YANGHAO CHAN, Physics Department, University of Michigan, YONGJIAN HAN, Key laboratory of quantum information, University of Science and Technology of China, LUMING DUAN, Physics Department, University of Michigan — We use the recently developed tensor network algorithm based on infinite projected entangled pair states (iPEPS) to study the phase diagram of frustrated antiferromagnetic J1-J2 Heisenberg model on a checkerboard lattice. The simulation indicates a Neel ordered phase when $J_2 < 0.88J_1$, a plaquette valence bond solid state when $0.88 < J_2/J_1 < 1.11$, and a stripe phase when $J_2 > 1.11J_1$, with two first-order transitions across the phase boundaries. The calculation shows the cross-dimer state proposed before is unlikely to be the ground state of the model, although such a state indeed arises as a metastable state in some parameter region.

S1.00255 Fabrication of organic spin-valve devices using indirect deposition, SHEN WANG, YUJUN SHI, LI LIN, BINBIN CHEN, FENJUAN YUE, DI WU, Nanjing University — The organic spin valves (OSVs) comprised of two ferromagnetic (FM) electrodes separated by an organic spacer are the principal device structures to study the spin-dependent transport. Normally, the top FM electrodes are directly deposited on top of the organic layer. The vaporized FM atoms can penetrate or diffuse into organic layer and form the so-called ill-defined layer, which is as thick as 80-100 nm. In this work we report a reliable method for fabricating high quality, reproducible OSVs. We use indirect deposition method, which relies on the scattering of the evaporated metallic atoms with inert gas to reduce kinetic energy, to deposit the Co electrode on top of the organic layer Alq₃. This method significantly suppresses the penetration of Co atoms into Alq₃ layer during deposition process, in comparison with devices fabricated by conventional direct deposition method. The improved Alq₃/Co interface is further confirmed by comparing the magnetic moment of depositing Co onto Alq₃ and Si substrates by indirect and direct deposition methods. And an OSV effect in La_{0.7}Sr_{0.3}MnO₃/Alq₃/Co devices is demonstrated at room temperature, indicating the improvement of spin injection efficiency at sharp Alq₃/Co interface.

S1.00256 Spin Transport in the XXZ Chain at Finite Temperature and Momentum¹, WOLFRAM BREINIG, Technical University Braunschweig, Germany, ROBIN STEINIGEWEG, J. Stefan Institute, Ljubljana, Slovenia — We investigate the role of momentum for the transport of magnetization in the spin-1/2 Heisenberg chain above the isotropic point at finite temperature and momentum [1]. Using numerical and analytical approaches, we analyze the autocorrelations of density and current and observe a finite region of the Brillouin zone with diffusive dynamics below a cut-off momentum, and a diffusion constant independent of momentum and time, which scales inversely with anisotropy. Lowering the temperature over a wide range, starting from infinity, the diffusion constant is found to increase strongly while the cut-off momentum for diffusion decreases. Above the cut-off momentum diffusion breaks down completely.

[1] Robin Steinigeweg and Wolfram Brenig, arXiv:1107.3103

¹Work supported in part by DFG FOR912, BR 1084/6-1, 1084/6-2, and EU MC-ITN LOTHERM PITN-GA-2009-238475.

S1.00257 Chemisorption of Co-based cyanol pyridyl valence tautomers on Au(111)¹, WANDERLA SCOPEL, YIFENG CHEN, MARCO BUONGIORNO NARDELLI, Department of Physics, North Carolina State University — Organic paramagnetic bistable molecules such as transition metal valence tautomers, where a magnetic transitions can be induced by an external perturbation, are attracting considerable attention due to their potential utilization in molecular electronic and spintronic devices. Using calculations from first principle based on density functional theory we have investigated the chemisorption of Co-based cyanol pyridyl valence tautomer (VT) molecules on the Au(111) surface via a thiol head group. Among the possible adsorption sites on the Au(111) surface, we considered both the fcc hollow site and the bridge site, which are suggested to be the two lowest energy adsorption configurations in previous investigations. We have characterized the stability and the influence of the substrate bonding on the electronic and magnetic properties of the VT molecule. Moreover, by adding a top Au contact, we have studied the electron and spin transport properties of these systems.

¹NSF Center for Chemical Innovation: Center for Molecular Spintronics (CHE-0943975)

S1.00258 Analysis on the Magnetic and Thermodynamic behavior of a Linear Magnetic Chain [Co(bpdc)(H₂O)₂].H₂O, YOUCEF HAMIDA, DUSAN DANILOVIC¹, TAN YUEN, Temple University, QIHAN GONG, JING LI, Rutgers University, DEPT. PHYSICS, TEMPLE UNIVERSITY COLLABORATION, DEPT. CHEMISTRY AND CHEMICAL BIOLOGY, RUTGERS UNIVERSITY COLLABORATION — [Co(bpdc)(H₂O)₂].H₂O (bpdc=biphenyldicarboxylate) was found to be a one dimensional ferromagnetic Co (II) chain system that orders below 5.5 K due to a weak antiferromagnetic inter-chain coupling. Classical Fisher Model (CFM), Mean Field Theory (MFT), and Ising Model (IM) were applied to the high temperature susceptibility data of [Co(bpdc)(H₂O)₂].H₂O. The fit to CFM yielded a $J/k_B = + 7.40$ K with $R^2 = 0.993$; MFT gave a $J/k_B = + 5.31$ K with a low $R^2 = 0.391$. The ratio interchain interactions (J') to that of intra-chain interactions was estimated to be $J'/J = - 0.005$. The magnetic specific heat was obtained via direct subtraction of the specific heat data for Zinc analogue from that of [Co(bpdc)(H₂O)₂].H₂O. The magnetic specific heat data was fit to the Ising Model for spin 1/2 yielding $J/k_B = + 15.27$ K. The interpretations on the spin state of the Co(II) at different temperatures in the compound are consistent with the behavior of Co(II) in other compounds with similar octahedral sites.

¹Current affiliation: Pitt Community College, Greenville, NC

S1.00259 Magnetic properties of 3d transition metal-phthalocyanine molecules on oxidized Cu(110) surface, JUN HU, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA 92697-4575 — After being extensively interesting topics in both fundamental researches and application practices for a decade, spintronics is now on its way of diversity. Molecular spintronics has attracted much attention in recent years, due to the accelerating miniaturization of electronic devices. In this work, based on first-principles calculations, we studied the electronic and magnetic properties of both isolated metal-phthalocyanines (commonly referred to as MPc) molecules (M=Mn, Fe and Co) and a single MPc molecule adsorbed on oxidized Cu(110) [O-Cu(110)] surface. We find that the easy axis of FePc molecule switches from in-plane direction to perpendicular direction when it is adsorbed on O-Cu(110) surface. However, such a switch of direction of magnetization could not be observed for MnPc and CoPc molecules which are two neighbors of FePc with one electron less and more, respectively. Furthermore, we find that the magnetization of these MPc molecules on O-Cu(110) surface are rather stable, so they could not be altered by moderate hole/electron doping. The e_g orbitals (d_{xz} and d_{yz}) of MPc molecules are found to be crucial for their magnetization on O-Cu(110) surface. **Acknowledgement.** This work was supported by DOE Grant DE-FG02-05ER46237.

S1.00260 Dependence of magnetic field and electronic transport of Mn4 Single-molecule magnet in a Single-Electron Transistor, ALVAR RODRIGUEZ, SIMRANJEET SINGH, FIROZE HAQUE, ENRIQUE DEL BARCO, University of Central Florida Department of Physics, TU NGUYEN, GEORGE CHRISTOU, University of Florida Department of Chemistry — Dependence of magnetic field and electronic transport of Mn4 Single-molecule magnet in a Single-Electron Transistor A. Rodriguez, S. Singh, F. Haque and E. del Barco Department of Physics, University of Central Florida, 4000 Central Florida Blvd., Orlando, Florida 32816 USA T. Nguyen and G. Christou Department of Chemistry, University of Florida, Gainesville, Florida 32611 USA Abstract We have performed single-electron transport measurements on a series of Mn-based low-nuclearity single-molecule magnets (SMM) observing Coulomb blockade. SMMs with well isolated and low ground spin states, i.e. $S = 9/2$ (Mn4) and $S = 6$ (Mn3) were chosen for these studies, such that the ground spin multiplet does not mix with levels of other excited spin states for the magnetic fields ($H = 0-8$ T) employed in the experiments. Different functionalization groups were employed to change the mechanical, geometrical and transport characteristics of the molecules when deposited from liquid solution on the transistors. Electromigration-broken three-terminal single-electron transistors were used. Results obtained at temperatures down to 240 mK and in the presence of high magnetic fields will be shown.

S1.00261 Magnetic characterization of a Mn6 Single-molecule Magnet, SIMRANJEET SINGH, ENRIQUE DEL BARCO, Department of Physics, University of Central Florida, Orlando, FL, MAHAMMAD ALI, Department of Chemistry, Jadavpur University, Kolkata, India — Single Molecule magnets (SMMs) are excellent candidates for the exploration of fundamental quantum effects at the nanoscale, as well as for potential applications in emerging technologies, such as quantum computation. Of particular interest are Mn6 SMMs, one of which has the highest effective energy barrier to magnetization reversal reported so far in the literature. We have performed Hall-effect magnetometry on single crystals of a new kind of Mn6 at cryogenic temperatures (>230 mK). We will discuss the dependence of the hysteresis loops on the temperature and different sweep rates of the applied magnetic field. The high saturation fields observed in this SMM will be discussed.

S1.00262 Stoner Instability in a Strongly Repulsive Fermi Gas¹, WUJIE HUANG, CHRISTIAN SANNER, EDWARD SU, AVIV KESHET, JONATHAN GILLEN, WOLFGANG KETTERLE, Center for Ultracold Atoms, Research Laboratory of Electronics, and Department of Physics, Massachusetts Institute of Technology — We study the existence of itinerant ferromagnetism using a ultracold Fermi gas with short range repulsion in a harmonic trap. A degenerate Fermi gas is rapidly quenched into the regime of strong effective repulsion near a Feshbach resonance. The spin fluctuations are monitored using speckle imaging and, contrary to several theoretical predictions, the samples remain in the paramagnetic phase for arbitrarily large scattering length. We also observe a rapid decay into bound pairs over times on the order of $10\hbar/E_F$ in a wide range of interaction strengths, which is intrinsic by the nature of Feshbach resonance and preventing the study of equilibrium phases of strongly repulsive fermions. Our work suggests that a Fermi gas with strong short-range repulsive interactions does not undergo a ferromagnetic phase transition.

¹This work was supported by NSF and ONR, AFOSR MURI, and under ARO from the DARPA Optical Lattice Emulator program.

S1.00263 Magnetism of Cobalt Dibromide Dihydrate and Monohydrate¹, G.C. DEFOTIS, A.S. HAMPTON, C.L. DESANTO, C.M. DAVIS, College of William and Mary — The magnetic properties of two hardly studied bromide compounds among the large family of 3d divalent transition metal halide hydrates are examined, with Co(II) the metal ion. Of interest is comparison between magnetic behaviors in the much more common dihydrate form and in the rarely made monohydrate form, as well as comparison between known properties of the far better studied chloride materials and those containing bromide. In the title dihydrate material a magnetic susceptibility maximum appears at 9.5 K, about half the temperature of a similar feature in the chloride dihydrate system. But in the title monohydrate material an enhanced susceptibility maximum appears at 15.5 K, virtually the same as in the similarly behaving chloride monohydrate system. As for chloride systems, a major difference between di- and monohydrates appears in that magnetic irreversibilities are far stronger in the latter. The magnetic susceptibility in both title systems is non-Curie-Weiss like at moderate to high temperatures, but can be accounted for well on the basis of a ground and an excited Kramers doublet, along with exchange interactions. The susceptibility in the vicinity of the maximum in the title dihydrate material is approximately accounted for with a three-dimensional Ising model.

¹Supported by the Petroleum Research Fund of the American Chemical Society

S1.00264 Crystal structure and ferromagnetic phase transitions in $\text{CeCu}_{1-x}\text{Ge}_{1+x}$ ($0.0 \leq x \leq 0.3$)¹, W.H. LEE, S.Y. SHIH, H.H. SUNG, K.J. SYU, S.C. CHEN, National Chung Cheng University, W.H. LEE TEAM — As revealed in the powder x-ray diffraction and crystallographic data, the single phase sample in the series $\text{CeCu}_{1-x}\text{Ge}_{1+x}$ ($0.0 \leq x \leq 0.3$) crystallizes in the AlB_2 -type structure with space group $P6_3/\text{mmc}$. The maximum ferromagnetic transition temperature T_c in $\text{CeCu}_{1-x}\text{Ge}_{1+x}$, as determined from the electrical- resistivity and magnetic susceptibility measurements, is 10.6 K for the compound $\text{CeCu}_{0.8}\text{Ge}_{1.2}$. The magnetic susceptibility for each sample in $\text{CeCu}_{1-x}\text{Ge}_{1+x}$ ($0.0 \leq x \leq 0.3$) follows Curie's behavior between 100 and 300 K with an effective moment $2.6 \pm 0.1 \mu_B/\text{Ce atom}$, a value close to that of Ce^{3+} . However, the observed saturation magnetic moment values ($0.96 \sim 1.15 \mu_B$) at low temperatures for all these compounds are well less than the theoretically expected value $2.14 \mu_B$ for the free Ce^{3+} ion tangling the entire six-fold $J = 5/2$ multiplet. Subtracting the estimated phonon contribution from LaCuGe , the entropy associated with the magnetic structure of CeCuGe is found to meet the theoretical value of $R \ln 2$, which would be expected for a doublet ground state of Ce^{3+} ion in the compound CeCuGe . The reduced saturation moment in $\text{CeCu}_{1-x}\text{Ge}_{1+x}$ is reasonably ascribed to partial lifting of the 4f-electron level degeneracy.

¹Supported by the National Science Council of Republic of China under Contract Numbers NSC 99-2112-M-194-006-MY3 and NSC 100-2811-M-194-015.

S1.00265 Deuterated Mn and Ni Dibromide Dihydrate and Contrast with Normal Water Systems¹, K.T. TROWELL, K.C. HAVAS, M.J. VAN DONGEN, C.H. KOMATSU, D.G. CHAN, Z.D. REED, G.C. DEFOTIS, College of William and Mary — First row transition metal hydrated bromide compounds are much less studied magnetically than chlorides, and for each of the common hydration states 2, 4 or 6 waters. Examination of rarer monohydrate chlorides was initiated only more recently. Quite intriguing similarities and differences in the magnetism, with respect to that of the most closely related dihydrates especially, occur. It is of interest to extend measurements to bromide systems, especially mono- and dihydrate forms. And given the role, structural and magnetic, that hydrogen bonding can play, deuteration effects are also worth exploring (and little studied in general). Magnetic measurements on the new deuterated title systems are presented. For the deuterated Mn compound the susceptibility is of similar general appearance to that of the normal water system, but with a maximum at 2.1 K, only one-third the 6.3 K of the latter; the maximum is much larger in the deuterated system. For the deuterated Ni compound a maximum appears about 10% lower than the 6.0 K location in the normal water system, and is of moderately larger size; it is however substantially broader. Comparisons with deuterated vs normal water behaviors in related materials, where differences are often far less striking, will be made.

¹Supported by a grant from the Solid State Chemistry Program of the DMR-NSF

S1.00266 Magnetic Domain Dynamics Study in Dysprosium, SAN-WEN CHEN, HONGYU GUO, XIANGSHUN LU, University of California San Diego, SUJOY ROY, KEOKI SEU, Lawrence Berkeley National Laboratory, KARINE DUMESNIL, University H. Poincare, France, SUNIL SINHA, University of California San Diego, UNIVERSITY OF CALIFORNIA SAN DIEGO TEAM, LAWRENCE BERKELEY NATIONAL LABORATORY COLLABORATION, UNIVERSITY H. POINCARÉ, FRANCE COLLABORATION — We have studied magnetic domain fluctuations in a Yttrium-Dysprosium-Yttrium tri-layer with X-ray photon correlation spectroscopy (XPCS) in conjunction with resonant soft x-ray magnetic scattering. Dysprosium possesses a helical antiferromagnetic ordering below its Néel temperature ($T_N = 180\text{K}$) and above its Curie temperature ($T_C \sim 85\text{K}$). With resonant x-ray scattering, we observed the magnetic satellite peak at $(0,0,q_m)$ due to the helical magnetic structure. We determined the transition temperature and found a shift in T_C from the bulk value and hysteresis behavior around T_C . The transverse correlation length showed a minimum at both T_C and T_N . With the coherent x-rays, we observed magnetic speckles from both static disorder and magnetic domains. The XPCS studies as a function of temperature showed that the magnetic domains are static up to 2000 seconds time scale when $T < 175\text{K}$. Close to T_N , there appears to be slow dynamics which might be due to domain wall fluctuation.

S1.00267 Giant Electromechanical Response in Graphene Nanoribbons, NABIL AL-AQTASH, RENAT SABIRIANOV, University of Nebraska at Omaha, HONG LI, Peking University, Beijing, P.R. China, LU WANG, WAI-NING MEI, University of Nebraska at Omaha, JING LU, Peking University, Beijing, P.R. China — The demonstration of spin injection into graphene has proposed that graphene could play a role in spintronic devices. Specifically, it has been found that zigzag graphene nanoribbons (ZGNR) have spin states at their edges. In this study, first principles quantum mechanical calculations have been performed to investigate the effect of twist on the electronic, magnetic and transport properties of ZGNR. We investigate the electronic and magnetic structures of nanoribbon of ZGNR in the flat geometry and with 180° twisting. Using density functional theory coupled with nonequilibrium Green's function method implemented in SIESTA code, we examine the local magnetic moments and the quantum conductance of twisted ZGNR in its ground state (antiferromagnetic) and in case of ferromagnetic spin orientations. Our calculations show that ZGNR in its ground state is insensitive to twisted deformation, since the conductance of the twisted ZGNR is almost unchanged, as well as, no band gap change. However, we observe electromechanical switch via twisting a ferromagnetic ZGNR in hypothetical ferromagnetic nanoribbons. The transmission in a hypothetical ferromagnetic state for 4-ZGNR is 2 quantum of conductance, while the transmission becomes zero in case of oppositely polarized leads (after twisting), i.e. we observe an ideal spin valve. We relaxed both the atomic positions and the spin directions in our calculations allowing for a Bloch/Neel-like domain wall in the latter case.

S1.00268 Simulations of random defects for fast domain wall motion in ferromagnetic nanowires¹, KYLE KIMMINAU, ANDREW KUNZ, Marquette University, PHYSICS DEPARTMENT TEAM — Domain walls in ferromagnetic nanowires move slowly when driven by large magnetic fields due to a process known as Walker breakdown. During Walker breakdown vortices are formed which slow the domain wall leading to low average speeds. Vortex formation is driven by the precessional motion of the magnetic moments in the domain wall. Techniques which disturb the coherent precession can be used to disrupt Walker breakdown and therefore recover fast domain wall speeds which could be useful for future technological devices. We used a combination of micromagnetic simulation and theoretical modeling to simulate the effects of random defects (voids) on the motion of a domain wall. Simulations find there is critical defect density associated with the destruction of the breakdown. We then use a magnetostatic charge model to calculate the strength of the perturbing field, created by the defects, necessary to disrupt the precessional motion of the moment in the domain wall. For an appropriate defect density the domain walls move quickly, without experiencing breakdown or a change in magnetic structure, for applied fields at least an order of magnitude greater than the typical breakdown field.

¹NSF DMR 1006947, NASA Wisconsin Space Grant Consortium

S1.00269 Anisotropic Magnetoresistance Effects in Fe, Co, Ni, Fe₄N, and Half-Metallic Ferromagnet: A Systematic Analysis, SATOSHI KOKADO, Faculty of Engineering, Shizuoka University, Japan, MASAKIYO TSUNODA, Graduate School of Engineering, Tohoku University, Japan, KIKUO HARIGAYA, Nanosystem Research Institute, AIST, Japan, AKIMASA SAKUMA, Graduate School of Engineering, Tohoku University, Japan — We theoretically analyze the anisotropic magnetoresistance (AMR) effects of bcc Fe (+), fcc Co (+), fcc Ni (+), Fe₄N (−), and a half-metallic ferromagnet (−) [1]. The sign in each () represents the sign of the AMR ratio observed experimentally. We here use the two-current model for a system consisting of a spin-polarized conduction state and localized d states with spin-orbit interaction. From the model, we first derive a general expression of the AMR ratio. The expression consists of a resistivity of the conduction state of the σ spin ($\sigma = \uparrow$ or $\downarrow$), $\rho_{s\sigma}$, and resistivities due to s-d scattering processes from the conduction state to the localized d states. On the basis of this expression, we next find a relation between the sign of the AMR ratio and the s-d scattering process. In addition, we obtain expressions of the AMR ratios appropriate to the respective materials. Using the expressions, we evaluate their AMR ratios, where the expressions take into account the theoretical values of $\rho_{s\downarrow}/\rho_{s\uparrow}$ of the respective materials. The evaluated AMR ratios correspond well to the experimental results.

[1] S. Kokado *et al.*, submitted to J. Phys. Soc. Jpn.

S1.00270 Molecular Dynamics Simulation of a Two Dimensional Heisenberg Fluid¹, B.V. COSTA, Universidade Federal de Minas Gerais, A.B. LIMA, E. CORREA, Universidade Federal do Triângulo Mineiro — In this work we use numerical Monte Carlo and Molecular Dynamics to study a classical two-dimensional compressible magnetic fluid. The magnetic interactions are realized through a Yukawa-like potential while particles interact through Lennard-Jones forces. Our preliminary results point to a very rich phase transition picture. At high density the system seems to undergo a magnetic transition, as suggested by the magnetization and susceptibility results.

¹Work was partially supported by CNPq and FAPEMIG.

S1.00271 ABSTRACT WITHDRAWN —

S1.00272 Ultrafast spin precession dynamics in exchange-biased FeNi/FeMn/FeNi films, JOO IN LEE, CHAN YONG HWANG, Korea Research Institute of Standards and Science — We investigated the spin precession dynamics in exchange-biased FeNi/FeMn/FeNi films by means of time-resolved magneto-optical Kerr effect (TR-MOKE). We observed the spin precession of all FeNi/FeMn/FeNi films in the TR-MOKE signals. The precession oscillations of the films changed rapidly as varying a thickness of antiferromagnet (FeMn). The period of the precession oscillations was not single and in the range of 10 to 20 ps. It is supposed that this is not only related to the exchange bias between ferromagnet and antiferromagnet but also double exchange biases in FeNi/FeMn/FeNi films.

S1.00273 Tilted polarizer devices with a generic spin torque efficiency coefficient¹, YA. B. BAZALIY, University of South Carolina, K.E. NEMCHENKO, Kharkiv University, Ukraine — Using the effective planar description [1-3] we study spin transfer devices with tilted polarizer. The dynamics of the free layer are investigated in the case of spin torque with substantially non-constant efficiency factor g . The switching diagram is constructed and discussed in qualitative terms.

[1] Ya. B. Bazaliy, Appl. Phys. Lett. **91**, 262510 (2007).

[2] Ya. B. Bazaliy, Phys. Rev. B **76**, 140402(R) (2007).

[3] Ya. B. Bazaliy, arXiv:1109.1331 (2011).

¹Supported by the NSF grant DMR-0847159.

S1.00274 Exchange coupled graded/soft/graded film with well-isolated grains fabricated by post-annealing, FANG WANG, University at Buffalo, Shanxi Normal University, JING ZHANG, JUN ZHANG, CHUNLING WANG, XIAOHONG XU, Shanxi Normal University — In order to solve the trilemma issue in perpendicular recording media, exchange spring and exchange coupled composite media have been proposed to reduce the coercivity of the hard magnetic layer without sacrificing the thermal stability. Thereafter, Suess proposed the graded media with a continuous variation in anisotropy to reduce the coercivity even further. Here we present an anisotropy-graded [FePt/C]5/Fe/[C/FePt]5 film, where C layer thickness gradually and symmetrically increases from two FePt ends to the soft Fe layer. In contrast with FePt/Fe bilayer, the graded/soft/graded film has a large reduction of 74% in coercivity. Adding C layers with different thickness not only tailors the Ku gradient, but also refines the grain size and weakens the intergranular exchange interaction. Micromagnetic simulation reveals that the magnetization reversal is initiated by domain wall formation at the center of the soft Fe layer followed by domain wall propagation in two FePt layers simultaneously. This work was supported by the National Science Foundation for Distinguished Young Scholars (Grant No. 51025101), NSFC (Grant No. 60776008, 51101095).

S1.00275 Anomalous magnetic anisotropy in Mn₃O₄ investigated by ⁵⁵Mn²⁺ and ⁵⁵Mn³⁺ Nuclear magnetic resonance, CHANGSOO KIM, JEONG HYUN SHIM¹, EUNA JO, SOONCHIL LEE, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea — Mn₃O₄ has Yafet-Kittel type spin structure below Neel Temperature (41K). The magnetization along the c-axis is smaller than that along the ab-plane even in external magnetic field of 30 Tesla, implying huge magnetic anisotropy in the ab-plane. We measured ⁵⁵Mn²⁺ and ⁵⁵Mn³⁺ Nuclear Magnetic Resonance (NMR) of a Mn₃O₄ single crystal in external magnetic field. The canting angles of Mn²⁺ and Mn³⁺ magnetic moments were calculated from the spectral shift obtained for various magnetic field directions between the a, b and c-axes. With the canting angle data, we estimated the anisotropy energies of the Mn²⁺ and Mn³⁺ magnetic moments and the exchange energy between them. The result also shows that Mn³⁺ spins in the Yafet-Kittel structure lie in the ab-plane contrary to the previous reports.

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S1.00276 Magnetic property enhancement of modified nanocrystalline ZrCo₅-based magnets¹, WENYONG ZHANG, XINGZHONG LI, RALPH SKOMSKI, JEFF SHIELD, DAVID J SELLMYER, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE68588, NANOMAGNETICS AND MAGNETOELECTRONIC MATERIALS TEAM — The metastable ZrCo₅ compound may be a good candidate for the development of rare-earth-free high-performance hard magnetic materials because of its high magnetocrystalline anisotropy field. Melt spinning is a good approach to synthesize metastable phase because of its high quench rate. In this work, the effect of Zr and Fe addition on structure and magnetic properties of melt-spun nanocrystalline Zr_{1+x}Co₅(0–0.3) alloys has been investigated. All the samples consist of orthorhombic ZrCo₅ hard magnetic and Co/Zr₆Co₂₃ soft magnetic phases. Proper Zr addition causes nanostructure refinement and the increase of the hard magnetic phase content, which strengthens intergrain exchange coupling. As a result, coercivity and maximum energy product of ZrCo₅-based magnet are significantly enhanced. The best magnetic properties: $iH_c = 2.8$ kOe, $(BH)_{max} = 4$ MGOe, which is the best value among Co-Zr binary alloys, are achieved in Zr_{1.1}Co₅. The temperature coefficient of its coercivity between 10 and 380K is -0.05%/K. The saturation magnetization of nanocrystalline Zr_{1.1}Co₅ is greatly increased due to 16 at% Fe addition.

¹Research supported by BREM/DOE/Ames Lab and ARO.

S1.00277 Competing magnetic interactions and interfacial frozen spin in Ni-NiO core-shell nano-rods¹, YUAN-CHIEH TSENG, HAO-CHUN HSU, CHIH-CHIEH LO, National Chiao Tung University, NATIONAL CHIAO TUNG UNIVERSITY TEAM — This work investigates the complex interfacial magnetism of free-standing Ni-NiO core-shell rods fabricated by electrodeless plating and an anodic aluminum oxide template. Vertical magnetization shift, arising from opposite field cooling conditions, suggests frozen spin (FS) at the Ni-NiO interface. The FS was related to the pinning effects of the NiO on the Ni, which mediated the interfacial antiferromagnetic (AFM)-ferromagnetic (FM) coupling, leading to the temperature-dependent properties of the rods. The FS was evident below 100 K, at which point the NiO-AFM dominated the properties with a suppressed coercive field and non-saturated magnetization. Above 100 K, however, the Ni-FM dominated and the FM phase was restored, due to the disappearance of the FS.

¹The work is supported by the National Science Council of Taiwan under Grant No. NSC 98-2112-M-009 022-MY3.

S1.00278 Magnetic Properties of Nanostructured Mn_xTaS₂, PAUL SHAND, ZACH GRIFFITH, STROH LESLIE, TIM KIDD, LAURA STRAUSS, University of Northern Iowa — We have fabricated tapelike nanostructures of Mn_xTaS₂ that consist of bundles of TaS₂ nanotubes intercalated with Mn. The magnetic properties of samples with Mn concentrations of 15% and 23% (nominal 25%) were investigated. The Mn_{0.23}TaS₂ sample exhibited ferromagnetic characteristics with a Curie temperature near 90 K, which is close to that of bulk Mn_{0.25}TaS₂ crystals; however, the behavior of the linear and nonlinear ac susceptibility in the vicinity of the transition indicates departures from standard 3D ferromagnetic behavior. The Mn_{0.15}TaS₂ sample exhibits a spin-glass-like transition near 8 K, with a frequency-dependent ac susceptibility near the transition and hysteretic and aging effects below the transition. The imaginary part of the ac susceptibility becomes non-zero at temperatures significantly higher than the transition temperature, which is unusual for spin glasses. Overall, our measurements indicate strong similarities between our nanostructured samples and their bulk crystalline counterparts but some intriguing differences as well. It is not yet clear whether these differences can be attributed to the quasi-one-dimensional nature of the nanostructured Mn_xTaS₂ samples.

S1.00279 The contactless measurement of forces which affect a magnetic particle in a fluid and its manipulation, SUSUMU TOKURA, MASAKAZU HARA, NORIHITO KAWAGUCHI, JUN IZAWA, Research Laboratory, IHI Corporation, NAOYUKI AMEMIYA, Department of Electrical Engineering, Kyoto University — The magnetic force has been used for the drug delivery, the cell/DNA manipulation, and other handlings of micro or nanoparticles. When magnetic particles are suspended in a fluid, they are influenced by the magnetic force caused by the magnetic field gradient, the gravity force, and the buoyance force. The magnetic torque also affects them to align their magnetic moments to the direction of the applied magnetic field. Furthermore, the viscous force or the force between the magnetized magnetic particles themselves cannot be neglected. In this study, methods of the quantitative measurement of these forces and the manipulation of a magnetic particle were developed. Four electromagnets were used to apply magnetic fields to ferrite particles (300nm-300 μ m) in a fluid in a vessel. The particle tracking velocimetry method was used to visualize the behavior of the particles. Based on the theory of the magnetic suspension and balance system, the vertical and horizontal forces affected a magnetic particle were estimated from the current in the coil of each electromagnet without any physical contact to it. And, the contactless manipulations of the magnetic particle suspended in the stagnated or flowing fluid by controlling the coil currents were demonstrated successfully.

S1.00280 Determination of second order phase transition temperature of monoclinic phase of $Gd_5(Si_xGe_{1-x})_4$, DAVID JILES, RAVI HADIMANI, Iowa State University, Y. MELIKHOV, Cardiff University, MAGNETIC RESEARCH GROUP TEAM, WOLFSON CENTRE FOR MAGNETICS TEAM — $Gd_5(Si_xGe_{1-x})_4$ has a first order phase transition from high temperature paramagnetic monoclinic to low temperature ferromagnetic orthorhombic phase for $0.4 < x < 0.51$. It is not possible to determine experimentally the second order phase transition temperature of orthorhombic or monoclinic phase. Previous studies have estimated second order phase transition temperature of the orthorhombic phase using a modified Arrott plot technique. The composition $0.3 < x < 0.4$ $Gd_5(Si_xGe_{1-x})_4$ has mixed monoclinic and orthorhombic phases without a clear transition between the two phases. We have determined the second order phase transition temperatures of both orthorhombic and monoclinic phases for $Gd_5Si_{1.5}Ge_{2.5}$ using modified Arrott plots. Magnetic moment vs. magnetic field for various temperatures was measured using a SQUID magnetometer. Arrott plots were plotted from $M^{1/\beta}$ and $(H/M)^{1/\gamma}$ isotherms using critical exponents of $1/\gamma = 0.85$ and $1/\beta = 1.85$. We obtained two sets of parallel lines for the orthorhombic phase and the monoclinic phase. The temperature of the isotherm that passes through the origin for both orthorhombic and monoclinic phase was estimated to be 299.5 K and 197 K respectively.

S1.00281 Boron diffusion due to annealing in CoFeB/MgO/CoFeB interfaces: A combined HAXPES and NEXAFS study, ABDUL RUMAIZ, NSLS, Brookhaven National Laboratory, CHERNO JAYE, JOSEPH WOICIK, NIST, WEIGANG WANG, Department of Physics, Johns Hopkins University, DANIEL FISCHER, NIST, C.L. CHIEN, Department of Physics, Johns Hopkins University — We report the hard x-ray photo-electron spectroscopy (HAXPES) and near edge x-ray absorption fine structure (NEXAFS) of CoFeB|MgO|CoFeB tunnel junctions as a function of annealing time. Upon annealing, the oxidation state of B changes from predominantly elemental (0 valence) boron in the as deposited sample to higher oxidation in annealed samples as evident from HAXPES spectra. The NEXAFS spectroscopy results showed that upon heating, B species migrate towards the MgO and interact with it. A comparison of the tunnel junction NEXAFS signature with some standards suggests that the B forms a 3-fold coordinated boron compound in the MgO environment and 4-fold coordinated boron resembling Kotoite mineral in the CoFe/MgO interface.

S1.00282 Mössbauer study of corrosion and abrasion products in oil transporting pipes, RAUL W. GOMEZ, JOSE LUIS PEREZ MAZARIEGO, VIVIANNE MARQUINA, MA. LUISA MARQUINA, ROSALIA RIDAURA, Facultad de Ciencias, UNAM, Mexico D.F. 04510, LORENZO MARTINEZ, ICF, UNAM, Cuernavaca, Mor. — It is known that one of the main technological problems in carbon steel oleoducts is the corrosion produced by different substances, such as water, carbon dioxide, sulfur, and microorganisms. In addition, if in such mixture there is sand, aggressive sludge can be form that abrasions material from the oleoduct. A room temperature Mössbauer study of corroded material taken from different sites of oleoducts is presented. Most of the Mössbauer spectra reveal the presence of nanoparticles, indicating that in these pipes the abrasion problem is severe. A preliminary identification of the oxidized samples suggests the presence of magnetite, and some Iron hydroxides. Further studies are in course in order to identify unambiguously the products present in the corroded materials.

S1.00283 STRONGLY CORRELATED SYSTEMS, INCLUDING QUANTUM FLUIDS AND SOLIDS —

S1.00284 Performance of hybrid density functional theory for α versus δ -Pu¹, SARAH C. HERNANDEZ, ASOK K. RAY, University of Texas at Arlington — Hybrid density functional theory, which replaces a fraction of density functional theory exchange with exact Hartree-Fock exchange, has been used to study the electronic, geometric, and magnetic properties of α -Pu and compared with our previous results for δ -Pu. A non-magnetic (NM) ground state was realized for $\alpha=0.55$ (α indicating the fraction of the HF exchange) for δ -Pu but the equilibrium atomic volume deviated from experiment by 19%, the 5f electron population was close to 4 and a 5f DOS that shows anomalous localization and failed to match experimentally obtained PES data.² For α -Pu, a NM ground state was obtained at 40% HF exchange. Comparing the two phases at the NM ground state, the 5f population is about the same, but energy differences between the different magnetic configurations for the two phases are observed. For δ -Pu NM-FM and NM-AFM ΔE are 86.33 and 82.28 mRy/atom, respectively, and for α -Pu the NM-FM and NM-AFM ΔE are 144.98 and 60.72 mRy/atom, respectively. The 5f DOS for δ -Pu show no DOS at the Fermi level but the presence of localized states, while for α -Pu DOS show delocalization. Though hybrid density functional theory might not perform better compared to DFT for δ -Pu, it shows promise for α -Pu.

¹This work is partially supported by the Welch Foundation (Grant No. Y-1525) and by the LSAMP-BD Program.

²R. Atta-Fynn and A. K. Ray, Europhys. Lett. 85, 27008 (2009)

S1.00285 Mott behavior of ultrathin epitaxial LaNiO₃ films and interfaces via hard x-ray and standing-wave excited photoemission, ALEXANDER GRAY, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, ALEXANDER KAISER, Department of Physics, University of California, Davis, JUNWOO SON, ANDERSON JANOTTI, Materials Department, University of California, Santa Barbara, SEE-HUN YANG, IBM Almaden Research Center, AARON BOSTWICK, Advanced Light Source, LBNL, SHIGENORI UEDA, KEISUKE KOBAYASHI, NIMS Beamline Station at SPring-8, CHRIS VAN DE WALLE, SUSANNE STEMMER, Materials Department, University of California, Santa Barbara, CHARLES FADLEY, Department of Physics, University of California, Davis — In this study we apply several emerging x-ray photoemission techniques to study Mott behavior of ultrathin LaNiO₃ films and interfaces in a depth-resolved manner. In order to understand the effects of thickness and strain on the electronic structure, we apply hard x-ray photoemission (HAXPES) at 6 keV to epitaxial LaNiO₃ films of varying thickness under compressive and tensile strain. Mott metal-to-insulator transition is observed for the thinnest films. Furthermore, standing-wave-excited photoemission is used to study the electronic structure of ultrathin LaNiO₃ in a SrTiO₃/LaNiO₃ superlattice. Standing-wave measurements of core-level and valence band spectra are used to derive layer-resolved densities of states, revealing a suppression of electronic states near the Fermi level in the multilayer as compared to bulk LaNiO₃. Further analysis shows that the suppression of these states is not homogeneously distributed over the LaNiO₃ layers but is more pronounced near the interfaces.

S1.00286 Depth-resolved ARPES of buried layers and interfaces via soft x-ray standing-wave excited photoemission, ALEXANDER GRAY, Stanford Institute for Materials and Energy Sciences, SLAC Linear Accelerator Laboratory, JAN MINAR, Physical Chemistry Institute, Ludwig Maximilian University, LUKASZ PLUCINSKI, Research Center Jülich, MARK HUIJBEN, University of Twente, AARON BOSTWICK, ELI ROTENBERG, Advanced Light Source, LBNL, SEE-HUN YANG, IBM Almaden Research Center, CLAUS SCHNEIDER, Research Center Jülich, HUBERT EBERT, Physical Chemistry Institute, Ludwig Maximilian University, CHARLES FADLEY, Department of Physics, University of California Davis — We introduce a new depth-selective photoemission technique, achieved by combining soft x-ray ARPES with standing-wave (SW) excited photoelectron spectroscopy, wherein the intensity profile of the exciting x-ray radiation is tailored within the sample. This effect is accomplished by setting-up an x-ray standing-wave field within the sample by growing it on a synthetic periodic multilayer mirror substrate, which in first-order Bragg reflection acts as the standing-wave generator. The antinodes of the standing wave function as epicenters for photoemission and can be moved vertically through the buried layers and interfaces by scanning the x-ray incidence angle. The new SW-ARPES technique is then applied to the investigation of the electronic properties of the buried interface within a magnetic tunnel junction $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{SrTiO}_3$. The experimental results are compared to the state-of-art one-step photoemission theory including matrix element effects.

S1.00287 Dependence of Polarization and Dielectric response on Epitaxial Strain in $(\text{Ba}_x\text{Sr}_{1-x})\text{TiO}_3$ Ultrathin Films from First-Principles, SAAD BIN-OMRAN, King Saud University — A first-principles-derived schemes is used to use a first-principles-derived technique to construct the temperature-versus-misfit strain phase diagrams for the whole BST composition rang (i.e., $x=0.00, 0.20, 0.40, 0.60, 0.80, 1.00$). Moreover, we investigate the dependence of their dielectric and ferroelectric properties on the strain and the concentration. Our results reveal that the predicated phase diagrams show a topology similar to those calculated by Shirokov et. al. *Phy. Rev. B.* **79** 144118 (2009) with quantitative discrepancies that will be revealed and explained. Our results also indicate that in-plane strain increases (respectively, decreases) the in-plane (respectively, out-of-plane) dielectric constants. Furthermore, the out-of-plane component of dielectric permittivity ϵ_{33} enhances with lowering x in $(\text{Ba}_x\text{Sr}_{1-x})\text{TiO}_3$ films. We hope that our results will be benefits to many scientists and will lead to new strategies for material design.

S1.00288 A first principles thermodynamic study of Si-HfO₂ and Pt-HfO₂ interfaces, HONG ZHU, RAMPI RAMPRASAD, University of Connecticut — Atomic-level control of dielectric-semiconductor and dielectric-metal interfaces has become critical in determining the properties of the emerging high- k oxide-based MOSFETs. Using Si-HfO₂ and Pt-HfO₂ as an example, we investigate the evolution of these interface structures and electronic properties as a function of processing conditions by combining density functional theory results and statistical thermodynamics. Firstly, using first principles thermodynamics (FPTs), we determine the phase diagrams of Si-HfO₂ and Pt-HfO₂ interfaces. The vibrational and configurational entropic contributions to the free energies of the condensed phases are explicitly included. We demonstrate that the predictions of the FPT approach are in quantitative agreement with experiments for the interfaces considered. Secondly, a parameter-free methodology to determine the work function shift (or effective work function, EWF) of metal when interfaced with oxide is developed. This strategy is combined with statistical thermodynamics to predict the most probable EWF at given processing condition. The favorable agreement between the computed and experimental EWFs under generally adopted conditions is indicative of the usefulness of such full first-principles property-processing relationship studies.

S1.00289 Spiral spin order induced ferroelectricity in various type-II multiferroics, JUNMING LIU, YUAN LIU, Nanjing University, Department of Physics — In the past decade, one of the milestones associated with multiferroicity researches has been the experimental and theoretical identification of spin orders induced ferroelectricity in various spin frustrated oxide materials. These specific orders include the noncollinear spiral spin order, collinear spin order of exchange striction, E -type antiferromagnetic (AFM) order of double-exchange nature, and so on. Both the cross-product type and dot-product type spin interactions may contribute to the ferroelectricity generation. In consequence, experimentally observable multiferroic phenomena can be complex and reflected in multifold dimensions. In this talk, we address the spiral spin order induced ferroelectricity in various multiferroics where the cross-product type spin interaction is believed to contribute to the ferroelectricity. A modulation of such spiral spin order by various approaches is investigated and in particular the complex spin interactions in RMnO_3 with magnetic and non-magnetic doping at the R-site and Mn site will be discussed. Hopefully this talk may allow additional facts to our comprehensive understanding of the multifold interactions which eventually have impact on the magnitude of ferroelectric polarization in those multiferroics.

S1.00290 Ultrafast Photoinduced Magnetic Phase Transition in Manganites, TIANQI LI, AARON PATZ, Ames Laboratory and Dept of Physics and Astro, Iowa State University, JIAQIANG YAN, THOMAS LOGRASSO, Department of Physics and Astronomy, Iowa State University, ILIAS PERAKIS, Department of Physics, University of Crete, Greece, JIGANG WANG, Ames Laboratory and Dept of Physics and Astro, Iowa State University — The process of manipulating collective spin ordering and inducing magnetic phase transitions in highly *non-equilibrium, non-thermal* states at *femtosecond* time scales has received much current interest. These ultrafast processes offer opportunities for significant improvement over modern magneto-optical recording and magnetic storage/logic devices. One prominent system for such femtosecond magnetism is the strongly correlated manganites, which are truly responsive near the phase boundary, exhibiting extreme sensitivity to external stimuli such as light, electric and magnetic fields. Here, using ultrafast two-color magnetic circular dichroism spectroscopy, we observed distinct fs spin dynamics and critical behaviors in the strongly correlated manganites. We will discuss the origin of the responses as well as present a thorough study on differently doped and thin film samples.

S1.00291 δ -doped SrTiO_3 heterostructure in high magnetic fields, SCOTT RIGGS, MINU KIM, Stanford University, CHRIS BELL, Stanford University, IAN FISHER, Stanford University, ROSS MACDONALD, National High Magnetic Field Lab, HAROLD HWANG, Stanford University — High mobility 0.1% δ -doped STO magneto-transport has been measured in high magnetic fields as a function of angle. The Nb:SrTiO₃ doping layer is 25 nm thick and sandwiched between insulating SrTiO₃ buffer and cap layers on an SrTiO₃ substrate, putting it well within the 2-dimensional limit. The system exhibits Shubnikov-de Haas oscillations over the entire angle range measured. The resulting interplay between multiple sub-bands as the system approaches the quantum limit will be discussed.

S1.00292 Magnetic order and structural phase transition in strained ultrathin $\text{SrRuO}_3/\text{SrTiO}_3$ superlattice¹, MINGQIANG GU, XIAOSHAN WU, Nanjing University, GUOPING ZHANG, Indiana State University — Strain is one of the key parameters to control the properties of functional materials in fabrication. With first-principles simulations, we find for the first time that $\text{SrRuO}_3/\text{SrTiO}_3$ superlattice undergoes robust phase transitions with the in-plane lattice strain ranging from -4.5% to 6%. In the high tensile strain region, the magnetic ordering among neighboring Ru ions changes from a ferromagnetic to an antiferromagnetic phase, together with a metal-to-Mott-insulator transition, a unique character in our superlattice which is absent in the bulk. On the other hand, in the low strain region, the suppression of the octahedra tilting was also observed. The driving force of the suppression of tilting was investigated and found to be the charge redistribution in the Sr-O plane. All of these are important to the strategy of controlling the structural, electronic and magnetic properties in Ru-based perovskite systems.

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S1.00293 Unexpected high conductivity at emerging twin boundaries in LSMO thin films, BENJAMIN MARTINEZ, LUIS GARZON, LUIS PENA, REGINA GÁLGERAN, ZORICA KONSTANTINOVIC, ALBERTO POMAR, BERNAT BOZZO, FELIP SANDIUMENGE, LUIS BALCELLS, CARMEN OCAL, ICMAB-CSIC. Campus de Bellaterra, Bellaterra 08193. SPAIN, NANOSTRUCTURED MAGNETIC MATERIALS COLLABORATION, SCANNING FORCE MICROSCOPY COLLABORATION — Transport properties of high quality $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ (LSMO) thin films are studied by using Conducting Scanning Force Microscopy (C-SFM) measurements. Current images were acquired in a non-invasive manner by using the contact operation mode at the lowest possible applied load needed. LSMO thin film surface consists of one unit cell steps separating atomically flat terraces, with a low surface roughness on the terraces reproducing the STO substrate morphology. The existence of twin boundaries within the film is evidenced by conducting scanning force microscopy data. I(V) characteristics curves obtained at specific surface points indicate an important enhancement of the electronic response at the twin boundaries locations as compared to that measured on the twin surface. The absolute values of the measured current for a given voltage may differ by up to nearly one order of magnitude depending on whether the tip contacts the location where the twin boundary emerges at the surface or it is placed on a region on top of one of the twin crystallites. The origin of this large difference is not clear yet, but preliminary analysis seems to indicate that an increase in the density of states (DOS) at the boundaries might have an important contribution.

S1.00294 The role of correlations on oxygen orbitals in late transition-metal oxides, BAYO LAU, HUNG T. DANG, EMANUEL GULL, ANDREW J. MILLIS, Department of Physics, Columbia University, NY, NY — We investigate the effect on transition-metal oxide physics of including interactions on the oxygen sites as well as on the transition-metal site using a generalization of the single-site Dynamical Mean Field method. On-site repulsive and Hund's interactions in the full Slater-Kanamori form are treated using a numerically exact continuous-time quantum Monte-Carlo solver. We determine the metal-insulator and magnetic phase diagrams as a function of charge-transfer tendency and interaction strengths. The results are compared directly to models with no oxygen correlations, yielding insights about the role of oxygen-specific correlations.

S1.00295 Dynamical mean-field embedding of the dual fermion dynamical cluster approach for strongly correlated systems, ZI YANG MENG, SANDEEP PATHAK, SHUXIANG YANG, HANNA TERLETSKA, JUANA MORENO, MARK JARRELL, Louisiana State University — We extend the recently developed dual fermion dynamical cluster approach with a further embedding of the dual fermion lattice into a larger, third length scale. The resulting approach is a complete multi-scale many-body technique for strongly correlated electron systems. It treats the short length scales explicitly by the dynamical cluster approach, intermediate length scales diagrammatically with the dual fermion technique, and the largest length scales approximately at a dynamical mean-field level. This technique iterated to self-consistency on all the three length scales. To illustrate the implementation and applicability of this method, we test it with the one and two dimensional Falicov-Kimball model. We will specifically address the convergence and critical scaling behavior of the charge-density-wave transition temperature.

S1.00296 Single domain VO_2 single crystals exhibiting metal-insulator transition and insulator-insulator transition, JOONSEOK YOON, Physics Dept., Yonsei Univ., BONGJIN MUN, Applied Physics Dept., Hanyang Univ., KAI CHEN, Advanced Light Source, LBNL & CAMP-Nano, Xi'an Jiaotong Univ., CATHERINE DEJOIE, NOBUMICHI TAMURA, MARTIN KUNZ, ZHI LIU, SUNG-KWAN MO, Advanced Light Source, LBNL, KYUNGSUN MOON, Physics Dept., Yonsei Univ., CHANGWOO PARK, Hanbat National Univ. & Advanced Nano Products, HONGLYOUL JU, Physics Dept., Yonsei Univ. — Electrical transport, optical microscopy, and synchrotron-based x-ray micro-diffraction measurements have been carried out on single domain VO_2 single crystals, exhibiting an abrupt first-order metal-insulator transition (MIT) with a high resistance ratio $\sim 10^5$ near $\sim 67^\circ\text{C}$ and a gradual insulator-insulator transition (IIT) at $\sim 48^\circ\text{C}$. Low temperature ($T < 45^\circ\text{C}$), intermediate ($\sim 50^\circ\text{C} < T < \sim 67^\circ\text{C}$), above MIT ($T > 67^\circ\text{C}$) phases were insulating monoclinic M2 with half vanadium ion dimerization, monoclinic M1 with full vanadium ion dimerization, and rutile (R) phases, respectively. In this poster, we will present unusual structural phases of M1, M2, and R of single-domain VO_2 single crystals and discuss the relationships between structures and the characteristics of the MIT of VO_2 .

S1.00297 Mechanism of orbital-selective phase transition by different magnetic states, HUNPYO LEE, YU-ZHONG ZHANG, HARALD O. JESCHKE, ROSER VALENTI, None — Using a dynamical cluster approximation we analyzed the behavior a degenerated two-orbital anisotropic Hubbard model at half-filling where both orbitals have equal bandwidths and one orbital is in paramagnetic (PM) state while the other one is in antiferromagnetic (AF) solution. We found an orbital-selective metal-insulator transition in which the PM orbital undergoes a transition from a Fermi liquid (FL) to a Mott insulator through a non-FL, while the AF orbital displays a transition from a FL to an AF insulator through an AF metallic phase. Finally, we would discuss that our intermediate phases are possibly related to the puzzling AF metallic state iron-pnictide superconductors.

S1.00298 Lattice-Symmetry-Driven Phase Competition in Vanadium Dioxide¹, ALEXANDER TSELEV, Oak Ridge National Laboratory, Oak Ridge, TN, USA, IGOR A. LUK'YANCHUK, University of Picardie Jules Verne, Amiens, France, ILIA N. IVANOV, JOHN D. BUDAI, JONATHAN Z. TISCHLER, Oak Ridge National Laboratory, Oak Ridge, TN, USA, EVGHENI STRELCOV, ANDREI KOLMAKOV, Southern Illinois University Carbondale, Carbondale, IL, USA, SERGEI V. KALININ, Oak Ridge National Laboratory, Oak Ridge, TN, USA — We performed group-theoretical analysis of the symmetry relationships between lattice structures of R, M1, M2, and T phases of vanadium dioxide in the frameworks of the general Ginzburg-Landau phase transition theory. The analysis leads to a conclusion that the competition between the lower-symmetry phases M1, M2, and T in the metal-insulator transition is pure symmetry driven, since all the three phases correspond to different directions of the same multi-component structural order parameter. Therefore, the lower-symmetry phases can be stabilized in respect to each other by small perturbations such as doping or stress.

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S1.00299 Valence fluctuation driven quantum phase transition¹, PRAMOD KUMAR², N.S. VIDHYADHIRAJA³, Jawaharlal Nehru Centre for advanced Scientific Research (JNCASR), Bengaluru — In recent years quantum critical phenomenon have acquired a great interest in the condensed matter community. Many rare earth intermetallic compounds, which are also heavy fermions can be tuned easily to quantum critical point by application of external perturbations like magnetic field and pressure. YbRh_2Si_2 and CeCu_2Si_2 are a few examples. The periodic Anderson model (PAM) is a paradigm for studying these kind of systems. We investigate the extended periodic anderson model (EPAM), which includes Coulomb interaction of conduction and localised electrons using local moment approach (LMA) within dynamical mean field theory (DMFT) with the objective of developing an understanding of quantum phase transitions due to valence fluctuations. We show that tuning c-f interaction and on-site energy of localised electron (which can be achieved by varying external perturbation like pressure) leads to some exotic phenomena like vanishing of Fermi liquid scale. We study transport properties near quantum critical point and highlight the anomalies due to the proximity of QCP.

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S1.00300 Band Insulators and Hubbard interactions, GUN SANG JEON, Department of Physics, Ewha Womans University, ARA GO, Department of Physics and Astronomy and Center for Theoretical Physics, Seoul National University — We investigate the theoretical models which are band insulators in the absence of interaction and evolve into Mott insulators under strong mutual repulsive interaction. We use the cellular dynamical mean-field theory to study the nature of the interaction-driven transitions in the systems. In various systems we compute the renormalized band gap which is defined by the self-energy corrected band gap and show that it is a convenient measure to characterize band insulating phases in such systems; the spectral gap is fully explained by the renormalized band gap when the systems remain in the band insulating phase. Finally we discuss interesting transition behavior from a band insulator to a Mott insulator.

S1.00301 Electronic structure of $\text{Lu}_{1-x}\text{La}_x\text{VO}_3$ single crystals using soft x-ray spectroscopy¹, BO CHEN, JUDE LAVEROCK, JAMES MCNULTY, DAVE NEWBY, KEVIN SMITH, Boston University, ANDERS GLANS, JINGHUA GUO, Advanced Light Source, GEETHA BALAKRISHNAN, RAVI SINGH, University of Warwick — The rare-earth vanadates, RVO_3 , offer a rich phase diagram of both orbital and spin ordering phenomena, stemming from their two-fold occupation of the three-fold degenerate V t_{2g} orbitals. It has been discussed that, in RVO_3 , which shows the t_{2g} orbital ordering, the Jahn-Teller coupling suppression is much weaker than that in the e_g electron systems. In order to address the orbital ordering effects, we report soft x-ray measurements of $\text{Lu}_{1-x}\text{La}_x\text{VO}_3$ single crystals, which approach both the smallest and largest rare-earth ionic sizes. X-ray absorption spectroscopy and x-ray emission spectroscopy, which reveal both the unoccupied and occupied partial density of states, are employed to observe the changes in the V $3d$ and O $2p$ states, across the orbital ordering transitions and R-site ionic radii. Also, resonant inelastic x-ray scattering is applied to probe the O $2p$ -V $3d^*$ charge transfer excitations and V $3d$ - $3d^*$ transitions. Together, these complementary techniques provide a picture of the electronic structure of $\text{Lu}_{1-x}\text{La}_x\text{VO}_3$ to test the role of the orbital ordering during phase transitions with varying rare-earth ionic sizes.

¹The Boston University program is supported in part by the U.S. Department of Energy under Contract No. DE-FG02-98ER45680. The Advanced Light Source is supported by the Department of Energy under Contract No. DE-AC02-05CH11231.

S1.00302 Singularity in self-energy and composite fermion excitations of interacting electrons¹, JIAN-XIN ZHU, LIJUN ZHU, Los Alamos National Laboratory — We propose that a composite fermion operator $f_{i\sigma}(2n_{i\bar{\sigma}} - 1)$ could have coherent excitations, where $f_{i\sigma}$ is the fermion operator for interacting electrons and $n_{i\bar{\sigma}}$ is the number operator of the opposite spin. In the two-impurity Anderson model, it is found that the excitation of this composite fermion has a pseudogap in the Kondo regime, and has a finite spectral weight in the regime where the excitation of the regular fermion $f_{i\sigma}$ has a pseudogap. In the latter regime, the self-energy of $f_{i\sigma}$ is found to be singular near Fermi energy. We argue that this composite fermion could develop a Fermi surface with Fermi liquid behaviors but "hidden" from charge excitations in lattice generalizations. We further illustrate that this type of excitations is essential in addressing the pseudogap state and unconventional superconductivity.

¹This work was supported by the National Nuclear Security Administration of the U.S. DOE at LANL under Contract No. DE-AC52-06NA25396, the U.S. DOE Office of Basic Energy Sciences, the LANL LDRD Program, and the DOE CINT at LANL.

S1.00303 Finite pulse relaxation calorimetry and specific heat of $\text{NdOs}_4\text{Sb}_{12}$ ¹, B. SOMSANUK, U.I. URBINA, P.-C. HO, Physics/California State University, Fresno, M.B. MAPLE, Physics/University of California, San Diego, T. YANAGISAWA, Hokkaido University, Japan — The compound $\text{NdOs}_4\text{Sb}_{12}$ is a mean-field ferromagnet at about 1 K. As inferred from specific heat measurements below 10 K, the electronic specific heat coefficient of this compound is very large (~ 520 mJ/mol-K²). Intriguingly, a recent ultrasonic measurement shows that this compound has double ultrasonic dispersions at ~ 15 K and 40 K. We have used our newly developed relaxation calorimeter to measure the specific heat of $\text{NdOs}_4\text{Sb}_{12}$ in the temperature range 11 K to 300 K. In this presentation, we will describe the experimental setup used for the finite pulse relaxation calorimetry in a cryocooler and the results of our measurements on the $\text{NdOs}_4\text{Sb}_{12}$ sample.

¹Research at CSU-Fresno is supported by NSF DMR-1104544; at UCSD by NSF DMR-0802478 and US DOE DE FG02-04ER46105; at Hokkaido U by MEXT, Japan.

S1.00304 Magnetization measurements in site disordered UCu_4Ni ¹, ARIANA VALDEZ, E. SOTO, O.O. BERNAL, Department of Physics and Astronomy, California State University, Los Angeles, CA 90032, D.E. MACLAUGHLIN, Department of Physics and Astronomy, University of California, Riverside, CA 92125, G.R. STEWART, J.S. KIM, Department of Physics, University of Florida, Gainesville, FL 32611 — UCu_4Ni is a non-Fermi liquid, quantum critical system, obtained from dilution of Cu for Ni in antiferromagnetic (AFM) UCu_5 . Introduction of Ni in the lattice structure of the parent compound suppresses the AFM transition temperature from 16.5 Kelvin down to zero at $x = 1$. Because Ni ions are slightly smaller than Cu ones (Pd and Cu ions are similar in size), Ni can be expected to distribute itself randomly between the two available crystal sites. UCu_4Ni is therefore a site-disordered material. We present a magnetization study of a random powder of UCu_4Ni as a function of applied magnetic field (-9.0 – 9.0 T) and temperature (2–300 K). We analyze the data from the point of view of magnetic disorder, as would be produced by a distribution of local magnetic susceptibilities, within the context of the Kondo Disorder Model. Comparison with similar existing studies in polycrystalline samples by others will be discussed.

¹Work supported by NSF/DMR-0604015 and 1105380.

S1.00305 Finite Size Effects on Electrical Transport of Nanoribbons of the Charge Density Wave Conductor NbSe_3 ¹, ADAM STABILE, Department of Physics, SUNY at Buffalo, LUISA WHITTAKER, Department of Chemistry, SUNY at Buffalo, TAI-LUNG WU, Department of Physics, SUNY at Buffalo, PETER MARLEY, Department of Chemistry, SUNY at Buffalo, ZHENZHONG SHI, Department of Physics, SUNY at Buffalo, SARBAJIT BANERJEE, Department of Chemistry, SUNY at Buffalo, G. SAMBANDAMURTHY, Department of Physics, SUNY at Buffalo — NbSe_3 is a textbook example of a charge density wave material, and although its properties are well known in bulk, its nanoscale characteristics are relatively unexplored. In particular, owing to the chain-like atomic structure of NbSe_3 , electric transport studies on quasi-one-dimensional devices remain a new frontier in scientific research in which unique finite size effects occur as a result of geometrical confinement and lattice reconstruction in the nanoscale. We used a novel, facile chemical vapor transport method for synthesizing nanoscale, single-crystalline NbSe_3 nanoribbons. This bottom-up method for preparing free-standing nanoribbon devices avoids potential sample degradation observed in top-down approaches. Typical ribbons have cross sectional area 10^4 nm² or less and lengths 10 – 50 μm . Single nanoribbon electrical transport measurements show expected charge density wave transitions at 59 and 141 K. We also observe significant enhancement in the depinning effect and sliding regimes mainly attributed to finite size effects.

¹Stabile, A. A.; Whittaker, L.; Wu, T. L.; Marley, P. M.; Banerjee, S.; and Sambandamurthy, G., Nanotechnology, 22, 485201 (2011)

S1.00306 The magnetoelectric effect on the novel multiferroic Co_3TeO_6 , C.C. CHOU, S. MUKHERJEE, J.H. ZHANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, J.L. HER, Division of Natural Science, Center for General Education, Chang Gung University, Tao-Yuan 333, Taiwan, H. BERGER, Institutes of Physics of Complex Matter, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland, H.D. YANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan — The magnetic, thermal, and dielectric measurements were performed on a single crystal sample Co_3TeO_6 . Two anomalies are observed at $T_1 \sim 26$ K and $T_2 \sim 18$ K in magnetic susceptibility and specific heat measurements. Dielectric constant data show a step anomaly at 18 K, which does not display frequency-dependent behavior but a magnetoelectric effect. Furthermore, the values of the magnetoelectric coupling constant γ were calculated, which are 0.0268 and 0.0239 at 7 K and 13 K, respectively. The temperature-dependent X-ray diffraction suggests that the lattice parameters slightly deviate from linear trend as temperature down to 26 K, and then shows an anomalous variation around 18 K, where a structural distortion probably appears. All phenomena of our results indicate that Co_3TeO_6 is one member of multiferroic materials

S1.00307 Quantum phase transition of the sub-Ohmic rotor model, MANAL AL-ALI, THOMAS VOJTA, Missouri University of Science and Technology — We investigate the behavior of an N -component quantum rotor coupled to a bosonic dissipative bath having a sub-Ohmic spectral density $J(\omega) \propto \omega^s$ with $s < 1$. With increasing dissipation strength, this system undergoes a quantum phase transition from a delocalized phase to a localized phase. We determine the exact critical behavior of this transition in the large- N limit. For $1 > s > 1/2$, we find nontrivial critical behavior corresponding to an interacting renormalization group fixed point while we find mean-field behavior for $s < 1/2$. The results agree with those of the corresponding long-range interacting classical model. The quantum-to-classical mapping is therefore valid for the sub-Ohmic rotor model.

S1.00308 Pomeranchuk instability from a black hole¹, KA WAI LO, University of Illinois at Urbana Champaign, MO-HAMMAD EDALATI, University of Texas at Austin, PHILIP PHILLIPS, University of Illinois at Urbana Champaign — Within the AdS/CFT correspondence, we introduce a probe spinor field and a neutral symmetric traceless spin-two field which are dual to a fermionic operator and a neutral tensor order parameter in the boundary field theory. By considering a certain coupling between the two probe fields, we show that a transition induced by condensation of the neutral order parameter dual to the neutral spin-two field can lead to the breaking of rotational symmetry of Fermi surface and hence a Pomeranchuk instability. The critical properties of this transition are computed.

¹National Science Foundation Division of Material Research -0940992

S1.00309 Superfluidity Without Boson Condensation, A.M. KADIN, Princeton Junction, NJ — Superfluidity is generally attributed to condensation of boson wavefunctions. He-4 atoms have zero net spin in the nucleus and in the electrons, and so are bosons, while He-3 atoms have a nuclear spin of $1/2$, and are fermions. This fits the conventional understanding that the superfluid transition of He-4 at 2.2 K is due to boson condensation, while the lack of such a transition in He-3 is due to the absence of bosons until atomic pairing into boson-like Cooper pairs occurs in the mK range. However, Kadin [1] has extended a novel non-boson superconducting condensation mechanism to superfluids. This is based on an interleaved two-phase structure of close-packed electron orbitals (analogous to an ionic liquid), whereby each orbital is surrounded by multiple anti-phase orbitals, with nodes between them to maintain orthogonality. This entire structure moves together as a superfluid, preserving long-range phase coherence. The lack of superfluidity in He-3 is attributable *not* to these atoms being fermions, but rather to the presence of unpaired nuclear spins that destroy the phase coherence due to spin-flip scattering. This is consistent with the behavior of mixtures of He-3 and He-4. Only at mK temperatures, when the nuclear spins order and spin-flip scattering is suppressed, is superfluidity again possible. A similar picture may also be extended to “Bose-Einstein condensates” in dilute concentrations of alkali metal atoms, but *only* if one assumes the presence of close-packed atomic clusters or droplets, rather than a dilute gas. [1] A.M. Kadin, <http://arxiv.org/abs/0909.2901> (2009); <http://arxiv.org/abs/1107.5794> (2011).

S1.00310 ^3He - ^4He liquid mixtures investigated by neutron imaging technique at low temperatures¹, PATRICK GUMANN, University of Waterloo, JULIA SCHERSCHLIGT, DANIEL HUSSEY, DAVID JACOBSON, NIST Center for Neutron Research, DAVID CORY, IVAR TAMINIAU, University of Waterloo — Helium is a unique element which exhibits a variety of different phases and unusual behaviors. It can be found in nature in two stable isotopic forms: ^3He and ^4He . One of the most profound quantum mechanical effects, superfluidity, occurs below 2.17 K in liquid helium ^4He and 0.003 K in liquid ^3He . There are also interesting phenomena occurring in mixtures of the two isotopes. One demonstrative example is the finite solubility of liquid ^3He (a Fermi system) in superfluid ^4He (a Bose system) even at $T = 0$ K. This is the basic principle in the operation of a ^3He - ^4He dilution refrigerator capable of continuously producing 2 mK. While much has been done in studies of the thermodynamical, quantum properties of liquid helium mixtures, there has not been any attempt to visualize the dynamics of ^3He in liquid ^4He . Presented results of neutron imaging experiments on 0.3 bar liquid ^3He - ^4He mixtures, at 1.5 K have shown a clear diffusion of ^3He driven by the difference in chemical potential. The data were taken for over 12 hours using a high resolution CCD camera.

¹Supported NIST Center for Neutron Research, U.S. Commerce Department

S1.00311 Traces of Vortices in Superfluid Helium Droplets¹, LUIS F. GOMEZ, Department of Chemistry, University of Southern California, Los Angeles, CA, EVGENY LOGINOV, SICPA SA, Prilly, Switzerland, ANDREY F. VILESOV, Department of Chemistry and Department of Physics, University of Southern California, Los Angeles, CA — We report on the observation of vortices in superfluid ^4He droplets produced by a free fluid-jet expansion. The vortices were traced by introducing silver atoms into the droplets, which clustered along the vortex lines. The silver clusters were subsequently surface deposited and imaged via electron microscopy. The prevalence of elongated track-shaped deposits shows that vortices are ubiquitous in droplets larger than about 300 nm and that their lifetime exceeds a few milliseconds. In these experiments the droplets become superfluid within a few microseconds, which is at least 10^6 times faster than in previous bulk helium experiments. We discuss possible formation mechanisms and the stability of the vortices obtained during this rapid phase transition.

¹This work was supported by NSF grant CHE-1112391.

S1.00312 POST-DEADLINE ABSTRACTS —

S1.00313 Size effect of properties in hybrid of gold nanoparticles and calamitic mesogen¹, CHIH-HAO YU, CHRIS WELCH, BAI J. TANG, CHRISTOPHER J. SCHUBERT, GEORG H. MEHL, Department of Chemistry, University of Hull — In this contribution we describe the synthesis and investigation of Au NPs functionalized with organic mesogenic groups which self-assemble into liquid crystalline phases. A nematic mesogenic liquid crystalline laterally reacts with functionalized gold via a siloxane group using Karstedt's catalyst. Compared to earlier work where NPs were in the size of 1.5-2.5 nm, we report here on larger than 5 nm sized particles. The synthesis of the particles is based on a new methodology using digestive ripening and synthesis functionalisation of the organic groups. This example may open up a protocol for liquid crystal molecules encapsulated in nanoparticles. Properties of the calamitic mesogen encapsulated gold nanoparticles have been investigated by HRTEM, NMR, UV/Vis, differential scanning calorimetry (DSC), optical polarizing microscopy (OPM).

¹Funded by the European Union's Seven Framework Programme (FP7 2007) under Grant Agreement no 228455 (NANOGOLD)

S1.00314 Trimeric surfactant as superior boundary lubricant, NIR KAMPF, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, Israel, CHUNXIAN WU, YILIN WANG, Key Laboratory of Colloid and Interface Science, Institute of Chemistry, Chinese Academy of Sciences, Beijing, China, JACOB KLEIN, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, Israel — Surfactants are widely used to modify surfaces and interfaces properties. A unique cationic trimeric surfactant, tri(dodecyltrimethylammonioacetox)-diethyltri-amine trichloride (DTAD), was found to form liposome-like aggregates in solution or a highly ordered bilayer patterns on mica surface [1,2]. We have investigated the normal and shear forces between two atomically smooth mica surfaces across this surfactant using the surface force balance (SFB) technique. Shear forces measured across the trimeric surfactant solution demonstrate ultra-low friction coefficient ($\mu=5 \times 10^{-5}$) under pressure of tens of atmospheres. AFM scans under the trimeric surfactant solution demonstrate the presence of large spheres (ca. 100nm in diameter) on the mica. The contribution of the compressed charged spheres to the ultra-low friction measured can be explained by the efficient hydration lubrication mechanism exist between the hydrated surfactant head-groups and the mica surface. A weak dependence of the friction coefficient to the shear rate or amplitude was observed.

[1] Hou et al., *Langmuir*, **24**, 10572 (2008).

[2] Wu et al., *Langmuir*, **26**, 7922 (2010).

S1.00315 Freely Suspended Smectic Films in Aqueous Environment, KARTHIK PEDDIREDDY, CHRISTIAN BAHAR, Max Planck Institute for Dynamics and Self Organization — Smectic liquid crystals easily form thin films which are freely suspended on a solid frame in air. These systems have been thoroughly studied for various purposes such as structural studies of smectic phases, investigating phase transitions in two-dimensional systems, and studying various physical properties of liquid crystals. In the present study, we explore the preparation of freely suspended smectic films in water. A prerequisite is the presence of a surfactant which accumulates at the liquid-crystal/water interface and induces a homeotropic anchoring of the director, so that the smectic layers align parallel to the two film surfaces. The presence of the surfactant might also serve as a handle to tune properties such as the surface tension of the films (which is hardly possible for freely suspended films in air). We study the formation of films in water using different frames and different surfactants, and we focus especially on the thinning behaviour which occurs when the temperature is increased towards the smectic - nematic or smectic - isotropic transition.

S1.00316 Stiffness Dependent Separation of Cells in a Microfluidic Device, TODD SULCHEK, GONGHAO WANG, WENBIN MAO, CAITLIN HENEGAR, ALEXANDER ALEXEEV, Georgia Tech — Abnormal cell mechanical stiffness can point to the development of various diseases including cancers and infections. We report a new high-throughput technique for continuous cell separation utilizing variation in cell stiffness. We use a microfluidic channel decorated by periodic diagonal ridges to separate K562 lymphoblastic cell line modified to different mechanical stiffness values. Diagonal ridges within the microfluidic flow channel compress and deform the cells in rapid succession to translate each cell perpendicular to the channel axis in proportion to its stiffness. Atomic force microscopy (AFM) was used to directly measure the Young's modulus of modified K562 cells to verify the stiffness variation. We demonstrate that soft cells can be separated from stiff cells at physiological concentrations with a fivefold enrichment of cell populations. This microfluidic device opens the way for conducting rapid and low-cost cell analysis and purification through physical markers.

S1.00317 Spin-orbital models using dipolar fermions in zig-zag optical lattices¹, TEIMURAZ VEKUA, GAOYOUNG SUN, GEORGE JACKELI, LUIS SANTOS, none — Ultra-cold dipolar spinor fermions in zig-zag type optical lattices can mimic spin-orbital models relevant in solid-state systems, as pyroxene titanium and layered vanadium oxides, with the interesting advantage of reviving the quantum nature of orbital fluctuations. We discuss two different physical systems in which these models may be simulated, showing that the interplay between lattice geometry and spin and orbital quantum dynamics produces a wealth of novel quantum phases.

¹This work has been supported by QUEST (Center for Quantum Engineering and Space-Time Research). Support from SCOPES Grant IZ73Z0-128058 (T.V.) and GNSF/ST09-447 (G.J.) is acknowledged.

S1.00318 Spin-dependent low-energy ⁴He⁺ ion scattering on non-magnetic surfaces¹, TAKU SUZUKI, YASUSHI YAMAUCHI, SYUNICHI HISHITA, National Institute for Materials Science — We investigated electron-spin-polarized ⁴He⁺ ion scattering on various non-magnetic surfaces at kinetic energies below 2 keV [1]. It was observed that the scattered He⁺ ion yield depends on the He⁺ ion spin. We interpret this spin-dependent scattering in terms of the spin-orbit coupling (SOC) that acts transiently on the He⁺1s electron spin in the He⁺-target binary collision. This interpretation qualitatively explains the relationship between the spin-dependent scattering and the scattering geometry, incident velocity, and magnetic field arrangement. This is the first study to report SOC caused by projectile electron spin in ion scattering.

[1] T.Suzuki, Y.Yamauchi, and S.Hishita, *Phys.Rev.Lett.* 107(2011)176101.

¹Sentan-JST, Kakenhi 22760032

S1.00319 Iron chalcogenide photovoltaic absorbers – problems and opportunities, ROBERT KOKENYESI¹, VORRANUTCH JIERATUM, EMMELINE ALTSCHUL, DOUGLAS KESZLER, Department of Chemistry, Oregon State University, Corvallis, OR, RAM RAVICHANDRAN, BRIAN PELATT, JOHN WAGER, School of EECS, Oregon State University, Corvallis, OR, LIPING YU, STEPHAN LANY, National Renewable Energy Laboratory, Golden, CO, ALEX ZUNGER, University of Colorado at Boulder, Boulder, CO, CENTER FOR INVERSE DESIGN, EFRC COLLABORATION — Realizing new, efficient solar absorbers containing earth-abundant materials represents a critical element for expanding the reach of photovoltaic (PV) technologies, meeting growing energy needs. The use of Fe in PV was proposed more than 25 years ago in the form of FeS₂ pyrite. We report a concerted and integrated theoretical and experimental study that provides new insight into the problem of FeS₂. Computational results on FeS₂ reveal high formation energies for bulk point defects and small formation energies for S vacancies near the surface. These findings are consistent with the formation of metallic S-deficient binary Fe-S phases at low temperatures that affect the electrical and optical properties of thin films. We have used this new understanding to propose and implement design rules for identifying new Fe-containing materials—Fe₂SiS₄ and Fe₂GeS₄—that may circumvent the limitations of pyrite. These ternary materials are *p*-type with direct allowed optical band gaps near 1.5 eV.

¹formerly Robert Kykyneshi

S1.00320 Normal force and interpenetration between polyelectrolyte brushes¹, MARK MATSEN, University of Reading — We examine the normal force between two opposing polyelectrolyte brushes and the interpenetration of their chains that is responsible for sliding friction. We focus on the special case of semi-dilute brushes in a theta solvent, for which the classical strong-stretching theory (SST) can be solved analytically. Interestingly, SST predicts that the brushes contract as they are compressed together maintaining a polymer-free gap, which provides an explanation for the ultra-low frictional forces observed in experiment. We examine the degree to which the SST predictions are affected by chain fluctuations by employing self-consistent field theory (SCFT). While the normal force is relatively unaffected, fluctuations are found to have a strong impact on brush interpenetration. Even still, the contraction of the brushes does significantly prolong the onset of interpenetration, implying that a sizeable normal force can be achieved before the sliding friction becomes significant.

¹EPSRC (grant no. EP/F068425/1)

S1.00321 Optical Properties of III-V Semiconductors in Wurtzite Phase, AMRIT DE, University of California - Riverside, CRAIG PRYOR, University of Iowa — A number of recent experiments have shown that the photoluminescence intensity in free standing nanowires is polarization dependent. One contribution to this effect is the optical anisotropy arising from the tendency of the nanowires to crystallize in wurtzite form. We calculate the frequency dependent dielectric functions for nine non-Nitride wurtzite phase III-V semiconductors (AlP, AlAs, AlSb, GaP, GaAs, GaSb, InP, InAs and InSb), based on our maximally constrained empirical pseudopotential bulk band structure calculations. Their complex dielectric functions are calculated in the dipole approximation for polarization perpendicular and parallel to the c-axis of the crystal. We also predict their reflectivity spectra and the static dielectric constants. Optical selection rules are used to explain key features of the dielectric functions. In general it is seen that the III-V wurtzite phase semiconductors exhibit strong optical anisotropy which suggests that they could be potentially useful as nonlinear optical crystals.

S1.00322 Studies to Enhance Superconductivity in Thin Film Carbon, BENJAMIN PIERCE, LYLE BRUNKE, JACK BURKE, DAVID VIER, ANDREW STECKL, TIMOTHY HAUGAN, None, WPAFB/AFRL COLLABORATION, UNIVERSITY OF CINCINNATI COLLABORATION, UNIVERSITY OF CALIFORNIA SAN DIEGO COLLABORATION — With research in the area of superconductivity growing, it is no surprise that new efforts are being made to induce superconductivity or increase transition temperatures (T_c) in carbon given its many allotropic forms. Promising results have been published for boron doping in diamond films, and phosphorus doping in highly oriented pyrolytic graphite (HOPG) films show hints of superconductivity. Following these examples in the literature, we have begun studies to explore superconductivity in thin film carbon samples doped with different elements. Carbon thin films are prepared by pulsed laser deposition (PLD) on amorphous SiO_2/Si and single-crystal substrates. Doping is achieved by depositing from $(\text{C}_{1-x}\text{M}_x)$ single-targets with $\text{M} = \text{B}_4\text{C}$ and BN , and also by ion implantation into pure-carbon films. Previous research had indicated that Boron in HOPG did not elicit superconducting properties, but we aim to explore that also in thin film carbon and see if there needs to be a higher doping in the sample if trends were able to be seen in diamond films. Higher onset temperatures, T_c , and current densities, J_c , are hoped to be achieved with doping of the thin film carbon with different elements.

S1.00323 Anomalous resistivity peak in a ferromagnetic nanowire proximity-coupled to superconducting electrodes¹, SO TAKEI, VICTOR GALITSKI, University of Maryland — Motivated by the recent experiment of Wang et al. [Nature Physics 6, 389 (2010)], we study temperature-dependent transport in such a mesoscopic structure consisting of a ferromagnetic nanowire proximity-coupled to two conventional superconducting electrodes. It is assumed that the asymmetry in the tunneling barrier gives rise to the Rashba spin-orbit-coupling in the barrier that enables induced p-wave superconductivity in the ferromagnet to exist. First, we develop a microscopic theory of Andreev scattering at the spin-orbit-coupled interface, derive a set of self-consistent boundary conditions, and find an expression for the p-wave minigap in terms of the microscopic parameters of the contact. Second, we study temperature-dependence of the resistance near the superconducting transition and find that it should generally feature a fluctuation-induced peak. The upturn in resistance is related to the suppression of the single-particle density of states due to the formation of fluctuating pairs, whose tunneling is suppressed. We find a good agreement between the data and our fluctuation theory. Then, we discuss this and related setups involving ferromagnetic nanowires in the context of one-dimensional topological superconductors.

¹V. G. is grateful to Simons Foundation for support through the “Simons Distinguished Visiting Scholars” program. S.T. and V.G. were also supported by NSF-CAREER award.

S1.00324 ABSTRACT MOVED TO W21.00007 —

S1.00325 Soft phonon mode and superconducting properties of 2H-NbS₂ compared to 2H-NbSe₂, MAXIME LEROUX, CNRS / UJF, Institut NÉEL, 38042 Grenoble cedex 9, France, MATHIEU LE TACON, Max Planck Institut für Festkörperforschung, D-70569 Stuttgart, Germany, MATTEO CALANDRA, CNRS / IMPMC Université Paris 6, 75252, Paris cedex 05, France, THIERRY KLEIN, CNRS / UJF, Institut NÉEL, 38042 Grenoble cedex 9, France, LAURENT CARIO, CNRS / IMN Jean-Rouxel, Université de Nantes, 44322 Nantes, France, PIERRE RODIÈRE, CNRS / UJF, Institut NÉEL, 38042 Grenoble cedex 9, France — I will report on several recent results on 2H-NbS₂. This compound is the only superconducting 2H-dichalcogenide which does not develop a charge density wave (CDW). I will start with the temperature dependence of the phonon spectra of 2H-NbS₂ measured by Inelastic X-ray Scattering (IXS). Along ΓM , a huge softening of two phonon modes was observed on a wide part of the Brillouin zone. This is almost the same as the CDW precursor soft phonons modes that appear above $T_{CDW} \approx 33\text{ K}$ in 2H-NbSe₂[Weber11]. It clearly indicates that 2H-NbS₂ is also at proximity of a CDW instability. In the second part I will show measurement of H_{c1} and magnetic penetration depth, which show signs of a small energy scale in the superconducting gap of 2H-NbS₂, very similar to 2H-NbSe₂ [Fletcher07], and also in good agreement with STS measurement[Guillamon08]. In view of these two facts and as an open question, we would like to discuss the hypothesis of a quantum critical point (QCP) lying between 2H-NbS₂ and 2H-NbSe₂, where the 2nd order phase transition would be the CDW instability.

S1.00326 Evidence for a hidden-order pseudogap in URu₂Si₂¹, J.T. HARALDSEN, Los Alamos National Laboratory, Y. DUBI, Tel Aviv University, N.J. CURRO, University of California - Davis, A.V. BALATSKY, Los Alamos National Laboratory — Through an analysis and modeling of data from various experimental techniques, we present evidence for the presence of a hidden order pseudogap in URu₂Si₂ in the temperature range between 25 K and 17.5 K. Considering fluctuations of the hidden order energy gap at the transition as the origin of the pseudogap, we evaluate the effects that gap fluctuations would produce on observables like tunneling conductance, neutron scattering, and nuclear resonance, and relate them to the experimental findings. We show that the transition into hidden order phase is likely second order and is preceded by the onset of non-coherent hidden order fluctuations.

¹Work was carried out under the help and support of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396 and the Center for Integrated Nanotechnology.

S1.00327 In Situ Electronic Characterization of Graphene Nanoconstrictions Fabricated in a Transmission Electron Microscope¹, YE LU, CHRISTOPHER MERCHANT, MARIJA DRNDIC, A.T. CHARLIE JOHNSON, University of Pennsylvania, UNIVERSITY OF PENNSYLVANIA TEAM — We report electronic measurements on high quality graphene nanoconstrictions (GNCs) fabricated in a transmission electron microscope (TEM), and the first measurements on GNC conductance with an accurate measurement of constriction width down to 1 nm. To create the GNCs, freely suspended graphene ribbons were fabricated using few-layer graphene grown by chemical vapor deposition. The ribbons were loaded into the TEM, and a current-annealing procedure was used to clean the material and improve its electronic characteristics. The TEM beam was then used to sculpt GNCs to a series of desired widths in the range 1-700 nm; after each sculpting step, the sample was imaged by TEM and its electronic properties were measured in situ. GNC conductance was found to be remarkably high, comparable to that of exfoliated graphene samples of similar size. The GNC conductance varied with width approximately as $G(w) = (e^2/h)w^{0.75}$, where w is the constriction width in nanometers. GNCs support current densities greater than $120 \mu\text{A}/\text{nm}^2$, 2 orders of magnitude higher than that which has been previously reported for graphene nanoribbons and 2000 times higher than that reported for copper.

¹National Science Foundation through Grant #DMR-0805136 (Y.L. and A.T.C.J.) and NIH Grant R21HG004767 and R21HG 557611 (C.M. and M.D.).

S1.00328 One-dimensional Si nanolines in hydrogenated Si(001), BIANCO FRANÇOIS, SIGRUN A. KÖSTER, JAMES G. H. OWEN, CHRISTOPH RENNER, University of Geneva, DPMC - MaNEP Quai Ernest-Ansermet 24, 1211 Geneva 4, DAVID R. BOWLER, University College London, London Centre of Nanotechnology — We present a detailed study of the structural and electronic properties of a self-assembled silicon nanoline embedded in the H-terminated silicon (001) surface, known as the Haiku stripe. The nanoline is a perfectly straight and defect free endotaxial structure of huge aspect ratio; it can grow micrometre long at a constant width of exactly four Si dimers (1.54 nm). Another remarkable property is its capacity to be exposed to air without suffering any degradation. The nanoline grows independently of any step edges at tunable densities, from isolated nanolines to a dense array of nanolines. In addition to these unique structural characteristics, scanning tunnelling microscopy and density functional theory reveal a one-dimensional state confined along the Haiku core. This nanoline is a promising candidate for the long sought after electronic solid-state one-dimensional model system to explore the fascinating quantum properties emerging in such reduced dimensionality. Phys. Rev. B, 84, 035328 (2011)

S1.00329 Formation of complex emulsion in microfluidic channel, CHANG-HYUNG CHOI, JONGMIN KIM, CHANG-SOO LEE, Chungnam National University — We first report a novel emulsification method using two binary mixtures that produces complex emulsion by phase separation, triggered by external diffusion of separation agent dissolved in continuous phase. A disperse phase consists of monomer and D-solvent (good solvent for disperse phase), while mixture of separation-triggering agent (SA) and C-solvent (good solvent for continuous phase) is used as a continuous phase. Individual droplet was formed by microfluidic system, allowing how the separation dynamically occurs as a function of time. This system consists of the three major steps involving the transformation of a single droplet into the complex emulsion. In the first, when two immiscible phases meet at cross-junction, droplets are generated and dispersed in continuous phase containing the SA. Since the SA is only selectively soluble in the monomer of disperse phase, external diffusion of SA into the droplets through the interface occurs which initiates phase separation. In transient state, the external diffusion of the SA generates both partial separated region and SA/monomer complex at the near interface of partial separated region. In the last step, where the phase separation fully occurs, single droplets transform into complex emulsion such as double emulsion or multiple emulsion with high order. In addition, we demonstrate a capability for generation of complex emulsions gives a great opportunity to fabricate functional materials using template synthesis.

S1.00330 Heralded entanglement between two single atoms at remote locations, MARKUS WEBER, JULIAN HOFMANN, WENJAMIN ROSENFELD, LMU Munich and Max Planck Institute of Quantum Optics, Germany, CHRISTIAN KURTSTIEFER, University of Singapore, NORBERT ORTEGEL, MICHAEL KRUG, HARALD WEINFURTER, LMU Munich and Max Planck Institute of Quantum Optics, Germany — Entanglement between single trapped atoms at large distances is a key resource for future applications in quantum communication, like quantum networks and the quantum repeater. We have set up two independently operating atomic traps situated in two neighboring laboratories separated by 20 meter. On each side we capture a single Rb-87 atom in an optical dipole trap and generate a spin-entangled state between the atom and a single spontaneously emitted photon [1]. These photons are collected with high-NA objectives, coupled into single-mode optical fibers, and guided to the same fiber beam splitter (BS) where they interfere. A coincident detection of two orthogonally polarized photons leaving the BS allows us to project them onto two out of four maximally entangled Bell states. This Bell-state-projection on the photons swaps the entanglement onto the atoms. Here we report the faithful generation and analysis of entanglement between two single trapped atoms at remote locations. The observed entanglement fidelity is high enough, opening up the possibility for a first loophole-free test of Bell's inequality [2].

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[2] W. Rosenfeld, et al., Adv. Sci. Lett. 2, 469 (2009).

S1.00331 Quantum network with trusted and untrusted relays, XIONGFENG MA, University of Toronto, RAZIEH ANNABESTANI, University of Waterloo, CHI-HANG FRED FUNG, University of Hong Kong, HOI-KWONG LO, University of Toronto, NORBERT LÜTKENHAUS, DAVID PITKÄNEN, University of Waterloo, MOHSEN RAZAVI, University of Leeds — Quantum key distribution offers two distant users to establish a random secure key by exploiting properties of quantum mechanics, whose security has proven in theory. In practice, many lab and field demonstrations have been performed in the last 20 years. Nowadays, quantum network with quantum key distribution systems are tested around the world, such as in China, Europe, Japan and US. In this talk, I will give a brief introduction of recent development for quantum network. For the untrusted relay part, I will introduce the measurement-device-independent quantum key distribution scheme and a quantum relay with linear optics. The security of such scheme is proven without assumptions on the detection devices, where most of quantum hacking strategies are launched. This scheme can be realized with current technology. For the trusted relay part, I will introduce so-called delayed privacy amplification, with which no error correction and privacy amplification is necessarily to be performed between users and the relay. In this way, classical communications and computational power requirement on the relay site will be reduced.

S1.00332 Entanglement witness operator for quantum teleportation¹, ARCHAN S. MAJUMDAR, S. N. Bose National Centre for Basic Sciences, Kolkata, SATYABARTA ADHIKARI, Institute of Physics, Bhubaneswar, NIRMAN GANGULY, JYOTISHMAN CHATTERJEE, Dept. of Mathematics, Heritage Institute of Technology, Kolkata — The ability of entangled states to act as resource for teleportation is linked to a property of the fully entangled fraction. We show that the set of states with their fully entangled fraction bounded by a threshold value required for performing teleportation is both convex and compact. This feature enables for the existence of hermitian witness operators the measurement of which could distinguish unknown states useful for performing teleportation. We present an example of such a witness operator illustrating it for different classes of states. We further discuss the experimental measurability of the witness operator. (arXiv:1108.1493v2 [quant-ph]; to appear in Phys. Rev. Lett.)

¹ASM acknowledges support from the Project IR/S2/PU-16/2007, DST, India.

S1.00333 Entanglement Entropy in 1-D integrable chains , FABIO FRANCHINI, Massachusetts Institute of Technology/SISSA/INFN, STEFANO EVANGELISTI, Oxford University/University of Bologna/INFN, ELISA ERCOLESSI, FRANCESCO RAVANINI, University of Bologna/INFN, ANDREA DE LUCA, SISSA/INFN — We study analytically the Renyi entropy of a bipartite lattice in the limit of two semi-infinite chains joined at the origin, for a few integrable 1-dimensional models, by using the techniques of Corner Transfer Matrices of the corresponding 2-D classical systems, namely the 8-vertex model and the RSOS. In the scaling limit, close to a conformal point, we reproduce the leading behavior expected from CFT prediction. The sub-leading corrections, however, differ from naïve expectations and we show that lattice effect can give rise to additional relevant terms in any numerical approach. Moreover, in the vicinity of a non-conformal (ferromagnetic) point, we observe a violation of universality and a behavior of the entropy characteristic of an *essential singularity*.

S1.00334 Constant Tip-Surface Distance with Atomic Force Microscopy via Quality Factor Feedback , LIN FAN, DANIEL POTTER, TODD SULCHEK, Georgia Institute of Technology — The atomic force microscope (AFM) is a powerful and widely used instrument to image topography and measure forces at the micrometer and nanometer length scale. Because of the high degree of operating accuracy required of the instrument, small thermal and mechanical drifts of the cantilever and piezoactuator systems hamper measurements as the AFM tip drifts spatially relative to the sample surface. To compensate for the drift, we control the tip-surface distance by monitoring the cantilever quality factor (Q) in a closed loop. Brownian thermal fluctuations provide sufficient actuation to accurately determine cantilever Q by fitting the thermal noise spectrum to a Lorentzian function. We show that the cantilever damping is sufficiently affected by the tip-surface distance so that the tip position of soft cantilevers can be maintained within 70 nm of a setpoint in air and within 3 nm in water with 95 percent reliability. Utilizing this method to hover the tip above a sample surface, we have the capability to study sensitive interactions at the nanometer length scale over long periods of time.

S1.00335 Fractal contours of scalar in smooth flows , MARIJA VUCELJA, Courant Institute of Mathematical Sciences, NYU, GREGORY FALKOVICH, Department of Physics of Complex Systems, Weizmann Institute of Science, 76100 Rehovot, Israel, KONSTANTIN TURITSYN, Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA — A passive scalar field was studied under the action of pumping, diffusion and advection by a smooth flow with a Lagrangian chaos. We present theoretical arguments showing that scalar statistics is not conformal invariant and formulate a new effective semi-analytic algorithm to model scalar turbulence. We then carry out massive numerics of scalar turbulence focusing on nodal lines. The distribution of contours over sizes and perimeters is shown to depend neither on the flow realization nor on the resolution (diffusion) scale for scales exceeding this scale. The scalar isolines are found fractal/smooth at the scales larger/smaller than the pumping scale. We characterize the statistics of bending of a long isoline by the driving function of the Loewner map, show that it behaves like diffusion with diffusivity independent of resolution yet, most surprisingly, dependent on the velocity realization and time (beyond the time on which the statistics of the scalar is stabilized).

S1.00336 Laplace pressure induced droplet generation in micromold for synthesizing monodisperse microspheres. , CHANG-HYUNG CHOI, Chungnam National University, JINKEE LEE, Sungkyunkwan University, CHANG-SOO LEE, Chungnam National University — Microspheres are widely used in applications such MEMS, chemical release systems, optical materials and various biological applications. Here, we report the new micromolding technique for synthesizing spherical monodisperse particles through surface-tension-induced flow. The spherical droplets were prepared using Laplace pressure difference, which is highly depending on geometries of the mold shape, without any pumping system to make flow. We calculated the minimum pressure difference to make the flow moves and form the droplets. It provides a synthetic tool for generating the microspheres using different reaction schemes; UV-polymerization, sol-gel reaction and colloidal assemblies. The monodisperse spherical particles, which are made of various materials, were successfully generated without any surfactant because each droplet can be separately positioned in mold patterns during solidification process.

S1.00337 Tuning the Ferroelectric Properties through a Magnetic Field , JEFFERY CARVELL, RUIHUA CHENG, Indiana University Purdue University Indianapolis — Preparation and characterization of multiferroic materials in which ferroelectricity and ferromagnetism coexist would be a milestone for functionalized materials and devices. We have demonstrated that the electric polarization of ferroelectric polymer, poly(vinylidene fluoride) (PVDF), can be controlled by applying an external magnetic field. Samples were created in a layered heterostructure, with the key part of a PVDF layer sandwiched by two layers of Fe thin films. We found that as the applied magnetic field is changed, the switching of electric polarization for the PVDF displayed a dependence on the external magnetic field. We also noticed that both coercivity and polarization for the PVDF polymer display hysteretic features according to the change of an applied magnetic field. Our study showed that the thickness of both the iron layer and the PVDF layer have an effect on the magnetoelectric coupling in our samples. The same magnetostriction strain applied to a thicker PVDF layer becomes tougher to flip the polarization compared to a thinner PVDF layer. As the iron film thickness increases, the magnetoelectric strain also increases, and the PVDF polymer can be easily saturated and the polarization is more easily flipped. We have shown that it is possible to control the ferroelectric properties of a PVDF film by tuning the magnetic field in heterostructures. Our study shows that this system could have show promising applications for new information technology and devices.

S1.00338 Anderson localization and correlation-induced delocalization in N-leg optical lattices , TIGRAN SEDRAKYAN, Fine Theoretical Physics Institute, University of Minnesota, JASON KESTNER, SANKAR DAS SARMA, University of Maryland, College Park — Recent experiments demonstrated localization of ultracold neutral atoms in a disordered optical potential. The great advantage of these atomic systems is the control of disorder form and strength, interactions, dimensionality, etc., in principle allowing for unambiguous observation of the phenomenon under a variety of circumstances. However, the localization observed so far is qualitatively indistinguishable from classical localization of particles in a disordered trapping potential. We propose a realization of the one-dimensional random dimer model and certain N-leg generalizations using cold atoms in an optical lattice. These models exhibit multiple delocalization energies that depend strongly on the symmetry properties of the corresponding Hamiltonian. We demonstrate that the N-leg systems possess similarities with their 1D ancestors but are demonstrably distinct. The existence of critical delocalization energies leads to dips in the momentum distribution which serve as a clear signal of the localization-delocalization transition.

S1.00339 Multidimensional scaling of ideological landscape on social network sites , DEOKJAE LEE, Department of Physics and Astronomy, Seoul National University, KYU S. HAHN, Department of Communication, Seoul National University, JUYONG PARK, Department of Physics, Kyung Hee University — Social network sites (SNSs) are valuable source of information on various subjects in network science. Recently, political activity of SNSs users has increasing attention and is an interesting interdisciplinary subject of physical and social science. In this work, we measure ideological positions of the legislators of U.S. and South Korea (S.K.) evaluated by Twitter users, using the information employed in the bipartite network structure of the legislators and their Twitter followers. We compare the result with ideological positions constructed from roll call record of the legislators. This shows there is a discrepancy between the ideological positions evaluated by Twitter users and actual positions estimated from roll call votes in S.K. We also assess the ideological positions of the Twitter users themselves and analyze the distribution of the positions.

S1.00340 Some Recent Developments in Structure and Glassy Behavior of Proteins¹, CHIN-KUN HU, Institute of Physics of Academia Sinica, Taipei, Taiwan — We have used ARVO developed by us to find that the ratio of volume and surface area of proteins in Protein Data Bank distributed in a very narrow region [1]. Such result is useful for the determination of protein 3D structures. It has been widely known that a spin glass model can be used to understand the slow relaxation behavior of a glass at low temperatures [2]. We have used molecular dynamics and simple models of polymer chains to study relaxation and aggregation of proteins under various conditions and found that polymer chains with neighboring monomers connected by rigid bonds can relax very slowly and show glassy behavior [3]. We have also found that native collagen fibrils show glassy behavior at room temperatures [4]. The results of [3] and [4] about the glassy behavior of polymers or proteins are useful for understanding the mechanism for a biological system to maintain in a non-equilibrium state, including the ancient seed [5], which can maintain in a non-equilibrium state for a very long time. (1) M.-C. Wu, M. S. Li, W.-J. Ma, M. Kouza, and C.-K. Hu, EPL, in press (2011); (2) C. Dasgupta, S.-K. Ma, and C.-K. Hu. Phys. Rev. B 20, 3837-3849 (1979); (3) W.-J. Ma and C.-K. Hu, J. Phys. Soc. Japan 79, 024005, 024006, 054001, and 104002 (2010), C.-K. Hu and W.-J. Ma, Prog. Theor. Phys. Supp. 184, 369 (2010); S. G. Gevorgian, A. E. Allahverdyan, D. S. Gevorgyan and C.-K. Hu, EPL 95, 23001 (2011); S. Sallon, et al. Science 320, 1464 (2008).

¹Supported by Grant NSC 100-2112-M-001-003-MY2.

S1.00341 Effective spectral dimension of hub in scale-free networks, SUNGMIN HWANG, Department of Physics and Astronomy, Seoul National University, DEOK-SUN LEE, Department of Natural Medical Sciences and Department of Physics, Inha University, BYUNGNAM KAHNG, Department of Physics and Astronomy, Seoul National University — Exploring the World Wide Web has become one of the key issues in information science, specifically in context of its application to the PageRank-like algorithms used in search engine. The random walk approach has been employed to study such a problem. The probability of the return to the origin (RTO) of random walks is inversely related to how information can be accessed during random surfing. We find analytically that the RTO probability for a given starting node shows a crossover from a slow to a fast decay behavior with time and the crossover time increases with the degree of the starting node. Furthermore, the RTO probability is almost constant in the early-time regime as the degree exponent approaches two. This result indicates that a random surfer can be effectively trapped at the hub and supports the necessity of the random jump strategy empirically used in the Google's search engine.

S1.00342 Rings and boxes in dissipative environments, BARUCH HOROVITZ, Ben-Gurion University, Israel — We study a particle on a ring in presence of a dissipative Caldeira-Leggett environment and derive its response to a DC field [1]. We find, through a 2-loop renormalization group analysis, that a large dissipation parameter η flows to a fixed point $\eta^R = \hbar/2\pi$. We also reexamine the mapping of this problem to that of the Coulomb box and show that the relaxation resistance, of recent interest, has a certain average that is quantized for $\eta > \eta^R$, leading to quantized noise. We propose a box experiment to detect this noise. When the particle carries a spin with spin-orbit interactions [2] we find that the spin correlations in the direction perpendicular to the ring are finite at long times, i.e. do not dephase, while the parallel components may decay as a power law at strong dissipation.

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[2] G. Zaránd, G. T. Zimányi and F. Wilhelm, Phys. Rev. B **62**, 8137 (2000).

S1.00343 JV Annealing Study of P3HT:PCBM OPV, ROY MURRAY, University of Delaware, STEVE HEGEDUS, IEC, University of Delaware, S. ISMAT SHAH, Department of Physics and Department of Materials Science, University of Delaware — Current-voltage (JV) analysis of poly (3-hexylthiophene) (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM) organic photovoltaics (OPV) yield valuable insight into the internal physics of devices. A simple lumped circuit model, previously used to analyze various thin film photovoltaics and more recently applied to OPV has been used to study annealing parameters. An annealing study of P3HT:PCBM blend OPV was carried out using the lumped circuit model. Limiting carrier lifetime-mobility product information and barrier data were extracted from the JV analysis of these devices. Collection loss characteristics were also obtained. The data was used to better characterize annealing effects.

S1.00344 Hydrogen adsorption around a hydrogen atom anchored in a graphene vacancy, GERARDO VAZQUEZ, FERNANDO MAGANA, Instituto de Fisica, UNAM, EDUARDO RANGEL, Instituto de Investigacion en Materiales, UNAM — In this work, we study the adsorption of hydrogen molecules around a hydrogen atom anchored in a graphene vacancy. We used density functional theory and molecular dynamics. To study the adsorption of hydrogen molecules on the system we used three hydrogen molecules around each hydrogen atom. It was found that raising the temperature of the system up to 900 K the hydrogen molecules remained linked to the system of graphene doped with hydrogen. The results show that doping graphene with atomic hydrogen can be useful to store hydrogen molecules in the system.

S1.00345 Beyond the Hubbard model: best effective single dressed band description of interacting atoms in optical lattices¹, ULF BISSBORT, FRANK DEURETZBACHER, WALTER HOFSTETTER, Goethe Universität Frankfurt a.M. — We construct the effective lowest-band Bose-Hubbard model incorporating interaction-induced on-site correlations. The model is based on ladder operators for local correlated states, which deviate from the usual Wannier creation and annihilation operators, allowing for a systematic construction of the most appropriate single-band low-energy description in form of the extended Bose-Hubbard model. A formulation of this model in terms of ladder operators not only naturally contains the previously found effective multi-body interactions, but also contains multi-body induced single particle tunneling, pair tunneling and nearest-neighbor interaction processes of higher orders. An alternative description of the same model can be formulated in terms of occupation-dependent Bose-Hubbard parameters. These multi-particle effects can be enhanced using Feshbach resonances, leading to corrections which are well within experimental reach and of significance to the phase diagram of ultracold bosonic atoms in an optical lattice. We analyze the energy reduction mechanism of interacting atoms on a local lattice site and show that this cannot be explained only by a spatial broadening of Wannier orbitals on a single particle level, which neglects correlations.

¹DFG Forschergruppe 801 grant

S1.00346 Doping-induced evolution of superconducting gap in iron-based superconductors: a point-contact Andreev reflection study of BaNi-122 single crystals¹, CONG REN, ZHAOSHENG WANG, BING SHEN, HUIQIAN LUO, XINGYE LU, ZHENYU WANG, JUN ZHU, JUN GONG, XINGYUAN HOU, CHUNHONG LI, LEI SHAN, Laboratory for Superconductivity, Institute of Physics, HUAN YANG, HAIHU WEN, Department of Physics, Nanjing University — We report a systematic investigation on c-axis point-contact Andreev reflection (PCAR) in superconducting $\text{BaFe}_{2-x}\text{Ni}_x\text{As}_2$ single crystals from underdoped to overdoped regions ($0.075 < x < 0.15$). At optimal doping ($x = 0.1$) the PCAR spectrum feature a dip-hump structure at the edge of the conductance gap, which corresponds to electron-boson coupling mode in energy scale. Two-superconducting-gap structure is resolved in the PCAR spectroscopy. In the $s_{\pm}$ scenario, quantitative analysis using a generalized Blonder-Tinkham-Klapwijk (BTK) formalism with two gaps: one isotropic and another angle dependent, suggest a nodeless state in strong-coupling limit with gap minima on the Fermi surfaces. Upon crossing above the optimal doping ($x > 0.1$), the PCAR spectrum show an in-gap sharp narrow peak at low bias, in contrast to the case of underdoped samples ($x < 0.1$), signaling the onset of deepened gap minima or nodes in the superconducting gap. This result provides evidence of the modulation of the gap amplitude with doping concentration, consistent with the calculations for the orbital dependent pair interaction mediated by the antiferromagne

¹This work is supported by the National Science Foundation of China, the Ministry of Science and Technology of China, and Chinese Academy of Sciences.

S1.00347 Discontinuous percolation transition in hidden in continuous percolation transition, YOUNG SUL CHO, BYUNGNAM KAHNG, Seoul National University — Diffusion limited cluster aggregation model is the well known model which describes the aggregation of diffusive clusters. In this model, time t is defined so as to describe the situation in which clusters follow Brownian motion. Thus t defined in this model can be regarded as real time. In this presentation, we introduce a new variable p which increases as much as $\delta p = 1/N$ whenever two distinct clusters aggregate. We use p instead of t to study a percolation problem in diffusion limited cluster aggregation model. Then, we find that a discontinuous percolation transition occurs if we observe the growth of the largest cluster as a function of the transformed variable p . This result implies that a continuous percolation transition can be observed as a discontinuous percolation transition when a controlled parameter is changed.

S1.00348 The magnetic flux periodicity in SNS square ring., HONG-YI CHEN, National Taiwan Normal University, CHUNG-PIN CHOU, Academia Sinica, Taiwan — In this work, we study the magnetic flux periodicity of d-wave superconductor-normal-superconductor square ring. The Hamiltonian of the SNS square ring is solved by using self-consistent Bogoliubov-de Gennes equations. The total current as a function of flux exhibits the hc/e period. As we increase the length of the normal metal, the hc/e period becomes $hc/2e$ period. Furthermore, we also investigate the behavior of the supercurrent in SNS and SIS junctions and the phase variation of the Josephson current.

S1.00349 High Pressure Ultrasonic and Transport Studies of Cerium Skutterudite Thermoelectrics¹, MATTHEW JACOBSEN, WEI LIU, WEI ZHU, Mineral Physics Institute, Stony Brook University, QIANG LI, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, BAOSHENG LI, Mineral Physics Institute, Stony Brook University — In the effort to find more efficient thermoelectric materials, some skutterudite materials based on CoSb_3 have shown that these materials have the potential of being effective at elevated temperatures. This work will present high pressure ultrasonic and transport measurements on the cerium filled versions of this parent compound, $\text{CeFe}_4\text{Sb}_{12}$ and $\text{CeFe}_3\text{CoSb}_{12}$. A previous study on these materials showed an anomaly in the equation of state for these materials originally attributed to the vitrification of a Methanol:Ethanol pressure medium. However, the studies performed as a part of this work demonstrate that, while this may be partly to blame, there is some contribution due to a real effect in this material.

¹This work was supported by DoE/NNSA (DEFG5209NA29458 to BL). Portions of this work were carried out at the National Synchrotron Light Source, which is supported by the US DoE, Divisions of Materials and Chemical Sciences under Ct. No. DE-AC02-76CH00016

S1.00350 Topological Superfluid in P-band Optical Lattice¹, YA-JIE WU, JING HE, CHUN-LI ZANG, SU-PENG KOU, Department of physics, Beijing Normal University, CONDENSED MATTER PHYSICS GROUP TEAM — By studying p-band fermionic system with nearest neighbor attractive interaction we find translation symmetry protected Z_2 topological superfluid (TSF) that is characterized by a special fermion parity pattern at high symmetry points in momentum space $k = (0, 0)$, $(0, \pi)$, $(\pi, 0)$, (π, π) . Such Z_2 TSF supports the robust Majorana edge modes and a new type of low energy excitation - (supersymmetric) Z_2 link-excitation.

¹The authors would like to thank W. M. Liu, C. Wu, H. Zhai, S. Chen for helpful conversations. This work is supported by NFSC Grant No. 10874017, 11174035, National Basic Research Program of China (973 Program) under the grant No. 2011CB921803.

Wednesday, February 29, 2012 2:30PM - 5:30PM –
Session T1 DAMOP: Hybrid Systems, Optomechanics and Macroscopic Systems at the Quantum Limit II 203

2:30PM T1.00001 Coupling propagating acoustic waves to quantum circuits, MARTIN GUSTAFSSON, Chalmers University of Technology, PAULO SANTOS, Paul-Drude-Institut für Festkörperelektronik, GÖRAN JOHANSSON, PER DELSING, Chalmers University of Technology — We present a method for coupling propagating Surface Acoustic Waves (SAW) to charge sensitive quantum circuits, by direct piezoelectric charge induction. Using an RF-Single Electron Transistor¹ as a high-performance electrometer, and employing an on-chip mixing technique², we demonstrate ultra-high displacement sensitivity in the gigahertz frequency range, and an averaged detection sensitivity below the single-phonon level. Based on these experimental results, we discuss how the method can be enhanced and extended to superconducting qubits, and what roles Surface Acoustic Waves could potentially play in novel hybrid quantum devices.

¹R.J. Schoelkopf, P. Wahlgren, A.A. Kozhevnikov, P. Delsing, and D.E. Prober, Science. **280**, 1238 (1998).

²R. Knobel, C.S. Yung, and A.N. Cleland, Appl. Phys. Lett. **81**, 532 (2002).

2:42PM T1.00002 Single Crystal Diamond Mechanical Resonators¹ , PREETI OVARTCHAIYAPONG, BRYAN MYERS, PAUL LAURIA, ANIA BLESZYNSKI JAYICH, University of California Santa Barbara — We report on the fabrication and measurement of single crystal diamond mechanical resonators. This is an important step towards realizing diamond photonics, optomechanics, and diamond-based scanning magnetometers. We present measurements of mechanical quality factors in excess of 10,000 as well as estimates of the coupling to embedded nitrogen-vacancy (NV) centers through strain. Strain tuning the NV's zero-phonon line could facilitate coupling its spin state to a photonic network. We also discuss strain as a coupling mechanism between the spin and mechanical degree of freedom in a diamond based resonator.

¹This work was supported by UCSB and the AFOSR, FA9550-11-1-0013

2:54PM T1.00003 Resonant Optical Forces in Silicon Carbide Nanostructures , DONGFANG LI, RASHID ZIA, Brown University — Silicon carbide (SiC) materials are widely used for their exceptional electronic, mechanical, and thermal properties. For example, given its high stiffness to density ratio, SiC is an ideal material for mechanical resonators, and it has been explored for applications in nanoelectromechanical systems (NEMS). SiC also supports strong surface phonon-polariton resonances in the infrared region, which could enable its use for optomechanics. Similar to surface plasmon-polaritons supported by metal-dielectric interfaces, these surface waves at a SiC-vacuum interface can be used to guide and confine intense electromagnetic energy. Here, we investigate the resonant optical forces induced by phonon-polariton modes in different SiC nanostructures. Specifically, we calculate optical forces using the Maxwell Stress Tensor for three geometries: spherical particles, slab waveguides, and rectangular waveguides. We find that the high quality factor phonon-polariton modes in SiC can produce very large forces, more than two orders of magnitude larger than the plasmonic forces in similar metal nanostructures. These strong resonant forces, combined with its mechanical and thermal properties, make SiC a promising material for optomechanical applications.

3:06PM T1.00004 Quantum Mechanical Scattering in Nanoscale Systems¹ , A.G. GIANFRANCESCO, A. ILYASHENKO, C.R. BOUCHER, L.R. RAM-MOHAN, Worcester Polytechnic Institute — We investigate quantum scattering using the finite element method. Unlike textbook treatments employing asymptotic boundary conditions (BCs), we use modified BCs, which permits computation close to the near-field region and reduces the Cauchy BCs to Dirichlet BCs, greatly simplifying the analysis. Scattering from any finite quantum mechanical potential can be modeled, including scattering in a finite waveguide geometry and in the open domain. Being numerical, our analysis goes beyond the Born Approximation, and the finite element approach allows us to transcend geometric constraints. Results of the formulation will be presented with several case studies, including spin dependent scattering, demonstrating the high accuracy and flexibility attained in this approach.

¹This work was supported by AFRL/DARPA under contract #FA8650-10-1-7046, and by the National Science Foundation #ECS-0725427.

3:18PM T1.00005 Modeling time domain spectroscopy of electron-phonon coupled systems out of equilibrium , MICHAEL SENTEF, A.F. KEMPER, BRIAN MORITZ, T.P. DEVEREAUX, Stanford Institute for Materials and Energy Science, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA — Recent advances in Terahertz large-electric field generation and pump-probe spectroscopies resolving pico- and even femtosecond time scales allow to study the behavior of photoexcited solids out of equilibrium. The relaxation after the pump pulse typically involves very fast processes related to purely electronic degrees of freedom, but for the slower return back to equilibrium it is essential to understand the interplay of electronic and lattice degrees of freedom. We present a theoretical investigation of electron-phonon coupled systems out of equilibrium, with results for various quantities (electronic distribution function, time-resolved angle-resolved photoemission, charge current). Our results show that the experimentally observed behavior can be related to the underlying microscopic properties of the system.

3:30PM T1.00006 Modeling lattice interaction in non-equilibrium pump-probe experiments , A.F. KEMPER, MICHAEL SENTEF, BRIAN MORITZ, T.P. DEVEREAUX, Stanford Institute for Materials and Energy Science — In past years, advances in experimental laser technology have allowed for the study of materials at ever shorter timescales. In these pump-probe experiments, after excitation by the pulse, the systems evolve back to equilibrium through its inherent relaxation processes, which are typically temporally separated by their characteristic timescales. Among the slower processes are the electron-phonon interactions, which carry the majority of the energy transferred to the electrons away into the lattice. We present a direct calculation of the characteristic timescales for systems driven out of equilibrium via a short pulse and allowed to relax via electron-phonon interactions. We make a direct connection between the observable timescales and the microscopic specifics, both via decay rates and oscillations in various photon-spectroscopies.

3:42PM T1.00007 Fluctuation Induced Forces for Surface Relief Gratings , JEF WAGNER, ROYA ZANDI, University of California Riverside, THORSTEN EMIG, Laboratoire de Physique Theorique et Modeles Statistiques Universite Paris Sud — In 1948 H. G. B. Casimir predicted that two flat parallel neutral perfectly conducting plates would attract each other due to the quantum fluctuations of the electromagnetic field. Since then progress has been made to allow one to calculate the interaction energy due to both quantum and thermal fluctuations between two objects of almost arbitrary shape and material properties. This work focuses on interaction with at least one object described by a surface relief grating. The Casimir energy is calculated using the scattering matrix approach, and the scattering matrix of the periodic surface is calculated using the C method from electromagnetic grating theory. The strengths and limitations of the method with regards to calculating the Casimir energy are discussed, and the results for simple 1-D and 2-D periodic structures are shown.

3:54PM T1.00008 Superfluid to Mott-Insulator Transition in Thermodynamic Limit of 1D Coupled Cavity Array , ADAM G. D'SOUZA, BARRY C. SANDERS, DAVID L. FEDER, IQIS, University of Calgary — In recent years, there has been great interest in simulating condensed matter models with quantum optical systems, which are usually characterized by a high degree of experimental control. One such model is the Jaynes-Cummings-Hubbard (JCH) model, an analog for the Bose-Hubbard (BH) model, in which mobile photons interact with atoms localized within a regular lattice of weakly coupled cavities. Finite system Density Matrix Renormalization Group (DMRG) studies have predicted a superfluid (SF) to Mott insulator (MI) transition in the phase diagram of the JCH model, and finite-size scaling has been used to determine the phase boundary in the thermodynamic limit. In this work, we directly numerically investigate the JCH model in the thermodynamic limit using infinite-system DMRG. The preliminary results indicate that the properties of the expected SF state are not wholly consistent with those of a conventional superfluid.

4:06PM T1.00009 Dirac Exciton-Polariton Condensates in a Triangular Lattice , NA YOUNG KIM, Stanford University, KENICHIRO KUSUDO, National Institute of Informatics, SVEN HOEFLING, ALFRED FORCHÉL, University of Wuerzburg, YOSHIHISA YAMAMOTO, Stanford University — Microcavity exciton-polaritons are quantum bose particles arising from the strong light-matter coupling between cavity photons and quantum well excitons. Recently, we have investigated the behavior of condensates in artificial lattice geometries in two-dimension (2D). Coherent *p*- and *d*-orbital state in a 2D square lattice is recently observed. Here we investigate exciton-polariton condensates at Dirac points formed in a 2D triangular lattice and experimental mapping of Dirac dispersion and discuss the interaction effect. We anticipate that the preparation of high-orbital condensates can be further extended to probe dynamical quantum phase transition in a controlled manner as quantum simulation applications.

4:18PM T1.00010 Numerical Study of the Bose-Einstein Condensation of Exciton-Polaritons ,

ASLAN KASIMOV, JESUS SIERRA, King Abdullah University of Science and Technology, RADA-MARIA WEISHÄUPL, Vienna University — Using the complex Gross-Pitaevskii equation (cGPE) with pumping and decay terms that models the Bose-Einstein condensate of exciton-polaritons, we numerically investigate the dynamics of instability of its radially symmetric steady solutions. We develop accurate algorithms for computing the steady state solution, the linear stability spectra, as well as the full nonlinear solutions of the cGPE. We accurately compute the thresholds of instability that depend, e.g. on the strength and size of the polariton pumping spot and observe the formation of vortices and such complex dynamics as the formation of vortex lattices and nucleation.

4:30PM T1.00011 Formation and decay of a Bose-Einstein condensate of trapped dipole ex-

citons , GERMAN KOLMAKOV, OLEG BERMAN, ROMAN KEZERASHVILI, New York City College of Technology CUNY, YURII LOZOVIK, Institute of Spectroscopy RAS — We study the nonlinear dynamics of formation and decay of a Bose-Einstein condensate of dipole excitons trapped in an external confining potential in coupled quantum wells. The problem is considered within an analytical approach and in numerical simulations. The trap restricts the spatial distribution of excitons and results in non-uniform density distribution in the exciton cloud. We demonstrate that under typical experimental conditions, regardless of a long-range nonlocal interaction of the dipole excitons, the system can be described by a generalized Gross-Pitaevskii equation with the local interaction between the excitons, and we find the effective interaction constant. In the numerical simulations, we account for the finite lifetime of dipole excitons and generation of the excitons due to continuous laser pumping. We also discuss formation and decay of vortex states in the condensate.

4:42PM T1.00012 Measurement of Casimir force with magnetic materials Alexandr Banishev, Chia-Cheng Chang, Umar Mohideen Department of Physics and Astronomy, University of Cal-

ifornia, Riverside, USA , ALEXANDR BANISHEV, CHIA-CHENG CHANG, UMAR MOHIDEEN , Department of Physics and Astronomy, University of California, Riverside — The Casimir effect is important in various fields from atomic physics to nanotechnology. According to the Lifshitz theory of the Casimir force, the interaction between two objects depends both on their dielectric permittivity and magnetic permeability. Thus the role of magnetic properties on the Casimir force is interesting particularly due to the possibility of a reduction the Casimir force. In this report we will present the results of a Casimir force measurement between a magnetic material such as nickel coated on SiO₂ plate and a Au-coated sphere.

4:54PM T1.00013 Geometry and fluctuation induced (Casimir) forces ,

SHOMEK MUKHOPADHYAY, EHSAN NORUZIFAR, UMAR MOHIDEEN, University of California , Riverside — Since the original prediction of attraction between parallel, perfectly conducting plates by Casimir there has been significant amount of work done in extending the calculations to real materials, finite temperatures and micro or nanostructured geometries. Majority of the experimental work has been carried out in the sphere-plane geometry. In this talk we will present ongoing experimental work on sphere-cylinder and sphere-cone geometries using frequency modulated atomic force microscopy. We will discuss numerical results in the sphere cylinder geometry and the range of validity of the point force approximation(PFA).

5:06PM T1.00014 Temperature dependence of Casimir force ,

JUN XU, University of California, Riverside, RODRIGO CASTILLO-GARZA, University of Texas,Austin, ROBERT SCHAFER, SHOMEK MUKHOPADHYAY, UMAR MOHIDEEN, University of California, Riverside — Most of the experimental work till date on Casimir forces have been performed at or near room temperature. We report on our measurements of Casimir forces performed at liquid helium and liquid nitrogen temperatures using gold coated sphere and plate. These measurements were performed on a home built Atomic Force Microscope with a phase locked loop to track the frequency shift. We will discuss the results in the context of current theoretical understanding of temperature dependence in the sphere – plate geometry.

5:18PM T1.00015 Enhanced light-matter interactions of a single emitter coupled to a slot waveguide ,

MAIKEN H. MIKKELSEN, NITIPAT PHOLCHAI, PAVEL KOLCHIN, NSF Nanoscale Science and Engineering Center (NSEC), 3112 Etcheverry Hall, University of California, Berkeley, CA 94720, USA, JINYONG OH, M. SAIF ISLAM, Department of Electrical and Computer Engineering, 2064 Kemper Hall, University of California, Davis, CA95616, USA, XIANG ZHANG, NSF Nanoscale Science and Engineering Center (NSEC), 3112 Etcheverry Hall, University of California, Berkeley, CA 94720, USA — Traditionally, enhanced light-matter interactions are achieved using either plasmonic structures or photonic crystals. However, these structures suffer from inherent metal losses or narrow operating bandwidth. Instead, here we use an all-dielectric waveguide structure with ultra-small mode volume and low-loss and broadband capabilities. A slot-waveguide architecture is used for deep sub-wavelength light confinement in a low-index material surrounded by high-index barriers. Individual colloidal quantum dots are controllably coupled to this waveguide mode. A large Purcell enhancement is observed from lifetime measurements of the spontaneous emission rate of the quantum dot before and after coupling to the waveguide. Second order intensity correlation measurements verify that the observed fluorescence is indeed due to a single quantum dot. The demonstrated system is a promising broadband and low-loss platform for quantum information applications.

Wednesday, February 29, 2012 2:30PM - 5:30PM –

Session T2 FIP: Invited Session: PIRE in Condensed Matter 204AB

2:30PM T2.00001 Terahertz Dynamics in Carbon Nanomaterials¹ ,

JUNICHIRO KONO, Rice University — This NSF Partnerships for International Research and Education (PIRE) project supports a unique interdisciplinary and international partnership investigating terahertz (THz) dynamics in nanostructures. The 0.1 to 10 THz frequency range of the electromagnetic spectrum is where electrical transport and optical transitions merge, offering exciting opportunities to study a variety of novel physical phenomena in condensed matter. By combining THz technology and nanotechnology, we can advance our understanding of THz physics while improving and developing THz devices. Specifically, this PIRE research explores THz dynamics of electrons in carbon nanomaterials, namely, nanotubes and graphene — low-dimensional, *sp*²-bonded carbon systems with unique finite-frequency properties. Japan and the U.S. are global leaders in both THz research and carbon research, and stimulating cooperation is critical to further advance THz science and to commercialize products developed in the lab. However, obstacles exist for international collaboration — primarily linguistic and cultural barriers — and this PIRE project aims to address these barriers through the integration of our research and education programs. Our strong educational portfolio endeavours to cultivate interest in nanotechnology amongst young U.S. undergraduate students and encourage them to pursue graduate study and academic research in the physical sciences, especially those from underrepresented groups. Our award-winning International Research Experience for Undergraduates Program, NanoJapan, provides structured research internships in Japanese university laboratories with Japanese mentors — recognized as a model international education program for science and engineering students. The project builds the skill sets of nanoscience researchers and students by cultivating international and inter-cultural awareness, research expertise, and specific academic interests in nanotechnology. U.S. project partners include Rice University, the University of Florida, the University of Tulsa, the State University of New York at Buffalo, Southern Illinois University at Carbondale, and Texas A&M University. Japanese partners include: Osaka University, Chiba University, Shinshu University, Tohoku University, the University of Tokyo, the National Institute of Information and Communications Technology, the National Institute of Materials Science, Hokkaido University, RIKEN, and the University of Aizu.

¹This PIRE project is cofunded by the Office of International Science and Engineering, the Division of Electrical, Communications, and Cyber Systems, and the Division of Materials Research of the National Science Foundation.

3:06PM T2.00002 Petascale Many Body Methods for Complex Correlated Systems, THOMAS PRUSCHKE, Georg-August-Universität Göttingen — Correlated systems constitute an important class of materials in modern condensed matter physics. Correlation among electrons are at the heart of all ordering phenomena and many intriguing novel aspects, such as quantum phase transitions or topological insulators, observed in a variety of compounds. Yet, theoretically describing these phenomena is still a formidable task, even if one restricts the models used to the smallest possible set of degrees of freedom. Here, modern computer architectures play an essential role, and the joint effort to devise efficient algorithms and implement them on state-of-the-art hardware has become an extremely active field in condensed-matter research. To tackle this task single-handed is quite obviously not possible. The NSF-OISE funded PIRE collaboration “Graduate Education and Research in Petascale Many Body Methods for Complex Correlated Systems” is a successful initiative to bring together leading experts around the world to form a virtual international organization for addressing these emerging challenges and educate the next generation of computational condensed matter physicists. The collaboration includes research groups developing novel theoretical tools to reliably and systematically study correlated solids, experts in efficient computational algorithms needed to solve the emerging equations, and those able to use modern heterogeneous computer architectures to make them working tools for the growing community.

3:42PM T2.00003 Polymers at Interfaces: US-Korea International Research and Education Partnership¹, CHANG YEOL RYU, Rensselaer Polytechnic Institute — Our NSF program of Partnership for International Research and Education (PIRE) is focused on the development and training of graduate, undergraduate students and faculty members in the field of polymer physics by promoting both domestic and international research collaborations with specific exchange opportunities for both US and Korean participants. This collaborative effort by a group of 5 US faculty members is motivated by the global partnership with Korean polymer physicists to promote novel opportunities in polymer science research and education. Our PIRE program involves a focused research plan at the forefront of polymer physics based on the synthesis, separation, characterization, and theory of synthetic polymers in bulk and at interfaces. The multifaceted research activities spanning the areas of polymer synthesis, characterization, property modifications and their modeling will be presented to advance our knowledge on polymer behaviors at interfaces.

¹NSF OISE PIRE 0730243

4:18PM T2.00004 SPIRE, the “Spin Triangle”: Athens, Hamburg, Buenos Aires: Advancing Nanospintronics and Nanomagnetism¹, ARTHUR R. SMITH, Ohio University Nanoscale and Quantum Phenomena Institute — Future technological advances at the frontier of ‘elec’tronics will increasingly rely on the use of the spin property of the electron at ever smaller length scales. As a result, it is critical to make substantial efforts towards understanding and ultimately controlling spin and magnetism at the nanoscale. In SPIRE, the goal is to achieve these important scientific advancements through a unique combination of experimental and theoretical techniques, as well as complementary expertise and coherent efforts across three continents. The key experimental tool of choice is spin-polarized scanning tunneling microscopy – the premier method for accessing the spin structure of surfaces and nanostructures with resolution down to the atomic scale. At the same time, atom and molecule deposition and manipulation schemes are added in order to both atomically engineer, and precisely investigate, novel nanoscale spin structures. These efforts are being applied to an array of physical systems, including single magnetic atomic layers, self-assembled 2-D molecular arrays, single adatoms and molecules, and alloyed spintronic materials. Efforts are aimed at exploring complex spin structures and phenomena occurring in these systems. At the same time, the problems are approached, and in some cases guided, by the use of leading theoretical tools, including analytical approaches such as renormalization group theory, and computational approaches such as first principles density functional theory. The scientific goals of the project are achieved by a collaborative effort with the international partners, engaging students at all levels who, through their research experiences both at home and abroad, gain international research outlooks as well as understandings of cultural differences, by working on intriguing problems of mutual interest. A novel scientific journalism internship program based at Ohio University furthers the project’s broader impacts.

¹The NSF PIRE program is gratefully acknowledged.

4:54PM T2.00005 Super-PIRE: International Consortium for Proving Novel Superconductors¹, YASUTOMO UEMURA, Department of Physics, Columbia University — The Super-PIRE project aims to study high-T_c cuprates, FeAs, heavy-fermion and other unconventional superconductors by using neutron scattering, muon spin relaxation, X-ray scattering, optical conductivity, ARPES and STM measurements in international collaboration. The project includes US PI’s Billinge, Pasupathy, Uemura (Columbia), and Dai (UTK/ORNL), Project Partner (PP) Balatsky (LANL), and foreign PI’s Uchida, Tajima, Maekawa, Eisaki (Japan), Hayden (UK), Wang (China), Luke (Canada), and about 40 additional “Local Experts” from institutions of the PI/PP’s. In this talk, we introduce the organization of the project, initial scientific products including 4 papers published in Nature group journals, and the out-reach effort centered in organizing special graduate and undergraduate courses at Columbia recorded as voice-synchronized ppt presentations, and then broadcasted in a class-room of Tokyo University. Homepage address: <http://www.phys.utk.edu/superpire/members.html>

¹NSF OISE-0968226

Wednesday, February 29, 2012 2:30PM - 5:30PM – Session T4 DAMOP: Vortices, Rotation, and Synthetic Gauge Fields 205C

2:30PM T4.00001 Rotating Ultracold Fermi Gases: Reduction in the Moment of Inertia Above the Superfluid Transition Temperature, K. LEVIN, VIVEK MISHRA, DAN WULIN, James Franck Institute, University of Chicago — There has been considerable interest in the viscosity of ultracold Fermi gases which is found to be anomalously suppressed even in the normal phase. This suppression, believed to derive from pseudogap effects, is also associated with a reduction in the moment of inertia, as measured by the Duke group. In this talk we address the relationship between viscosity and the reduced moment of inertia. We emphasize the very strong relation of the latter to the anomalous normal state diamagnetism of the high temperature superconductors. We present a simple physical picture for the origin of these related phenomena. Our picture gains strong support from establishing sum rule compatibility and leads to testable predictions.

2:42PM T4.00002 Vortices in spin-orbit-coupled Bose-Einstein condensates, JURAJ RADIC, TIGRAN A. SEDRAKYAN, Joint Quantum Institute, University of Maryland, College Park, IAN B. SPIELMAN, Joint Quantum Institute, University of Maryland, College Park and NIST, Gaithersburg, VICTOR GALITSKI, Joint Quantum Institute, University of Maryland, College Park — We discuss realistic methods to create vortices in spin-orbit-coupled Bose-Einstein condensates. We show that, contrary to common intuition, rotation of the trap containing a spin-orbit-coupled condensate does not lead to an equilibrium state with static vortex structures but gives rise instead to intrinsically time-dependent Hamiltonian. We propose alternative methods to create stable static vortex configurations: (1) to rotate both the lasers and the anisotropic trap; and (2) to impose a synthetic Abelian field on top of synthetic spin-orbit interactions. We derive the effective Hamiltonians for spin-orbit condensates under such perturbations for most currently known realistic laser schemes that induce synthetic spin-orbit couplings and we solve the Gross-Pitaevskii equation for several experimentally relevant regimes. The new interesting effects include spatial separation of left- and right-moving spin-orbit condensates and the appearance of unusual vortex arrangements.

2:54PM T4.00003 2D Vortex Dynamics and Quantum Tunneling in the Lowest Landau Level Limit, ROHIT HEGDE, Department of Physics, University of Texas at Austin, CHARLES B. HANNA, Department of Physics, Boise State University, ALLAN H. MACDONALD, Department of Physics, University of Texas at Austin — We examine the collective excitation spectrum of a rapidly rotating cold Bose gas in the lowest Landau level regime. The Gross-Pitaevskii action can be equivalently expressed in terms of the angular momentum state expansion of the boson field or in terms of 2D vortex positions. We emphasize the very different role of visible and invisible vortices in the latter formulation and discuss the significance of non-standard non-local Berry phase coupling between separated vortices in the boson action. We also consider dissipative quantum tunneling of a single vortex, allowing for linear coupling to a bath of quadratic fluctuations of the lattice following the Caldeira-Leggett model, and comment on differences between the lowest Landau level limit and the case of vortices in a slowly rotating superfluid.

3:06PM T4.00004 Screening properties and phase transitions in unconventional plasmas for Ising-type quantum Hall states¹, EGIL V. HERLAND, Norwegian University of Science and Technology, EGOR BABAEV, UMass Amherst and KTH Stockholm, PARSA BENDERSON, Microsoft Research, Station Q, VICTOR GURARIE, University of Colorado, Boulder, CHETAN NAYAK, Microsoft Research, Station Q and University of California, Santa Barbara, ASLE SUDBO, Norwegian University of Science and Technology — Utilizing large-scale Monte-Carlo simulations, we investigate an unconventional two-component classical plasma in two dimensions that interacts with two different Coulomb interactions. This plasma controls the behavior of the norms and overlaps of the quantum-mechanical wavefunctions of Ising-type quantum Hall states. It also relates to a model for a rotating two-component Bose-Einstein condensate with an Andreev-Bashkin drag interaction. The plasma differs fundamentally from that which is associated with the two-dimensional XY model and Abelian fractional quantum Hall states. We find that this unconventional plasma undergoes a Berezinskii-Kosterlitz-Thouless phase transition from an insulator to a metal and that the parameter values corresponding to Ising-type quantum Hall states lie on the metallic side of this transition. This result verifies the required properties of the unconventional plasma used to demonstrate that Ising-type quantum Hall states possess quasiparticles with non-Abelian braiding statistics.

¹Supported by the Knut and Alice Wallenberg Foundation, NSF grants No. DMR-0955902, No. PHY-0904017, DARPA QuEST program, NRC Grant No. 205591/V30 (FRINAT).

3:18PM T4.00005 Edge excitations of bosonic fractional quantum Hall phases in optical lattices, JONAS KJALL, JOEL MOORE, University of California, Berkeley — With the rapid development in ultracold gases, the realization of a fractional quantum Hall state on a lattice draws nearer. We investigate the impact of finite size effects in these kind of systems including different trapping potentials. A good understanding of finite size effects is essential for designing experiments and the edge excitations will likely be the best way to experimentally determine the topological order of the bulk. We find different fractional quantum Hall phases for bosons in a circular harmonic trap as the flux of the synthetic gauge field is varied, including phases like $\nu = 1/2$ and $\nu = 2/3$ with different edge spectra.

3:30PM T4.00006 Finite temperature phase structures of hard-core bosons in an optical lattice with a synthetic magnetic field¹, KENICHI KASAMATSU, YUKI NAKANO, TETSUO MATSUI, Department of Physics, Kinki University — We study finite temperature phase structures of hard-core bosons in a two-dimensional optical lattice subject to a synthetic magnetic field by employing the gauged CP¹ model. Based on the extensive Monte Carlo simulations, we study their phase structures at finite temperatures for several values of the magnetic flux per plaquette of the lattice and mean particle density. Despite the presence of the particle number fluctuation, the thermodynamic properties are qualitatively similar to those of the frustrated XY model with only the phase as a dynamical variable.

¹One of the authors (K.K.) is supported in part by Grant-in-Aid for Scientific Research (Grant No. 21740267) from MEXT, Japan.

3:42PM T4.00007 Modulated superfluid phases of lattice bosons in a non-abelian gauge field¹, WILLIAM COLE, SHIZHONG ZHANG, NANDINI TRIVEDI, Department of Physics, The Ohio State University, Columbus OH 43210 — We consider the two-component Bose-Hubbard model subject to non-abelian gauge fields that give rise to spin-orbit coupling. We obtain the phase diagram based on an extended mean field theory and find many exotic superfluid phases (polarized, striped, checkerboard). We characterize the superfluid phases by finding their collective excitations within random phase approximation (RPA) and discuss the possibility of novel topological defects.

¹We acknowledge support from ARO W911NF-08-1-0338, DARPA OLE program (WC,SZ) and NSF DMR-0907275 (NT).

3:54PM T4.00008 ABSTRACT WITHDRAWN —

4:06PM T4.00009 Bosons under an artificial staggered magnetic field in an optical ladder, MIN-CHUL CHA, IN-HO JEON, TAE-YANG AN, Department of Applied Physics, Hanyang University, Ansan, Gyeonggi-do, 426-791 Korea, CCMPL TEAM — We calculate the ground state properties of cold bosons in an frustrated optical ladder due to an artificial staggered magnetic field. By investigating the momentum distribution of bosons via a Lanczos diagonalization method, we find the signature of the transition from the Meissner to vortex states as a function of the staggering strength of the field. Various states with different frustrations are discussed.

4:18PM T4.00010 Chiral Mott insulator of kinetically frustrated bosons¹, ARUN PARAMAKANTI, University of Toronto, ARYA DHAR, Indian Institute of Astrophysics, MAHESWAR MAJI, Indian Institute of Science, TAPAN MISHRA, Indian Institute of Astrophysics, SUBROTO MUKERJEE, Indian Institute of Science, RAMESH PAI, Goa University — We study the phase diagram of the fully frustrated Bose Hubbard (FFBH) model - the presence of a π -flux through each plaquette leads to kinetic frustration for the bosons making this a nontrivial model of quantum frustration. The FFBH model is equivalent to a model of frustrated quantum XY spins, or a fully frustrated Josephson junction array where one tunes the ratio of the charging energy to the Josephson coupling. Using Monte Carlo simulations and DMRG calculations on a ladder, we show that the ground state of this model is, at intermediate correlations, a Chiral Mott insulator which supports staggered loop currents. We characterize this Mott phase as a vortex supersolid or an exciton condensate and discuss experimental observables and generalizations.

¹NSERC of Canada, CIFAR, DST (Govt of India)

4:30PM T4.00011 Mean Field Dynamics of Spin-Orbit Coupled Bose-Einstein Condensates, YONGPING ZHANG, LI MAO, CHUANWEI ZHANG, Department of Physics and Astronomy, Washington State University, Pullman, WA — We derive the mean-field Gross-Pitaevskii equation for spin-orbit coupled Bose-Einstein condensates by taking account that the pseudospin states of atoms are superpositions of the hyperfine states with different scattering lengths. The ground state phases of the condensate in a harmonic trap are obtained numerically in various parameter regions. We find a new oscillation period in the center of mass motion of the condensate subject to a sudden shift of the harmonic trap. The oscillation period is dependent on the direction of the shift of the harmonic trap, linearly proportional to the spin-orbit coupling strength, and independent on the interaction strength.

4:42PM T4.00012 Rotation of supersolids in cold atomic condensates¹, SANKALPA GHOSH, RASHI SACHDEVA, Indian Institute of Technology, Delhi — In the framework of Gross Pitaevskii equation, with non-local interaction, we study the formation of Supersolid phase and the effect of rotation on such a system. The effect of rotation is to induce vortex patterns in such Supersolid phase, whose structures are in principle, different from the ordinary vortex in Superfluids. At sufficiently high rotation, these vortices arrange in the form of a lattice and thus, one has to take into account the interplay of two lattice structures, the Supersolid crystal lattice and the vortex lattice induced by rotation. We aim to study the elastic properties of such a system and compare it with the corresponding superfluid phase.

¹Physics Department, Indian Institute of Technology, Delhi

4:54PM T4.00013 Rashbons: Emergent bosonic fermion-pairs in synthetic non-Abelian gauge fields¹, JAYANTHA P. VYASANAKERE, VIJAY B. SHENOY, Indian Institute of Science Bangalore — In presence of a synthetic non-Abelian gauge field that produces a Rashba like spin-orbit interaction, a collection of weakly interacting fermions undergoes a crossover from a BCS ground state to a BEC ground state when the strength of the gauge field is increased [PRB 84, 014512 (2011)]. The BEC that is obtained at large gauge coupling strengths is a condensate of tightly bound bosonic fermion-pairs called rashbons. This study reveals a new qualitative aspect that the rashbon state ceases to exist when the center of mass momentum of the fermions exceeds a critical value of the order of the gauge coupling strength. The study allows us to estimate the transition temperature of the rashbon BEC, and suggests a route to enhance the exponentially small transition temperature of the system with a fixed weak attraction to the order of the Fermi temperature by tuning the strength of the non-Abelian gauge field. The absence of the rashbon states at large momenta, suggests a regime in parameter space where the normal state of the system will be a dynamical mixture of uncondensed rashbons and unpaired helical fermions. Such a state should show many novel features including pseudogap physics.

¹Supported by DST and DAE, India

5:06PM T4.00014 Evolution of the structure of vortex core across the BCS-BEC crossover induced by a synthetic non-Abelian gauge field¹, NABYENDU DAS, JAYANTHA P. VYASANAKERE, VIJAY B. SHENOY, Indian Institute of Science Bangalore — We study the evolution of the structure of vortex core of fermionic superfluids with increasing strength of a non-Abelian gauge field which induces a spin-orbit interaction. Using the Bogoliubov de-Gennes formulation, we study the spectrum of core states both in the BCS limit (small gauge coupling) and in the rashbon BEC limit where the superfluid is a condensate of rashbons. We show that the novel features of rashbon dispersion, the vanishing of the bound state at finite centre of mass momentum, result in a larger core region for vortices in the rashbon BEC.

¹Supported by DST and DAE, India

5:18PM T4.00015 ABSTRACT WITHDRAWN —

Wednesday, February 29, 2012 2:30PM - 5:18PM —
Session T5 DCMP: Assembly of Atoms and Molecules in Adsorption Systems 206A

2:30PM T5.00001 Chirality Recognition and Transition Mechanism of prochiral Molecules on metals¹, YELIANG WANG, BING YANG, HUANYAO CUN, NAN JIANG, SHIXUAN DU, HONG-JUN GAO, Institute of Physics, Chinese Academy of Sciences, Beijing100190, China, K-H ERNST COLLABORATION², YUE WANG COLLABORATION³ — The self-assemble behavior of prochiral species and the induced high-order chirality by 2D confinement on solid surfaces, including (1) QA16C molecules on a Au(111) surface and (2) molecule-metallic (TPA-Fe) complex on Cu(110) as well as their transferring process will be presented. Initial stages of a chiral phase transition in the molecule monolayer on metal surfaces were investigated by scanning tunneling microscopy (STM) at submolecular resolution. The prochiral QA16C molecules form a homochiral lamella phase at low coverages upon adsorption. A transition to a racemate lattice is observed with increasing coverage. Enantiomers of a homochiral lamella line become specifically substituted by opposite enantiomers such that a heterochiral structure evolves. A "chiral replacement" model is proposed for the transition: enantiomers replace QA molecules in enantiopure phase, leading to racemic one. Our findings are significant for the understanding and control of chiral phase transitions in related molecular systems like liquid crystals.

¹NSFC, China

²Empa, Swiss

³Jilin University, China

2:42PM T5.00002 A Library of the Nanoscale Self-Assembly of Amino Acids on Metal Surfaces, ERIN ISKI, ESMERALDA YITAMBEN, NATHAN GUISENGER, Argonne National Lab — The investigation of the hierarchical self-assembly of amino acids on surfaces represents a unique test-bed for the origin of enantio-favoritism in biology and the transmission of chirality from single molecules to complete surface layers. These chiral systems, in particular the assembly of isoleucine and alanine on Cu(111), represent a direct link to the understanding of certain biological processes, specifically the preference for some amino acids to form alpha helices vs. beta-pleated sheets in the secondary structure of proteins. Low temperature, ultra-high vacuum, scanning tunneling microscopy (LT UHV-STM) is used to study the hierarchical self-assembly of different amino acids on a Cu(111) single crystal in an effort to build a library of their two-dimensional structure with molecular-scale resolution for enhanced protein and peptide studies. Both enantiopure and racemic structures are studied in order to elucidate how chirality can affect the self-assembly of the amino acids. In some cases, density functional theory (DFT) models can be used to confirm the experimental structure. The advent of such a library with fully resolved, two-dimensional structures at different molecular coverages would address some of the complex questions surrounding the preferential formation of alpha helices vs. beta-pleated sheets in proteins and lead to a better understanding of the key role played by these amino acids in protein sequencing.

2:54PM T5.00003 Surface Patterning of Benzene Carboxylic Acids on Graphite: Influence of structure, solvent, and concentration on molecular self-assembly, GINA FLORIO, KIMBERLY STISO, JOSEPH CAMPANELLI, KIMBERLY DESSOURCES, TRUDI FOLKES, St. John's University — Scanning tunneling microscopy (STM) was used to investigate the molecular self-assembly of four different benzene carboxylic acid derivatives at the liquid/graphite interface: pyromellitic acid (1,2,4,5-benzenetetracarboxylic acid), trimellitic acid (1,2,4-benzenetricarboxylic acid), trimesic acid (1,3,5-benzenetricarboxylic acid), and 1,3,5-benzenetriacetic acid. A range of two dimensional networks are observed that depend sensitively on the number of carboxylic acids present, the nature of the solvent, and the solution concentration. We will describe our recent efforts to determine (a) the preferential two-dimensional structure(s) for each benzene carboxylic acid at the liquid/graphite interface, (b) the thermodynamic and kinetic factors influencing self-assembly (or lack thereof), (c) the role solvent plays in the assembly, (e) the effect of *in situ* versus *ex situ* dilution on surface packing density, and (f) the temporal evolution of the self-assembled monolayer. Results of computational analysis of analog molecules and model monolayer films will also be presented to aid assignment of network structures and to provide a qualitative picture of surface adsorption and network formation.

3:06PM T5.00004 Distinct Monolayer Structure of DH6T Films Grown on Untreated SiO₂¹, JOSEF SPALENKA, EHREN MANNEBACH, PHILLIP JOHNSON, University of Wisconsin-Madison, ZHONGHOU CAI, Advance Photon Source-Argonne National Laboratory, FRANZ HIMPSEL, PAUL EVANS, University of Wisconsin-Madison — Due to the relatively weak interactions between neighboring molecules, thin films of vacuum evaporated organic semiconductors can have different properties in monolayer films as compared to several monolayer and bulk-like films. We have structurally characterized monolayer and several monolayer films of dihexyl-sexithiophene (DH6T) using grazing incidence diffraction and near-edge x-ray absorption fine structure spectroscopy (NEXAFS), and electrically characterized low-coverage FET structures during deposition. The structural data indicate a distinct phase of DH6T in the monolayer which has a distorted unit cell and a distinct NEXAFS signature compared to thicker films. The hole mobility of $\sim 0.8 \text{ cm}^2/\text{V}\cdot\text{s}$ is approximately an order of magnitude higher than previously reported for vacuum deposited thick films of DH6T on unmodified SiO₂ surfaces.

¹This work supported by the National Science Foundation through the University of Wisconsin Materials Research Science and Engineering Center under Grant No. DMR-1121288

3:18PM T5.00005 Nucleation of C₆₀ on ultrathin SiO₂¹, BRAD CONRAD, Appalachian State University, MICHELLE GROCE, WILLIAM CULLEN, ALBERTO PIMPINELLI, ELLEN WILLIAMS, TED EINSTEIN, University of Maryland College Park — We utilize scanning tunneling microscopy to characterize the nucleation, growth, and morphology of C₆₀ on ultrathin SiO₂ grown at room temperature. C₆₀ thin films are deposited *in situ* by physical vapor deposition with thicknesses varying from <0.05 to ~ 1 ML. Island size and capture zone distributions are examined for a varied flux rate and substrate deposition temperature. The C₆₀ critical nucleus size is observed to change between monomers and dimers non-monotonically from 300 K to 500 K. Results will be discussed in terms of recent capture zone studies and analysis methods. Relation to device fabrication will be discussed. doi:10.1016/j.susc.2011.08.020

¹We gratefully acknowledge support and SEF support from the NSF MRSEC under grant DMR 05-20471, support from the University of Maryland CNAM, and support from Appalachian State University.

3:30PM T5.00006 Scanning Tunneling Spectroscopy of Self-assembled Nanoribbons of C₆₀-Diamantane Hybrid Molecules, J.C. RANDEL, F.C. NIESTEMSKI, Stanford University, S. MELINTE, UCL Belgium, H.C. MANOHARAN, Stanford University — As transistors approach the nanoscale, single molecules become viable alternatives for macroscopic devices. In terms of utilizing carbon, diamondoids – single cages of the bulk diamond lattice – have recently become available as the smallest units to explore these structures. We use low temperature scanning tunneling microscopy to perform electron mapping studies on self-assembled monolayers of novel hybrid molecules consisting of a single C₆₀ fused with the double diamond cage called diamantane. Unlike standard C₆₀ self-assembled monolayers, these hybrid molecules tend to form strips or nanoribbon assemblies as opposed to large-scale single sheets. We find spectroscopic differences between these hybrid molecules and the “parent” molecule C₆₀, and utilize spatial mapping to find electronic differences in the edge states of these ribbons. We discuss these results in terms of rectification and the potential of these hybrid molecules for molecular electronics.

3:42PM T5.00007 Pentacene pinwheels: chiral heterostructures between C₆₀ and pentacene¹, JEFFREY R. GUEST, JOSEPH A. SMERDON, OZGUN SUZER, NATHAN P. GUISSINGER, Center for Nanoscale Materials, Argonne National Laboratory — Pentacene and C₆₀ are archetypal molecules for optically active acceptor-donor molecular heterojunctions and for the study of self-assembly on surfaces. Using UHV STM, we demonstrate that these molecules - despite their high degree of symmetry - can self-assemble into *chiral* heterostructures when C₆₀ is deposited on a 'random-tiling' [1] of pentacene (Pn) on Cu(111). Two different chiral heterostructures with a central C₆₀ surrounded by 6 Pns in a 'pinwheel' formation are identified: one with interlocking Pns of mixed chirality and one with shared Pns of the same chirality. The latter is observed in single chirality domains that include hundreds of pinwheels. These complex structures are solved unambiguously through the analysis of the STM images and an understanding of Pn adsorption on Cu(111) [2]. Chiral light-absorbing acceptor-donor heterojunctions may provide a powerful platform for detecting and manipulating charge, spin, and optical polarization; we will discuss the electronic properties of these structures, and the prospect for studying the interaction of these types of systems with light using our laser-STM approach.

[1] J. A. Smerdon et al., Phys. Rev. B **84**, 165436 (2011).

[2] J. Lagoute et al, Phys. Rev. B **70**, 245415 (2004).

¹This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357 and “SISGR” Contract No. DE-FG02-09ER16109.

3:54PM T5.00008 Interaction of CO₂ with Oxygen Adatoms on Rutile TiO₂(110) Surface¹, XIAO LIN, YEOHOON YOON, ZHENJUN LI, ZHI-TAO WANG, BRUCE D. KAY, IGOR LYUBINETSKY, ROGER ROUSSEAU, ZDENEK DOHNALEK, Pacific Northwest National Laboratory — On TiO₂(110), oxygen vacancies (V_O's) act as the primary catalytic sites and as such they have been extensively investigated. However, only a few studies have been reported about the interactions of adsorbates with oxygen adatoms (O_a's) that are created by O₂ dissociation in V_O's. Here, we report a combined scanning tunneling microscopy (STM) / density functional theory (DFT) study of CO₂ on bare and O_a covered TiO₂(110). STM images of TiO₂(110) surfaces obtained before and after *in-situ* dose at ~ 50 K show that CO₂ molecules preferentially adsorb next to O_a's forming CO₂/O_a complexes. Temperature dependent studies further reveal that the CO₂ binding energy next to O_a's is similar to that on V_O's. Additional CO₂ molecules are found to diffuse rapidly along the Ti row between two CO₂/O_a complexes. Due to the slow STM sampling rate the images display a time average of all CO₂ binding configurations on the Ti rows and reveal differences in the populations found on ideal Ti sites and Ti sites next to V_O's.

¹X.L. is grateful for the support of the Linus Pauling Distinguished Postdoctoral Fellowship Program at PNNL. This work was supported by the US Department of Energy, Office of Basic Energy Sciences. The research was performed using EMSL.

4:06PM T5.00009 Adsorption of CO₂ in porous MCM-41 and MCM-48 using small angle scattering¹, BO WANG, Dept. of Physics and LENS, Indiana University, NARAYAN DAS, LENS, Indiana University, GARFIELD WARREN, Dept. of Physics, Indiana University, JOHN RUPP, MARIA MASTALERZ, Indiana Geological Survey, Indiana University, TIMOTHY PRISK, PAUL SOKOL, Dept. of Physics and LENS, Indiana University, DEPARTMENT OF PHYSICS AND LOW ENERGY NEUTRON SOURCE(LENS), INDIANA UNIVERSITY TEAM, INDIANA GEOLOGICAL SURVEY, INDIANA UNIVERSITY COLLABORATION — Adsorption of CO₂ onto the surface of nanopores in organic rich materials, such as shale and coals, is of great interest for understanding the processes associated with geological sequestration. These natural materials have complex pore structures which make the interpretation of experimental sorption measurements complicated. MCMs are synthetic materials with a well-defined regular porous structure that provides an ideal substrate to evaluate the models for the adsorption of gases (CO₂) into nanopores. Samples of MCM-41 and MCM-48 were synthesized at Indiana University and were characterized by nitrogen adsorption isotherms and Small Angle X-ray Scattering (SAXS). SANS studies were carried out on MCMs with different pore sizes as a function of pore filling and the results are interpreted in terms of layer growth models.

¹Construction of LENS was supported by the NSF grants DMR-0220560 and DMR-0320627, the 21st Century Science and Technology fund of Indiana, Indiana University, and the Department of Defense. Operation of LENS is supported by Indiana University.

4:18PM T5.00010 Self-Assembly of Metal Phthalocyanine on Silicon Studied by Scanning Probe Microscopy¹, SEAN WAGNER, PENG PENG ZHANG, Michigan State University — Integration of molecular electronics into modern electronics requires an improved understanding and control of hetero-interfaces between organic molecules and semiconductor surfaces. Supramolecular assembly provides flexibility in building up complex and functional materials with nanometer scale precision over large surface areas. To study behavior at the hetero-interface, we perform supramolecular assembly of Zinc Phthalocyanine (ZnPc) on deactivated Si(111)B $\sqrt{3}\times\sqrt{3}$ and on Si(111) 7×7 . Using scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) methods both the morphology and electronic structures of the self-assembled monolayer are investigated. Molecule-molecule and molecule-substrate interactions will be discussed.

¹This work was funded by the Office of Science Early Career Research Program (DE-SC0006400) through the Office of Basic Energy Sciences, U.S. Department of Energy.

4:30PM T5.00011 Decomposition of NH₃ and H₂ on ZrB₂ (0001) surface¹, WERONIKA WALKOSZ, Materials Science Division, Argonne National Laboratory, KEDAR MANANDHAR, MICHAEL TRENARY, Department of Chemistry, University of Illinois at Chicago, PETER ZAPOL, Materials Science Division, Argonne National Laboratory — Group III nitride semiconductors (AlN, GaN, InN, and their alloys) are important materials for applications in solid-state lighting, optoelectronics, and photovoltaics. However, the lack of lattice-matched substrates for their growth results in less than optimal material quality. In the last decade, zirconium diboride (ZrB₂) has been demonstrated as a promising substrate for GaN growth because of its similar lattice constant and thermal expansion properties when compared to the nitride. Moreover, the high electrical conductivity of ZrB₂ makes it desirable for many GaN-based device applications. In this talk, we present results of density functional theory calculations for the reactivity of the ZrB₂(0001) surface towards the N precursor, NH₃, and the carrier gas, H₂, commonly used in metal organic chemical vapor deposition and molecular beam epitaxy of nitrides. Two different terminations of ZrB₂(0001) surface, the Zr and B terminations, are considered and assessed in terms of their catalytic properties toward NH₃ and H₂ decomposition. The theoretical results are analyzed in connection with our recent XPS and RAIRS measurements.

¹Work supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357.

4:42PM T5.00012 Morphology of monolayer films on quasicrystalline surfaces from the phase field crystal model, JOERG ROTTLE, BENEDIKT ZIEBARTH, MICHAEL GREENWOOD, University of British Columbia — We present a computational study of the morphology of adsorbed monolayers on quasicrystalline surfaces with five- and seven-fold symmetry. The Phase Field Crystal model is employed to first simulate the growth of the quasicrystal surfaces and a two-dimensional film is then coupled elastically to the substrate. We find several different pseudomorphic phases for different types of surfaces and monolayer/substrate interactions, and quantify them by computing local order parameters. In agreement with recent experiments using colloids in quasiperiodic light fields, we find that the formation of quasicrystalline order is greatly inhibited on the seven-fold surfaces.

4:54PM T5.00013 Depolarization and bonding in quasi-one-dimensional Na structures on Cu(001), GUIDO FRATESI, ETSF, CNISM, Materials Science Department, Milano-Bicocca University, Milan, Italy — The formation of quasi-one-dimensional (Q1D) $p(n \times 2)$ -Na/Cu(001) structures is addressed by density-functional theory investigations for adsorbate coverage from low to the saturation one. A general dependence of the dipole moment on the given configuration is deduced by extending that for uniform distributions, and is greatly affecting the energetics of the Na overlayer. Larger stability for Q1D arrangements aligned along $[110]$ and $[\bar{1}\bar{1}0]$ holds at coverage larger than 0.2 ML, in agreement with low-temperature He scattering experiments, and can be explained by a reduced dipole-dipole repulsion for the $p(4 \times 2)$ with respect to hex-like distributions. Interatomic bonding charge displacements along zig-zag rows of Na atoms further support the Q1D structure and contribute significantly to the surface corrugation as seen by the He probe.

5:06PM T5.00014 Adsorption of In atoms on In/Si(111)- 8×2 studied by variable-temperature STM, HYUNGJOON SHIM, JONGHOON YEO, DONGCHUL SHIN, GEUNSEOP LEE, Department of Physics, Inha University — We have investigated adsorption of In atoms on In/Si(111) surface by using variable-temperature scanning tunneling microscope. At room temperature, the adsorbed In atoms on 4×1 are invisible due to its high mobility on a 4×1 phase. As the temperature decreases below the phase transition temperature, additional In atoms begin to appear being fixed on a 8×2 phase. The In atoms are mostly adsorbed as an isolated atoms (monomers) and paired ones (dimers) on In chains. The adsorbed In atom induces a local phase-flipping in the vicinity, resulting in a phase shift along the chain direction. Occasional hopping of isolated In atoms along the chain direction are observable at 80K. The hopping occurs preferentially in the direction of the local phase-flipping side. Formation of dimers in relation to the preferential hopping direction will be discussed.

Wednesday, February 29, 2012 2:30PM - 5:18PM —

Session T6 DMP: Focus Session: Graphene Devices - Spin, Charge, and Superconductivity

2:30PM T6.00001 Spin Relaxation and Spin Transport in Graphene , M.W. WU, Department of Physics, University of Science and Technology of China, Hefei, Anhui, 230026, China — In this talk we are going to present our theoretical investigations on spin dynamics of graphene under various conditions based on a fully microscopic kinetic-spin-Bloch-equation approach [1]. We manage to nail down the solo spin relaxation mechanism of graphene in measurements from two leading groups, one in US and one in the Netherland. Many novel effects of the electron-electron Coulomb interaction on spin relaxation in graphene are addressed. Our theory can have nice agreement with experimental data.
[1] M. W. Wu, J. H. Jiang, and M. Q. Weng, "Spin dynamics in semiconductors," Phys. Rep. **493**, 61 (2010).

3:06PM T6.00002 Spin and charge transport in high-mobility suspended graphene¹ , MARCOS GUIMARAES, PAUL ZOMER, ALINA VELIGURA, THOMAS MAASSEN, IVAN VERA-MARUN, NIKOLAOS TOMBROS, BART VAN WEES, Physics of Nanodevices, Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — Recent developments in graphene device fabrication techniques have made it possible to study the intrinsic properties of graphene by removing the substrate and making it suspended. Here we report electronic spin and charge transport measurements in high-mobility (over 70 000 cm²/Vs) suspended graphene devices. To achieve this high quality we apply a large DC current density to heat the graphene flake, removing contaminations. We show that using the current annealing technique it is possible to produce ballistic nanoconstrictions, where quantized conductance at zero magnetic field is observed [N. Tombros et al., Nat. Phys. **7**, 697 (2011)]. Studying the evolution of the position of the conductance plateaus in magnetic field we determine the width of the constriction. Spin transport measurements using ferromagnetic electrodes were also performed in our suspended graphene devices [M.H.D. Guimarães et al., in preparation]. Analyzing non-local Hanle precession measurements we extract the spin relaxation time and the spin diffusion constant as a function of the charge carrier density. Combining our measurements with computer simulations we show that the measured spin relaxation times are limited by the non-cleaned regions of the device.

¹This work was financially supported by the Dutch Foundation for Fundamental Research on Matter (FOM) and NWO and realized using NanoLab.NL facilities.

3:18PM T6.00003 Conductance Quantization in Graphene Nanoconstrictions , DRAGOMIR DAVIDOVIC, CHRISTOPHER MALEC, BRADLEY ELKUS, Georgia Institute of Technology — We present measurements of conductance quantization in a narrow Graphene constriction, of approximate width 200nm. Graphene is exfoliated on top of a Silicon Dioxide, and is not suspended. In high mobility samples ($>10000\text{cm}^2\text{V}^{-1}\text{s}^{-1}$), we observe pinch-off at the Dirac point, with a resistance at 4.2K of $\sim 40\text{k}\Omega$. As a function of gate voltage at zero magnetic field, the conductance displays a few plateaus with the quantized value close to $G_0=2e^2/h$, indicating valley degeneracy splitting. At high carrier density ($>5\times 10^{12}/\text{cm}^2$) in a weak magnetic field, conductance exhibits strong beating in the Shubnikov-de Haas oscillations, which is also attributed to the valley splitting, analogous the Rashba interaction beats observed in the Shubnikov-de Haas oscillations in semiconducting quantum wells. In the Quantum Hall regime, the conductance of the constriction has quantized values $nG_0, \dots$. In comparison, measurements in the leads of the constriction display normal graphene behavior without the valley splitting.

3:30PM T6.00004 Chiral orbital current and anomalous magnetic moment in gapped graphene , MIKITO KOSHINO, Dept. of Physics, Tohoku University — We present a low-energy effective theory to describe chiral orbital current and anomalous magnetic moment in graphene monolayer and multilayers with band gap. We show that an electronic state of general Bloch system may intrinsically contain a quantum mechanical current circulation due to interband matrix elements. In gapped graphene, the current circulation is opposite between different valleys (K,K'), and the corresponding magnetic moment accounts for valley splitting of Landau levels. In gapped bilayer and ABC-stacked multilayer graphenes, in particular, the valley-dependent magnetic moment causes a huge paramagnetism at low energy, and a full valley polarization is possible up to relatively high electron density. The formulation also applies to gapped surface states of three-dimensional topological insulator, where the chiral orbital current is related to the magneto-electric response of the system.

3:42PM T6.00005 Quantum coherence versus dephasing effects in the giant spin Hall current and nonlocal voltage in magnetotransport through multiterminal graphene bridges¹ , CHIEN-LIANG CHEN, CHING-RAY CHANG, Department of Physics, National Taiwan University, Taipei 10617, Taiwan, BRANISLAV K. NIKOLIC, Department of Physics and Astronomy, University of Delaware, Newark, DE 19716, USA — Motivated by the recent experiments [D. A. Abanin *et al.*, Science **323**, 328 (2011)] probing magnetotransport near the Dirac point in six-terminal graphene bridges from low to room temperature, we develop a nonequilibrium Green function (NEGF) theory of this phenomena. In the quantum-coherent regime, we find giant spin Hall (SH) conductance in four-terminal bridges, where the SH current is pure only at the Dirac point (DP), as well as the nonlocal voltage at a remote location in six-terminal bridges where the direct and inverse SH effect operate at the same time. The momentum-relaxing dephasing reduces their values at the DP by two orders of magnitude while washing out features away from the DP. Our theory is based on the linearized version of the Meir-Wingreen formula applied to multiterminal devices where dephasing is introduced through the self-energy within the active region of the bridge and currents and voltages are connected via generalized matrix of conductance coefficients.

¹This work was supported in part by the DOE Grant No. DE-FG02-07ER46374 through the Center for Spintronics and Biodetection at the University of Delaware.

3:54PM T6.00006 ABSTRACT WITHDRAWN —

4:06PM T6.00007 Magneto-transport studies of hydrogenated graphene¹ , BERNARD MATIS, National Research Council/Naval Research Laboratory, FELIPE BULAT, Sotera Defense Solutions, Inc., ADAM FRIEDMAN, BRIAN HOUSTON, JEFFREY BALDWIN, Naval Research Laboratory — We study the magnetoresistance of hydrogenated graphene devices on a SiO₂ substrate. A large negative magnetoresistance of up to 30% in a field of 2.5T is observed at low temperatures and at the film's charge neutrality point without any sign of saturation. A detailed analysis of the gate voltage dependence demonstrates a suppression of the large, negative magnetoresistance, which appears to be driven by a crossover from strong localization at low carrier concentrations to weak localization at higher carrier concentrations. Evidence of electron-hole symmetry breaking is found in the magnetic field traces at low temperature.

¹B. Matis performed this work courtesy of an National Research Council postdoctoral Fellowship. This work was supported by the Office of Naval Research.

4:18PM T6.00008 In-plane magnetotransport in gapped bilayer graphene, MATTHIAS STUDER, University of British Columbia, Canada, SIFANG CHEN, JOSHUA FOLK, University of British Columbia — The tunability of the band gap in bilayer graphene using a perpendicular electric field makes this material a promising candidate for future carbon electronics.¹ Recent studies show that the residual conductivity at low temperature in the gapped state with zero total carrier density is a result of hopping transport.² We have studied the transport in this regime as a function of an in-plane magnetic field. We find a strikingly strong positive magnetoresistance that leads to an increase of the resistance by an order of magnitude at 10 Teslas in-plane magnetic field compared to the value at 0 T. The temperature dependence of the resistance is well described by variable range hopping transport for all magnetic field values, and suggests that the hopping range is strongly dependent on the in-plane magnetic field.

¹J. B. Oostinga et al., *Nat. Mat.*, **7**, 151 (2007) Y. Zhang et al., *Nature*, **459**, 820 (2009)

²T. Taychatanapat and P. Jarillo-Herrero, *Phys. Rev. Lett.*, **105**, 166601, (2010)

4:30PM T6.00009 Direct measurements of the current-phase relation in graphene Josephson junctions, CHRISTOPHER ENGLISH, CIHAN KURTER, D.J. VAN HARLINGEN, NADYA MASON, University of Illinois at Urbana-Champaign — The current-phase relation (CPR) of a Josephson junction can provide key information about the microscopic processes and symmetries that influence the supercurrent. In this talk, we present CPR results on Josephson junctions containing single-layer graphene as a weak link. The measurements are based on a phase-sensitive SQUID technique in which we determine the supercurrent amplitude and phase as a function of both temperature and electrostatic doping (gate voltage). We present CPR measurements of narrow junctions (5 - 12 μm) in the diffusive regime spanning the temperature range of 25 - 800 mK. We compare these data with previous CPR measurements on wide junctions in the temperature range of 800 - 900 mK.

4:42PM T6.00010 Anomalous supercurrent switching in graphene under proximity e¹, ALEX LEVCHENKO, Michigan State University, U.C. COSKUN, M. BRENNER, T. HYMEL, University of Illinois at Urbana-Champaign, V. VAKARYUK, Argonne National Laboratory, A. BEZRYADIN, University of Illinois at Urbana-Champaign — We report a study of hysteretic current-voltage characteristics in superconductor-graphene-superconductor (SGS) junctions. The stochastic nature of the phase slips is characterized by measuring the distribution of the switching currents. We find that in SGS junctions the dispersion of the switching current scales with temperature as $\sigma_I \propto T^{\alpha_G}$ with $\alpha_G \approx 1/3$. This observation is in sharp contrast with the known Josephson junction behavior where $\sigma_I \propto T^{\alpha_J}$ with $\alpha_J = 2/3$. We propose an explanation using a modified version of Kurkijarvi's theory for the flux stability in rf-SQUID and attribute this anomalous effect to the temperature dependence of the critical current which persists down to low temperatures.

¹This work was supported by ONR grant N000140910689 and DOE grant DE-AC0298CH1088

4:54PM T6.00011 Gate Tuning of Different Phase-Particle Escape Regimes in Graphene-Based Josephson Junctions, GIL-HO LEE, DONGCHAN JEONG, JAE-HYUN CHOI, Dept. of Physics, POSTECH, YONG-JOO DOH, Dept. of Display and Semiconductor Physics, Korea University Sejong Campus, HU-JONG LEE, Dept. of Physics, POSTECH — Graphene-based Josephson junctions (GJJs) provide a unique system to investigate superconducting proximity effect with in-situ tunable Josephson coupling strength. While the phase-coherent behaviors of a GJJ under a magnetic field and microwave irradiation have been observed previously¹, we investigated the stochastic switching behavior of the supercurrent in this system. Here, we present the observation of the three different escaping regimes for a phase particle from a washboard potential of the GJJ; macroscopic quantum tunneling (MQT), thermal activation (TA), and phase diffusion (PD).² The crossover temperature (T_{MQT}^*) between the classical to quantum regime can be controlled by the gate voltage, implying that discrete energy levels of a phase particle are also gate-tunable. Moreover, direct observation of energy level quantization (ELQ) by microwave spectroscopy shows the consistent gate dependence of T_{MQT}^* . A new class of hybrid quantum devices such as a gate-tunable phase qubit is potentially realized by utilizing the MQT and ELQ behavior of the GJJs.

¹H. B. Heersche et al., *Nature* 446, 56 (2007); D. Jeong et al. *Phys. Rev. B* 83, 094503 (2011).

²G.-H. Lee et al., *Phys. Rev. Lett.* 107, 146605 (2011).

5:06PM T6.00012 Tunable resistance anomaly in graphene-superconductor hybrid structure¹, ATIKUR RAHMAN, JANICE WYNN GUIKEMA, NINA MARKOVIC, Johns Hopkins University — Junctions between superconductors and normal metals often exhibit a resistance anomaly: near the superconducting transition temperature, the resistance increases above the normal-state value. The magnitude of the excess resistance varies over a wide range, decreases in a magnetic field and can depend on the driving current and the history of thermal cycling. Several physical mechanisms have been proposed to explain the origin of the excess resistance, including the fluctuation-induced resistive state, nonequilibrium quasiparticle charge imbalance around NS boundary or phase-slip centers. Here we present an electronic transport study of superconductor-graphene hybrid structures that show a large resistance anomaly which survives even in presence of a relatively large magnetic field. We will show that, by changing the graphene resistance, we can tune the magnitude and position of the resistance peak and will examine the applicability of existing models to explain our results.

¹This work is supported in part by NSF DMR-1106167.

Wednesday, February 29, 2012 2:30PM - 5:06PM –
Session T7 DCOMP DMP: Focus Session: Computational Design of Materials: Electronic Structure Methods for Materials - Faster and More Accurate 207

2:30PM T7.00001 How accurate is Density Functional Theory in Predicting Reaction Energies Relevant to Phase Stability?, GEOFFROY HAUTIER, SHYUE PING ONG, ANUBHAV JAIN, CHARLES J. MOORE, GERBRAND CEDER, Massachusetts Institute of Technology — Density Functional Theory (DFT) computations can be used to build computational phase diagrams that are used to understand the stability of known phases but also to assess the stability of novel, predicted compounds. The quality and predictive power of those phase diagrams rely on the accuracy of DFT in modeling reaction energies and we will present in this talk the results of a large scale comparison between experimentally measured and DFT computed reaction energies. For starters, we will show that only certain reaction energies are directly relevant to phase stability of multicomponent systems and that very often those reaction energies are not the commonly studied reactions from the elements. Using data from different experimental thermochemical tables and DFT high-throughput computing, we will present the results of a statistical study based on more than 130 reaction energies relevant to phase stability and from binary oxides to ternary oxides. We will show that the typical error are around 30 meV/at and therefore an order of magnitude lower than the errors in reaction energies from the elements. Finally, we will discuss the broad implications of our results on the evaluation of ab initio phase diagrams and on the computational prediction of new solid phases.

2:42PM T7.00002 Correcting Density Functional Theory for Accurate Predictions of Compound Enthalpies of Formation:Fitted elemental-phase Reference Energies (FERE)¹, VLADAN STEVANOVIC, XIUWEN ZHANG, STEPHAN LANY, National Renewable Energy Laboratory, Golden CO, ALEX ZUNGER, University of Colorado, Boulder CO — The first step in the Inverse Design of materials is the assessment of their thermodynamic stability and the needed growth conditions. The compound enthalpy of formation (ΔH_f) is a quantity that provides these information. However, standard ab-initio approaches are known for their large errors in calculating ΔH_f of semiconducting and insulating compounds. In this talk I will present an approach, based on GGA+U total energies for compounds and fitted elemental-phase reference energies (FERE), that corrects GGA+U for the incomplete error cancellation between compound total energies and those of the pure elements, thereby resulting in ΔH_f values for insulating and semiconducting solids calculated with chemical accuracy. The FERE for 50 chemical elements we fit to a set of 252 measured ΔH_f of binary compounds (pnictides, chalcogenides and halides) and show accurate predictions also when applied to ternary compounds. I will discuss the application of the FERE approach in predicting new compounds, assess the accuracy of such predictions as well as comment on experimental efforts of our collaborators in growing some of the predicted materials.

¹Funded by DOE through Energy Frontiers Research Centers, Center for Inverse Design

2:54PM T7.00003 Correction to DFT Interaction Energies by an Empirical Dispersion Term Valid for a Range of Intermolecular Distances¹, CHRISTOS DELIGKARIS², JORGE H. RODRIGUEZ, Department of Physics, Purdue University — The computation of intermolecular interaction energies via commonly used density functionals is hindered by their inaccurate inclusion of medium and long range dispersion interactions. Computation of inter- and intra-molecule interaction energies as well as computational design of (bio)materials, requires a fairly accurate yet not overly expensive methodology. It is also desirable to compute intermolecular energies not only at their equilibrium (lowest energy) configurations but also over a range of distances. We present a method to compute intermolecular interaction energies by including an empirical correction for dispersion which is valid over a range of intermolecular distances. This is achieved by optimizing parameters that moderate the empirical correction by explicit comparison of density functional (GGA) energies with distance-dependent (DD) reference values obtained at the CCSD(T)/CBS limit. The resulting GGA-DD method yields interaction energies with an accuracy generally better than 1 kcal/mol for different types of noncovalent complexes, over a range of intermolecular distances and interaction strengths, relative to the expensive CCSD(T)/CBS standard

¹Supported, in part, by NSF CAREER award CHE-0349189

²Present address: Department of Physics, Drury University

3:06PM T7.00004 Accurate predictions of biomolecular interactions using density functional theory based semi-empirical alchemical derivatives in chemical compound space, ANATOLE VON LILIENFELD, Argonne National Laboratory — A small but relevant sub-set of chemical compound space is explored in terms of biomolecular interaction energies, and using analytical derivatives. When transmutating any two iso-electronic ligands their intermolecular energies are not necessarily monotonic functions, consequently the corresponding Hellmann-Feynman derivatives can fail to predict the right trends. Semi-empirical corrections, effectively linearizing the intermolecular energy in the interpolation parameter, promise to drastically improve the predictive power of these first order derivatives. For various biomolecules, including ellipticine interacting with DNA, we show that these semi-empirical derivatives yield predictions superior to alternative prediction schemes that are additive and derivative-free. As such, new evidence is presented in support of the conclusion that quantitative estimates of relevant properties of new molecules can be made without additional self-consistency calculations.

3:18PM T7.00005 Preliminary results in data mining for materials¹, DA GAO, YOUSEF SAAD, University of Minnesota at Twin Cities, JAMES CHELIKOWSKY, University of Texas at Austin — In recent years, materials scientists have started exploiting data mining techniques, i.e., methods for extracting meaningful information and patterns from data, for the discovery and design of materials. One of the grand challenges in this methodology is to establish correlations and intrinsic features in materials database in order to facilitate the extraction of useful information that can be exploited to discover new hypothetical materials. Using an atomic properties database of 110 elements, obtained from quantum mechanical calculations and several macroscopic properties database of binary compounds, we explored several sample data mining techniques to study the correlations among them with the goal of predicting macroscopic properties from knowledge of the atomic constituents. In this talk, preliminary results of such efforts will be presented to demonstrate how simple data mining can be applied in materials science and what they can achieve. These preliminary results indicate a good potential for data mining applications in materials science.

¹We would like to acknowledge support from the National Science Foundation under grants No. DMS-0810938, DMR-0940218, DMR-0941645 and OCI-1047997 and from the Welch Foundation under grant No. F-1708.

3:30PM T7.00006 Expediting Solutions for the Electronic Structure of Large Systems: A Spectrum Slicing Algorithm¹, GRADY SCHOFIELD, JAMES CHELIKOWSKY, University of Texas, YOUSEF SAAD, University of Minnesota — Solving the Kohn-Sham equation requires computing a set of low lying eigenpairs. The standard methods for computing such eigenpairs require two procedures: (a) maintaining the orthogonality of an approximation space, and (b) forming approximate eigenpairs with the Rayleigh-Ritz method. These two procedures scale cubically with the number of desired eigenpairs. We present a method, applicable to *any* large Hermitian eigenproblem, by which the spectrum is partitioned among distinct groups of processors. This “divide and conquer” approach serves as a parallelization scheme at the level of the solver, making it compatible with existing schemes that parallelize at a physical level, *e.g.*, k-points or symmetric representations, and at the level of primitive operations, matrix-vector multiplication. In addition, among all processor sets, the size of any approximation subspace is reduced, thereby reducing the cost of orthogonalization and the Rayleigh-Ritz method. We will explain the key aspects of the algorithm that give reliability, and demonstrate the accuracy of the algorithm by computing the electronic structure of a core-shell nanocrystal and a DNA segment. Overall scaling and the utility of the method for a wide variety of applications will be discussed.

¹We wish to acknowledge support from the National Science Foundation under grants No. DMR-0941645 and OCI-1047997 and from The Welch Foundation under grant No. F-1708.

3:42PM T7.00007 Density Functional Theory using Multiresolution Analysis with MADNESS, SCOTT THORNTON, ROBERT HARRISON, Joint Institute for Computational Sciences — We describe the first implementation of the all-electron Kohn-Sham density functional periodic solver (DFT) using multi-wavelets and fast integral equations using MADNESS (multiresolution adaptive numerical environment for scientific simulation; <http://code.google.com/p/m-a-d-n-e-s-s/>). The multiresolution nature of a multi-wavelet basis allows for fast computation with guaranteed precision. By reformulating the Kohn-Sham eigenvalue equation into the Lippmann-Schwinger equation, we can avoid using the derivative operator which allows better control of overall precision for the all-electron problem. Other highlights include the development of periodic integral operators with low-rank separation, an adaptable model potential for the nuclear potential, and an implementation for Hartree-Fock exchange.

3:54PM T7.00008 GPU speedup of the plane wave pseudopotential density functional theory calculations¹, LIN-WANG WANG, Material Science Division, Lawrence Berkeley National Lab, Berkeley, CA, 94720, WEILE JIA, ZONGYAN CAO, LONG WANG, XUEBIN CHI, Supercomputing Center, Computer Network Information Center, Chinese Academy of Sciences, Beijing, China, WEIGUO GAO, School of Mathematical Sciences, Fudan University, Shanghai, China — Plane wave (PW) pseudopotential density functional theory (DFT) calculation is the most widely used method for computational design of new materials. In this talk, we will present our recent work in using the graphics processing unit (GPU) to accelerate the PW-DFT calculations. Compared with the pure CPU calculation, the GPU machine with CUDA coding can speed up the calculation by 20 times for systems with a few hundred atoms, while still being able to scale to hundreds of CPU/GPU units. However, to reach this speedup, some algorithm changes are necessary. We will discuss these algorithm changes, and various computational kernels in a PW-DFT code, and their speedups in the GPU code. These include the FFT, the nonlocal projector, the orthogonalization and the diagonalization. We will also discuss the computational times for MPI communication, CPU/GPU memory copy, and floating point operation. We will present the hardware and library requirement to further speed up the calculations. Finally, the implication of the GPU speed up for new material design will be discussed.

¹This work is supported by SC/BES of U.S. Department of Energy under Contract No. DE-AC02-05CH11231, and NSF of China.

4:06PM T7.00009 Linear-scaling DFT+U applied to hole localization and Friedel oscillations in very dilute (Ga,Mn)As, ARASH MOSTOFI, Imperial College London, DAVID O'REGAN, Swiss Federal Institute of Technology Lausanne (EPFL), NICHOLAS HINE, Imperial College London, MICHAEL PAYNE, University of Cambridge — System-size and strong electronic correlation are two factors inhibiting the routine first-principles simulation of transition-metal doped nanostructures. Tackling these issues simultaneously, we have developed a linear-scaling implementation of the DFT+U method within the ONETEP code,¹ demonstrating scaling upto 7,000 atoms. Our implementation allows for nonorthogonal projectors,² which may be self-consistently optimized.³ We apply our approach to the prototypical dilute magnetic semiconductor (Ga,Mn)As. The ferromagnetic interaction between distant localized magnetic moments in (Ga,Mn)As is mediated by defect-induced holes, whose long-range character is critical. Our large-scale calculations on 1,728 atom super-cells enable us to study the localization and symmetry of the magnetization and hole in the very dilute (0.1%) limit, and to analyze the long-range Friedel oscillations.

¹Hine, Haynes, Mostofi, Skylaris & Payne, *Comp. Phys. Commun.*, **180**, 1041 (2009).

²O'Regan, Payne & Mostofi, *PRB* **83**, 245124 (2011).

³O'Regan, Hine, Payne & Mostofi, *PRB* **82**, 081102(R) (2010).

4:18PM T7.00010 G0W0 implementation using Lanczos algorithm and Sternheimer equation, JONATHAN LAFLAMME JANSSEN, NICOLAS BERUBE, GABRIEL ANTONIUS, MICHEL COTÉ, University of Montreal — The G0W0 approach is an accurate method to give a physical meaning to the eigenvalues obtained in density-functional theory (DFT) calculation. However, the calculation of such corrections with plane wave codes is currently prohibitive for systems with more than a few hundreds of electrons. What limits calculations to this system size is the need in current implementations to invert the dielectric matrix and the need to carry out summations over conduction bands. This talk presents a strategy to avoid both of these bottlenecks. In traditional plane wave implementations of G0W0, the dielectric matrix is expressed in a plane wave basis, which needs to be relatively big to properly describe the matrix. Here, we will explain how a Lanczos basis can be generated to substantially reduce the size of the matrix. Also, the number of conduction bands needed to reach convergence in the summations is usually an order of magnitude larger than the number of valence bands. Here, the calculation of the conduction states is avoided by reformulating the summations into linear equation problems (Sternheimer equations), which also substantially reduces the computation time. Preliminary results will be presented.

4:30PM T7.00011 Dynamical Cluster Approximation: Cluster Extension of CPA for Disordered System¹, CHINEDU EKUMA, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA, WEI KU, TOM BERLIJN, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York, 11973, USA, JUANA MORENO, MARK JARRELL, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA — The dynamical mean-field approximation (DMFA) or the coherent potential approximation (CPA) provides a convenient and effective method for studying disordered systems; however, non-local short range correlations of the disorder potential are neglected leading to a self-consistent single-site approximation. We combine the recently developed first principles method of Wei Ku and co-workers for the simulation of disordered systems with the dynamical cluster approximation (DCA) to develop a highly efficient means to treat disordered systems. We solve this model system using the DCA, which systematically incorporates short-range nonlocal correlations to the CPA. We apply this method to a number of model systems to illustrate where the DCA or a finite size simulation is more appropriate.

¹Work at LSU was funded in part by the National Science Foundation Award Number: EPS 1003897. Work at BNL is supported by the Department of Energy (DOE) CMSN

4:42PM T7.00012 Analyzing electron-electron correlations at nanoscale: a DFT+DMFT code for nanosystems¹, VOLODYMYR TURKOWSKI, ALAMGIR KABIR, TALAT S. RAHMAN, Physics Department and NSTC, University of Central Florida — We propose a DFT+DMFT approach to study electron-electron correlation effects in nanosized systems containing atoms with localized d- and f-electron states. For the purpose we have developed a nanoDFT+DMFT code which allows one to study the properties of systems containing up to several hundred atoms. The system geometry is first optimized using ab-initio electron structure calculations based on density-functional theory (DFT), and correlation effects are analyzed employing nonhomogeneous Dynamical Mean-Field Theory (DMFT) calculations with the iterated perturbation theory (IPT) approximation for the quantum impurity solver. To test the formalism we have evaluated the magnetic properties of several transition metal atom clusters and compared the results with those obtained from the exact diagonalization method (a few-atom clusters) and available experimental data (2-19 atom clusters). In particular, we find that the IPT-DMFT gives magnetic moments much closer to experimental values as compared to DFT calculations. We discuss possible extensions of the approach including application of more accurate quantum impurity solvers, such as Hirsch-Fye and Continuous-Time Quantum Monte Carlo. The application of the methodology to the nonequilibrium case is in progress.

¹Work supported in part by DOE Grants No. DOE-DE-FG02-07ER15842 and No. DOE-DE-FG02-07ER46354.

4:54PM T7.00013 Using Machine Learning to Accelerate Complex Atomic Structure Elucidation, WILLIAM BROUWER, LAZARO CALDERIN, JORGE SOFO, The Pennsylvania State University — Workers in various scientific disciplines seek to develop chemical models for extended and molecular systems. The modeling process revolves around the gradual refinement of model assumptions, through comparison of experimental and computational results. Solid state Nuclear Magnetic Resonance (NMR) is one such experimental technique, providing great insight into chemical order over Angstrom length scales. However, interpretation of spectra for complex materials is difficult, often requiring intensive simulations. Similarly, working forward from the model in order to produce experimental quantities via ab initio is computationally demanding. The work involved in these two significant steps, compounded by the need to iterate back and forth, drastically slows the discovery process for new materials. There is thus great motivation for the derivation of structural models directly from complex experimental data, the subject of this work. Using solid state NMR experimental datasets, in conjunction with ab initio calculations of measurable NMR parameters, a network of machine learning kernels are trained to rapidly yield structural details, on the basis of input NMR spectra. Results for an environmentally relevant material will be presented, and directions for future work.

Wednesday, February 29, 2012 2:30PM - 5:30PM – Session T8 DMP GMAG: Focus Session: Helical Phases and Skyrmions 208

2:30PM T8.00001 Spin waves in a skyrmion crystal¹, OLGA PETROVA, OLEG TCHERNYSHYOV, Johns Hopkins University — We derive the spectrum of low-frequency spin waves in skyrmion crystals observed recently in noncentrosymmetric ferromagnets [1-4]. We treat the skyrmion crystal as a superposition of three helices whose wavevectors form an equilateral triangle [1]. The low-frequency spin waves are Goldstone modes associated with displacements of skyrmions. Their dispersion is determined by the elastic properties of the skyrmion crystal and by the kinetic terms of the effective Lagrangian, which include both kinetic energy and a Berry phase term reflecting a non-trivial topology of magnetization. The Berry phase term acts like an effective magnetic field, mixing longitudinal and transverse vibrations into a gapped cyclotron mode and a twist wave with a quadratic dispersion [5].

- [1] Muehlbauer, Binz, Jonietz, Pfléiderer, Rosch, Neubauer, Georgii, Boeni, Science **323**, 915 (2009).
- [2] Muenzer, Neubauer, Adams, Muehlbauer, Franz, Jonietz, Georgii, et al., Phys. Rev. B **81**, 041203 (2010).
- [3] Yu, Onose, Kanazawa, Park, Han, Matsui, Nagaosa, Tokura, Nature **465**, 901 (2010).
- [4] Yu, Kanazawa, Onose, Kimoto, Zhang, Ishiwata, Matsui, Tokura, Nat. Mater. **10**, 106 (2011).
- [5] Petrova, Tchernyshyov, arXiv:1109.4990v2 [cond-mat.mes-hall]

¹This work was supported in part by the US National Science Foundation under Award No. DMR-1104753.

2:42PM T8.00002 Skyrmion contribution to thermopower of MnSi, ANA AKRAP, Department of Condensed Matter Physics, University of Geneva, CH-1211 Geneva 4, Switzerland, STEVAN ARSENIJEVIĆ, Institute of Condensed Matter Physics, Swiss Federal Institute of Technology, EPFL, CH-1015 Lausanne, Switzerland, CEDOMIR PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA, LÁSZLÓ FORRÓ, Institute of Condensed Matter Physics, Swiss Federal Institute of Technology, EPFL, CH-1015 Lausanne, Switzerland — Skyrmions have recently been theoretically predicted [1] and experimentally observed [2] in MnSi. To identify whether skyrmions contribute to thermoelectric transport, we present a detailed map of the temperature, pressure and magnetic field behavior of thermopower S in MnSi. $S/T(p, T)$ confirms the established phase diagram with Fermi liquid, non-Fermi liquid and partial order phases. In the high pressure non-Fermi liquid phase, $S(T)$ increases in the vicinity of the boundary with the Fermi liquid phase, at critical pressure $p_c \sim 14.5$ kbar. This may be linked to the scattering of conduction electrons on fluctuating amorphous skyrmions [1]. On the contrary, the thermopower decreases when an ordered lattice of skyrmions is established in the magnetic field. A small suppression of $S(T)$ is observed in a narrow region, for $27 \text{ K} < T < 29 \text{ K}$, and $0.1 \text{ T} < B < 0.3 \text{ T}$, corresponding to the ordered skyrmion A phase.

- [1] U. K. Rössler et al. Nature **442**, 797 (2006)
- [2] S. Mühlbauer, et al. Science **323**, 915 (2009)

2:54PM T8.00003 Quantum order-by-disorder near criticality and the secret of the partially ordered phase of MnSi, FRANK KRUGER, UNA KARAHASANOVIC, University of St Andrews, ANDREW GREEN, University College London — The vicinity of quantum phase transitions has proven fertile ground in the search for new quantum phases. We propose a physically motivated and unifying description of the phase reconstruction near metallic quantum-critical points using the idea of quantum order-by-disorder. Certain deformations of the Fermi surface associated with the onset of competing order enhance the phase space available for low-energy, particle-hole fluctuations and self-consistently lower the free energy. Applying the notion of quantum order-by-disorder to the itinerant helimagnet MnSi, we show that near to the quantum critical point, fluctuations lead to an increase of the spiral ordering wave vector and a reorientation away from the lattice favoured directions. The magnetic ordering pattern in this fluctuation-driven phase is found to be in excellent agreement with the neutron scattering data in the partially ordered phase of MnSi.

3:06PM T8.00004 Density-functional electronic structure and the origin of the Dzyaloshinskii-Moriya spin interaction in MnSi, K.V. SHANAVAS, S. SATPATHY, Department of Physics & Astronomy, University of Missouri — The metallic helimagnet MnSi has been found to exhibit skyrmionic spin textures when subjected to magnetic fields at low temperatures. The Dzyaloshinskii-Moriya (DM) interaction plays a key role in stabilizing the skyrmions, which arises from the anisotropic part of the super-exchange coupling and is of the form $\vec{D} \cdot (\vec{S}_i \times \vec{S}_j)$. The constant $\vec{D}$ depends on the strength of spin-orbit interaction of Mn d states and the orbital mixing induced by the distortion of MnSi₆ octahedra from the centrosymmetric rock salt phase. Using density functional theory based electronic structure calculations and symmetry analysis, we study the nature of the electronic ground state and the origin of the DM interaction in the B20 phase of MnSi. The ground state in the undistorted phase corresponds to d^6 configuration at Mn and p^2 at Si sites. The distortion reduces bandwidths and intermixes the ground state with the excited states, leading to a significant DM spin-orbit interaction.

3:18PM T8.00005 Criticality Induced First-Order Phase Transition in Dzyaloshinskii-Moriya Helimagnets, MARC JANOSCHEK¹, Los Alamos National Laboratory, MARKUS GARST, Universitaet zu Köln, ANDREAS BAUER, Technische Universitaet Muenchen, PASCAL KRAUTSCHEID, Universitaet zu Köln, ROBERT GEORGII, FRM II Technische Universitaet Muenchen, PETER BOENI, CHRISTIAN PFLEIDERER, Technische Universitaet Muenchen — Almost two centuries of research on phase transitions have repeatedly highlighted the importance of critical phenomena. One fascinating implication of critical phenomena is that critical fluctuations may drive the associated phase transition first order if symmetry allows them to assume enough phase space. As discussed by Brazovski, this is in particular the case if critical fluctuations become soft on a sphere in momentum space. By means of combined specific heat, magnetic susceptibility and neutron scattering measurements of the model helimagnet MnSi we show that this scenario is realized for the helimagnetic phase transition in Dzyaloshinskii-Moriya(DM) helimagnets with weak magnetic anisotropy. The remarkable agreement observed between experiment and theory clarifies the longstanding issue of the nature of the helimagnetic transition in MnSi, but more importantly, our calculations are entirely based on symmetry arguments, making this result relevant to DM helimagnets in general. This is in particular noteworthy in the light of a series of new discoveries that show that DM helimagnetism is at the heart of problems such as topological magnetism, multiferroics, and spintronics.

¹This work was performed while affiliated with UC San Diego, Technische Universitaet Muenchen, and Paul Scherrer Institut

3:30PM T8.00006 Tricriticality and giant magneto-elasticity in CoMnSi¹, KARL SANDEMAN, ZSOLT GERCSI, Imperial College London, ALEX BARCZA, University of Cambridge, KEVIN KNIGHT, ISIS, Rutherford Appleton Laboratory — Tricritical magnets have previously facilitated the study of different critical phenomena and scaling laws by varying external parameters (pressure, field and temperature) instead of composition. We have studied tricritical magnets driven by interest in the enhanced magnetocaloric effects seen at the first order side of a tricritical point where hysteresis can be minimised. Here we describe the results of microcalorimetry, Hall probe imaging, dilatometry, magnetometry and neutron diffraction experiments and density functional calculations. We build a picture of the relation between structure and magnetism in CoMnSi and find a giant magneto-elasticity that underpins the evolution of first order behavior in this metamagnetic helical antiferromagnet [2]. We are then able to use density functional theory to predict new metamagnets based on this insight. These have been successfully synthesized [3].

[1] K.G. Sandeman, *Magnetics Technology International* **1** 32 (2011).

[2] A. Barcza et al., *Phys. Rev. Lett.* **104** 247202 (2010).

[3] Z. Gercsi, K. Hono and K.G. Sandeman, *Phys. Rev. B* **83** 174403 (2011) and references therein.

¹The research leading to these results has received funding from the European Community's 7th Framework Programme under grant agreement 214864. K.G.S. gratefully acknowledges financial support from the Royal Society.

3:42PM T8.00007 Hall effect of spin-chirality origin in a triangular-lattice helimagnet Fe_{1.3}Sb, YUKI SHIOMI, MASAHIITO MOCHIZUKI, Department of Applied Physics, University of Tokyo, YOSHIO KANEKO, Multiferroics Project, ERATO, YOSHINORI TOKURA, Department of Applied Physics, University of Tokyo — We report on a topological Hall effect possibly induced by scalar spin chirality in a quasi-two-dimensional helimagnet Fe_{1+x}Sb. In the low-temperature region where the spins on interstitial-Fe (concentration $x \approx 0.3$) intervening the 120° spin-ordered triangular planes tend to freeze, a non-trivial component of Hall resistivity with opposite sign of the conventional anomalous Hall term is observed under magnetic field applied perpendicular to the triangular-lattice plane. The observed unconventional Hall effect is ascribed to the scalar spin chirality arising from the heptamer spin-clusters around the interstitial-Fe sites, which can be induced by the spin modulation by the Dzyaloshinsky-Moriya interaction.

3:54PM T8.00008 Vortex walls in helical magnets¹, FUXIANG LI, Dept. Physics and Astronomy, Texas A&M University, THOMAS NATTERMANN, Inst. Of Theoretical Physics, University of Cologne, D-50937, Cologne, Germany, VALERY POKROVSKY², Dept. Physics and Astronomy, Texas A&M University — The structure of domain walls determines to a large extent the properties of magnetic materials, in particular their hardness and switching behavior, it represents an essential ingredient of spintronics. In Bloch and Neel domain walls the magnetization rotates around a fixed axis in a one-dimensional magnetization profile. Surprisingly, domain walls in helical magnets, most relevant in multiferroics and metals, were never studied. We show that domain walls in helical magnets are fundamentally different from Bloch and Neel walls. They are generally two-dimensional patterns formed by a regular lattice of vortex singularities. Only at discrete exceptional orientations, domain walls are free of vortices, but still remain two-dimensional textures. In helical magnets with weak anisotropy the domain wall width and energy only weakly depend on the anisotropy, though domain wall does not exist without it. In conical phases vortices carry Berry phase flux resulting in the anomalous Hall effect. In multiferroics vortices are electrically charged allowing manipulating magnetic domain walls by the electric field. Our theory allows the interpretation of magnetic textures observed in helical magnetic structures.

¹This work has been supported by SFB 608 and by the DOE under the grant DE-FG02-06ER 46278.

²Landau Inst. for Theor. Physics, Russian Academy of Sciences, Chernogolovka, Moscow Distr, 142432

4:06PM T8.00009 Spin scalar chiral ordering and hidden positive biquadratic interaction in frustrated Kondo lattice systems, YUTAKA AKAGI, Dept. of Appl. Phys., Univ. of Tokyo, MASAFUMI UDAGAWA, Dept. of Appl. Phys., Univ. of Tokyo, MPI PKS, YUKITOSHI MOTOME, Dept. of Appl. Phys., Univ. of Tokyo — Recently, noncoplanar spin configurations with spin scalar chirality have drawn considerable attention as an origin of the anomalous Hall effect. In this mechanism, itinerant electrons acquire an internal magnetic field according to the solid angle spanning three spins through the so-called Berry phase, which can result in the anomalous Hall effect. In order to explore such nontrivial magnetic states in spin-charge coupled systems, we investigate a ferromagnetic Kondo lattice model on a triangular lattice by variational and perturbative calculations. As a result, we find that a noncoplanar four-sublattice spin ordering emerges near 1/4 filling, in addition to the 3/4 filling reported in the previous study. This new phase is stabilized in a wider parameter region compared to the 3/4 filling phase [1]. We also find that a kinetic-driven positive biquadratic interaction is critically enhanced and plays a crucial role on stabilizing a spin scalar chiral ordering near 1/4 filling. The origin of large positive biquadratic interaction is ascribed to the Fermi surface connection by the four sublattice ordering wave vectors, which we call the higher-order Kohn anomaly [2]. [1] Y. Akagi and Y. Motome, *J. Phys. Soc. Jpn.* **79** (2010) 083711. [2] Y. Akagi, M. Udagawa, and Y. Motome, submitted.

4:18PM T8.00010 First Principles Calculation of Helical Spin Order in Iron Perovskite SrFeO₃ and BaFeO₃, ZHI LI, Yukawa Institute for Theoretical Physics, Kyoto University — Motivated by recent discovery of ferromagnetism in cubic perovskite BaFeO₃ under small magnetic field, we investigate spin order in BaFeO₃ and isostructural SrFeO₃ by a first principles calculation using local spin density approximation (LSDA). We find that on-site Coulomb interaction U is necessary for obtaining helical spin order consistent with experiments. SrFeO₃ exhibits G-type helical order, while BaFeO₃ exhibits the A-type with very small wave vector. The A-type order is stabilized by lattice expansion. Small energy difference between the A-type and ferromagnetic orders explains ferromagnetism under small field. The LSDA+ U results are consistent with model calculation where negative charge-transfer energy in these compounds is explicitly taken into account.

4:30PM T8.00011 Investigation of the role of spin-texture on the Na_{0.46}CoO₂, J.W. KIM, E.-D. MUN, R. McDONALD, J. THOMPSON, I. MARTIN, C. BATISTA, V. ZAPF, LANL, P. MOLL, ETH-Zurich, A. MORPURGO, University of Geneva, D. ARGYRIOU, Helmholtz-Zentrum Berlin für Materialien und Energie — We will present magnetotransport properties and their relationship to a possible chiral spin texture in ultra-thin Na_{0.46}CoO₂ devices in high magnetic fields. This composition exhibits a weakly insulating state, with a frustrated local spin texture, unique, among the hexagonal Na_xCoO₂ family. Previous a large Hall effect was found for composition $x=0.5$ (M. Foo *et al.*, Phys. Rev. Lett. 92, 247001 (2004)) and prior high-field studies (L. Balicas *et al.*, Phys. Rev. Lett. 94, 236402 (2005).) have found the existence of a small Fermi surface in the system and a two-fold angular magnetoresistance. To date however, the Hall-conductivity has not been investigated in magnetic fields strong enough to suppress the charge-order, above 41 T. Herein, we investigate the role of local spin-texture (in the charge-ordered state) on the Hall conductance by measuring both bulk and devices with only several monolayers thick in strong magnetic fields. Our investigations under magnetic fields ($B < 60$ T) show that the high resistivity charge-order region is suppressed with out-of-plane field at $B \sim 41$ T with highly non-monotonic $-\rho_{xy}$ with a maximum at $B \sim 27$ T and rapidly decreases to zero. However, magnetization measurements show no significant features within measurement accuracy indicating that magnetization changes are small at the field-induced phase transition. Recent theoretical advances suggest that this compound exhibits a quantum Hall state coupled with spin chirality (I. Martin, C. D. Batista, Phys. Rev. Lett. 101, 156402 (2008)).

4:42PM T8.00012 Spin spiral state in hexagonal NiS¹, RAQUEL LIZARRAGA², ERIK HOLMSTROM³, Instituto de Ciencias Físicas y Matemáticas, LARS NORDSTROM⁴, OLLE ERIKSSON⁵, Department of Physics and Astronomy, SWARUP PANDA⁶, INDRA DASGUPTA⁷, D.D. SARMA⁸, Indian Institute of Science — Previous nesting function calculations on NiS have found instabilities for the magnetic ordering vectors $q=(2/3,2/3,0)$ and $q=(1/2,2/9,1)$ suggesting that the magnetic structure of NiS is non-collinear which does not agree with the experimentally determined antiferromagnetic state. We investigated the electronic and magnetic structure of NiS by means of a full-potential linearized augmented plane wave method within the local spin density approximation plus the Hubbard parameter U . Our method is specially suitable to study noncollinear magnetism where the magnetization density is allowed to vary in magnitude and direction continuously everywhere in space. Our results show that the ground state is metallic and that the antiferromagnetic state is almost degenerate with spin spirals along certain directions of the Brillouin zone.

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4:54PM T8.00013 Incommensurate antiferromagnetism in GdSi, YEJUN FENG, Argonne National Lab, JIYANG WANG, Univ. of Chicago, J.-W. KIM, Argonne National Lab, J.-Q. YAN, Univ. Tennessee & ORNL, NAYOON WOO, D.M. SILEVITCH, T.F. ROSENBAUM, Univ. of Chicago — Rare earth magnets are interesting model systems to study correlated spin, orbital and lattice degrees of freedom. Here we present a study of the antiferromagnetism in single crystal GdSi, using high-resolution, x-ray magnetic diffraction techniques. Our results clearly show an incommensurate magnetic structure at 6.5 K, with a lattice distortion from orthorhombic to monoclinic accompanying the magnetic phase transition in a second order fashion. We discuss implication to the anisotropic susceptibility in lights of the detailed magnetic structure.

5:06PM T8.00014 Spin-Orbital Locking, Emergent Pseudo-Spin, and Magnetic order in Na₂IrO₃, SUBHRO BHATTACHARJEE¹, University of Toronto, SUNG-SIK LEE², McMaster University, YONG BAEK KIM³, University of Toronto — The nature of magnetic order in the honeycomb lattice Iridate Na₂IrO₃ is explored by considering trigonal crystal field effect and spin-orbit coupling. An effective Hamiltonian is derived in terms of an emergent pseudo-spin-1/2, resulting from a spin-orbital locking, which is different from $j_{\text{eff}} = 1/2$ that is obtained when the spin-orbit coupling dominates. The resulting Hamiltonian is anisotropic and frustrated. Mean field theory suggests a ground state with 4-sublattice zig-zag magnetic order in the relevant parameter regime, in conformity with experiments. Various properties of the phase, the spin-wave spectrum and experimental consequences are discussed. Our approach contrasts with the recent proposal of a Heisenberg-Kitaev system for this material, and we point out the intrinsic difficulties with the latter approach for describing the magnetic properties of Na₂IrO₃.

¹Also at: McMaster University

²Also at: Perimeter Institute for Theoretical Physics

³Also at: Korea Institute of Advanced Study

5:18PM T8.00015 Magnetic order on a frustrated lattice due to orbital degrees of freedom in RO₂ hyperoxides¹, ANDRZEJ M. OLEŚ, Jagellonian University, Cracow, Poland, KRZYSZTOF WOHLFELD, MARIA DAGHOFER, IFW Dresden, Germany — The alkali RO₂ hyperoxides ($R=\text{Rb,Cs,K}$) crystallize in a frustrated bct lattice. Nevertheless, all of the members of the family of alkali RO₂ hyperoxides have long range layered C -type antiferromagnetic (C -AF) order at low temperature. We show that including the almost degenerate p -orbital degrees of freedom in a realistic spin-orbital model can resolve this contradiction [1]. Although *a priori* the orbital degrees of freedom do not remove frustration in spin system, we show that the anomalously large interorbital hopping together with the orbital order induced by the lattice stabilize the C -AF order in this class of compounds, in agreement with generalized Goodenough-Kanamori rules formulated here.

[1] K. Wohlfeld, M. Daghofer, and A.M. Oleś, EPL **96**, 27001 (2011).

¹We acknowledge support by Polish government Project No. N202 069639, Alexander von Humboldt Foundation and the Emmy-Noether Program.

Wednesday, February 29, 2012 2:30PM - 5:30PM –
Session T9 GMAG DMP: Focus Session: Magnetic Oxide Thin Films And Heterostructures - Interactions at Interfaces and in Superlattices 209

2:30PM T9.00001 Upper limit to magnetism in $\text{LaAlO}_3/\text{SrTiO}_3$ heterostructures, MICHAEL FITZSIMMONS, Los Alamos National Laboratory — In 2004 Ohtomo and Hwang reported unusually high conductivity in LaAlO_3 and SrTiO_3 bilayer samples. Since then, metallic conduction, superconductivity, magnetism, and coexistence of superconductivity and ferromagnetism have been attributed to $\text{LaAlO}_3/\text{SrTiO}_3$ interfaces. Very recently, two studies have reported large magnetic moments attributed to interfaces from measurement techniques that are unable to distinguish between interfacial and bulk magnetism. Consequently, it is imperative to perform magnetic measurements that by being intrinsically sensitive to interface magnetism are impervious to experimental artifacts suffered by bulk measurements. Using polarized neutron reflectometry, we measured the neutron spin dependent reflectivity from four $\text{LaAlO}_3/\text{SrTiO}_3$ superlattices. Our results indicate the upper limit for the magnetization averaged over the lateral dimensions of the sample induced by an 11 T magnetic field at 1.7 K is less than 2 G. SQUID magnetometry of the neutron superlattice samples sporadically finds an enhanced moment (consistent with past reports), possibly due to experimental artifacts. These observations set important restrictions on theories which imply a strongly enhanced magnetism at the interface between LaAlO_3 and SrTiO_3 . Work performed in collaboration with N.W. Hengartner, S. Singh, M. Zhernenkov (LANL), F.Y. Bruno, J. Santamaria (Universidad Complutense de Madrid), A. Brinkman, M.J.A. Huijben, H. Molegraaf (MESA+ Institute for Nanotechnology), J. de la Venta and Ivan K. Schuller (UCSD).

Work supported by the Office of Basic Energy Science, U.S. Department of Energy, BES-DMS and DMR under grant DE FG03-87ER-45332. Work at UCM is supported by Consolider Ingenio CSD2009-00013 (IMAGINE), CAM S2009-MAT 1756 (PHAMA) and work at Twente is supported by the Foundation for Fundamental Research on Matter (FOM).

3:06PM T9.00002 Magnetotransport behavior in $(\text{LaNiO}_3)_n/(\text{LaMnO}_3)_2$ superlattices, JASON HOFFMAN, Materials Science Division, Argonne National Laboratory, ANAND BHATTACHARYA, Materials Science Division and Center for Nanoscale Materials, Argonne National Laboratory — Recent advances in the deposition of epitaxial complex oxides have enabled the fabrication of a wide range of materials structures with atomically abrupt interfaces, that are characterized by novel electronic and magnetic ground states. In particular, superlattices that combine the paramagnetic metal, LaNiO_3 , with various band insulators, such as SrTiO_3 and LaAlO_3 , have attracted considerable theoretical and experimental interest. In this work, $(\text{LaNiO}_3)_n/(\text{LaMnO}_3)_2$ ($2 \leq n \leq 5$) superlattices that combine LaNiO_3 with an antiferromagnetic insulator are prepared on (001) SrTiO_3 substrates using ozone-assisted oxide molecular beam epitaxy. The total superlattice thickness is fixed at ~ 30 nm. X-ray reflectivity and x-ray diffraction reveal single-crystalline growth with interfacial and surface roughnesses of ~ 0.2 nm and ~ 0.5 nm, respectively. Electrical transport measurements carried out on superlattices with $n \leq 3$ show insulating behavior between 5 K and 300 K, while samples with $n = 4, 5$ are metallic with resistivity minima at 90 K and 30 K, respectively, below which we observe negative magnetoresistance. We discuss the role of charge transfer between LaNiO_3 and LaMnO_3 in understanding these results.

3:18PM T9.00003 Confinement induced metal-to-insulator transition in strained $\text{LaNiO}_3/\text{LaAlO}_3$ superlattices¹, ARIADNA BLANCA ROMERO, Ludwig Maximilians University Munich, Germany, ROSSITZA PENTCHEVA, Ludwig Maximilians University Munich — Using density functional theory calculations including a Hubbard U term we explore the effect of strain and confinement on the electronic ground state of superlattices containing the band insulator LaAlO_3 and the correlated metal LaNiO_3 . Besides a suppression of holes at the apical oxygen, a central feature is the asymmetric response to strain in single unit cell superlattices: For tensile strain a band gap opens due to charge disproportionation at the Ni sites with two distinct magnetic moments of $1.45\mu_B$ and $0.71\mu_B$. Under compressive strain, charge disproportionation is nearly quenched and the band gap collapses due to overlap of $d_{3z^2-r^2}$ bands through a semimetallic state. This asymmetry in the electronic behavior is associated with the difference in octahedral distortions and rotations under tensile and compressive strain. The ligand hole density and the metallic state are quickly restored with increasing thickness of the $(\text{LaAlO}_3)_n/(\text{LaNiO}_3)_n$ superlattice from $n = 1$ to $n = 3$.

¹We acknowledge support from the German Science Foundation, SFB/TR80.

3:30PM T9.00004 Electronic structure, charge modulation, and orbital polarization of $\text{LaNiO}_3/\text{SrTiO}_3$ superlattice¹, MYUNG JOON HAN, MICHEL VAN VEENENDAAL, Argonne National Lab and Northern Illinois University — First-principles density functional theory calculations have been performed to understand the detailed electronic structure for the various (m, n) combinations of $(\text{LaNiO}_3)_m/(\text{SrTiO}_3)_n$ superlattices. Due to the strong covalency of Ni-O bonds, the valence bands are dominated by Ni-d character and the electronic structure is mainly affected by the local environment rather than the ionic potential. Heterostructuring-induced quantum states and the interaction between them leads to the charge redistribution around the Fermi level, which may be responsible for the charge modulation and metal-insulator transition observed in the related systems.

¹This work was supported by the US Department of Energy (DOE) under Contract No. DE- FG02-03ER46097

3:42PM T9.00005 Electronic, magnetic, and structural coupling across oxide interfaces, CHARLES AHN, Yale University — Many complex oxide materials exhibit a strong interplay between spin, charge, and lattice effects. This coupling leads to a variety of novel electronic and magnetic properties, including charge ordered and magnetic states, “colossal” magnetoresistance (CMR), and a range of electron transport behavior. The possibility of integrating these different kinds behavior with other types of functionalities has motivated the development of new, artificially structured complex oxide-based materials systems, such as composite multiferroic heterostructures. In certain cases, the atomic-scale interface of these structures can dominate the observed behavior, with new physical properties emerging. For example, in epitaxial ferromagnetic/ferroelectric heterostructures, it is possible to achieve large magnetoelectric coupling that is controlled directly by the charge degrees of freedom. We have studied this coupling using a variety of techniques, including magnetization, magneto-optic Kerr effect magnetometry, and x-ray absorption spectroscopy. In addition, structural distortions that arise exclusively at the interface can influence simultaneously the interfacial electronic transport and magnetic properties. Using high resolution synchrotron scattering, we have determined the interplay between new interfacial structural motifs and the resulting electronic and magnetic function at the interface.

4:18PM T9.00006 Ferroelectric control of magnetocrystalline anisotropy and orbital magnetism in thin-film Fe/BaTiO_3 heterostructures, PAVEL LUKASHEV, J.D. BURTON, SITARAM JASWAL, EVGENY TSYMBAL, University of Nebraska - Lincoln — Correlations between magnetocrystalline anisotropy energy (MAE), ferroelectric (FE) polarization, and orbital magnetic moment are studied for ferroelectric/ferromagnetic heterostructures consisting of barium titanate (BaTiO_3) and thin-film iron (Fe). Using first-principles calculations we investigated different geometries of the BaTiO_3/Fe system, in particular with 1, 3, and 5 monolayers of Fe with either a free vacuum surface or Cu as a capping layer. We show that there is a large MAE change ($\sim 20\%$) upon switching of the polarization sign in the case of a vacuum layer, while the presence of Cu effectively removes the difference in MAE for opposite FE polarization directions in BaTiO_3 . This is explained by analyzing the correlation between MAE and orbital magnetic moments for different geometries and opposite polarization directions, as well as the film thickness. We show that the magnetoelectric coupling between MAE and FE polarization is directly linked to the degree of the magnetoelectric coupling between orbital moment and FE polarization.

4:30PM T9.00007 Electron-mediated ferromagnetic behavior in CoO/Al:ZnO multilayers¹

FRANCES HELLMAN, HYEON-JUN LEE, CATHERINE BORDEL, Physics Department, University of California, Berkeley, JULIE KAREL, Department of Materials Science and Engineering, University of California, Berkeley, DAVID W. COOKE, Physics Department, University of California, Berkeley, FRANCES HELLMAN'S GROUP TEAM — (111)-oriented epitaxial CoO/Al-doped ZnO (AZO) multilayers show a ferromagnetic behavior up to room temperature. Their magnetization exhibits an oscillatory behavior as a function of (i) the number of Co layers in the insulating antiferromagnetic CoO, and (ii) the thickness of the AZO layers. The ferromagnetism vanishes if AZO is replaced by intrinsic ZnO. This behavior can be explained by the existence of an RKKY-coupling, mediated by the free electrons of the non-magnetic AZO layers, between the uncompensated (111) ferromagnetic planes of insulating CoO when there is an odd number of planes in the layer. The oscillation period of the spontaneous magnetization as a function of the AZO layer thickness matches the Fermi wavevector calculated from the carrier concentration that was deduced from Hall effect measurements. The spin-polarization of the carriers in the AZO layer is confirmed via anomalous Hall effect.

¹This research was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Contract No. DE-AC02-05CH11231.

4:42PM T9.00008 Towards Room Temperature Spin Filtering in Oxide Tunnel Junctions¹

JODI IWATA-HARMS, FRANKLIN WONG, University of California, Berkeley, ELKE ARENHOLZ, Advanced Light Source, Lawrence Berkeley National Laboratory, YURI SUZUKI, University of California, Berkeley — Spin filtering, in which the magnetic tunnel barrier preferentially filters spin-up and spin-down electrons from a nonmagnetic electrode, has been demonstrated in junction heterostructures. By incorporating two spin filtering barriers, double spin filter magnetic tunnel junctions (DSF-MTJs) were predicted to yield magnetoresistance (MR) values orders of magnitude larger than that of conventional magnetic tunnel junctions. Recently, DSF-MTJs have exhibited spin filtering with magnetic electrodes at room temperature and at low temperature with nonmagnetic electrodes in EuS-based devices [1,2]. We have fabricated DSF-MTJs with nonmagnetic SrRuO₃ electrodes and room temperature ferrimagnets, NiFe₂O₄ and CoFe₂O₄, for spin filters in pursuit of room temperature functionality. Atomic force microscopy shows smooth films quantified by roughness values between 0.1–0.5nm. X-ray magnetic circular dichroism reveals ferromagnetic Ni²⁺ and Co²⁺, and element-specific hysteresis loops indicate the independent switching of the two spin filters. Transport data reveals junction MR and non-linear I-V characteristics consistent with tunneling.

[1] M.G. Chapline et al., PRB, 74, 014418 (2006).

[2] G.-X. Miao et al., PRL, 102, 076601 (2009).

¹NSF Grant No. 0604277 and 1104401

4:54PM T9.00009 Magnetic Behavior of Complex Oxide Magnetic Tunnel Junctions¹

SUZANNE G.E. TE VELTHUIS, YAOHUA LIU, J.W. FREELAND, Argonne National Laboratory, USA, M. ZHERNENKOV, M.R. FITZSIMMONS, Los Alamos National Laboratory, USA, C. VISANI, M. BIBES, A. BARTHÉLÉMY, Unité mixte de Physique CNRS/Thales, France, F. CUELLAR, Z. SEFRIQUI, C. LEON, J. SANTAMARIA, Universidad Complutense de Madrid, Spain — Half metallic manganese oxides have the potential of producing a large tunneling magnetoresistance (TMR) due to their high spin-polarization. To explore their applicability we investigated magnetic tunnel junctions (MTJs) with ferromagnetic La_{0.7}Ca_{0.3}MnO₃ (LCMO) electrodes and an insulating PrBa₂Cu₃O₇ (PBCO) barrier. In these MTJs, with temperature, the TMR peaks rather than increasing with decreasing T [1]. Our Polarized Neutron Reflectivity studies reveal differences in the magnetization, reversal behavior, and anisotropy, between the bottom and top LCMO layers. As was observed in the YBa₂Cu₃O₇ (YBCO)/LCMO system [2,3], with X-Ray Magnetic Circular Dichroism we have found a non-zero net moment on the Cu of PBCO at low temperature, originating at the interface. Unlike for YBCO, the Cu moment does not persist up to T_C of LCMO. These combined results provide a possible origin of the anomalous TMR behavior.

[1] Z. Sefrioui et al., Appl. Phys. Lett. 88, 022512 (2006) [2] J. Chakhalian et al., Nature Phys. 2, 244 (2006); Science 318, 1114 (2007) [3] C. Visani et al., Phys. Rev. B 84, 060405(R) (2011)

¹Work supported by US Department of Energy, Office of Science, Office of Basic Energy Sciences, under contract Nos. DE-AC02-06CH11357, DE-AC52-06NA25396 and the Spanish MICINN.

5:06PM T9.00010 Ferroelectric control of orbital occupancy in manganites¹

HANGHUI CHEN, Department of Physics, Yale University, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — Recent successful fabrication of epitaxial and coherent ferroelectric/manganite interfaces makes it possible to dynamically control charge and spin in manganites [1]. We demonstrate with *ab initio* calculations that in this system, *d*-orbital occupancies of the interfacial Mn atom can also be modulated by flipping the ferroelectric polarization (i.e. flippable orbital polarization). The underlying mechanism is the structural distortions of the oxygen octahedron and the Mn atom inside induced by the ferroelectric polarization. The in-plane orbital *d*_{x²-y²} is stabilized by rumpling in MnO₂ layers, while the Jahn-Teller distortion (*c/a* > 1) favors the out-of-plane orbital *d*_{3z²-r²}. This ferroelectric control of orbital occupancy serves as a new approach separate from strain for engineering orbital orderings in transition metal oxides.

[1] C.A.F.Vaz et al., Phys. Rev. Lett. 104, 127202 (2010)

¹This project is funded by NSF-MRSEC.

5:18PM T9.00011 Giant tunneling electroresistance (up to ~10,000%) in

La_{0.7}Sr_{0.3}MnO₃/BaTiO₃/La_{0.5}Ca_{0.5}MnO₃/La_{0.7}Sr_{0.3}MnO₃ ferroelectric tunnel junctions, YUEWEI YIN, QI LI, Department of Physics, Pennsylvania State University, University Park, PA 16802, USA, J.D. BURTON, E.Y. TSYMBAL, Department of Physics and Astronomy, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE 68588, USA, X.G. LI, Hefei National Laboratory for Physical Sciences at Microscale, Department of Physics, University of Science and Technology of China, Hefei 230026, PRC — Tunnel junction with a Ferroelectric (FE) barrier (FTJ) presents an opportunity for nanoelectronics because of the bi-stable electric field control of the tunneling resistance. FTJs of La_{0.7}Sr_{0.3}MnO₃/BaTiO₃/La_{0.5}Ca_{0.5}MnO₃/La_{0.7}Sr_{0.3}MnO₃ have been fabricated with pulsed-laser deposition. The special feature in the FTJ design is to insert an ultrathin (0.4 - 1.2 nm) La_{0.5}Ca_{0.5}MnO₃ film between La_{0.7}Sr_{0.3}MnO₃ Ferromagnetic (FM) electrode and BaTiO₃ FE barrier. A giant and reproducible tunneling electroresistance effect (~10,000%) was obtained with the reversal of FE polarization, about two orders of magnitude larger than the similar sized FTJ without the inserted La_{0.5}Ca_{0.5}MnO₃ layer. This result is consistent with the theoretical prediction [PRL 106, 157203 (2011)] that at a BaTiO₃/La_{0.5}Ca_{0.5}MnO₃ interface, an anti-FM insulating - FM metallic phase transition can occur in La_{0.5}Ca_{0.5}MnO₃ when the polarization of the BaTiO₃ is reversed due to the interfacial charge doping effect.

Wednesday, February 29, 2012 2:30PM - 5:30PM –

Session T10 DMP: Invited Session: Earth-Abundant Materials for Critical Technologies 210A

2:30PM T10.00001 An Overview of Rare Earth Science and Technology¹ , KARL GSCHNEIDNER, JR., Iowa

State University — Currently rare earth science and technology is robust: this includes all the major branches of science – biochemistry, chemistry, materials and physics. There are, however, currently some anomalies and distortions especially in the technology and applications sector of the rare earth field, which is caused by the dominance of China on the sales of rare earths and rare earth containing products. For the past 5 to 10 years ~95% of rare earths utilized in commerce came from China. Although Chinese actions have led to sudden and large price spikes and export embargoes, the rare earths are still available but at a higher cost. The start up of production in 2011 at mines in the USA and Australia will alleviate this situation in about two years. Basic and applied research on the condensed matter physics/materials science has hardly been impacted by these events, but new research opportunities are opening up especially with regard to the USA's military and energy security. Magnets seems to be the hottest topic, but research on battery materials, phosphors and catalysts are also (or should be) strongly considered.

¹This work is supported by the U.S. Department of Energy - Basic Energy Sciences under contract No. DE-AC02-07CH11358.

3:06PM T10.00002 Replacing critical rare earth materials in high energy density magnets¹ ,

R. WILLIAM MCCALLUM, Ames Laboratory USDOE / Iowa State University — High energy density permanent magnets are crucial to the design of internal permanent magnet motors (IPM) for hybride and electric vehicles and direct drive wind generators. Current motor designs use rare earth permanent magnets which easily meet the performance goals, however, the rising concerns over cost and foreign control of the current supply of rare earth resources has motivated a search for non-rare earth based permanent magnets alloys with performance metrics which allow the design of permanent magnet motors and generators without rare earth magnets. This talk will discuss the state of non-rare-earth permanent magnets and efforts to both improve the current materials and find new materials. These efforts combine first principles calculations and meso-scale magnetic modeling with advance characterization and synthesis techniques in order to advance the state of the art in non rare earth permanent magnets. The use of genetic algorithms in first principle structural calculations, combinatorial synthesis in the experimental search for materials, atom probe microscopy to characterize grain boundaries on the atomic level, and other state of the art techniques will be discussed. In addition the possibility of replacing critical rare earth elements with the most abundant rare earth Ce will be discussed.

¹Work at The Ames Laboratory was supported by the U.S. DOE under Contract No. DE-AC02-07CH11358.

3:42PM T10.00003 Solar to Fuel Conversion with Earth Abundant Materials , DANIEL G. NOCERA,

Massachusetts Institute of Technology — Studies in the Nocera group have led to the creation of a new earth-abundant catalyst that captures many of the functional elements of photosynthesis and in doing so provides a highly manufacturable and inexpensive method to effect a carbon-neutral and sustainable method for solar storage - solar fuels from water-splitting. This discovery enables an inexpensive 24/7 solar energy system for the individual, a capability that is attractive in the underdeveloped as well as the developed world.

4:18PM T10.00004 Organic-inorganic hybrid materials for energy efficiency , SETH COE-SULLIVAN, QD

Vision, Inc. — Quantum dot (QD) semiconductor nanocrystals are unique hybrid materials that have been considered in a broad range of energy production and energy efficiency applications including LEDs, displays, lighting and solar cells. In their photoluminescent mode of operation, QDs are currently in lighting products, and have the promise to be in liquid crystal display products in the near future, in both cases offering energy efficiency gains in the range of 25-40%. In electroluminescent mode, quantum dot light emitting devices (QLEDs) are an emerging class of thin-film hybrid organic-inorganic structures that can potentially achieve best-in-class performance amongst large-area emissive light sources. Indeed, efficiencies which double that of the most efficient OLEDs have been suggested. The hybrid nature of these materials offers the key design parameters that have enabled QD technology to reach market in lighting products, and promises to soon revolutionize the display industry.

4:54PM T10.00005 Photovoltaic devices using inexpensive, abundant inorganic materials: experiences with copper zinc tin sulfide (CZTS) , SUPRATIK GUHA, IBM Thomas J. Watson Research Center —

For photovoltaics to be able to contribute a significant percentage of global electricity, we ideally desire a cheap, efficient, safe, and abundant solar cell that can be treated more as a construction material than as a delicate semiconductor. We are not quite there yet, though thin film polycrystalline solar cells on cheap substrates represent a potential way to accomplish this objective. I will describe some of the requirements for a solar cell with this application objective, describe some of the challenges when we desire to transform a “polycrystalline,” “mineral-like” absorber into an efficient p-n junction solar cell, and in this context will describe our results with the kesterite compound copper zinc tin sulfide (CZTS).

Wednesday, February 29, 2012 2:30PM - 5:18PM –

Session T11 DMP: Focus Session: Graphene Structure, Stacking, Interactions: Twisted Layers

210B

2:30PM T11.00001 Continuum Model of the twisted graphene bilayer¹ , JOÃO LOPES DOS SANTOS, CFP

and DFA, Faculdade de Ciências, Universidade do Porto — The electronic structure of the twisted bilayer was first considered [1] in the context of a continuum description of the two layers, coupled by a spatially modulated hopping. The model's predictions were subsequently confirmed by experiments [2,3], including a scanning tunneling spectroscopy finding of two low energy Van-Hove peaks in the density of states [4], and by band structure calculations [5,6]. We discuss the extension of the model in several directions: the two families of commensurate structures discovered by Mele [7], will be characterized by elementary geometrical arguments; it will be shown that it is possible to calculate analytically *all* Fourier components of the hopping amplitudes for any kind of commensurate structure with large period; the calculations will be extended beyond the perturbative regime in the interlayer coupling to address the electronic structure and local density of states in the very small angle limit.

[1] J. M. B. Lopes dos Santos, *et. al*, Phys. Rev. Lett. **99**, 256802, (2007).

[2] Z. Ni, *et. al.*, Phys. Rev. B **77**, 235403, 2008.

[3] A. Luica, *et. al*, Phys. Rev. Lett. **106**, 126802 (2011).

[4] G. Li, *et. al*, Nature Physics **6**, 109 (2010).

[5] S. Shallcross, *et. al*, Phys. Rev. B **81**, 165105 (2010).

[6] G. de Laissardiere, *et. al*, Nano Letters **10**, 804 (2010).

[7] E. J. Mele, Phys. Rev. B **81**, 161405 (2010).

¹FCT, Portugal

3:06PM T11.00002 Moire Bloch Bands in Twisted Bilayer Graphene, ALLAN MACDONALD, University of Texas at Austin — A moiré superlattice pattern is formed when two copies of a periodic lattice are overlaid with a relative twist. I will address the electronic structure of a twisted two-layer graphene system by generalizing the Dirac equation continuum models that are used to describe single-layer graphene and untwisted bilayers. In the Dirac model electrons in graphene have a pseudospin degree-of-freedom corresponding to the honeycomb sublattice dependence of wavefunction amplitudes. The continuum model of twisted bilayers can be derived systematically [1] by assuming that interlayer tunneling amplitudes are non-local with a range that is large compared to the honeycomb lattice constant, and leads to an appealing picture in which the tunneling operator has a position-dependent pseudospin dependence that simply reflects the local registry between the two honeycombs. The continuum model twisted bilayer Hamiltonian is therefore periodic, with the periodicity of the moiré pattern, and insensitive to the incommensurability of the microscopic Hamiltonian. I will discuss the properties of the Bloch bands of this periodic Hamiltonian, which become highly non-trivial at small twist angles. In particular the Dirac velocity crosses zero several times as the twist angle is reduced and vanishes at a discrete set of magic angles. I will also briefly discuss the Hofstadter butterfly spectral patterns [2] created by incommensurability between the moiré pattern and magnetic lengths when a twisted bilayer is placed in an external magnetic field, and the electronic structure [3] of a single graphene layer that is twisted with respect to a boron nitride substrate.

[1] R. Bistritzer and A.H. MacDonald, PNAS **108**, 12233 (2011).

[2] R. Bistritzer and A.H. MacDonald, Phys. Rev. B **84**, 035440 (2011).

[3] A. Raoux and A.H. MacDonald, arXiv:1112.nnnn.

3:42PM T11.00003 Anomalies in the magneto-optical conductivity of twisted multilayer epitaxial graphene, ALEXEY B. KUZMENKO, IRIS CRASSEE, JULIEN LEVALLOIS, DIRK VAN DER MAREL, University of Geneva, Switzerland, ANDREW L. WALTER, Advanced Light Source, USA., THOMAS SEYLLER, University of Erlangen-Nuremberg, Germany — The nature of the electronic coupling between carbon layers in twisted multilayer graphene is an intriguing and hot-debated issue. We measured the Faraday rotation and optical absorption spectra of twisted graphene multilayers grown on the carbon face of SiC in the far-infrared range in magnetic fields up to 7 Tesla [1,2]. Multiple spectral components are identified, which include a quasi-classical cyclotron resonance, originating from the highly doped graphene layer closest to SiC, transitions between low-index Landau levels (LLs), which stem from quasineutral outer layers and a broad optical absorption background, which provenance is less obvious. Electron- and hole-type LL transitions are optically distinguished and shown to coexist. The variation of the Fermi velocity is about 10 percent across the layers. Our central observation is an anomalously small optical spectral weight of the individual LL transitions, which is likely caused by the unusual electronic coupling between randomly stacked graphene layers.

[1] I. Crassee *et al.* Nature Phys. **7**, 48 (2011).

[2] I. Crassee *et al.* Phys Rev B **84**, 035103 (2011).

3:54PM T11.00004 Quantum Hall Effect, Screening and Layer-Polarized Insulating States in Twisted Bilayer Graphene¹, JAVIER D. SANCHEZ-YAMAGISHI, Department of Physics, MIT, THITI TAYCHATANAPAT, Department of Physics, Harvard, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Tsukuba, Japan, AMIR YACOBY, Department of Physics, Harvard, PABLO JARILLO-HERRERO, Department of Physics, MIT — We present a study of electronic transport in dual-gated twisted bilayer graphene. Despite the sub-nanometer proximity between the layers, we identify independent contributions to the magnetoresistance from the graphene Landau level spectrum of each layer. We demonstrate that the filling factor of each layer can be independently controlled via the dual gates, which we use to induce Landau level crossings between the layers. By analyzing the gate dependence of the Landau level crossings, we characterize the finite inter-layer screening and extract the capacitance between the atomically-spaced layers. At zero filling factor, we observe magnetic and displacement field dependent insulating states, which indicate the presence of counter-propagating edge states with inter-layer coupling.

¹Research supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award de-sc0001819

4:06PM T11.00005 Formation of superlattice structures by interlayer bonding in twisted bilayer graphene, ANDRE MUNIZ, Universidade Federal do Rio Grande do Sul, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — We present a computational analysis of carbon nanostructure formation from twisted bilayer graphene, upon creation of interlayer covalent C-C bonds. The analysis is based on a combination of first-principles density functional theory calculations and classical molecular-dynamics simulations. We demonstrate that the resulting configurations constitute a novel class of stable structures and that their features are determined by the relative angle of rotation between the two graphene planes of the bilayer. For small angles of rotation (near 0 degrees), interlayer covalent bonding generates superlattices of diamond-like nanocrystals embedded within the graphene layers; for rotation angles near 30 degrees, superlattices of caged fullerene-like configurations are generated. We calculate the electronic band structure of these superlattices and show that their band gap can be controlled through selective hydrogenation and creation of interlayer bonds. We also show that the linear dispersion around the K point in the first Brillouin zone (Dirac cones), characteristic of single-layer and non-bonded twisted bilayer graphene, is preserved for some of these structures in spite of the introduction of sp³ bonds due to hydrogenation and interlayer C-C bonding.

4:18PM T11.00006 Phonon mediated conductance in misoriented graphene bilayers, VASILIOS PEREBEINOS, JERRY TERSOFF, PHAEDON AVOURIS, IBM - Watson — Electrical transport in a misoriented graphene bilayer is facilitated by umklapp processes whose strength is known to decrease rapidly with the number of atoms in the commensurate cell. As the misorientation angle is reduced, the number of atoms increases, and the umklapp conductance in an ideal (infinitely large and defect free) bilayer becomes negligible. We show that at room temperature coupling to the out-of-plane phonon vibrations leads in a conductance several orders of magnitude larger than that produced by pure electronic umklapp. The most relevant phonons originate from the flexural modes of the monolayer, vibrating out-of-phase in the bilayer, with energies around 80 cm⁻¹ near the Γ -point. These phonon modes disperse nearly quadratically away from the center of the Brillouin zone. As the misorientation angle is reduced, the relevant phonon wavevector connecting the two Fermi surfaces in monolayers is reduced as well, which results in larger phonon mediated conductance. This is the opposite behavior to that expected from the umklapp conductance. We will present calculations of phonon mediated conductance as a function of misorientation angle, doping, temperature, and applied bias, for a tight-binding electron-phonon Hamiltonian.

4:30PM T11.00007 Probing interlayer interactions in twisted bilayer graphene with Raman spectroscopy, ROBIN HAVENER, Applied and Engineering Physics, Cornell University, LOLA BROWN, Chemistry and Chemical Biology, Cornell University, HOULONG ZHUANG, Materials Science and Engineering, Cornell University, MICHAL WOJCIK, Chemistry and Chemical Biology, Cornell University, CARLOS RUIZ-VARGAS, Applied and Engineering Physics, Cornell University, RICHARD G. HENNIG, Materials Science and Engineering, Cornell University, JIWOONG PARK, Chemistry and Chemical Biology, Cornell University — Chemical vapor deposition (CVD) growth or artificial layer-by-layer assembly of graphene typically produces multi-layer regions in which the layers are twisted with respect to each other, but the electronic and optical properties of this new material are still under investigation. In particular, little is known about how the twist angle affects the Raman signature of this material. We use a combination of dark-field transmission electron microscopy (DF-TEM) and widefield Raman imaging (WRI) to study the Raman signature of bilayer CVD graphene regions with known twist angles. We find that the intensities of the G and 2D peaks vary predictably with twist angle. In particular, we observe a strong G band enhancement at a specific twist angle that depends on our excitation energy. To explain this behavior, we model the electronic band structure of twisted bilayer graphene; the interaction between layers creates new saddle point van Hove singularities, and these energy states can enable a fully resonant G band pathway for a specific angle and excitation energy. This G band resonance feature is a very sensitive probe of twist angle and interlayer interactions.

4:42PM T11.00008 Strong Rotational Angle Dependence of Raman Spectroscopy in Rotated Double-Layer Graphene, KWANPYO KIM, SINISA COH, LIANG Z. TAN, WILLIAM REGAN, JONG MIN YUK, ERIC CHATTERJEE, M. F. CROMMIE, MARVIN L. COHEN, STEVEN G. LOUIE, A. ZETTL, Department of Physics, UC Berkeley — We perform a complementary Raman spectroscopy and transmission electron microscopy (TEM) study, as well as electronic-structure and Raman calculations, on suspended rotated double-layer graphene. Graphene Raman spectra show a strong dependence on the rotational angles between two stacked layers. For low-angle mis-orientations (~ 10 degrees), double-layer graphene exhibits Raman signature closer to AB-stacked bilayer graphene. Double-layers with high rotational angles ($> \sim 15$ degrees), on the other hand, display Raman spectra similar to monolayer graphene. Rotational angle dependent modifications of the electronic band structure in double-layer graphene can explain this trend and a G peak enhancement at certain middle angles. The computed electronic band structures and key features of the graphene Raman peaks including the blue shift, width and intensity of the 2D peaks agree well with experimental data.

4:54PM T11.00009 Effect of stacking on the transport properties of few-layer graphene: NEGF-DFT investigation, MATHEUS LIMA, JOSÉ EDUARDO PADILHA, RENATO PONTES, ANTÔNIO J. R. DA SILVA, ADALBERTO FAZZIO, University of São Paulo (IFUSP) — We study the effect of the stacking order on the electronic transport properties of few-layer graphene (FLG) by performing ab initio calculations based on the formalism that combines non-equilibrium green's functions and density functional theory. The stacking of the layers - Bernal (ABA), Rhombohedral (ABC) or even a combination between them - have to be considered as an extra degree of freedom and consequently the FLG properties are highly sensitive to the stacking configuration. In particular, the band structures and the transport properties of FLG present a behavior markedly distinct from that for single layer. We consider FLG from trilayer to dodecalayer in both stacks. We show that for FLG, in the Rhombohedral stacking, a simple counting of bands cannot be used to predict the amount of conducting channels. We also show that for FLG, in the Rhombohedral stacking, the outermost layers dominate the contribution to the transmittance whereas for the Bernal stacking the innermost layers also present a significant contribution to the transmittance. Moreover, we investigate the effect of bias voltage and the temperature in the transport properties of FLG. We acknowledge the INCT/CNPq, CAPES and FAPESP for the financial support.

5:06PM T11.00010 First principles study of trilayers of graphene-BN-graphene¹, XIAOLIANG ZHONG, RODRIGO AMORIM, RAVINDRA PANDEY, Michigan Technological University, SHASHI KARNA, US Army Research Laboratory, Weapons and Materials Research Directorate, ATTN: RDRL-WM — The stability, electronic structure and electronic transport properties of graphene-BN-graphene (C-BN-C) trilayers are studied in the framework of density functional theory. Different stacking formats, i.e., AAA, ABA and ABC stackings are considered. The ABA stacking is found to be most energetically favorable, followed by ABC and AAA stackings. The interlayer spacing of trilayers are close to those of corresponding C-BN bilayers, while the intralayer bond length can be regarded as the weighted mean of constituent layers. All considered configurations are found to be metallic, independent of stacking formats. When an external electric field is applied perpendicularly, electronic band structures undergo stacking-dependent variations. While both AAA and ABA stackings show good tunability of energy gap, ABC stacking shows less flexibility of gap tuning. We will also present the results of the electronic transport properties which are modeled by sandwiching trilayers between gold contact electrodes.

¹The work at Michigan Technological University was performed under support by the Army Research Laboratory through Contract No. W911NF-09-2-0026-133417.

Wednesday, February 29, 2012 2:30PM - 5:18PM —
Session T12 DMP: Focus Session: Graphene: Growth, Mechanical Exfoliation, and Properties - CVD on Metals 210C

2:30PM T12.00001 Characterization of Few Layer Graphene films Grown on Cu, Cu-Ni and SiC Substrates¹, P. TYAGI, J.D. MCNEILAN, J. ABEL, F.J. NELSON, Z.R. ROBINSON, R.L. MOORE, A.C. DIEBOLD, V.P. LABELLA, C.A. VENTRICE, JR., Univ. at Albany, A. SANDIN, D.B. DOUGHERTY, J.E. ROWE, North Carolina State Univ., C. DIMITRAKOPOULOS, A. GRILL, C.Y. SUNG, IBM T.J. Watson, S. CHEN, A. MUNSON, C.W. MAGNUSON, R.S. RUOFF, Univ. of Texas — The electronic structure of graphene depends on the number of graphene layers and the stacking sequence between the layers. Therefore, it is important to have a non-destructive technique for analyzing the overlayer coverage of graphene directly on the growth substrate. We have developed a technique using angle-resolved XPS to determine the average graphene thickness directly on metal foil substrates and SiC substrates. Since monolayer graphene films can be grown on Cu substrates, these samples are used as a standard reference for a monolayer of graphene. HOPG is used as a standard reference for bulk graphite. The electron mean free path of the C-1s photoelectron can be determined by analyzing the areas under the C-1s peaks of monolayer graphene/Cu and bulk graphite. With the electron mean free path, the graphene coverage of a film of arbitrary thickness can be determined by analyzing the area under the C-1s of that sample. Analysis of graphene coverages for graphene films grown on Cu-Ni substrates and of the thickness of both the graphene overlayer and intermediate buffer layer on SiC will be presented.

¹Support from the NSF (1006350/1006411) and ONR is appreciated.

2:42PM T12.00002 Investigation of large-area graphene synthesized on palladium surface, XIAOHONG AN, FANGZE LIU, Department of Physics, Northeastern University, YUNGJOON JUNG, Department of Mechanical and Industrial Engineering, Northeastern University, SWASTIK KAR, Department of Physics, Northeastern University, DEPARTMENT OF PHYSICS COLLABORATION, DEPARTMENT OF MECHANICAL AND INDUSTRIAL ENGINEERING COLLABORATION — We present a detailed study of large-area growth of graphene on palladium substrates. By studying the growth at different stages through appropriate variations of the temperature and time intervals of growth, and by investigating the growth at different regions of the metal substrate we have been able to observe a number of important properties of graphene growth on Pd surfaces. We have explored the nature of the as-synthesized graphene through a combination of electron microscopy and Raman spectroscopic analysis. Raman analysis of the graphene enables us to identify different kinds of as-synthesized graphene, including monolayer, turbostratic multi-layer, and mixed Bernal-turbostratic graphene layers. We further demonstrate a systematic study of the evolution of these different types of graphene as a function of temperature and growth-time.

2:54PM T12.00003 Crystallographic effects of copper substrate on graphene growth and fluorination, JOSHUA WOOD, SCOTT SCHMUCKER, GREGORY DODGE, THADDEUS KRAWCZYK, AUSTIN LYONS, ERIC POP, JOSEPH LYDING, University of Illinois at Urbana-Champaign — Graphene grown by chemical vapor deposition (CVD) on Cu is appealing due to supposed large-area monolayer growth and the low cost of the Cu foil substrate. However, this Cu substrate is inherently polycrystalline, with low and high index facets, annealing twins, and rough sites. We characterize CVD graphene growth on the Cu surfaces by combining Raman spectroscopy, electron-backscatter diffraction (EBSD), and scanning electron microscopy (SEM). We find that graphene growth on Cu(100) is multilayered and of low-quality, while growth on Cu(111) is monolayer and of high-quality. High index Cu facets containing a high percentage of (111) terraces are more monolayer-like than Cu(100). Graphene has a higher growth rate on (111) surfaces, growing the fastest on Cu(111). At temperatures below 900 °C, compact islands of graphene form from lowered growth rate. To open a bandgap in graphene, quantum confinement or covalent chemistry must be used. We do the latter by exposing our graphene films to XeF₂ gas, terminating in an insulating C₄F stoichiometry and covalent C-F bonds. Rougher facets fluorinate first, which allows possible bandgap engineering by the Cu crystallography. Additionally, film defects assist in fluorination effectiveness. We also show preliminary results on Cu crystallography effects for CVD of hexagonal boron nitride (h-BN).

3:06PM T12.00004 Barrier-Guided Growth of Micro- and Nano-Structured Graphene, NATHANIEL SAFRON, MYUNGWOONG KIM, PADMA GOPALAN, MICHAEL ARNOLD, University of Wisconsin: Madison — The patterning of graphene is necessary for tuning its physical and electronic structure and for device-integration. Traditionally, patterning has been achieved via *top-down* chemical or physical etching, which induces defects and disorder that degrades performance. In this work, we overcome these challenges through a fundamentally new *bottom-up* growth method for the rational synthesis of patterned graphene called Barrier-Guided Chemical Vapor Deposition (BG-CVD). We deposit patterned barriers on the Cu surface, using scalable lithography methods, which guide the growth of graphene around them into any desired shape. The barriers locally passivate the surface, (i) preventing the decomposition of the methane, and (ii) blocking the growth of graphene on the barrier. By designing appropriate barrier layers, we have grown arbitrary patterns, nanoribbons, and nanoporated graphene with features down to 25 nm with high mobility ($215 \text{ cm}^2/\text{Vs}$). These materials are highly crystalline with domain size $>4 \mu\text{m}$ and have 2-10x less edge defects than comparable top-down etched materials. The pattern reproducibility is $<1 \text{ nm}$ and thus, ultimately, should enable the bottom-up synthesis of sub-5 nm features. These results indicate BG-CVD as a superior production route to patterned graphene.

3:18PM T12.00005 Synthesis of Large-grain, Single-crystalline Graphene by a Novel Chemical Vapor Deposition Method and Electrical properties, YI ZHANG, LUYAO ZHANG, PYOJAE KIM, MINYUAN GE, CHONGWU ZHOU, University of Southern California — Graphene, a two dimensional, honey comb arrangement of carbon atoms has drawn significant attention with its interesting physical and electronic properties. Tremendous efforts have been made to synthesize large-scale, high quality, single-layer graphene (SLG). Based on previous studies, CVD graphene with large grain size (less grain boundaries) and low defect density would show an enhancement of device mobility. Here we report a novel CVD method to synthesize graphene with grain size up to several hundreds of micrometers on copper foil. Raman surface map of individual graphene grain indicated that the large-grain graphene was single-layer and with very low defect density. Selected Area Electron Diffraction (SAED) also confirmed that the each individual graphene island was a single grain. Morphology study was also performed to investigate the relation between the shape of graphene and growth parameters. Furthermore, the large-grain graphene was transferred to SiO_2/Si for the field effect study, and the device mobility derived from the large-grain graphene was $\sim 5,200 \text{ cm}^2/\text{V.s}$. The achieved high device mobility indicates that the large-grain single-crystalline graphene is of great potential for graphene-based nanoelectronics.

3:30PM T12.00006 Mesoscale STM Study of Thermally Annealed Copper Foils¹, OLESYA SARAJLIC, RAMESH MANI, Georgia State University — The growth of high quality graphene has become a topic of significance. There have been utilized several methods of material growth including the epitaxial growth on SiC, method of exfoliation of graphite, and chemical vapor deposition (CVD). The CVD approach typically utilizes foils of copper or nickel that are exposed to organic compounds at a high temperature. The purpose of the study is to investigate the role of the metal surface morphology during the growth process, relative grain size before and after thermal treatment, and relative flatness of the substrate after annealing. We investigated the effects of thermal annealing of polycrystalline Cu foil at the mesoscale using an ultrahigh vacuum (UHV) scanning tunneling microscope (STM). Prolonged low-temperature and rapid high-temperature annealing of the samples is being carried out and the resulting surface morphology will be reported. The STM observations reveal that the film quality is limited by grain boundaries.

¹ARO:W911NF-07-01-0158,DOE:DE-SC0001762

3:42PM T12.00007 Graphene Crystal Growth and Device Integration, LUIGI COLOMBO, Texas Instruments Incorporated — Graphene has unique electronic, chemical, thermal and physical properties and this is opening many opportunities for its use. However, to date the majority of the experiments have been performed on exfoliated graphene. There is a need to develop high quality, large area single crystal graphene for electronic applications. The discovery of graphene growth copper by chemical vapor deposition (CVD) has led to the growth of polycrystalline large area (square meters) films. The domain size for the baseline process is a few tens of microns in diameter but large "crystals," 0.25 square mm, have been grown. However, even though the films are not yet fully single crystals the transport properties are equivalent to those of exfoliated graphene. The ultimate usefulness of any material for electronics is the ability to integrate it with dielectrics and metals. Graphene is chemically inert and will require special processes to integrate it with dielectrics and metals without interrupting its band structure. The objective of this presentation is to review and present new data on large area graphene crystal growth and integration of dielectrics and metals. Surface analysis of graphene with dielectrics and metals under various processing conditions will also be presented.

4:18PM T12.00008 In Situ Characterization of Alloy Catalysts for Low-Temperature Graphene Growth, ROBERT WEATHERUP, BERNHARD BAYER, BRUNO DLUBAK, PIRAN KIDAMBI, Dept. Engineering, University of Cambridge, RAOUL BLUME, Helmholtz-Zentrum Berlin, CATERINA DUCATI, Dept. Materials Science and Metallurgy, University of Cambridge, CARSTEN BAEHTZ, Helmholtz-Zentrum Dresden-Rossendorf, ROBERT SCHLOEGL, Fritz Haber Institute, STEPHAN HOFMANN, Dept. Engineering, University of Cambridge — Chemical vapor deposition (CVD) on transition metal catalysts offers a low-cost method of producing large-area graphene, but due to limited understanding of the underlying mechanism(s), growth control remains rudimentary. We use in situ X-ray photoelectron spectroscopy (XPS) and X-ray diffraction (XRD) to monitor catalytic CVD on Ni based catalysts under typical reactor conditions. We thus develop a coherent model for graphene formation and show that graphene growth occurs during isothermal hydrocarbon exposure and is not limited to precipitation upon cooling. We introduce alloy catalysts to improve graphene growth by tuning reactivity and selectivity. We show that alloying polycrystalline Ni with Au allows low temperature ($<450^\circ\text{C}$) CVD of predominantly monolayer ($>74\%$) graphene films with an average D/G peak ratio of ~ 0.24 and domain sizes in excess of $220 \mu\text{m}^2$ [1]. We suggest that Au decorates a majority of high reactivity Ni surface sites, such as step edges, and lowers the stability of surface C. Au alloying thereby drastically lowers the graphene nucleation density, allowing more uniform and controlled growth at CMOS compatible temperatures. [1] Weatherup et al. Nano Lett. 11, 4154 (2011)

4:30PM T12.00009 ACCVD growth of mono- and bi-layer graphene and mechanism study, XIAO CHEN, PEI ZHAO, BO HOU, ERIK EINARSSON, SHOHEI CHIASHI, SHIGEO MARUYAMA, Maruyama-Shiomi Lab, Department of Mechanical Engineering, The University of Tokyo — CVD on metal substrates has been proved to be effective in the synthesis of graphene. But before utilization in graphene electronics, the quality of the consequential graphene needs to be improved, and a reliable method to grow large-scale, high-quality bi-layer graphene is required. Besides, the mechanism of growth is not fully understood. Here we report utilizing Alcohol catalytic CVD (ACCVD) to produce mono- and bi-layer graphene. By applying alcohol as carbon source, we carefully studied how each parameter affects the growth process, and the defects and grain size of graphene. By changing growth conditions we could efficiently control the layer number (1 or 2). Afterwards, we conducted and compared the transfer procedures utilizing three commonly used mediators—PVA, PDMS and PMMA. We also employed ^{12}C , ^{13}C , and $2\text{-}^{13}\text{C}$ ethanol to synthesize graphene, and with the spectroscopy characterization results we are able to explain the growth mechanism on Cu and Ni substrates to a certain extent.

4:42PM T12.00010 Synthesis and sensing application of large scale bilayer graphene, SUNG JU HONG, JUNG HOON YOO, SEUNG JAE BAEK, YUNG WOO PARK, Seoul National University — We have synthesized large scale bilayer graphene by using Chemical Vapor Deposition (CVD) in atmospheric pressure. Bilayer graphene was grown by using CH_4 , H_2 and Ar gases. The growth temperature was 1050°C . Conventional FET measurement shows ambipolar transfer characteristics. Results of Raman spectroscopy, Atomic Force microscope (AFM) and Transmission Electron Microscope (TEM) indicate the film is bilayer graphene. Especially, adlayer structure which interrupt uniformity was reduced in low methane flow condition. Furthermore, large size CVD bilayer graphene film can be investigated to apply sensor devices. By using conventional photolithography process, we have fabricated device array structure and studied sensing behavior.

4:54PM T12.00011 ABSTRACT WITHDRAWN —

5:06PM T12.00012 CVD growth of graphene at low temperature, CHANGGAN ZENG, Department of Physics, University of Science and Technology of China — Graphene has attracted a lot of research interest owing to its exotic properties and a wide spectrum of potential applications. Chemical vapor deposition (CVD) from gaseous hydrocarbon sources has shown great promises for large-scale graphene growth. However, high growth temperature, typically 1000°C, is required for such growth. In this talk, I will show a revised CVD route to grow graphene on Cu foils at low temperature, adopting solid and liquid hydrocarbon feedstocks. For solid PMMA and polystyrene precursors, centimeter-scale monolayer graphene films are synthesized at a growth temperature down to 400°C. When benzene is used as the hydrocarbon source, monolayer graphene flakes with excellent quality are achieved at a growth temperature as low as 300°C. I will also talk about our recent progress on low-temperature graphene growth using paraterphenyl as precursor. The successful low-temperature growth can be qualitatively understood from the first principles calculations. Our work might pave a way to economical and convenient growth route of graphene, as well as better control of the growth pattern of graphene at low temperature.

Wednesday, February 29, 2012 2:30PM - 5:06PM —

Session T13 DMP GMAG: Focus Session: Low-Dimensional and Molecular Magnetism - Molecular Ferromagnetism and 2D Magnetism 211

2:30PM T13.00001 Magnetic phase diagram of quasi-2D quantum Heisenberg antiferromagnets with XY anisotropy, FAN XIAO, CHRISTOPHER LANDEE, Department of Physics, Clark University, Worcester MA 01610, MARK TURNBULL, Carlson School of Chemistry and Biochemistry, Clark University, Worcester, MA 01610, NATHANAEL FORTUNE, Department of Physics, Smith College, Northampton MA 01063, SCOTT HANNAHS, National High Magnetic Field Lab, Tallahassee, FL 32310 — The magnetic phase diagram of a quasi-2D quantum Heisenberg antiferromagnetic compound $\text{Cu}(\text{pz})_2(\text{ClO}_4)_2$ [1] has been determined by experimental measurements; TN shows a strong field dependence. The data reveal the presence of a small (0.5%) amount of XY anisotropy. QMC simulations have been performed to examine the role of the anisotropy and the interlayer exchange (') upon the phase diagram [2,3]. Comparison of the QMC results with the experimental phase diagram will be presented.

- [1] F. Xiao, F. M. Woodward, C. P. Landee, M. M. Turnbull, C. Mielke, N. Harrison, T. Lancaster, S. J. Blundell, P. J. Baker, P. Babkevich, and F. L. Pratt. Phys. Rev. B, 79(13): 134412 (2009)
[2] A. Cuccoli, T. Roscilde, R. Vaia, and P. Verrucchi. Phys. Rev. B, 68(6):060402 (2003).
[3] A. Cuccoli, T. Roscilde, R. Vaia, and P. Verrucchi. Phys. Rev. Lett., 90(16): 167205 (2003).

2:42PM T13.00002 Magnetic excitations of the $S=1/2$ square lattice antiferromagnet $\text{CuF}_2(\text{H}_2\text{O})_2(\text{pyz})$ ($\text{pyz}=\text{pyrazine}$), CUIHUA WANG, MARK D. LUMSDEN, RANDY S. FISHMAN, GEORG EHLERS, TAO HONG, Oak Ridge National Laboratory, JOHN A. SCHLUETER, CORTNEY DUNMARS, Argonne National Laboratory, JAMIE L. MANSON, Eastern Washington University, ANDREW D. CHRISTIANSON, Oak Ridge National Laboratory — We have studied the magnetic structure and excitations of the two dimensional $S=1/2$ square lattice antiferromagnet deuterated $\text{CuF}_2(\text{H}_2\text{O})_2(\text{pyz})$. The neutron diffraction measurements show that the antiferromagnetic structure is collinearly arranged with the estimated magnetic moment of $0.60 \pm 0.07 \mu_B/\text{Cu}$. This value is much smaller than the single ion magnetic moment, reflecting the presence of strong quantum fluctuations. The spin wave dispersion from magnetic zone center to the zone boundary point ($\pi/2 \pi/2$) can be roughly described by a 2d Heisenberg model with a magnetic exchange constant $J_{2d} = 1.099 \pm 0.002 \text{ meV}$ and a tiny contribution from an inter-plane interaction (J_{perp} is about 1% of J_{2d}). This is close to the first principles DFT calculations while about two times larger than the value extracted by fitting of the magnetic susceptibility. Compared to ($\pi/2 \pi/2$), preliminary measurements of the spin excitation at the zone boundary point ($\pi 0$) shows an obvious suppression of the excitation energy. This suppression is expected on the basis of quantum Monte Carlo and series expansion calculations for the quantum corrections of linear spin wave theory.

2:54PM T13.00003 Edge state and its stability of 2D antiferromagnetic quantum spin systems, TAKAFUMI SUZUKI, Research Center for Nano-Micro Structure Science and Engineering, University of Hyogo, MASAHIRO SATO, Department of Physics, Aoyama Gakuin University — Topological insulators (TIs) [1] have been of great interest in condensed matter physics. One of the most important points is that TIs are characterized by non-local quantities such as topological quantities of the bulk or gapless surface states [2]. The TI phase and the surface states are quite stable for any time-reversal symmetric perturbations. On the other hand, the Haldane-gap state in quantum spin systems is another class of the topological state [3], because, similarly to TIs, this gapped state has no local order and is characterized by the non-local (string) order parameter or free spins at the edges. In this study, motivated by the recent development of theories for topological phases and surface states, we consider properties of edge states in 2D quantum spin systems by applying the quantum Monte Carlo method. Particularly, we focus on the three points; (1) which spin systems can have gapless edge states, (2) the stability of the gapless edge states, and (3) the difference between the edge modes of TIs and spin systems.

- [1] See, for example, M. Z. Hasan and C. L. Kane, RMP82, 3045 (2010).
[2] A. P. Schnyder, et al., PRB 78, 195125 (2008), A. Kitaev, AIP Conf. Proc. 1134, 22 (2009).
[3] F.D.M. Haldane, Phys. Lett. 93A, 464 (1983); PRL50, 1153 (1983).

3:06PM T13.00004 Absence of magnetic order in low-dimensional (RKKY) systems, FABIO PEDROCCHI, University of Basel, Department of Physics, ANTHONY LEGGETT, University of Illinois at Urbana-Champaign, Department of Physics, DANIEL LOSS, University of Basel, Department of Physics — We extend the Mermin-Wagner theorem to a system of lattice spins which are spin-coupled to itinerant and interacting charge carriers. We use the Bogoliubov inequality to rigorously prove that neither (anti-) ferromagnetic nor helical long-range order is possible in one and two dimensions at any finite temperature. Our proof applies to a wide class of models including any form of electron-electron and single-electron interactions that are independent of spin. In the presence of Rashba or Dresselhaus spin-orbit interactions (SOI) magnetic order is not excluded and intimately connected to equilibrium spin currents. However, in the special case when Rashba and Dresselhaus SOIs are tuned to be equal, magnetic order is excluded again. This opens up a new possibility to control magnetism electrically.

References: D. Loss, F. L. Pedrocchi, and A. J. Leggett, Phys. Rev. Lett. **107**, 107201 (2011).

3:18PM T13.00005 Continuous and Discontinuous Quantum Phase Transitions in a Model Two-Dimensional Magnet, SARA HARAVIFARD, Argonne National Laboratory / The University of Chicago, ARNAB BANERJEE, The University of Chicago, JONATHAN LANG, GEORGE SRAJER, Argonne National Laboratory, DANIEL SILEVITCH, The University of Chicago, BRUCE GAULIN, McMaster University, HANNA DABKOWSKA, Brockhouse Institute for Material Research, THOMAS ROSENBAUM, The University of Chicago — The Shasty-Sutherland model consists of a set of spin 1/2 dimers on a 2-dimensional square lattice which are predicted to change from isolated, gapped excitations to a collective, ordered ground state by tuning the ratio of the intra to inter-dimer coupling. We compress the model Shastry-Sutherland material, $\text{SrCu}_2(\text{BO}_3)_2$, in a diamond anvil cell at cryogenic temperatures to continuously tune the coupling energies and induce changes in state. High-resolution x-ray measurements exploit a remarkably strong spin-lattice coupling to ascertain the physics of the magnetic transition. The singlet-triplet gap energy is suppressed continuously with increasing pressure, vanishing completely by 2 GPa. This continuous quantum phase transition is followed by a structural distortion at higher pressure corresponding to the onset of long-range order.

3:30PM T13.00006 Late-time Domain Growth in the Compressible Triangular Ising Net¹, MENG MENG, DAVID LANDAU, Center for Simulation Physics, University of Georgia — We perform large scale Monte Carlo simulations of the long-time domain growth behavior in a compressible, triangular Ising net. Unlike previous work,² our model has no bond angle interactions or lattice mismatch. The system is quenched below the critical temperature from a homogenous disordered state to an ordered phase where multiple domains coexist. We include an elastic energy part in the Hamiltonian to adjust the rigidity of the model. Theory expects the domain size $R(t)$ grows as a power law $R(t) = A + Bt^n$, where t is the time after the quench. For the rigid model we find the late-time domain size growth factor n has Lifshitz-Slosov value of $\frac{1}{3}$. For weak flexible models, we get slight reduction from $\frac{1}{3}$. For the strongly flexible model, we get a bimodal distribution of bond lengths and a dramatically reduced value of n , which has similar behavior as the mismatch model.³

¹Research supported by NSF

²Mitchell and DP Landau, PRL 97, 025701 (2006)

³Ibid.

3:42PM T13.00007 Atomic-scale antiferromagnets with stable Neel states, ANDREAS HEINRICH, IBM Research — A macroscopic antiferromagnet is characterized by long-range magnetic order, for example with the spin of neighboring atoms alternating their direction. Here we will discuss how far such concepts can be extended towards the atomic scale. We use low-temperature scanning tunneling microscopy with spin-polarized tips to investigate antiferromagnets consisting of a small number of Fe atoms on a thin Cu₂N substrate. As few as 8 Fe atoms show two stable magnetic states in which the spin between neighboring atoms alternates. The STM can be used to switch between these two magnetic states. When heating the spins to about 10K, spontaneous switching occurs from which the switching dynamics is deduced. Small structures show a second switching mechanism that is not dependent on temperature but strongly dependent on the length of the antiferromagnetic chain, suggesting switching by quantum tunneling of magnetization (the Neel vector).

3:54PM T13.00008 Contrasting low-dimensional magnetism in the 3D metal-organic frameworks $[\text{Cu}(\text{VF}_6)(\text{pyz})_2] \bullet 4\text{H}_2\text{O}$ and $[\text{Cu}(\text{HF}_2)(\text{pyz})_2]\text{SbF}_6$ (pyz = pyrazine)¹, JAMIE MANSON, Department of Chemistry and Biochemistry, Eastern Washington University, Cheney, WA 99004 USA, JOHN SCHLUETER, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439 USA, PAUL GODDARD, Clarendon Laboratory, Department of Physics, University of Oxford, Oxford OX1 3PU UK, JOHN SINGLETON, ROSS MCDONALD, OSCAR AYALA-VALENZUELA, MPA-NHMFL, Los Alamos National Laboratory, Los Alamos, NM 87545, TOM LANCASTER, STEPHEN BLUNDELL, Clarendon Laboratory, Department of Physics, University of Oxford, Oxford OX1 3PU UK — $[\text{Cu}(\text{VF}_6)(\text{pyz})_2] \bullet 4\text{H}_2\text{O}$ (**1**) and $[\text{Cu}(\text{HF}_2)(\text{pyz})_2]\text{SbF}_6$ (**2**) form tetragonal frameworks that consist of 2D $[\text{Cu}(\text{pyz})_2]^{2+}$ square lattices that are linked in 3D by bridging VF_6^{2-} (**1**) or HF_2^- (**2**) anions. Magnetic susceptibility data shows apparent paramagnetism, although not simple Curie-Weiss behavior, in **1**. For **2**, a broad maximum in $\chi(T)$ at 12.5 K and a sharp kink at 4.3 K indicate short- (SRO) and long-range (LRO) magnetic ordering, respectively. Additional experimental data for **1** (e.g., heat capacity and $\mu^+\text{SR}$) however, indicate that a LRO state occurs below 3.6 K whereas pulsed-field magnetization data suggest a superposition of AFM Cu^{2+} layers and fluctuating V^{4+} moments. The structural and magnetic behavior of **1** and **2** will be described as well as possible new directions.

¹The work at EWU was supported by the National Science Foundation under grant No. DMR-1005825

4:06PM T13.00009 ABSTRACT WITHDRAWN —

4:18PM T13.00010 Strong Exchange Anisotropy in Heavy Atom Radical Ferromagnets¹, STEPHEN WINTER, University of Waterloo — The discovery twenty years ago of ferromagnetic ordering in “light atom” p-block (N, O based) radicals appeared to provide a major conceptual advance, suggesting the possibility of a new era in non-metal molecular magnetism. However, the weak through-space magnetic exchange interactions present in these early radical-based ferromagnets afforded very low Curie temperatures T_C (< 2 K), and the localization of spin density on light atoms ensured low coercive fields H_c (< 100 Oe). In this context, the observation of ferromagnetic ordering in “heavy atom” (Se) radicals, with T_C as high as 17 K and coercive fields H_c up to 1370 Oe (at 2 K), represents a significant improvement in properties. This presentation will provide a theoretical and experimental examination of the source of the large coercive fields reported for these “heavy atom” radical ferromagnets. High-field ferromagnetic resonance (FMR) measurements, interpreted in the context of the anisotropic exchange interactions between the radicals in the solid state, leads to the conclusion that spin-orbit effects are responsible for the large observed magnetic anisotropy. This conclusion is supported by detailed analysis of the symmetry and magnitude of the spin-orbit interactions. An interesting discussion is the extent to which these anisotropic exchange terms also contribute to the enhancement of T_C . That is, in the field of organic magnetism, where low dimensional magnetic structures are commonly found, long range ordering may depend crucially on such anisotropy.

See JACS **130**, 8414-8425 (2008), JACS **133**, 8126-8129 (2011).

¹Coauthors: S. Hill, A. Kovalev, S. Datta (NHMFL), R. T. Oakley (Waterloo). We thank the NSERC of Canada and the U.S. NSF (Grant DMR0804408) for financial support.

4:54PM T13.00011 FMR Study of the Field Dependence of the Ferromagnetic Transition in an Organic Magnet, ALEXEY KOVALEV, NHMFL, Tallahassee, FL32310, STEPHEN WINTER, University of Waterloo, Ontario N2L 3G1, Canada, STEPHEN HILL, NHMFL and Florida State University, Tallahassee, FL32310, RICHARD OAKLEY, University of Waterloo, Ontario N2L 3G1, Canada — Organic heterocyclic thia/selenazyl radicals have unique magnetic properties. First and foremost, in their crystalline form, they experience a transition to a ferromagnetic state at temperatures that are the highest for any material containing only non-metallic elements. Second, their low temperature uniaxial anisotropy field is the highest among purely organic ferromagnets [Winter et al., JACS 133, 8126 (2011)]. To investigate the effect of a magnetic field on the transition in the mixed Se-S compound ($T_c = 12.5$ K) at zero field, we employ ferromagnetic resonance (FMR) absorption as a measure of the anisotropy field for a single crystal. We also focus on the temperature and field dependence of the FMR linewidth. Our main finding is that the application of a field significantly broadens the ferromagnetic transition, with a noticeable FMR signal observed to as high as $2T_c$ in fields of a few tesla. Meanwhile, the FMR linewidth is relatively insensitive to frequency/field, though it becomes narrower upon decreasing the temperature and saturates below T_c . We will discuss the broadening of the ferromagnetic transition within the framework of scaling theory.

Wednesday, February 29, 2012 2:30PM - 4:42PM –
Session T14 GMAG DMP FIAP: Focus Session: Spins in Semiconductors - Spins and Edge States 212

2:30PM T14.00001 Controlled coupling of spin-resolved quantum Hall edge states, BISWAJIT KARMAKAR¹, NEST-CNR Istituto Nanoscienze and Scuola Normale Superiore. Pisa. Italy — Spin resolved edge states in quantum Hall systems at filling fraction $\nu = 2$ possess large coherence [1] and relaxation [2] lengths. They are ideal candidates for the implementation of dual-rail quantum computation architectures [3] by encoding the qubit in the spin degree of freedom of the co-propagating spin resolved edge states. An important element for realization of such architectures is a coherent beam splitter that controllably mixes the two co-propagating spin-resolved edge channels to create any superposition of the two logic states. In this talk we demonstrate a new method to controllably couple spin resolved edge states and induce inter-edge charge transfer associated to spin-flip scattering events [4]. The process exploits the coupling of the electron spin with a spatially-dependent periodic in-plane magnetic field that is created by an array of Cobalt nano-magnets placed at the boundary of the GaAs/AlGaAs modulation doped heterostructure. The maximum charge/spin transfer of 28 ± 1 % is achieved at 250 mK by fine tuning the perpendicular magnetic field. These results are key steps towards the realization of a scalable quantum interferometric device currently under investigation in our group.

[1] Y. Ji et al. Nature 422 (2003) 415.

[2] G. Muller et al. Phys. Rev. B 45 (1992) 3932.

[3] V. Giovannetti et al., Phys. Rev. B 77 (2008) 155320.

[4] B. Karmakar et al., (accepted in PRL).

¹The work is done in collaboration with D. Venturelli, L. Chirrolfi, F. Taddei, V. Giovannetti, R. Fazio, S. Roddaro, G. Biasiol, L. Sorba, V. Pellegrini and F. Beltram.

3:06PM T14.00002 Theory of Temperature-dependent Spin Dynamics with Electron-Phonon Interaction, JIMMY HUTASOIT, TUDOR STANESCU, West Virginia University — We develop a theory of temperature-dependent spin dynamics in spin-orbit coupled semiconductors that includes the effects of electron-phonon interaction. A set of coupled kinetic equations for the spin density matrix are derived starting from the quantum Liouville equation. The spin-conserving and spin-flipping scattering terms due to electron-phonon interaction in the presence of spin-orbit coupling are derived explicitly using an effective low-energy Hamiltonian for the conduction and valence bands. From the solution of the kinetic equations, we extract the temperature dependence of spin transport and relaxation in various parameter regimes. In particular, we discuss the effect of electron-phonon interaction on the persistent spin helix lifetime.

3:18PM T14.00003 Absence of intrinsic spin splitting in 1D quantum wires of tetrahedral semiconductors¹, JUN-WEI LUO, LIJUN ZHANG, National Renewable Energy Laboratory, Golden, Colorado 80401, USA, ALEX ZUNGER, University of Colorado, Boulder, Colorado 80309, USA — The energy bands of 3D, 2D, and 1D structures are generally split at certain wavevector values into spin-components, a spin splitting that occurs even without external magnetic field and reflects the effect of spin-orbit interaction on certain symmetries. We show via atomistic theory that 1D quantum-wires made of conventional zincblende semiconductors have unexpected zero SS for all electron and hole bands if the wire is oriented along (001) (belonging to D_{2d} symmetry), and for some of bands if the wire is oriented along (111) (belonging to C_{3v} symmetry). We find that the predicted absence of Dresselhaus SS in both (001)-oriented and (111)-oriented 1D wires is immune to perturbations lowering their original D_{2d} and C_{3v} structural symmetries, such as alloying of the matrix around the wire or application of an external electric field. Indeed, such perturbations induce only Rashba SS. We find that the scaling of the SS with wavevector is dominated by a linear term plus a minor cubic term.

J.W. Luo, L. Zhang, and A. Zunger, Phys. Rev. B 84, 121303(R) (2011).

¹Funded by DOE-SC-BES-MSED under Contract No. DE-AC36-08GO28308 to NREL

3:30PM T14.00004 chiral magnon edge mode in a magnonic crystal, RYUICHI SHINDOU, RYO MATSUMOTO, SHUICHI MURAKAMI, Tokyo Institute of Technology — A bosonic system with a periodically crystalline potential has a Chern integer associated with its magnetic Bloch wavefunction. As in its fermionic counterpart like integer quantum Hall states, the Chern number thus introduced is defined for each bosonic energy band which is energetically separated from the others. When two bosonic systems having different Chern integers are connected, or when a bosonic system with non-zero Chern integer is terminated with the vacuum, chiral bosonic edge modes appear in their boundaries. We argue that a simple magnonic crystal can realize such magnonic chiral edge modes. Based on this example, we show how to design spin-wave guides in a magnonic crystal and how to channelize, split and manipulate them.

3:42PM T14.00005 Anomalous Hall and Nernst effects in electron and hole-doped semiconductors, EUGEN DUMITRESCU, CATALINA MARINESCU, Clemson University, CHUANWEI ZHANG, Washington State University, SUMANTA TEWARI, Clemson University — Recently it has been proposed that Majorana fermions may exist in a thin film semiconductor with proximity induced s-wave superconductivity. We compute anomalous Hall and anomalous Nernst coefficients for both electron and hole-doped semiconducting systems in the presence of an in-plane magnetic field and Rashba and Dresselhaus spin-orbit coupling. The anomalous Nernst coefficient vanishes and has plateaus as a function of the chemical potential corresponding to carrier densities which realize the topological state.

3:54PM T14.00006 The Origin of Dirac Cones for Classical Waves in Periodic Systems, JUN MEI, Department of Physics, South China University of Technology, Guangzhou 510641, China, YING WU, Division of Mathematical and Computer Sciences and Engineering, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia, CHE TING CHAN, ZHAO-QING ZHANG, Department of Physics and William Mong Institute of Nano Science and Technology, Hong Kong University of Science and Technology, Hong Kong — By using a perturbation method, we propose a general theory to understand the origin of Dirac cone dispersions for classical waves in periodic structures. A selection rule for the existence of Dirac cones is established under the group theory analysis, which reveals the relation between the unusual linear dispersions and the symmetry of the degenerate Bloch states at the Dirac point. The theory is capable of accurately predicting the linear slopes at various symmetry points in the Brillouin zone, independent of frequency and lattice structure. Furthermore, it can be also used to construct the Hamiltonian, which is in consistent with the Berry phase calculations.

4:06PM T14.00007 Exactly Solvable Topological Chiral Spin Liquid with Random Exchange¹, VICTOR CHUA, GREGORY A. FIETE, Department of Physics, University of Texas at Austin — We extend the Yao-Kivelson decorated honeycomb lattice Kitaev model [Phys. Rev. Lett. 99, 247203 (2007)] of an exactly solvable chiral spin liquid by including disordered exchange couplings. We have determined the phase diagram of this system and found that disorder enlarges the region of the topological non-Abelian phase with finite Chern number. We study the energy level statistics as a function of disorder and other parameters in the Hamiltonian, and show that the phase transition between the non-Abelian and Abelian phases of the model at large disorder can be associated with pair annihilation of extended states at zero energy. Analogies to integer quantum Hall systems, topological Anderson insulators, and disordered topological Chern insulators are discussed.

¹ARO grant W911NF-09-1-0527 and NSF grant DMR- 0955778

4:18PM T14.00008 Lie algebras for time-dependent Rashba-Dresselhaus materials, JEAN-FRANCOIS VAN HUELE, MANUEL BERRONDO, Brigham Young University — We study the spin dynamics of Rashba and Dresselhaus interactions in systems with unconfined and confined geometries. We show how Lie algebra factorization of the evolution can be used to describe systems with arbitrary time-dependence in the parameters.

4:30PM T14.00009 Quantum Spin Holography with Surface State Electrons, OLEG BROVKO, VALERI S. STEPANYUK, Max Planck Institute of Microstructure Physics, Halle, Germany — Recently Moon et al. have shown that information can be stored in a fermionic state of a two-dimensional electron gas and have dubbed the proposed concept quantum holographic encoding. They have constructed molecular holograms of CO molecules on a Cu(111) surface, hosting a surface state (SS) [2]. Interference of electron waves scattered at the molecules leads to formation of an electron density pattern representing an information page [1]. This page has then been read out with an STM. It has been also shown that using the innate energy dispersion of SS electrons one can project the hologram not only in two spatial degrees of freedom but also in the energy dimension. In our contribution we expand the concept and show that the spin of the electron can also act as a new dimension for information storage. If the molecules or atoms used for a hologram are magnetic then the scattering of surface state electrons becomes spin-dependent, allowing one to store different information pages in different spin channels. As an example we demonstrate the possibility of simultaneous encoding two different information pages with electrons of the same energy but opposite spins.

[1] C.R. Moon et al., Nature Nano. 4, 167 (2009)

[2] W. Shockley, Phys. Rev. 56, 317 (1939)

Wednesday, February 29, 2012 2:30PM - 5:30PM –
Session T15 DMP GMAG: Focus Session: Magnetic Nanostructures-Exchange Bias and Exchange-Coupled Systems 213

2:30PM T15.00001 Investigation of CoO/Fe/Ag(001) and NiO/Fe/Ag(001) epitaxial thin films X-ray magnetic dichroism, Z.Q. QIU, University of California at Berkeley — Interfacial coupling at antiferromagnetic (AFM)/ferromagnetic (FM) interface is less understood because of the so-called magnetic frustration and the lack of direct measurement on AFM thin films. These difficulties have been partially overcome by recent development of X-ray Magnetic Dichroism on single crystalline magnetic thin films. In this talk, I will report our study on epitaxial CoO/Fe/Ag(001) system using X-ray Magnetic Circular Dichroism (XMCD) and X-ray Magnetic Linear Dichroism (XMLD). XMCD was used to measure the Fe hysteresis loops and XMLD was used to measure the response of the AFM CoO spins in response to the Fe magnetization reversal. We find that the CoO spins consist of rotatable and frozen spins with respect to the Fe spin rotation, and only the Fe uniaxial magnetic anisotropy follows the CoO frozen spins. By using focused ion beam to pattern the films into microstructures, we also observed vortex state in CoO disk imprinted from the Fe vortex state.

3:06PM T15.00002 Mirror symmetry in magnetization reversal and coexistence of positive and negative exchange bias in Ni/FeF₂ heterostructures, XAVIER BATLLE, M. KOVYLINA, A. LABARTA, Dept. Fisica Fonamental, Universitat de Barcelona, 08028 Barcelona, Catalonia, Spain, R. MORALES, Basque Foundation for Science, IKERBASQUE, 48011 Bilbao, Spain, M. EREKHINSKY, IVAN K. SCHULLER, Physics Department, University of California San Diego, La Jolla 92093 CA, USA — Positively and negatively exchange biased (PEB and NEB) magnetoresistance (MR) loops in Ni/FeF₂ ferromagnetic/antiferromagnetic (AF) heterostructures proceed through exactly the same reversal mechanisms. The MR curves exhibit striking mirror symmetry: the increasing (decreasing) field branch of the PEB (NEB) loop is identical to the decreasing (increasing) branch of the NEB (PEB) loop. The latter suggests that, on average, similar but opposite sign EB domain configurations are reached for low or high cooling fields, with equal interfacial density of pinned uncompensated AF spins responsible for NEB or PEB. Micromagnetic simulations are in agreement with experimental results and imply the coexistence of EB domains of opposite sign for all cooling fields, which results in a new reversal mechanism not previously reported. The persistence of NEB (PEB) domains even at high (low) cooling fields may be produced by the size distribution and density of pinned uncompensated moments in the bulk of the AF. The support of the Spanish MICINN, Catalan DURSI, IKERBASQUE and the US Department of Energy are recognized.

3:18PM T15.00003 Phase separation and giant exchange bias in Mn-based binary alloys¹, F. JIMENEZ-VILLACORTA, J.L. MARION, L.H. LEWIS, Department of Chemical Engineering, Northeastern University — The ability to tailor, control and modify the magnetic properties of Mn-based alloys opens the possibility of developing exchange bias systems for permanent magnet and sensor technologies. Rapid solidification of AgMn, CuMn and AlMn manganese-based alloys, with significant Mn concentration (~ 30 -70 at%), has produced alloys that all exhibit a remarkable exchange bias at $T = 10$ K, of the order of ~ 10 kOe. Structural characterization confirms the formation of a phase-separated nanostructure (*fcc* for AgMn and CuMn and *hcp* for AlMn) of 40-80 nm in all alloys as characterized by phase-specific crystallographic texture and lattice parameters. The observed exchange bias is highly reduced upon moderate annealing ($T = 250$ °C) accompanied by homogenization of the Mn concentrations in the alloys. These results are tentatively attributed to different metastable incorporation of Mn within the two phases, yielding slightly different unit cell volumes, which provides an antiferromagnetic (Mn-rich phase) and ferromagnetic (Mn-poor phase) character in these two phases.

¹This research has been funded by the Office of Naval Research (ONR) under Grant # N00014-10-1-0553.

3:30PM T15.00004 Exchange Bias and Large Vertical Magnetization Shift in FM/V₂O₃ Interfaces¹, JOSE DE LA VENTA, MIKHAIL EREKHINSKY, SIMING WANG, IVAN K. SCHULLER, Univ of California - San Diego, RAFAEL MORALES, Universidad del País Vasco and IKERBASQUE — We have investigated exchange bias in different combinations of V₂O₃ thin films with ferromagnetic layers. The exchange bias is accompanied by a large vertical shift in the magnetization. These effects are only observed when V₂O₃ is grown on top of Ni₈₀Fe₂₀ permalloy (Py). The magnitude of the vertical shift is as large as 60% of the total magnetization which has never been reported in any system. The exchange bias and the vertical shift are related to the formation of a Fe₃O₄ interlayer. We will show evidence that the Fe₃O₄ Verwey transition is responsible for the appearance of the exchange bias and the vertical shift in the magnetization.

¹This work has been supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences under Award FG03-87ER-45332 and Spanish MICINN and IKERBASQUE.

3:42PM T15.00005 Exchange Bias in Ni/Co Multilayers with Perpendicular Anisotropy¹, SCOTT M. CAMPBELL, Department of Physics, University of South Florida, S.M. MOHSENI², T.N. ANH NGUYEN, Materials Physics, School of Information and Communication Technology, KTH Royal Institute of Technology, R.K. DUMAS, JOHAN AKERMAN³, Department of Physics, University of Gothenburg, CASEY W. MILLER, Department of Physics, University of South Florida — We have studied exchange bias in Ta(5nm)/Au(10)/[Ni(t)/Co(0.4)] $\times$ 5/IrMn(8)/Ta(5) multilayers for Ni thicknesses of 0.8-1.2 nm. The samples were deposited via sputtering and no deposition field was used. The samples were annealed at 200 °C in an applied field of 1500 Oe for different durations, then measured by polar Magneto-Optical Kerr Effect at room temperature. We find that the field annealing significantly alters the hysteresis loop shape, giving it more single domain character while simultaneously inducing exchange bias in the direction of the annealing field. After 34 (2 and 32) hrs annealing, the exchange bias of the samples each reach a maximum value ranging from 100 Oe for the thickest Ni to 35 Oe for the thinnest Ni. We find that the samples with the thinner Ni layers approach their exchange bias maximum values for shorter annealing times.

¹Supported by NSF, The Swedish Institute, The Swedish Foundation for Strategic Research, The Swedish Research Council and the Knut and Alice Wallenberg Foundation.

²NanOsc AB

³Materials Physics, School of Information and Communication Technology, KTH Royal Institute of Technology, NanOsc AB

3:54PM T15.00006 Electrical measurement of antiferromagnetic moments in exchange-coupled IrMn/NiFe stacks, H. REICHOVA, X. MARTI, Institute of Physics ASCR, v.v.i., Cukrovarnicka 10, Praha 6, Czech Republic, B.G. PARK, J. WUNDERLICH, Hitachi Cambridge Laboratory, Cambridge CB3 0HE, UK, Y. KUROSAKI, M. YAMADA, H. YAMAMOTO, A. NISHIDE, J. HAYAKAWA, H. TAKAHASHI, Hitachi Ltd, Advanced Research Laboratory, 1-280 Higashi-koigakubo, Kokubunju-shi, Tokyo 185-8601, Japan, T. JUNGWIRTH, Institute of Physics ASCR, v.v.i., Cukrovarnicka 10, Praha 6, Czech Republic — A great attention is currently focused on the development of new spintronic devices. One crucial technological issue is the coupling phenomena between thin antiferromagnetic (AFM) and ferromagnetic (FM) layers. Despite the exchange coupling was for the first time observed already in 1956, yet the effect is not fully understood. Certainly, the zero macroscopic magnetic moment in the AFM materials hinders the investigation, in contrast to the exhaustive studies on the FM counterpart. Only a very few experiments at large scale facilities explored the status of the AFM layer. Here, we will address the study of both FM and AFM moments in the archetypical IrMn/NiFe exchange-coupled system. Using common laboratory magnetization and transport tools, we found a direct link between reversal of FM moments in NiFe and rotation and pinning of AFM moments in IrMn [1]. We will show that a full rotation of AFM moments in IrMn occurs at high temperatures, in contrast to only partial rotation of AFM at low temperatures. We will discuss the experimental results in the framework of different exchange coupling models. [1] <http://arxiv.org/abs/1108.2189>

4:06PM T15.00007 Exchange bias of conetic thin films¹, TATIANA EGGERS, HILLARY KIRBY, PRIYANGA JAY-ATHILAKA, SCOTT CAMPBELL, CASEY MILLER, University of South Florida — In this work, we study the exchange bias and coercivity of Ni₇₇Fe₁₄Cu₅Mo₄ (Conetic, also known as mu-metal) exchange coupled with FeMn as functions of Conetic thickness and buffer layer material. The samples studied were BL(30nm)/Conetic(9nm-30nm)/FeMn(10nm)/Ta(5nm), where BL = Cu or Ta. All samples were grown by magnetron sputtering in a deposition field of ~ 150 Oe during growth to set the exchange bias axis. Room temperature hysteresis loops were measured by a magneto-optical Kerr effect magnetometer as a function of applied-field angle. For each variety of sample, the exchange bias and coercivity were inversely proportional to Conetic thickness. With Cu buffer layers grown on Si, the H_{eb} decreased from 300 Oe to 62 Oe, and H_c decreased from 99 Oe to 9 Oe. Similar results were found when the Cu buffer layer was grown on SiO_x, though the maximum coercivity was only 67 Oe. For the samples grown on Si(001)/Ta(5nm), the exchange bias decreased from 80 Oe to 14 Oe, while the coercivity increases only slightly from 2 Oe to 10 Oe. These results indicate a trade-off between preserving the softness of the ferromagnet and having a large exchange, which may be useful for tuning the performance of low-field sensing materials

¹Supported by NSF.

4:18PM T15.00008 Effect of Cu Layer on Exchange Bias in FeMn, DOGAN KAYA, Texas A&M University, PRIYANGA JAYATHILAKA, CASEY W. MILLER, University of South Florida, IGOR V. ROSHCHIN, Texas A&M University — One of the most important puzzles related to the mechanism of exchange bias is the origin and role of uncompensated magnetization in the antiferromagnet. We study effects of a Cu layer on the uncompensated magnetization and exchange bias in FeMn, the material with a high potential for applications in magnetic recording. The multilayers of Ta(50 Å)/[FeMn(50 Å – 150 Å)/Cu(50 Å)]₁₀/Ta(50 Å) are deposited by UHV DC magnetron sputtering on top of Si/SiO_x 3 mm x5 mm substrates. Samples with a single layer of FeMn of the same thickness, Ta(50 Å)/FeMn(50 Å – 150 Å)/Ta(50 Å) are used as control samples. The samples are cooled in a field of 7 T and their magnetization is measured using a SQUID magnetometer. All the samples have uncompensated magnetization that exhibits a hysteresis at 10 K. The hysteresis loops for FeMn/Cu multilayers are exchange bias shifted, while FeMn without Cu exhibits no exchange bias. Dependence of coercive field (H_c), exchange bias (H_e), and saturated magnetization (M_s) on the FeMn thickness and on temperature will be discussed. Work is supported by Texas A&M University, TAMU-CONACYT Collaborative Research Program, and by NSF (USF).

4:30PM T15.00009 Interface coupling between ferromagnets and random and dilute antiferromagnets¹, DAVID LEDERMAN, KINESHMA MUNBODH, MIYEON CHEON, West Virginia University, Morgantown, WV 26506-6315, M.R. FITZSIMMONS, Los Alamos National Laboratory, Los Alamos, NM 87545, NEIL R. DILLEY, Quantum Design, Inc., San Diego, CA 92121 — Depth profiles for pinned and unpinned magnetizations were determined across the interface between a ferromagnet (F) and random and dilute antiferromagnets (RAF and DAF) exemplified by $\text{Fe}_{0.45}\text{Ni}_{0.55}\text{F}_2/\text{Co}$ and $\text{Fe}_{0.34}\text{Zn}_{0.66}\text{F}_2/\text{Co}$ bilayers, respectively, using polarized neutron reflectivity (PNR). PNR measurements were complemented by magnetometry using applied fields as large as 160 kOe to assure saturation of the entire sample, including magnetic moments that are normally pinned at lower fields. The locations of pinned and unpinned magnetization in the ferro- and antiferromagnets were identified. The origin of exchange bias in the RAF system is noticeably different than that of the DAF system. In the RAF system, a domain wall is formed at the RAF/F interface when the ferromagnet's magnetization is reversed. In the DAF system, some domains within the bulk of the DAF are reversed upon reversal of the ferromagnet with others remaining pinned, while the interface magnetization is entirely reversed. This work was supported by the National Science Foundation.

¹This work was supported by the National Science Foundation

4:42PM T15.00010 A study of the magnetic interlayer coupling between CoO(NiO) and Fe films across MgO spacer layer in CoO(NiO)/MgO/Fe/Ag(001) using MOKE and XMLD, ALI TAN, JIA LI, YANG MENG, University of California Berkeley, ELKE ARENHOLZ, Advanced Light Source, Lawrence Berkeley National Laboratory, CHANYONG HWANG, Advanced Industrial Technology Group, Korea Research Institute of Standards and Sciences, ZI QIANG QIU, University of California Berkeley — CoO(NiO)/MgO/Fe/Ag(001) films were grown epitaxially and studied by Magneto Optical Kerr Effect (MOKE) and X-ray Magnetic Linear Dichroism (XMLD). The enhancement of the Fe layer coercivity due to its coupling to the AFM (NiO) overlayer was studied as a function of the MgO spacer layer thickness using MOKE. We found that the Fe coercivity enhancement persists to ~ 2 ML MgO thickness, after which the AFM-FM interlayer coupling becomes too weak to affect the Fe coercivity. Below 2ML MgO thickness, the Fe coercivity enhancement depends both on the MgO and NiO thicknesses. To further understand the effect of interlayer coupling, the rotatable CoO spins in CoO/MgO/Fe/Ag(001) after field cooling along the Fe(100) axis were determined using the XMLD measurement as a function of the MgO thickness. We found that 2 ML MgO thickness sets a critical value beyond which the CoO/MgO/Fe interlayer coupling no longer rotates the CoO spins.

4:54PM T15.00011 Modification of thickness dependent magnetic properties of perpendicular anisotropy Co/Pd multilayer upon hydrogenation¹, KINESHMA MUNBODH, FELIO PEREZ, DAVID LEDERMAN, West Virginia University — We have studied the change in saturation magnetization (M_S) and effective perpendicular anisotropy (K_{eff}) upon hydrogenation at room temperature and a pressure of one atmosphere in (Co/Pd)₂₅ multilayers, with Co thickness ≤ 5 Å and Pd thickness ranging from 0 Å to 25 Å. The change in M_S and K_{eff} was studied as a function of the x-ray scattering length density profile, generated from the x-ray reflectivity fits. The results show that when the Pd thickness ≤ 10 Å, the films were highly interdiffused, resulting in no measurable change in M_S and K_{eff} . As the thickness of Pd increases, the contrast between the Co and Pd layers increases, leading to a decrease in M_S and an increase in the component of magnetization in the plane of the samples and hence causing K_{eff} to decrease. The results clearly demonstrate that the solubility of hydrogen in the multilayer samples decreases with increasing alloying effects as it decreases the vacancy in the Pd 4d band leading to no electronic transfer from the hydrogen atoms to the Pd.

¹This work was supported by the Department of Energy.

5:06PM T15.00012 Momentum transfer resolved memory in a magnetic system with perpendicular anisotropy, KEOKI SEU, SUJOY ROY, Advanced Light Source, Lawrence Berkeley National Laboratory, RUN SU, DAN PARKS, Physics Department, University of Oregon, ERIK SHIPTON, ERIC FULLERTON, Physics Department, University of California at San Diego, STEPHEN KEVAN, Physics Department, University of Oregon — We have used resonant, coherent soft x-ray scattering to measure wave vector resolved magnetic domain memory in Co/Pd multilayers. The technique uses angular cross correlation functions and can be applied to any system with circular annuli of constant values of scattering wave vector q . In our Co/Pd film, the memory exhibits a maximum at $q=0.0384$ nm⁻¹ near initial reversal that decreases in magnitude as the magnetization is further reversed. The peak is attributed to bubble domains that nucleate reproducibly near initial reversal and which grow into a labyrinth domain structure that is not reproduced from one magnetization cycle to the next.

5:18PM T15.00013 Measure of magnetization anisotropy by AMR in electrodes of Co/Pd multilayers¹, AMOS SHARONI, YANIV KACHLON, NOA KURZWEL, Department of Physics and Institute of Nanotechnology, Bar Ilan University, Ramat Gan, Israel — We studied the anisotropic magnetoresistance (AMR) properties of multilayered Co/Pd thin film electrodes as function of magnetic field. The perpendicular magnetization anisotropy (PMA) in these films is found to modify the AMR. The magnetoresistance (MR) for fields out-of-plane (ρ_{op}) is considerably different than for in-plane fields transverse to current direction (ρ_{ip}), although in both cases current is perpendicular to the magnetic field. Moreover, opposed to other thin films, where ρ_{op} is smaller than ρ_{ip} , our films show an opposite effect, the origin of which is not clear. We can understand the AMR properties of the electrodes by an expanded Stoner-Wolfarth model, where we introduce an additional energy scale related to the PMA. Through a numerical refinement process, we can extract anisotropic energy constants of the films. This is done by reconstructing the MR behavior of the electrodes, using the linear terms in the dependence of resistivity on magnetization orientation. Our anisotropic constants coincide remarkably with other bulk measurements. Thus, our refinement process is an excellent method to extract anisotropic constants also in nano-scale systems, which cannot be measured otherwise.

¹Work supported by EU-FP7 People IRG #268357.

Wednesday, February 29, 2012 2:30PM - 5:30PM — Session T16 DCMP: Kondo Lattice Theory 251

2:30PM T16.00001 A new paradigm for heavy electron materials, YI-FENG YANG, Institute of Physics, Chinese Academy of Sciences, DAVID PINES, University of California, Davis — Recent experiments on the emergence of heavy electrons that display universal behavior below a characteristic temperature T^* have shown that the well-known Doniach phase diagram does not apply to most materials. Here we introduce the concept of hybridization effectiveness as the organizing principle and show that it makes possible a consistent and quantitative description of the low temperature emergent behaviors of a number of heavy electron materials. We propose a new phase diagram and predict a delocalization line in the pressure/temperature phase diagram that is to be examined in future experiment.

2:42PM T16.00002 Superconductivity in Heavy Fermion Materials, JOHN VAN DYKE, JEREMY FIGGINS, DIRK MORR, University of Illinois at Chicago — Superconductivity in heavy fermion materials is a complex phenomenon since it often emerges from a strongly entangled state, the Kondo screened heavy Fermi liquid. In this talk, we discuss possible pairing interactions that arises in the heavy Fermi liquid, and the resulting symmetries and momentum dependencies of the superconducting order parameter. In particular, we show that the interplay between the large Fermi surface of the Fermi liquid state and the momentum dependence of the pairing interaction naturally leads to an unconventional symmetry of the superconducting order parameter in general, and a $d_{x^2-y^2}$ -symmetry in particular. Moreover, we identify the signatures of unconventional pairing in the differential conductance, dI/dV , measured in scanning tunneling spectroscopy as well as in the quasi-particle interference pattern. Finally, we discuss the effects of impurities on the spatial dependence of both the superconducting order parameter and the hybridization.

2:54PM T16.00003 Single-particle and optical self-energies of a Fermi liquid revisited, DMITRII MASLOV, University of Florida, ANDREY CHUBUKOV, University of Wisconsin — We discuss the conditions under which the imaginary part of the single-particle self-energy at the Fermi surface $\Sigma(\omega, T)$ and the optical scattering rate $1/\tau(\Omega, T)$ have particular simple scaling forms $\text{Im}\Sigma(\omega, T) \propto \omega^2 + \pi^2 T^2$ and $1/\tau(\Omega, T) \propto \Omega^2 + 4\pi^2 T^2$. We show that these relations follow from particular analytic properties of the effective fermion-fermion interaction and are only satisfied when the single-particle and optical self-energies are analytic functions of the frequency. When they are not, the scaling forms are more complex even if the system remains a Fermi liquid. We also address recently observed violation of the $\Omega^2 + 4\pi^2 T^2$ form of $1/\tau$ in URu_2Si_2 and discuss possible mechanisms of this violation.

3:06PM T16.00004 Singular Valence Fluctuations at a Kondo Destroyed Quantum Critical Point¹, JEDEDIAH PIXLEY, Rice University, STEFAN KIRCHNER, Max Planck Institute for the Physics of Complex Systems, KEVIN INGERSENT, University of Florida, QIMIAO SI, Rice University — Recent experiments on the heavy fermion superconductor $\beta\text{-YbAlB}_4$ have indicated that this compound satisfies quantum critical scaling [1]. Motivated by the observation of mixed valency in this material [2], we study the Kondo destruction physics in the mixed-valence regime [3] of a particle-hole asymmetric Anderson impurity model with a pseudogapped density of states. In the vicinity of the quantum critical point we determine the finite temperature spin and charge susceptibilities by utilizing a continuous time quantum Monte Carlo method [4] and the numerical renormalization group. We show that this mixed-valence quantum critical point displays a Kondo breakdown effect. Furthermore, we find that both dynamic spin and charge susceptibilities obey frequency over temperature scaling, and that the static charge susceptibility diverges with a universal exponent. Possible implications of our results for $\beta\text{-YbAlB}_4$ are discussed. [1] Matsumoto et al, Science **331**, 316 (2011). [2] Okawa et al, Physical Review Letters **104**, 247201 (2010). [3] J. H. Pixley, S. Kirchner, Kevin Ingersent and Q. Si, arXiv:1108.5227v1 (2011). [4] M. Glossop, S. Kirchner, J. H. Pixley and Q. Si, Phys. Rev. Lett. **107**, 076404 (2011).

¹Funding for this work is provided by NSF and the Welch Foundation.

3:18PM T16.00005 Kondo Physics in a Rare Earth Ion with well localized $4f$ electrons¹, JOLANTA STANKIEWICZ, Instituto de Ciencia de Materiales de Aragon, CSIC-Universidad de Zaragoza, ZACHARY FISK, Department of Physics, University of California at Irvine, MARCO EVANGELISTI, Instituto de Ciencia de Materiales de Aragon, CSIC-Universidad de Zaragoza, PEDRO SCHLOTTMAN, Department of Physics, Florida State University — We observe a rise in the low temperature resistivity of dilute $\text{La}_{1-x}\text{Nd}_x\text{B}_6$ single crystals. The specific heat data for the same samples show that there is an entropy of $R\ln 4$ per mole Nd involved in the excess specific heat above that of LaB_6 . All these features are consistent with a Kondo scale of $T_K = 1$ K. However, Nd has a well localized $4f^3$ $J = 9/2$ Hund's Rule configuration which is not expected to be Kondo coupled to the conduction electrons in LaB_6 . We conjecture that the unexpected Kondo effect arises via participation of $4f$ quadrupolar degrees of freedom of the Nd crystal field ground state quartet. Raman experiments as well as detailed theoretical studies do indicate that one expects strong quadrupolar influence in the properties of NdB_6 .

¹Supported by grant MAT2008/03074, from MICINN of Spain, and by NSF grant DMR-0854781.

3:30PM T16.00006 Partial disorder in the periodic Anderson model on a triangular lattice, SATORU HAYAMI, Dep. Appl. Phys., Univ. Tokyo, MASAFUMI UDAGAWA, Dep. Appl. Phys., Univ. Tokyo, MPI PKS, YUKITOSHI MOTOME, Dep. Appl. Phys., Univ. Tokyo — In Kondo lattice systems, keen competition between the Kondo coupling and RKKY interaction leads to a quantum critical point between a magnetically-ordered state and a Fermi liquid state. This is a source of novel phenomena, such as a non-Fermi liquid behavior and a superconductivity. In the present study, we explore a new quantum phase related to the competition by introducing a new parameter, geometrical frustration of the lattice structure. Especially, we focus on the possibility of a partial disordered (PD) state, in which a magnetically ordered and nonmagnetic sites coexist. We consider a fundamental model for the rare-earth systems, a periodic Anderson model on a frustrated triangular lattice, and investigate the ground-state phase diagram by the Hartree-Fock approximation with assuming three-site unit cell. As a result, we find a PD state at half filling between a noncollinear antiferromagnetic metal and a Kondo insulator [1]. The PD state is stabilized by relaxing the frustration by forming collinear antiferromagnetic order on an unfrustrated honeycomb subnetwork, while leaving remaining sites non-magnetic. We will also discuss the effects of spin anisotropy and carrier doping to the PD state.

[1] S. Hayami, M. Udagawa, and Y. Motome, J. Phys. Soc. Jpn. **80**, 073704 (2011).

3:42PM T16.00007 Quantum critical Kondo destruction of the Bose-Fermi Kondo model in the presence of a local transverse field, EMILIAN NICA, Rice University, KEVIN INGERSENT, University of Florida, QIMIAO SI, Rice University — Recent studies of the global phase diagram of quantum critical heavy fermion metals [1] have motivated us to consider the interplay between the quantum fluctuations within the local-moment system and those associated with the Kondo interaction. Towards this goal, we study a Bose-Fermi Kondo model with Ising anisotropy in the presence of a local transverse field. We apply the numerical renormalization group method for the case with a sub-ohmic bosonic bath exponent and a constant conduction electron density of states [2]. Upon increasing the strength of the transverse field in the Kondo screened phase we find a crossover from a fully screened to a fully polarized impurity spin with no transition in between. Increasing the strength of the transverse coupling in the localized phase, on the other hand, we identify signatures for a continuous transition into a partially polarized Kondo phase. We discuss the implications of our results for the global phase diagram of the Kondo lattice system.

[1] Q. Si and F. Steglich, Science **329**, 1161 (2010).

[2] M. T. Glossop and K. Ingersent, Phys. Rev. B **75**, 104410 (2007).

3:54PM T16.00008 A spin-selective Kondo-insulator: Cooperation between Ferromagnetism and Kondo-effect, ROBERT PETERS, NORIO KAWAKAMI, Kyoto University, THOMAS PRUSCHKE, University of Goettingen — Taking ferromagnetic heavy fermion compounds as motivation we analyze the mechanism stabilizing the ferromagnetic state in the antiferromagnetically coupled Kondo lattice model. We find that even for this ferromagnetic state Kondo screening plays an essential role in stabilizing the ferromagnetic state at zero temperature leading to very interesting properties: while the majority-spin electrons are metallic, the minority-spin electrons form an insulating state. We clarify that this state is due to partial Kondo screening, so that parts of the local moments are bound to the electrons, resulting in a dynamically-induced commensurability which is essential for producing the gap in the minority-spin electrons. We believe that the mechanism proposed here, the dynamically generated commensurability, is generic for the ferromagnetic phase in the antiferromagnetically coupled Kondo lattice model, thus providing new insights into the zero temperature physics for the Kondo lattice model.

4:06PM T16.00009 Phase diagram of half-filled $J_1 - J_2$ -Heisenberg Kondo lattice model on honeycomb lattice¹

, QIMIAO SI, Rice University, PALLAB GOSWAMI, National High Magnetic Field Laboratory and Florida State University — Recent studies in quantum critical heavy fermion metals have opened up a rich phase diagram. The zero-temperature global phase diagram involves a combination of phases, featuring Kondo screening/destruction and antiferromagnetic order/disorder as the quantum fluctuations of the local moments are tuned relative to their Kondo coupling with the spins of the conduction electrons. Recently, we have studied a one-dimensional Heisenberg-Kondo model to reveal a competition between a Kondo-screened paramagnetic phase with a large Fermi surface and a Kondo-destroyed paramagnetic spin-Peierls phase with a small Fermi surface [1]. To take advantage of the intuitions gained through that work, we study here a half-filled, $J_1 - J_2$ Heisenberg-Kondo lattice model on a honeycomb lattice. We have obtained a rich phase diagram as a function of magnetic frustration and Kondo coupling. Apart from antiferromagnetic and Kondo insulators, we also find Kondo-destroyed phases that are semi-metallic with Fermi points. There are also particular critical points which are gapless in both charge and spin sectors.

[1] P. Goswami and Q. Si, Phys. Rev. Lett. **107**, 126404 (2011).

¹NSF

4:18PM T16.00010 Cluster dynamical mean-field study of charge ordering in the Kondo lattice model at quarter filling

, JUNKI YOSHITAKE, TAKAHIRO MISAWA, YUKITOSHI MOTOME, Dept. of Appl. Phys., Univ. of Tokyo — The Kondo lattice model is one of fundamental models for heavy-fermion systems, where exchange interactions between itinerant electrons and localized spins play an important role. Among many different phases described by this model, an interesting possibility is a charge-ordered state, in particular when considering the fact that the model does not include any bare repulsive interaction between electrons. The possibility was first pointed out by a perturbation expansion in the strong Kondo coupling limit at quarter filling [1], and recently examined by the dynamical mean-field theory in infinite dimensions [2]. However, it remains unclear whether the charge-ordered state still survives in two or three dimensions and what type of magnetic order is accommodated in the charge-ordered state. To clarify these issues, we investigate the quarter-filled Kondo lattice model on a square lattice by using cluster dynamical mean-field theory, which can include both spatial and dynamical correlations. We found that charge-ordered state appears in the intermediate coupling region. We will discuss electronic and magnetic properties in the charge-ordered state in detail.

[1] H. E. Hirsch, Phys. Rev. B **30**, 5383 (1984).

[2] J. Otsuki *et al.*, J. Phys. Soc. Jpn. **78**, 034719 (2009).

4:30PM T16.00011 Phase diagram of the non-centrosymmetric Kondo lattice model

, LEONID ISAEV, Louisiana State University, DANIEL AGTERBERG, University of Wisconsin-Milwaukee, ILYA VEKHTER, Louisiana State University — Kondo lattice model is prototypical for studying materials with localized f-electrons such as heavy-fermion compounds that exhibit a competition between Kondo screening and magnetism. This competition was argued to be crucial for superconductivity in these systems. We study the effects of spin-orbit interaction (SOI) in the conduction band (due to the lack of inversion symmetry), on the interplay between Kondo, superconducting and magnetic phases by considering the $S = 1/2$ 2D Kondo lattice with short-range Heisenberg coupling between localized moments and utilizing a pseudo-fermion hybridization mean-field theory. In particular, we demonstrate that the heavy-fermion state, and hence superconductivity, is suppressed with increasing SOI. Our results are of relevance for Ce- and U-based heavy-fermion superconductors without inversion symmetry.

4:42PM T16.00012 Simulation of the triangular Kondo-lattice model using the gradient kernel polynomial method

, KIPTON BARROS, YASUYUKI KATO, Theoretical Division, Los Alamos National Laboratory — We introduce a method to study systems, such as the Kondo-lattice model, where a classical field is coupled to fermionic degrees of freedom. Such systems are computationally challenging because each change to the classical field requires recalculation of the density of states for the bilinear fermionic Hamiltonian. The kernel polynomial method (KPM) is a useful tool to approximate the density of states at a cost linear in the system size. We extend KPM to approximate the gradient of the density of states at the same cost, allowing fast updates of the entire classical field. Simulations of the triangular Kondo-lattice model indicate phases with exotic non-coplanar spin ordering and spontaneous quantum Hall effect.

4:54PM T16.00013 Monte Carlo simulations of magnetic clustering at a quantum critical point¹

, TOM HEITMANN, University of Missouri Research Reactor, JOHN GADDY, JAGAT LAMSAL, WOUTER MONTFROOIJ, Department of Physics and Astronomy, University of Missouri — We present the results of Monte Carlo simulations on a percolating magnetic system with relevance to quantum critical point materials. It has previously been shown that, for heavily doped quantum critical point compounds such as $\text{Ce}(\text{Ru}_{0.24}\text{Fe}_{0.76})_2\text{Ge}_2$, the formation and dynamics of magnetic clusters strongly influences the physical response of the system at low temperature. Our simulation is based on the idea that finite-size effects force small magnetic clusters to order at comparatively high temperatures and, once formed, are impervious to Kondo shielding. Disorder acts to introduce a distribution of Kondo temperatures which, in turn, governs the formation of clusters as the temperature is lowered. We implement a percolation model based on such a distribution— first introduced by Bernal *et al.*— and with a restriction whereby Kondo shielding is allowed to remove moments from the infinite cluster *only*. We investigate how this influences thermodynamic quantities as well as how well the simulations align with our analytic theory that is based on the same restriction.

¹This research is supported by the U.S. Department of Energy, Basic Energy Sciences, and the Division of Materials Sciences and Engineering under Grant No. DE-FG02-07ER46381

5:06PM T16.00014 Monte Carlo study of a spin-ice type Kondo lattice model on a pyrochlore lattice

, HIROAKI ISHIZUKA, Dept. of Appl. Phys., Univ. of Tokyo, MASAFUMI UDAGAWA, Dept. of Appl. Phys., Univ. of Tokyo, MPI-PKS, Dresden, YUKITOSHI MOTOME, Dept. of Appl. Phys., Univ. of Tokyo — Recent experiments on geometrically frustrated metallic oxides, such as pyrochlore oxides $\text{R}_2\text{Mo}_2\text{O}_7$ and $\text{R}_2\text{Ir}_2\text{O}_7$, have drawn increasing interest in the effect of geometrical frustration in itinerant electron systems. In these systems, the coupling between electrons and frustrated magnetism leads to various fascinating phenomena. However, much less theoretical studies have been done by treating the interplay of localized spins and itinerant electrons in an unbiased manner. To clarify electronic and magnetic behaviors in such spin-charge coupled systems on frustrated lattice structures, we investigate a spin-ice type Kondo lattice model on a pyrochlore lattice by a real-space Monte Carlo simulation. By employing a sophisticated algorithm, we conduct calculations up to 2048 sites. We show that the system exhibits keen competition between various magnetic phases depending on the spin-charge coupling and electron density. As a consequence, the system shows rich phase diagram with complex magnetic orderings and phase separations between them. Furthermore, in applied magnetic field, we identify a magnetization plateau for one of the novel magnetic phases. In the presentation, the phase diagram and the mechanism of the magnetic orderings will be discussed in details.

5:18PM T16.00015 O(3)-symmetric variational wave functions for the Kondo lattice model

, JOHAN NILSSON, University of Gothenburg — We construct and investigate a class of correlated wave functions for the Kondo lattice model. The construction is based on the faithful fermionic representation of the Kondo lattice model that was introduced recently by the author in PRB **83**, 235103 (2011). In the limit of small exchange coupling the wave functions allow for both local singlet correlations between the localized moments and the conduction electrons, as well as an essentially arbitrary spin correlation function for the localized moments. We compare and contrast our results with those of previous studies.

Wednesday, February 29, 2012 2:30PM - 5:18PM –

Session T17 DMP: Focus Session: Electron, Ion, and Exciton Transport in Nanostructures - Quantum Transport II 252A

2:30PM T17.00001 AC Bias Spectroscopy of the Kondo Singlet in a Single Electron Transistor¹

, BRYAN HEMINGWAY, TAI-MIN LIU², ANDREI KOGAN, University of Cincinnati, STEVEN HERBERT, Xavier University, MICHAEL MELLOCH, Purdue University — We have measured the nonlinear differential conductance, G , of a single electron transistor in the spin 1/2 Kondo regime in presence of an oscillating source voltage. In two distinct regimes, $hf > k_B T_K$ and $hf \ll k_B T_K$, where f is the oscillation frequency and T_K is the Kondo temperature, comparison to the static model of Kondo transport reveals agreement at very low frequencies and an increasing systematic departure at high frequencies. When $hf \lesssim k_B T_K$, the G defined as the derivative of the time averaged current through the device with respect to the average bias drastically differs from the static model. We show that the effect cannot be explained by an increase in the electron temperature.

¹Research is supported by the NSF DMR Grant No. 0804199 and the University of Cincinnati

²Currently at the University of Basel, Switzerland

2:42PM T17.00002 Connection between Local moment and Underscreened Kondo effect in parallel double quantum dots¹

, SERGIO ULLOA, NANCY SANDLER, Ohio U, ARTURO WONG, KEVIN INGERSENT, U of Florida, WILLIAM LANE, Jacksonville U, LUIS DIAS, U of Sao Paulo — Double quantum dots connected in parallel to a single channel, have been studied theoretically in two disparate limits: (I) Systems in which each dot has strong Coulomb interactions, exhibiting an underscreened spin-1 Kondo effect [1]; (II) An interacting dot 1 and a non-interacting dot 2, showing a quantum phase transition between Kondo phase and non-Kondo local-moment [2]. In this work, we use the numerical renormalization group approach to study a strongly interacting “quantum dot 1” and a weakly interacting “dot 2” connected in parallel to metallic leads. Gate voltages can drive the system between Kondo-quenched and free-moment phases separated by Kosterlitz-Thouless quantum phase transitions. As interactions in dot 2 become stronger relative to the dot-lead coupling, the free moment evolves from an isolated spin-1/2 in dot 1 to a many-body doublet arising from an underscreened Kondo effect. These limits, which feature very different entanglements between dot and lead electrons, can be distinguished by conductance measurements at finite temperatures.

[1] D. E. Logan, C. J. Wright, and M. R. Galpin, PRB 80, 125117 (2009).

[2] L. G. G. V. Dias da Silva et al., PRL 97, 096603 (2006).

¹Supported by NSF MWN/CIAM.

2:54PM T17.00003 Temperature Dependence of a Double Quantum Dot Kondo Effect

, ANDREW J. KELLER, SAMI AMASHA, ILEANA G. RAU, Stanford University, JORDAN A. KATINE, Hitachi Global Storage Technologies, HADAS SHTRIKMAN, Weizmann Institute, DAVID GOLDBABER-GORDON, Stanford University — Lateral quantum dots are highly tunable experimental systems ideal for exploring the interplay of orbital, spin, and charge correlations. We present studies of a double quantum dot system in a GaAs/AlGaAs heterostructure where transport through each dot may be measured independently. In the limit of negligible inter-dot tunneling, the conductance through both dots is enhanced along inter-dot charge degeneracy lines, where the energy cost for an electron to be on either dot is the same [A. Hübner, et al. PRL 101, 186804 (2008)]. With spin degeneracy, there are expected to be four or five-fold degenerate states, depending on the parity of the electron occupation number of each dot. We attribute the enhanced conductance to a double-dot Kondo effect that screens these localized, degenerate states. The temperature dependence of this Kondo effect is studied as a function of the coupling strength of each dot to its leads and the parity of the electron occupation numbers.

3:06PM T17.00004 Phase-dependent coherence and transport effects in a double-dot Aharonov-Bohm interferometer¹

, SAVANNAH GARMON, SALIL BEDKHAL, DVIRA SEGAL, University of Toronto — We study coherence dynamics between two sites comprising a double-dot interferometer attached to non-equilibrium leads. We demonstrate via numerical simulation that a magnetic flux passing through the interferometer results in phase-dependent decoherence in the case of degenerate dots. The precise details of these effects relies on an interplay between Markovian and non-Markovian dynamics. We employ various methods to further investigate these effects analytically, including the derivation of a quantum Langevin equation and a direct calculation of the relevant correlation functions. In addition, we investigate multi-particle scattering states in the same system.

¹Center for Quantum Information and Quantum Control (CQIQC), Sloan Fellowship of Dvira Segal

3:18PM T17.00005 Electrostatic modulation of periodic potentials in a two-dimensional electron gas: from antidot lattice to quantum dot lattice

, SRIJIT GOSWAMI, MOHAMMAD ALI AAMIR, SAQUIB SHAMIM, Department of Physics, Indian Institute of Science, CHRISTOPH SIEGERT, Cavendish Laboratory, University of Cambridge, MICHAEL PEPPER, Department of Electronic and Electrical Engineering, University College London, IAN FARRER, DAVID RITCHIE, Cavendish Laboratory, University of Cambridge, ARINDAM GHOSH, Department of Physics, Indian Institute of Science — We use a dual gated device structure to introduce a gate-tunable periodic potential in a GaAs/AlGaAs two dimensional electron gas (2DEG). Using a suitable choice of gate voltages we can controllably alter the potential landscape in the 2DEG, thereby inducing either a periodic array of antidots or quantum dots. Antidots are artificial scattering centers, and therefore allow for a study of electron dynamics. On the other hand, a quantum dot lattice provides the opportunity to study correlated electron physics. We use a variety of electrical measurements such as magneto-resistance, thermo-voltage and current-voltage characteristics to probe these two contrasting regimes.

3:30PM T17.00006 Universal out-of-equilibrium transport in Kondo-correlated quantum dots: a renormalized superperturbation theory on the Keldysh contour, STEFAN KIRCHNER, Max Planck Institute for Physics of Complex Systems, Germany, ENRIQUE MUNOZ, Pontificia Universidad Catolica de Valparaiso, Chile, C.J. BOLECH, University of Cincinnati — The non-linear conductance of semiconductor heterostructures and single molecule devices exhibiting Kondo physics has recently attracted attention [1,2]. We address the observed sample-dependence across various systems by considering additional electronic contributions present in the effective low-energy model underlying these experiments. To this end we develop a novel version of the superperturbation theory [3] in terms of dual fermions on the Keldysh contour. We analyze the role of particle hole asymmetry on the transport coefficients. Our approach [4] systematically extends the work of Yamada and Yosida and others to the particle-hole asymmetric Anderson model and reproduce the exactly solvable resonant level model and the special case considered in [5]. It correctly describes the strong coupling physics and is free of internal inconsistencies that would lead to a breakdown of current conservation.

- [1] M. Grobis et al., Phys. Rev. Lett. 100, 246601 (2008).
- [2] G. D. Scott et al., Phys. Rev. B 79, 165413 (2009).
- [3] H. Hafermann et al., EPL 85, 27007 (2009).
- [4] Enrique Munoz, C.J. Bolech, and Stefan Kirchner, submitted (2011).
- [5] K. Yamada, Prog. Theo. Phys. 62, 354 (1979).

3:42PM T17.00007 Multi-state operation in quantum dot channel FETs incorporating spatial wavefunction-switching¹, F. JAIN, K. BASKAR, S. KARMAKAR, P-Y. CHAN, E. SUAREZ, B. MILLER, J. CHANDY, University of Connecticut, E. HELLER, RSoft Design Group — Three-state behavior has been demonstrated in Si and InGaAs quantum dot gate (QDG) field-effect transistors^{2,3} (FETs). Recently, spatial wavefunction switched⁴ (SWS) and quantum dot channel⁵ (QDC) FETs have been reported to exhibit four-state operation. This paper presents simulations of versatile combinations of SWS features in QDC channels to optimally design multi-state transport in FETs that have the potential of scaling to sub-12nm regime. A QDC-FET channel is modeled as having superlattice-like mini-energy bands where the carrier wavefunctions are transferred across the channel as drain voltage is changed, producing step-like multi-state electrical characteristics. This behavior is analogous to that of single electron transistors.⁶ The difference is that QDC devices use more than a few electrons and operate at room temperature. The SWS feature additionally provides carrier transfer from lower to upper dot layer(s) in a QDC having more than one layer of quantum dots.

- ¹Support in part by NSF and ONR.
- ²S. Karmakar, *et al.*, J. Electronic Materials, 40, 1746, 2011.
- ³F Jain, J. Electronic Materials, 40, 1717, 2011.
- ⁴Ibid.
- ⁵F. Jain et al., Proc. II-VI Workshop, Oct.2011.
- ⁶S. J. Shin, et al., Appl. Phys. Lett. 97, 103101, 2010.

3:54PM T17.00008 Tunneling in double quantum dots and rings: search for chaos assistance¹, IGOR FILIKHIN, SERGEI MATINYAN, BRANISLAV VLAHOVIC, North Carolina Central University — Semiconductor heterostructures as quantum dots (QD) or quantum rings (QR) demonstrate discreet atom-like energy level structure. In the case of double QD (DQD) or double concentric QR (DCQR), a single electron spectrum is composed of a set of quasi-doublets [1]. We study influence of these specific spectrum properties on electron tunneling related to the electron transport through DQD (DCQR). The double InAs/GaAs quantum dots (rings) are considered within three dimensional single sub-band effective approach [2]. Tunneling between dots (rings) is evaluated by effect of inter-dot distance and QD (QR) geometry. We show that the quasi-doublets of the electron spectra define tunneling properties of the DCQR. Violation of symmetry of the DCQR geometry leads to increase of tunneling. Discussed will be also the chaos assisted tunneling in the double QD (DCQR).

- [1] I. Filikhin, S. G. Matinyan and B. Vlahovic, Phys. Lett. A 375, 620 (2011); I. Filikhin, S. G. Matinyan, J. Nimmo and B. Vlahovic, Physica E 43, 1669 (2011).
- [2] I. Filikhin, V. M. Suslov and B. Vlahovic, Phys. Rev. B 73, 205332 (2006).

¹This work is supported by the NSF (HRD-0833184) and NASA (NNX09AV07A).

4:06PM T17.00009 First-principles study of orbital-dependent quantum confinement in Si/Ge nanowire superlattices, MIN-KOOK KIM, HYOUNG JOON CHOI, Yonsei University — We study electronic structures of H-passivated Si/Ge nanowire superlattices (NWSLs) oriented along [110] direction, using an *ab-initio* pseudopotential density-functional method with the local density approximation. Obtained electronic structures of the Si/Ge NWSLs show both dispersive and non-dispersive bands in conduction and valence bands due to band-selective quantum confinement: the highest valence band and the lowest conduction band are not confined in either the Si- or Ge-nanowire segment but they are extended throughout the whole NWSLs, while there exist non-dispersive bands confined in either Si- or Ge-nanowire segment below the top of the valence band and above the bottom of the conduction band. This feature originates from strong orbital-dependence of quantum confinement of electronic states, making conventional band-offset diagrams for superlattices invalid in Si/Ge NWSLs. Effects of atomic geometries on the confinement are studied with different diameters and superlattice periodicities. This work was supported by NRF of Korea (Grant Nos. 2009-0081204 and 2011-0018306). Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2011-C3-05).

4:18PM T17.00010 One-dimensional physics in transition-metal nanowires¹, JUNICHI OKAMOTO, ANDREW MILLIS, NADER ZAKI, CHRIS MARIANETTI, Columbia University — One atom wide transition-metal nanowires can now be fabricated on Cu step edges. We present a theoretical study of the electronic properties of such systems. While the systems fall within the broad class of Luttinger liquids, about which much is known, characteristic features of transition metals including orbital degeneracy and interactions which favor locally high-spin configurations lead to new physics. Density functional calculations indicate that Co nanowires on Cu surfaces are half metals and are not electronically isolated from the substrate material. The multi-orbital and local high-spin physics are elucidated by Hartree-Fock approximations and bosonization calculations of the multi-orbital Hubbard model.

¹This work is supported by Department of Energy Contract Nos. DE-FG02-04ER46157 (J.O.), and DE-FG02-04ER46169 (A.J.M.).

4:30PM T17.00011 Detection of spin states in a quantum dot by random telegraph signal analysis with the hidden Markov model, MATTHEW HOUSE, HONGWEN JIANG, University of California, Los Angeles, MING XIAO, GUOPING GUO, HAIYOU LI, GANG CAO, TAO TU, GUANGCAN GUO, Key Laboratory of Quantum Information, Chinese Academy of Sciences, University of Science and Technology of China — A lateral GaAs quantum dot with an adjacent quantum point contact charge sensor was tuned so that its chemical potential is close to the Fermi level of an adjacent electron reservoir. In this configuration electrons tunnel back and forth between the quantum dot and the reservoir due to thermal fluctuations, characteristic switching known as a random telegraph signal (RTS). The charge state of the quantum dot is directly observable, but spin and orbital state information is not. Such extra states may reveal themselves in the statistics of the timing of tunneling events. We present a statistical analysis approach based on the Hidden Markov Model (HMM) for extracting information about the internal structure of the quantum dot from RTS data, particularly focusing on determining the electronic spin state. We demonstrate on simulated and experimental data that this technique can detect electron spin states and measure their tunneling rates individually when the energy level difference is less than or comparable to the thermal energy scale. This opens a new regime for studying quantum dot spin physics because other experiments require a Zeeman energy difference greater than the thermal energy in order to distinguish the spin states.

4:42PM T17.00012 Impact of adsorbed organic monolayers on vacuum electron tunneling contributions to electrical resistance at an asperity contact, DIANA BERMAN, MATTHEW WALKER, JACQUELINE KRIM, North Carolina State University — Electrical Contact Resistance measurements are reported for RF MEMS switches situated within an ultrahigh vacuum system equipped with *in situ* oxygen plasma cleaning capabilities. Measurements were performed on Au/Au permanently adhered switches, and functioning Au/RuO₂ switches in the presence and absence of adsorbed monolayers of pentane and dodecane. The data are analyzed to explore how adsorbed molecules in regions close to the contact may impact vacuum tunneling contributions to the experimentally measured resistance: (1) The resistance associated with direct contact in parallel with a vacuum tunneling path, which upon uptake of the monolayer is replaced by the molecular resistance, and (2) A series connection of the direct contact resistance with the molecular layer after adsorption occurs, with the vacuum tunneling path assumed to be negligible. The results favor scenario (1), whereby uptake of the molecular layer effectively shuts down the vacuum tunneling path, which in this case is effectively ~30 Ohms in the absence of an adsorbed film. The methods constitute a new and original approach to documenting vacuum tunneling levels in regions of close proximity. Funding agencies: NSF, AFOSR MURI, DARPA.

[1] D. Berman, M. Walker, C. Nordquist, J. Krim, *J. Appl. Phys.*, in press

4:54PM T17.00013 Dependence of Conductance Resonances and Modulations on Channel Length in Asymmetric Quantum Point Contacts (QPCs)¹, HAO ZHANG, Duke University, PHILLIP WU, Lund University, ALBERT CHANG, Duke University — Transport features below $2e^2/h$ show resonance peaks in highly asymmetric QPCs. As we increase the channel length, the number of peaks observable also increases. We characterize the number of peaks and/or oscillations as a function of channel length, when the QPC is tuned to or below the first quantum channel. The number of peaks/oscillations appears to increase on average as the channel length increases. In addition, we find preliminary evidence that there is a correspondence between the resonance peaks and the zero-bias anomaly (ZBA) in the differential conductance. These behaviors are consistent with an interpretation based on the formation of quasi-bound-states within the QPC channel in the single-mode limit.

¹Work support by NSF DMR 0701948

5:06PM T17.00014 New scenario of shuttling mechanism in magnetic nano-electromechanical single-electron tunneling systems, HEE CHUL PARK, School of Computational Science, Korea Institute for Advanced Study, ANATOLI M. KADIGROBOV, ROBERT I. SHEKHTER, MATS JONSON, Department of Physics, University of Gothenburg — We investigate a new shuttling scenario in the electro-mechanics of a movable quantum dot between a nonmagnetic lead and a magnetic lead. In this device, the quantum dot has two energy levels due to the Zeeman energy splitting under magnetic field with Coulomb blockade. The electromechanical instability is shown to depend on the external voltage when the vibrating energy overcomes the dissipation energy of the system. In addition to the normal shuttling behavior, the shuttling current can be suppressed and then recovered depending on the external voltage. It is also found that the nano-electromechanical oscillation significantly improves the spin polarized current compared with one in the fixed quantum dot due to the interplay between the spin polarized transport and mechanical degree of freedom.

Wednesday, February 29, 2012 2:30PM - 5:18PM –
Session T18 DMP: Focus Session: Interfaces in Complex Oxides - Superconductivity and Magnetism at Interfaces 252B

2:30PM T18.00001 Local imaging of the superfluid density at the LAO/STO interface as a function of gate voltage, JULIE A. BERT, BEENA KALISKY, CHRIS BELL, YASUYUKI HIKITA, HAROLD Y. HWANG, KATHRYN A. MOLER, Stanford Institute for Materials and Energy Sciences, Stanford University — The interface between two insulating oxides, LaAlO₃ and SrTiO₃, exhibits a two-dimensional electron system with high mobility, magnetism, superconductivity at low temperatures, and an electric-field-tuned superconductor-insulator transition. This interface has been studied extensively using transport and magnetization, which do not directly probe potential variation on a local length scale. We use a scanning SQUID microscope to locally probe superconductivity and magnetism in LAO/STO heterostructures. We measure the local diamagnetic susceptibility and critical temperature as a function of position and gate voltage. Our local susceptibility measurement is related to the density of superconducting carriers which gives us a map of superfluid density. We find that the superfluid density is inhomogeneous, showing regions of susceptibility that varies over a large fraction of the total response while the critical temperature remains relatively uniform across the sample. Tracking the evolution of both of these parameters as a function of gate voltage and position enables investigation of the local onset of the superconductor-insulator transitions on both sides of the dome.

2:42PM T18.00002 Magnetism and superconductivity at LAO/STO-interfaces: the role of Ti 3d interface electrons¹, NATALIA PAVLENKO, Institute of Physics, University of Augsburg (Germany); Institute for Condensed Matter Physics, Lviv (Ukraine), THILO KOPP, Institute of Physics, University of Augsburg (Germany), E.Y. TSYMBAL, Department of Physics and Astronomy, University of Nebraska-Lincoln, G.A. SAWATZKY, Department of Physics and Astronomy, University of British Columbia, Vancouver, JOCHEN MANNHART, Max Planck Institute for Solid State Research, Stuttgart (Germany) — Ferromagnetism and superconductivity are in most cases adverse. However, recent experiments reveal that they coexist at interfaces of LaAlO_3 and SrTiO_3 [1]. We analyze the ferromagnetic state within density functional theory and provide evidence that it is also generated by Ti 3d interface electrons, as is the two-dimensional electron liquid at the interface which gives rise to superconductivity [2]. We demonstrate that oxygen vacancies in the TiO_2 interface layer enhance the tendency for ferromagnetism considerably. This allows for the notion that areas with increased density of oxygen vacancies produce ferromagnetic puddles and account for the previous observation of a superparamagnetic behavior in the superconducting state [3].

[1] Lu Li, C. Richter, J. Mannhart, and R.C. Ashoori, *Nature Physics* **7**, 762 (2011).

[2] N. Reyren et al., *Science* **317**, 1196 (2007).

[3] N. Pavlenko, T. Kopp, E.Y. Tsymbal, G.A. Sawatzky, and J. Mannhart, *cond-mat/arXiv:1105.1163* (2011)

¹This work was supported by the DFG (TRR-80), the EC (oxIDES), Nebraska MRSEC (NSF DMR-0820521), NSF-EPSCoR (EPS-1010674).

2:54PM T18.00003 Superconductivity and magnetism in the presence of interface-induced Rashba spin-orbit coupling¹, FLORIAN LODER, ARNO KAMPF, THILO KOPP, University of Augsburg, Germany, TRR 80 TEAM — Two dimensional electron systems at oxide interfaces are often influenced by a Rashba type spin-orbit coupling (SOC), which is tunable by a transverse electric field. Ferromagnetism at the interface can simultaneously induce strong local magnetic fields. This combination of SOC and magnetism leads to anisotropic two-sheeted Fermi surfaces, on which superconductivity with finite-momentum pairing is favored. The superconducting order parameter is derived within a generalized pairing model realizing both, the FFLO superconductor in the limit of vanishing SOC and a mixed-parity pairing state with zero pair momentum if the magnetism vanishes. The nature of the pairing state is discussed in the context of interface superconductivity and ferromagnetism at LAO-STO interfaces [1,2].

[1] Lu Li, C. Richter, J. Mannhart, and R. C. Ashoori, *Nature Physics* **7**, 762 (2011)

[2] J. A. Bert, B. Kallisky, C. Bell, M. Kim, Y. Hikita, H. Y. Hwang, and K. A. Moler, *Nature Physics* **7**, 767 (2011)

¹This work was supported by the DFG through TRR 80.

3:06PM T18.00004 Superconductivity and magnetism in a three-band model of the LAO/STO interface from a weak-coupling perspective, MARK FISCHER, Cornell University, SRINIVAS RAGHU, Stanford University, EUN-AH KIM, Cornell University — Recent experiments on LAO/STO interfaces have shown the occurrence of both superconductivity and magnetism in this system. Motivated by these experiments, we analyze various Fermi-liquid instabilities in a three-band model of the LAO/STO interface with purely repulsive interactions by calculating susceptibilities for superconducting, magnetic and nematic orders. In light of recent transport experiments proposing a Lifshitz transition between d orbitals, we particularly study how the susceptibilities depend on the chemical potential. Further, we investigate the interplay of these different orders.

3:18PM T18.00005 Magnetism of $\text{LaAlO}_3/\text{SrTiO}_3$ Heterostructure Interface, LU LI¹, Department of Physics, Massachusetts Institute of Technology, C. RICHTER, University of Augsburg, D-86135 Augsburg, Germany, J. MANNHART, Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany, R.C. ASHOORI, Department of Physics, Massachusetts Institute of Technology — The $\text{LaAlO}_3/\text{SrTiO}_3$ heterostructure is a potential candidate for a high mobility two-dimensional electron system with novel electronic and magnetic properties. Magnetic ordering has been proposed to arise from d-shell electrons transferred by the polarization discontinuity at the interface. However the magnetization of this system cannot easily be detected with standard techniques due to the small volume of the interfacial region. Using torque magnetometry, we measure the magnetic moment of the interface system directly. Our results indicate the existence of a magnetic ordering at the two-dimensional conductive interface. The ferromagnetic-like ordering state persists up to 200 K. Such a state is hardly explained by ion-exchange at the interface, since LaTiO_3 is antiferromagnetic. Moreover, the same magnetic behavior persists even when the sample is superconducting, which suggests an unconventional two-dimensional superconducting phase.

¹Current address: University of Michigan, Dept. of Physics

3:30PM T18.00006 Signatures of local superconducting islands at elevated temperatures in $\text{LaAlO}_3/\text{SrTiO}_3$ Heterostructure Interface, R.C. ASHOORI, LU LI¹, Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02138, C. RICHTER, University of Augsburg, D-86135 Augsburg, Germany, J. MANNHART, Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — Superconductivity has been observed in $\text{LaAlO}_3/\text{SrTiO}_3$ heterostructures below 300 mK in resistivity measurements and later confirmed with Meissner effect. Our detailed magnetization measurements in several $\text{LaAlO}_3/\text{SrTiO}_3$ samples indicate a quasi superconducting state persisting up to 4 K. In these samples, we discovered large nonreversible magnetization vs. field curves. Moreover, the magnitude of the nonreversible loop is proportional to sweep rates, suggesting that it is caused by local magnetic moments generated by eddy currents. Based on this eddy current picture, the inferred conductance is found to be 7 orders of magnitude larger than the conductance across the whole interface. This contrast suggests the existence of small local quasi superconducting regions at a temperature of 4 K, well above the long range superconducting transition temperature.

¹Current address: University of Michigan, Dept. of Physics

3:42PM T18.00007 Superconductivity and Ferromagnetism in Oxide Interface Structures: Possibility of Finite Momentum Pairing, KAREN MICHAELI, ANDREW POTTER, PATRICK LEE, Massachusetts Institute of Technology — We present a model that captures the physical properties of the interface between two oxides, LaAlO_3 and SrTiO_3 . Despite extensive experimental studies of these systems, no clear theoretical picture has emerged so far. The model that we suggest for the interface electrons explains the main experimental observations. In particular, we address one of the most intriguing phenomena observed in these system: the coexistence of ferromagnetism and superconductivity. Ordinarily this ferromagnetism would destroy superconductivity, but due to strong spin-orbit coupling near the interface, the magnetism and superconductivity can coexist by forming an FFLO-type condensate of Cooper pairs at finite momentum. Surprisingly, this unconventional superconducting state survives even at strong disorder.

3:54PM T18.00008 Tuning the ferromagnetism in $\text{LaAlO}_3/\text{SrTiO}_3$, BEENA KALISKY, Stanford University, USA; Bar-Ilan University, Israel, JULIE A. BERT, BRANNON B. KLOPPER, CHRISTOPHER BELL, Stanford University, USA, HIROKI SATO, Stanford University, USA; University of Tokyo, Japan, YASUYUKI HIKITA, HAROLD Y. HWANG, KATHRYN A. MOLER, Stanford University, USA — The interface of $\text{LaAlO}_3/\text{SrTiO}_3$ heterostructures exhibits both conductivity and magnetism. Significant effort has been invested researching the details and characteristics of the conductivity, such as conductance only above a critical LaAlO_3 thickness. However, reports of ferromagnetism differ in a variety of details requiring further investigation into the material properties that control magnetism. In this study we use a scanning SQUID microscope to locally image the landscape of ferromagnetism as a function of several tuning parameters including the LaAlO_3 thickness, back gate voltage, local strain and surface treatment. We find that the ferromagnetism is inhomogeneous within each sample, varies considerably between samples, and appears only in samples whose LaAlO_3 layer is thicker than a threshold value, similar to the conductance critical thickness. The ferromagnetism changes with local strain, surface treatment with polar solvents and applied field. However it is not affected by changing the gate voltage or cycling the temperature up to 300K. These results provide experimental input for determining and controlling the mechanisms of magnetism in engineered complex oxide interfaces.

4:06PM T18.00009 Strong magnetic interaction in localized two-dimensional electron gas in $\text{LaAlO}_3/\text{SrTiO}_3/\text{NdGaO}_3$ heterostructures¹ , Z. HUANG, X. WANG, Z.Q. LIU, W.M. LV, S.W. ZENG, A. ANNADI, W.L. TAN, T. VENKATESAN, - ARIANDO, NUSNNI-NanoCore, National University of Singapore, Singapore — Via reducing the thickness of SrTiO_3 layer, strong localization of two-dimensional electron gas is artificially introduced at $\text{LaAlO}_3/\text{SrTiO}_3$ interface grown on NdGaO_3 (110) substrates. This localization is characterized by the low carrier density, robust insulating ground state and variable range hopping behavior at low temperature. Given the spatially-limited conducting channel in the thin SrTiO_3 layer, the degeneration of Ti 3d orbitals at the interface should be responsible for this strong localization. Moreover, the typical butterfly-like hysteresis loop and unusual anisotropic features in magnetoresistance observed in the thinner SrTiO_3 samples indicate the enhanced magnetic interaction in this strongly localized two-dimensional electron gas.

¹We thank National Research Foundation (NRF) Singapore under the Competitive Research Program (CRP) “Tailoring Oxide Electronics by Atomic Control” NRF2008NRF-CRP002-024 and Ministry of Education (MOE) FRC-ARF Grant No. R-144-000-278-112.

4:18PM T18.00010 Investigation of electric field induction of superconductivity at complex oxide interfaces¹ , J.T. HARALDSEN, Los Alamos National Laboratory, P. WOLFLE, Karlsruhe Institute of Technology, A.V. BALATSKY, Los Alamos National Laboratory — We examine the modified electronic states and change in carrier density at the interfaces of complex oxide films produced by an external electric field. Using a Ginzburg-Landau formalism and ab-initio calculations, we show that linear coupling of an electric potential can influence the superconducting order parameter and induce a transition to a superconducting phase. Further, we examine the correlation between carrier density and the superconducting critical temperature T_c by investigating capacitance and density of states with changing electric potential. We will discuss implications of this work in the context of interfaces formed by LaAlO_3 and SrTiO_3 thin films. This approach points to an alternative path to superconducting devices with tunable transition temperature. Work was carried out under the help and support of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

¹Work was carried out under the help and support of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

4:30PM T18.00011 Evidence for charge-vortex duality at the $\text{LaAlO}_3\text{-SrTiO}_3$ interface¹ , MANAN MEHTA, DIMITRY DIKIN, Department of Physics and Astronomy, Northwestern University, Evanston, IL, CHUNG WUNG BARK, CHAD FOLKMAN, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, Madison, WI, VENKAT CHANDRASEKHAR, Department of Physics and Astronomy, Northwestern University, Evanston, IL — The conducting gas formed at the interface between LaAlO_3 and SrTiO_3 undergoes a superconductor to insulator transition (SIT) on the application of a back gate voltage, V_g . The system also shows evidence of ferromagnetic order coexisting with superconductivity.² The juxtaposition of the ferromagnet with the conducting gas allows for the observation of a novel manifestation of charge-vortex duality. The field due to the magnetization dynamics in the ferromagnet causes a sharp *increase* in resistance on the superconducting side of the transition, in the magnetoresistance measurements, and a sharp *decrease* in resistance on the insulating side. The system can be modeled as an array of Josephson junctions, with two characteristic energy scales: a Josephson coupling energy E_J , and a Coulomb charging energy E_C . V_g then tunes the ratio, E_J/E_C , to cause the transition. We will present external field sweep-rate dependent magnetoresistance data on both sides of the transition to elucidate the nature of the superconducting and insulating states.

¹Funded by the DOE through grant number DE-FG02-06ER46346.

²Dikin *et al*, PRL **107**, 056802 (2011)

4:42PM T18.00012 Single-Mode Cooper Pair Channel in $\text{LaAlO}_3/\text{SrTiO}_3$ Nanowires , JOSHUA VEAZEY, GUANGLEI CHENG, PATRICK IRVIN, MENGCHEN HUANG, U. of Pittsburgh, CHUNG WUNG BARK, SANGWOO RYU, CHANG-BEOM EOM, U. of Wisconsin-Madison, JEREMY LEVY, U. of Pittsburgh — The conducting $\text{LaAlO}_3/\text{SrTiO}_3$ interface becomes superconducting¹ below a critical temperature $T_c \sim 100\text{-}400$ mK. Here, we investigate the transport characteristics of $\text{LaAlO}_3/\text{SrTiO}_3$ structures formed from ~ 10 nm-wide nanowire segments produced by a conductive atomic force microscope lithography technique². Above $T_c \sim 200$ mK we find a characteristic four-terminal conductance $G \sim e^2/h$ that is independent of the channel length. Below T_c we find that the conductance increases to $G \sim 4e^2/h$. This increase is attributed to the formation of Cooper pairs that propagate in a single mode. We also discuss the interactions between Cooper pairs and spin-polarized transport in these structures. This work is supported by AFOSR (FA9550-10-1-0524).

¹N. Reyren, *et al.*, Science **317**, 1196-9 (2007).

²C. Cen, S. Thiel, K. E. Andersen, C. S. Hellberg, J. Mannhart, and J. Levy, Nature Materials **7**, 2136 (2008).

4:54PM T18.00013 Two doped holes with different distributions in $\text{Sr}_2\text{CuO}_{4-\delta} - \text{La}_2\text{CuO}_4$ superlattices¹, S. SMADICI, J.C.T. LEE, P. ABBAMONTE, University of Illinois at Urbana-Champaign, IL 61801, USA, A. RUSYDI, National University of Singapore, 11754, Singapore, G. LOGVENOV, Max-Planck-Institut for Solid State Research, D-70569, Germany, I. BOZOVIC, Brookhaven National Laboratory, NY 11973, USA — X-ray absorption in $\text{Sr}_2\text{CuO}_{4-\delta} - \text{La}_2\text{CuO}_4$ (SCO-LCO) superlattices shows a variable occupation with doping of two hole states. In addition to the holes doped for $x < x_{\text{optimal}}$ in bulk $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, a variation with doping of a second hole state is observed at higher energy. Measurements suggest that this hole is located on apical oxygen atoms and polarized in the $a - b$ plane. Considering the surface reflectivity gives a good qualitative description of the line shapes of resonant soft X-ray scattering. The interference between the superlattice and surface reflections was used to distinguish between scatterers in the SCO and the LCO layers, with the two hole states maximized in different layers of the superlattice. This suggests that the states emptied preferentially in the SCO layers are the additional states in the extension of the Zhang-Rice singlet-upper Hubbard band model to higher doping levels.

¹This work was supported by Grants DE-FG02-06ER46285, DE-AC02-98CH10886, MA-509-MACA, DE-FG02-07ER46453 and DE-FG02-07ER46471.

5:06PM T18.00014 Highly Spin-Polarized Conducting State at the Interface between Non-magnetic Band Insulators: $\text{LaAlO}_3/\text{FeS}_2$ (001), J.D. BURTON, E.Y. TSYMBAL, University of Nebraska - Lincoln, Nebraska Center for Materials and Nanoscience — Interface engineering of complex oxide heterostructures allows creating interfaces with properties and functionalities distinct from those typical for the respective bulk constituents. In the spirit of the well known conducting $\text{LaAlO}_3/\text{SrTiO}_3$ interface we study a similar interface with the added functionality of being unambiguously ferromagnetic. Our first-principles density functional calculations demonstrate that such a spin-polarized two-dimensional conducting state can be realized at the (001) interface between the two non-magnetic band insulators FeS_2 and LaAlO_3 . The (001) surface of FeS_2 (pyrite), a diamagnetic insulator, supports a localized surface state deriving from the Fe d-orbitals near the conduction band minimum. We find that, similar to the $\text{LaAlO}_3/\text{SrTiO}_3$ system, the deposition of a few unit cells of the polar perovskite oxide LaAlO_3 leads to electron transfer into these surface bands, thereby creating a conducting interface. The occupation of these narrow bands leads to an exchange splitting between the spin sub-bands, yielding a highly spin-polarized conducting state quite distinct from the rest of the non-magnetic, insulating bulk. [Ref: J. D. Burton and E. Y. Tsympal, Phys. Rev. Lett. 107, 166601 (2011).]

Wednesday, February 29, 2012 2:30PM - 5:30PM —

Session T19 APS: Kavli Foundation Special Session: Emergent Physics at the Mesoscale Ballroom East

2:30PM T19.00001 Mesoscopic Lawlessness, R.B. LAUGHLIN, Stanford University — Whether physics will contribute significantly to unraveling the secrets of life, the grandest challenge of them all, depends critically on whether proteins and other mesoscale objects exhibit emergent law. By this I mean quantitative relationships among their measured properties that are always true. The jury is still out on the matter, for there is evidence both for and against, but it is spotty, on account of the difficulty of measuring 100 nm - 1000 objects without damaging them quantum mechanically. It is therefore not clear that history will repeat itself. Physics contributed mightily to 20th century materials science through its identification and mastery of powerful macroscopic emergent laws such as crystalline rigidity, superconductivity and ferromagnetism, but it cannot do the same thing in biology, regardless of how powerful computers get, unless nature cooperates. The challenge before us as physicists is therefore not to amass more and more terabytes of data and computational output but rather to search for and, with luck, find operating principles at the scale of life greater than those of chemistry, which is to say, greater than a world ruled by nothing but miraculous accidents.

3:06PM T19.00002 Ultracold, trapped atomic gases as material systems¹, WILLIAM D. PHILLIPS², Joint Quantum Institute, University of Maryland and National Institute of Standards and Technology, 100 Bureau Drive, Stop 8424, Gaithersburg MD 20899 — Laser cooling and evaporative cooling of neutral atomic gases has led to the creation of quantum degenerate Bose and Fermi gases that constitute a new class of material systems. Many of the features of the Hamiltonians governing the behavior of these systems can be controlled and manipulated in experiments. The necessarily finite sizes of such systems are often mesoscopic in the sense that they are large enough that collective effects are important, yet small enough that the size plays a role in determining the systems' behavior. Among the experimental tools available are optical lattices, synthetic fields, and the ability to change the size and dimensionality of the system. Ultracold gases can realize some of the idealized Hamiltonians used to model condensed matter systems, creating a quantum simulation of such models, which may be computationally intractable. Atomic gases can also provide new condensed-matter-like systems that have no analogs in real condensed matter.

¹This work was supported by the ONR, DARPA, ARO, and the NSF through the PFC@JQI.

²In collaboration with Gretchen K. Campbell, Paul D. Lett, James V. Porto, and Ian B. Spielman, JQI, University of Maryland and NIST.

3:42PM T19.00003 Self Assembly on the Mesoscale, ANGELA BELCHER, MIT Dept of Materials Science and Engineering — No abstract available.

4:18PM T19.00004 The mesoscale interface between physics and biology, WILLIAM BIALEK, Princeton — No abstract available.

4:54PM T19.00005 Biological physics on the mesoscale, GEORGE WHITESIDES, Harvard — No abstract available.

Wednesday, February 29, 2012 2:30PM - 5:30PM —

Session T20 FIAP: Invited Session: Advanced Characterization of Transistor Gate Stacks and Interfaces 253C

2:30PM T20.00001 Directions in High-k Gate Stacks: From Silicon Chips to Carbon Nano-materials, MATTHEW COPEL, IBM — The successful implementation of high-k/metal gates for silicon CMOS has culminated a decade of research on metal-oxide interactions with silicon. The ability to profile materials on a nanometer length scale has greatly assisted our ability to tailor electrical properties to create functional devices. Initial concerns addressed with composition profiling (e.g. Si content, Hf diffusion, thermal stability) have been replaced by more advanced questions. For example, gate-first technologies often use threshold-modifying layers, whose electrical properties are closely linked with their depth distribution. Oxygen diffusion is another complex problem of current concern, where physical characterization by isotopic tracing has given valuable insights. A similar set of challenges will confront us in creating carbon-based devices. Much effort is focused on nucleation of dielectrics, along with stability and interactions with the channel. This parallels work in the early development of high-k/Si. This talk will review some important lessons from the past decade, and discuss how we can apply this knowledge to creating improved graphene-channel devices.

3:06PM T20.00002 Nanometer-scale properties of metal/oxide interfaces and “end-on” metal contacts to Si nanowires studied by ballistic electron emission microscopy (BEEM)¹, JON PELZ, The Ohio State University, Dept. of Physics, Columbus, OH 43210 — BEEM is a hot-electron (HE) technique based on scanning tunneling microscopy that can probe buried metal/semiconductor and metal/dielectric interfaces with nm-scale spatial resolution and energy resolution of a few meV. BEEM is a three-terminal technique, so the HE energy and interface electric field can be varied independently. I will discuss two studies of interest for future transistor technologies. The first concerns the band structure and alignments in a 20 nm-thick film of the high-k dielectric material Sc_2O_3 grown epitaxially on Si(111). Sc_2O_3 and related rare-earth/transition metal oxide films on Si were found to have similar band alignments and bandgap, and also “tailing” conduction band (CB) states extending ~ 1 eV below the primary CB. We combined BEEM with internal photoemission to measure the band alignment and to study electron transport through these “tail” states.² Surprisingly, these tail states were found to form a robust band of extended states that supports elastic hot-electron transport even *against* an applied electric field. The second study concerns HE injection and transport through “end-on” metal contacts made to ~ 100 nm diameter vertical Si nanowires (NWs) embedded in a SiO_2 dielectric. At low HE flux, We observed *lateral variations* of the local Schottky Barrier Height (SBH) across individual end-on Au Schottky contacts, with the SBH at the contact edge found to be ~ 25 meV lower than at the contact center. Finite-element electrostatic simulations suggest that this is due to a larger interface electric field at the contact edge due to positively charged Si/native-oxide interface states near the Au/NW contact, with this (equilibrium) interface state charge induced by local band bending due to the high work function Au contact. We also observed a strong *suppression* of the hot-electron transmission efficiency at larger HE flux, likely due to (non-equilibrium) *steady-state negative charge accumulation* in metastable traps at the Si/oxide interface located near the injecting metal contact. Ongoing BEEM measurements of metal contacts to SrTiO_3 substrates and films may also be discussed.

In collaboration with W. Cai, Y. Che, L. F. Edge, D. G. Schlom, E. R. Hemesath, and L. J. Lauhon.

¹Work supported by NSF Grant No. DMR-0805237

²W. Cai, S. E. Stone, J. P. Pelz, L. F. Edge, and D. G. Schlom, Appl. Phys. Lett **91**, 042901 (2007).

3:42PM T20.00003 Metropolis Prize Talk: Defects in Al_2O_3 and their impact on III-V/ Al_2O_3 MOS-based devices, JUSTIN R. WEBER, Intel Corporation, Hillsboro, OR — As the dimensions of conventional silicon devices continue to shrink, novel approaches are required to achieve increasing performance demands. Recently Intel announced the implementation of a 3-D MOSFET geometry known as the tri-gate transistor for their 22 nm technology. In addition to different geometries, new materials will also be needed for future technologies. In this talk, we will consider the use of III-V channel materials, and novel gate dielectrics. Al_2O_3 is a promising dielectric for III-V devices. However, the presence of deep levels and fixed charge in the Al_2O_3 layer is a concern, with native defects being a potential source of traps, leakage, and fixed charge. We will present the results of hybrid density functional calculations for such defects. The energetic positions of defect-induced levels will be discussed in the context of the III-V/ Al_2O_3 interface. We find that native defects are a source of border traps, and fixed charge in the dielectric. We will also discuss the interaction of hydrogen with such defects, in the context of passivation. Our results indicate that hydrogen is effective at removing border traps, and helps to alleviate the problem of fixed charge. This work was performed in collaboration with A. Janotti and C. G. Van de Walle.

4:18PM T20.00004 Charge Traps at and near High-K Oxide/III-V Interfaces¹, PAUL MCINTYRE, Stanford University — The effort to achieve higher performance metal-oxide-semiconductor (MOS) devices prompts interest in new semiconductor channel materials such as indium gallium arsenide that can achieve larger drive currents than state-of-the-art Si field effect transistors, at low operating voltages. In order for InGaAs-channel transistors to approach their performance limits, however, high permittivity (high-k) metal oxide gate dielectrics must be prepared on the III-V surface in a manner that produces a minimal areal density of charge-trapping defects. This presentation will review different experimental approaches to prepare relatively passive interfaces between deposited oxides and GaAs or InGaAs. Both pre-oxide deposition and post-deposition methods will be summarized. It will also describe the influence of near-interface defects in the oxides (border traps) and why these particular defects are so significant for arsenide MOS devices. An attempt will be made to associate electrically-active traps detected at different energies in the III-V semiconductor bandgap with specific surface and point defects, based on prior reported experimental and computational observations. The difficulty of quantifying trap densities using typical capacitance-voltage and conductance-voltage methods developed for silicon MOS will be discussed.

¹Support by the SRC Non-Classical CMOS Center is gratefully acknowledged.

4:54PM T20.00005 Electrical characterization of interfacial defects, GENNADI BERSUKER, SEMATECH — Aggressive transistor scaling to achieve better chip functionality calls for the introduction of new dielectric and metal materials into traditional device gate stacks. The advanced gate stacks represent multilayer structures, the materials of which may strongly interact (primarily during high temperature processing), generating structural defects in these layers. These complex structures pose new challenges in interpreting electrical measurements, which are sensitive to even extremely small concentrations of electrically active defects. The critical task is, thus, to link the structural and electrical characteristics of these multicomponent gate stacks in order to identify and control defects affecting device performance. In this presentation, we focus on analyzing interfacial defects affecting electrical characteristics of the metal/high-k (HK) gate stacks, which are of major interest to the semiconductor industry. We first developed models of the physical processes governing the measurements of the electrical techniques we used that allowed us to extract the structural parameters of the defects from the electrical data. By comparing the extracted parameters to those obtained by ab initio calculations of the material structures, we identified the nature of the contributing defects. A recently proposed model for random telegraph noise (RTN) and frequency-dependent charge pumping (CP) measurements that takes into consideration the multi-phonon lattice relaxation induced by charge trapping/detrapping at the defect sites was employed to extract characteristics of the traps in the interfacial SiO_2 layer in HfO_2 -based HK devices. Our results indicate that the electron capture/emission times are controlled by the lattice re-arrangement (caused by the trapped electrons) rather than by electron tunneling to/from the trap as generally assumed. The strong dependency of the measured values on defect relaxation and ionization energies allows these values to be extracted; the values can then be used as a defect identifier. Complementary modeling of the gate leakage current in HK devices during electrical stress using the same approach yields characteristics of the traps in the interfacial SiO_2 layer contributing to trap-assisted tunneling (TAT). Based on the values obtained by RTN, CP, and TAT measurements, the electrically active defects were tentatively assigned to oxygen vacancies in various charged states. In all cases, stress-induced traps were generated exclusively in the interfacial layer of the HK stacks, consistent with earlier findings that HK dielectrics are more resistant to defect generation than SiO_2 . Based on these findings, as well as an earlier TEM/EELS study of the elemental composition of the breakdown path, we proposed that the breakdown path formation/evolution in the interfacial layer is associated with the growth of an oxygen-deficient filament facilitated by the grain boundaries in the overlaying high-k film. This model successfully describes the temperature-dependent evolution of interfacial layer degradation through various breakdown phases.

Wednesday, February 29, 2012 2:30PM - 5:30PM – Session T21 DCMP: Magnetic Ordering and Dynamics in Cuprates 254A

2:30PM T21.00001 Two Dimensional Incommensurate and Three Dimensional Commensurate Magnetic Order and Fluctuations in $La_{2-x}Ba_xCuO_4$ ¹, JEROD WAGMAN, GREG VAN GASTEL, KATE ROSS, McMaster University, ZAHRA YAMANI, Chalk River Laboratories, YANG ZHAO, National Institute of Standards and Technology, ANN KALLIN, EMMA MAZUREK, Brockhouse Institute for Materials Research, YIMING QIU, JOHN COPLEY, National Institute of Standards and Technology, HANNA DABKOWSKA, Brockhouse Institute for Materials Research, BRUCE GAULIN, McMaster University — We present neutron scattering measurements on single crystals of $La_{2-x}Ba_xCuO_4$, with $0 \leq x \leq 0.035$. These experiments reveal the evolution of the magnetism: from a three dimensional (3D) commensurate (C) antiferromagnet, with a relatively high T_N , to a two dimensional (2D) incommensurate (IC) antiferromagnet with finite range static correlations, with relatively low effective T_N s. At low temperatures, the 2D IC magnetism co-exists with the 3D C magnetism for Ba concentrations as low as $x = 0.0125$. We find that 3D C magnetism disappears by $x = 0.025$; consistent with the limit of $x \sim 0.02$ observed in the sister family of doped Mott insulators $La_{2-x}Sr_xCuO_4$. We construct a phase diagram based on magnetic order parameter measurements, which displays much of the complexity of standard high temperature superconductivity phase diagrams discussed in the literature. Analysis of high energy-resolution inelastic neutron scattering shows the low energy dynamic susceptibility to fall off with temperature on a scale much higher than the effective 2D IC T_N s in the sample. This effect is such that appreciable dynamic 2D IC magnetic fluctuations inhabit much of the “pseudogap” regime of the phase diagram.

¹NSERC

2:42PM T21.00002 ABSTRACT WITHDRAWN —

2:54PM T21.00003 Novel magnetic excitations in the high-temperature superconductor $HgBa_2CuO_{4+\delta}$, MUN CHAN, University of Minnesota, YUAN LI, Max Planck Institute for Solid State Research, Germany, V. BALÉDENT, Laboratoire Léon Brillouin, N. BARIŠIĆ, University of Minnesota, K. HRADIL, Forschungsneutronenquelle Heinz Maier-Leibnitz, Germany, YANGMU LI, University of Minnesota, R.A. MOLE, Forschungsneutronenquelle Heinz Maier-Leibnitz, Germany, Y. SIDIS, Laboratoire Léon Brillouin, P. STEFFENS, Institut Laue Langevin, France, G. YU, University of Minnesota, X. ZHAO, Jilin University, China, P. BOURGES, Laboratoire Léon Brillouin, M. GREVEN, University of Minnesota — We report on the observation of novel magnetic excitations in the pseudogap phase of the cuprate superconductor $HgBa_2CuO_{4+\delta}$ ($Hg1201$) using neutron scattering, and on their relationship with antiferromagnetic (AF) fluctuations. Following polarized neutron diffraction experiments that demonstrated a novel ($q=0$) magnetic order in the pseudogap phase [B. Fauqué *et al.* PRL 96, 197001 (2006); Y. Li *et al.*, Nature 455, 372 (2008)], our inelastic measurements revealed two weakly-dispersive magnetic excitation branches in $Hg1201$ [Y. Li *et al.*, Nature 468, 283 (2010), and preprint]. These excitations are observed in the pseudogap phase and appear to be associated with the $q=0$ magnetic order. In our optimally-doped sample, the magnetic resonance occurs at the dispersion maximum of the higher-energy branch. In under-doped $Hg1201$, the two excitation branches exhibit local intensity maxima at q_{AF} , and we find evidence for an hourglass dispersion associated with the lower branch. These results reveal a profound connection between the novel excitations and the conventional AF fluctuations.

3:06PM T21.00004 Stripe order in $La_{2-x}Ba_xCuO_4$ in high magnetic fields¹, M. HUECKER, BNL, M. VON ZIMMERMANN, HASYLAB at DESY, Z.J. XU, J.S. WEN, G.D. GU, I.A. ZALIZNYAK, BNL, J.-H. CHUNG, NCNR at NIST, E.S. CHOI, NHMFL, J.M. TRANQUADA, BNL — The observation of enhanced spin stripe order in the vortex cores of $La_{2-x}Sr_xCuO_4$ has been a landmark experiment that revealed the intimate connection between superconductivity and incommensurate antiferromagnetism. Only recently we have observed a corresponding field dependence of the spin and, more importantly, of the charge stripe order in $La_{2-x}Ba_xCuO_4$. Here we present our recent results from neutron diffraction, x-ray diffraction, and torque measurements in high magnetic fields. These helped us to establish the field versus temperature and doping phase diagrams for spin and charge order, and to further corroborate the stripe model as the more appropriate description than for example spiral and vortex states.

¹Work at Brookhaven was supported by the Office of Science, U.S. Department of Energy.

3:18PM T21.00005 Pressure study of local tilts and their correlation to stripe order in single crystal $La_{1.875}Ba_{0.125}CuO_4$, GILBERTO FABBRIS, Argonne National Laboratory and Washington University in St. Louis, MARKUS HÜCKER, GENDA GU, JOHN TRANQUADA, Brookhaven National Laboratory, DANIEL HASKEL, Argonne National Laboratory — The strong T_c suppression in $LaBaCuO$ at $x=0.125$ is widely believed to be related to formation of static stripes, at least partially driven by a strong electron-lattice coupling in a low temperature tetragonal (LTT) phase (Tranquada *et al.*, Nature 375, 561 (1995)). A recent high-pressure experiment appears to challenge this view as it was observed that static stripe order persists to pressures higher than required to induce LTT to HTT transition (Hucker *et al.*, PRL 104, 057004 (2010)). We carried out high-pressure La K-edge polarized XAFS measurements in $LaBaCuO$ ($x=0.125$) single crystals in a diamond anvil cell to probe local CuO_6 tilts. We observe that the local tilts remain LTT-like at high pressure, even though the macroscopic structure is HTT. The results suggest a significant order-disorder component to this pressure-induced phase transition, whereby the local LTT tilts remain present in the local scale but disorder over long range resulting in HTT symmetry seen by diffraction. The result may help explain why the stripe order is largely unaffected by the LTT to HTT pressure-induced transition. Work at Argonne (BNL) is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357 (DE-AC02-98CH10886).

3:30PM T21.00006 Gutzwiller Charge and Magnetic Phase Diagrams of Cuprates¹, ROBERT MARKIEWICZ, Northeastern University, JOSE LORENZANA, Sapienza, University of Rome, GOETZ SEIBOLD, University of Cottbus, Germany, ARUN BANSIL, Northeastern University — We extend our previous analysis of the magnetic phase diagram of the cuprates to look for charge instabilities, either purely electronic or involving electron-phonon coupling, employing Gutzwiller approximation $GA+RPA$ calculations of the Hubbard model. In the absence of phonons we find an overscreening instability for large doping at (π, π) . In the presence of electron-phonon coupling, we find a rich response to Fermi surface nesting, very similar to the magnetic case, and in this case the instability criterion can be formulated as a generalized Stoner criterion. In the hole-doping regime, where evidence exists for a nonmagnetic (stripe) pseudogap, we find competing instabilities. Since the same susceptibility peaks are present for both spin and charge excitations, differences in preferred q -vectors arise from the q -dependence of the interaction $U_{eff,q}$.

¹Supported in part by the US DOE.

3:42PM T21.00007 The impact of incommensurate bond centered density waves in underdoped cuprates, LIANG NIESTEMSKI, Colgate University, ZIQIANG WANG, Boston College — We study the particle-particle channel and the particle-hole channel of the valence bond fluctuations away from half filling in cuprates. Based on strong-coupling analysis of the t-J model, we argue that the superexchange interaction J induced incommensurate bond centered density wave order is the driving mechanism for the pseudogap state. We show that the interplay between the incommensurate bond centered density wave instability and the intrinsic electronic inhomogeneity in real cuprates materials is responsible for the observed pseudogap phenomena.

3:54PM T21.00008 Two-component electron fluid and pseudogap asymmetry in underdoped high-Tc cuprate superconductors, JAMES STOREY, Victoria University of Wellington, New Zealand, JEFFERY TALLON, Industrial Research Ltd., New Zealand, GRANT WILLIAMS, Victoria University of Wellington, New Zealand — Evidence from NMR of a two-component spin system in the cuprate high-Tc superconductors is shown to be paralleled by similar evidence from the total electronic entropy so that a two-component quasiparticle fluid is implicated. We propose that this two-component behavior arises from reconstruction of the energy-momentum dispersion into two branches in the pseudogap regime. If correct then it follows that single-component electronic behavior will be recovered when the pseudogap closes in the overdoped regime. We illustrate this by calculating the spin susceptibility using the resonating valence bond spin liquid model developed by Yang, Rice and Zhang, finding excellent agreement with the NMR results. In addition, we find that the particle-hole asymmetric pseudogap of this model accounts for both the large thermoelectric power, and the downturn in resistivity observed in underdoped cuprates.

4:06PM T21.00009 Spin excitations in a layered antiferromagnetic metal, WENYA ROWE, Department of Physics, University of Florida, Gainesville, FL, JOHANNES KNOLLE, Max-Planck-Institut für Physik komplexer System, D-01187 Dresden, Germany, ILYA EREMIN, Institute für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany, PETER HIRSCHFELD, Department of Physics, University of Florida, Gainesville, FL — The proximity of antiferromagnetic order in high-temperature superconducting materials is considered a possible clue to the electronic excitations which form superconducting pairs. Here we study the transverse and longitudinal spin excitation spectrum in a one-band model in the pure spin density wave (SDW) state and in the coexistence state of SDW and superconductivity. We start from a Stoner insulator which is similar to the case of cuprate parent compounds. By changing the chemical potential and the SDW order parameter, we study the evolution of the spectrum with different Fermi surfaces, such as the one with only hole pockets, with only electron pockets and with pockets of both types. We also compute the spin excitations in the coexistence of the AF and d-wave superconductivity, motivated by electron-doped cuprates.

4:18PM T21.00010 Coexistence of Superconductivity and Magnetic Order in $\text{RuGd}_2\text{Sr}(\text{Cu}_{1-x}\text{Fe}_x)_2\text{O}_8$ probed by ^{99}Ru and ^{57}Fe Mössbauer Effects¹, D. COFFEY, Dept. of Physics, Buffalo State College, NY, G. LONG, Dept. of Physics, SUNY Buffalo, M. DEMARCO, Dept. of Physics, Buffalo State College, NY, M. S. TORIKACHVILI, Dept. of Physics, San Diego State University — $\text{RuGd}_2\text{Sr}_2\text{Cu}_2\text{O}_8$ develops magnetic order at about 137K and becomes a superconductor at lower temperatures ($T_{SC} \sim 40\text{K}$). T_{SC} decreases with increasing Fe doping in $\text{RuGd}_2\text{Sr}_2(\text{Cu}_{1-x}\text{Fe}_x)_2\text{O}_8$ and is zero by $x = .03$. We measure the ^{99}Ru and ^{57}Fe Mössbauer Effects for $x=0, 0.1, 0.2$, and 0.3 . The ^{57}Fe Mössbauer spectra (MS) show that there are two different Fe sites at 4.2K with very similar hyperfine magnetic fields, $H_{\text{hyper}} \sim 48\text{ T}$. However H_{hyper} goes to zero at $\sim$ half the Fe sites in a temperature range between 30K and 40K in superconducting and non-superconducting samples. There is no significant change in H_{hyper} in the ^{99}Ru MS in this temperature range. We conclude that the Fe sites whose H_{hyper} does not change are in the magnetically ordered RuO planes. We assume that the Fe's which see the transition between 30K and 40K are in the CuO planes and investigate how this transition arises.

¹The work was supported by USDOE(DE-FG02-03ER46064) at BSC and by NSF-DMR-085335 at SDSU.

4:30PM T21.00011 NMR Studies of the pseudogap in BSCCO-2212, J. CROCKER, A.P. DIOGUARDI, N. APROBERTS-WARREN, A.C. SHOCKLEY, UC Davis, H.-J. GRAFE, IFW Dresden, Z. XU, J. WEN, G. GU, BNL, N.J. CURRO, UC Davis — We present O-17 NMR measurements on a single crystal of overdoped BSCCO-2212 ($T_c = 82\text{K}$). As a function of temperature we measure the planar oxygen's: resonance linewidths, Knight shift (K), electronic field gradient (EFG), and spin lattice relaxation rate ($1/T_1$) along each principle axis. Our analysis shows that their temperature dependence can be explained by a suppression of the density of states in the pseudogap region $T < T^* = 94\text{K}$.

4:42PM T21.00012 ^{17}O and ^{199}Hg NMR measurements of $\text{HgBa}_2\text{CuO}_{4+y}$ single crystals¹, A.M. MOUNCE, S. OH, W.P. HALPERIN, Northwestern University, P.L. KUHNS, A.P. REYES, National High Magnetic Field Laboratory, D. XIA, X. ZHAO, University of Minnesota, Jilin University, M. CHAN, L. JI, M. GREVEN, University of Minnesota — The high superconducting transition temperature and the simple tetragonal structure of $\text{HgBa}_2\text{CuO}_{4+y}$ ($\text{Hg}1201$) makes this material an ideal candidate to study unconventional superconductivity in the cuprates[1]. Nuclear magnet resonance has been performed on $\text{Hg}1201$ single crystals which have been annealed in an ^{17}O atmosphere to various dopings. Preliminary results of the NMR spectra and relaxation of both ^{17}O and ^{199}Hg are presented. Narrow linewidths allow for the resolution of both ^{17}O lattice sites and a doping dependent ^{199}Hg spectral splitting[2]. This work is supported by DOE/BES: DE-FG02-05ER46248 and the NHMFL by NSF and the State of Florida.[1] N. Barišić *et al*, PRB **78**, 054518 (2008) [2] J. Haase *et al*, arXiv:1110.601v1 (2011)

¹This work is supported by DOE/BES: DE-FG02-05ER46248 and the NHMFL by NSF and the State of Florida.

4:54PM T21.00013 Magnetic susceptibility analysis on Zn-doping in the high T_c superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{7-1}$, ZACHARY C.M. WINTER, MICHAEL G. SMITH, ALWYN REBELLO, JOHN J. NEUMEIER, Montana State University — Localized magnetic moments are known to destroy superconductivity in conventional superconductors. In the case of $\text{YBa}_2\text{Cu}_3\text{O}_7$ (YBCO), the nonmagnetic ion Zn has a very strong impact on suppressing the superconducting transition temperature (T_c). YBCO loses all superconductivity when only 10% of the Cu is substituted with Zn.² In this project, we have investigated the magnetic susceptibility for a number of Zn doping levels in samples with the nominal composition $\text{YBa}_2(\text{Cu}_{1-x}\text{Zn}_x)_3\text{O}_7$. We observe the development of Curie-Weiss paramagnetism for some Zn compositions, and will address whether the associated paramagnetic moments might cause magnetic pair-breaking.

¹This material is based upon work supported by the National Science Foundation (DMR-0907036).

²R. E. Walstedt *et al*. Phys. Rev. B, **48**, 10646 (1993)

5:06PM T21.00014 Observable NMR signal from orbital current order in YBCO, SAMUEL LEDERER, STEVEN KIVELSON, Stanford University — Assuming, as suggested by recent neutron scattering experiments, that a broken symmetry state with orbital current order occurs in the pseudo-gap phase of the cuprate superconductors, we show that there must be associated equilibrium magnetic fields at various atomic sites in the unit cell, which should be detectable by NMR experiments.

5:18PM T21.00015 Numerical study of magnetic excitations probed by photon spectroscopies in families of high-temperature superconductors, CHUNJING JIA, CHENG-CHIEN CHEN, BRIAN MORITZ, ADAM SORINI, THOMAS DEVEREAUX, SIMES, SLAC National Accelerator Laboratory and Stanford University — Magnetic excitation in high-temperature superconductors has been a topic of cutting edge research for many years. In photon spectroscopies, single- and two-magnon excitations can be created and measured efficiently using techniques such as resonant inelastic x-ray scattering and optical Raman scattering. We present numerical studies of the magnetic excitations for different families of high-temperature superconductors, including both copper and iron based superconductors. These magnetic excitations and their dispersions provide important information in understanding the magnetic properties of these materials.

Wednesday, February 29, 2012 2:30PM - 5:30PM –
Session T22 DMP DCOMP: Focus Session: Fe-based Superconductivity - Properties of 122 phases 254B

2:30PM T22.00001 Combined effects of chemical doping and pressure on physical properties of CaFe_2As_2 ¹, SHENG RAN, SERGEY BUD'KO, PAUL CANFIELD, Ames Laboratory U.S. DOE and Department of Physics and Astronomy, Iowa State University, MILTON TORIKACHVILI, Department of Physics, San Diego State University — The AFe_2As_2 compounds (A = alkaline earth) are the most extensively studied materials among the FeAs-based superconductors, and CaFe_2As_2 is the most pressure sensitive among them. The structural/magnetic phase transition near 170K is suppressed rapidly under pressure and a nonmagnetic, collapsed tetragonal phase is stabilized. Depending on the hydrostaticity of the pressure medium, the superconducting phase may or may not be induced. In this talk we will present the combined effects of chemical doping and pressure on the structural/magnetic phase transition as well as the collapsed tetragonal structure phase transition in an attempt to better understand the interactions between these phases.

¹Supported by U.S. DOE (DE-AC02-07CH11358), AFOSR-MURI (FA9550-09-1-0603), and NSF (DMR-0805335).

2:42PM T22.00002 First Principles Calculations of the Pnictide CaFe_2As_2 under Pressure, KHANDKER QUADER, Kent State University, MICHAEL WIDOM, Carnegie-Mellon University — We carry out first principles calculations of the effects of pressure on the structural and magnetic properties of the pnictide CaFe_2As_2 and compare with experiments. Our PBE-GGA calculations accurately reproduce the experimentally observed structural and magnetic ordering at zero pressure. Enthalpic considerations show that antiferromagnetic orthorhombic phase is favored over the non-magnetic tetragonal phase at pressure $P=0$, while the “collapsed” tetragonal phase is favored for pressures greater than 0.4 GPa, in good agreement with experiments. The calculated pressure dependences of the lattice parameters and the Fe-As bond lengths agree with experimental trends. We will discuss the nature of bonding and antibonding orbitals near the Fermi surface and we will evaluate the interplanar magnetic exchange interaction J.

2:54PM T22.00003 Evidence for domain wall superconductivity in antiferromagnetic CaFe_2As_2 , ADAM P. DIOGUARDI, UC Davis Physics, HONG XIAO, T. HU, Department of Physics, University of Crete and FORTH, NICHOLAS APROBERTS-WARREN, ABIGAIL SHOCKLEY, JOHN CROCKER, DAVID M. NISSON, Department of Physics, UC Davis, Z. VISKADOURAKIS, Department of Physics, University of Crete and FORTH, XIANYANG TEE, Division of Physics and Applied Physics, Nanyang Technology University, I. RADULOV, Department of Physics, University of Crete and FORTH, C.C. ALMASAN, Department of Physics, Kent State University, NICHOLAS J. CURRO, Department of Physics, UC Davis, CHRISTOS PANAGOPOULOS, Department of Physics, University of Crete and FORTH — ⁷⁵As nuclear magnetic resonance (NMR), resistivity, and magnetization measurements in the antiferromagnetic state of the iron-based superconductor parent compound CaFe_2As_2 exhibit anomalous features consistent with the collective freezing of domain walls. Below $T^* \approx 10$ K, the ⁷⁵As NMR measurements reveal the presence of low fluctuations of the hyperfine field, the resistivity shows an enhancement and subsequent suppression, and the bulk magnetization shows a sharp increase. These features in both the charge and spin response are strongly field dependent, are fully suppressed by $H^* \approx 15$ T, and suggest the presence of filamentary superconductivity nucleated at the antiphase domain walls.

3:06PM T22.00004 Local atomic structure of BaFe_2As_2 by neutron powder diffraction, JENNIFER NIEDZIELA, Dept. of Physics and Astronomy, U. Tennessee, Knoxville; ORNL - Neutron Sciences Directorate, TAKESHI EGAMI, Dept. of Mat. Science and Engineering, Dept. of Physics and Astronomy, U. Tennessee, Knoxville; ORNL - Joint Institute for Neutron Sciences — All structures of iron-based superconductors (FeSC) have planar layers of iron, tetrahedrally coordinated by pnictogens or chalcogens, and the structural details of this layer impact the superconducting and magnetic properties. Local structural studies of the iron-coordinated layer show evidence for local distortions resulting from models that allow for overall reductions in local symmetry. BaFe_2As_2 , a parent compound of several families of FeSC, undergoes a transition at $T \approx 140$ K, resulting in the onset of AFM ordering following a small lattice distortion. Here we report the results of a by time of flight neutron diffraction study on BaFe_2As_2 , analyzed using Rietveld and pair distribution function techniques. This work produces a comprehensive view of the local structure of BaFe_2As_2 as a function of temperature. The results are consistent with previous work showing stratification of the As-As bond length, and show that models accounting for an overall reduction in local symmetry provide the best fit to the experimental data. Further, the results show that local distortions are present up to room temperature. Details of the experiment and implications for the paramagnetic and magnetic states will be discussed.

3:18PM T22.00005 First principles study of uniaxial pressure-induced phase transitions in CaFe_2As_2 and BaFe_2As_2 , ROSER VALENTI, MILAN TOMIC, HARALD O. JESCHKE, Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, 60438 Frankfurt, Germany — We consider density functional theory methods to determine the equilibrium structures of CaFe_2As_2 and BaFe_2As_2 under the effect of uniaxial pressure. We compare the results with calculations for hydrostatic pressure as well as with available experimental results. In CaFe_2As_2 , we observe a unique phase transition from a magnetic orthorhombic phase to a nonmagnetic collapsed tetragonal phase for both pressure conditions and no indication of a tetragonal phase at intermediate uniaxial pressures. In contrast, for both uniaxial and hydrostatic pressure, BaFe_2As_2 shows two phase transitions from a magnetic orthorhombic to a collapsed tetragonal phase through an intermediate nonmagnetic tetragonal phase. We predict the critical transition pressures under uniaxial conditions to be much lower than those under hydrostatic conditions which implies that the systems are highly sensitive to uniaxial stress. We compare our results to available experimental measurements.

3:30PM T22.00006 Temperature-Pressure Phase Diagram of Lightly Hole-doped BaFe_2As_2 ¹, BALAZS SIPOS, ATHENA SAFA-SEFAT, BRIAN C. SALES, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831 USA, CORRELATED ELECTRON MATERIALS GROUP, MATERIALS SCIENCE AND TECHNOLOGY DIVISION, ORNL TEAM — Chemical doping and application of pressure are the two common tools to tune the electronic structure of a material. Although electron-doping on Fe-site in BaFe_2As_2 gives superconductivity up to ~ 22 K, it is puzzling that hole-doping does not. For this reason, we decided to carry out pressure studies on a few lightly Cr- or Mo-doped crystals of BaFe_2As_2 . We have applied pressures of up to 2 GPa using a cylinder cell, and Fluorinert as pressure medium. Our preliminary findings reveal the shift of antiferromagnetic ordering temperatures to lower with pressure, and a down-turn in resistivity at low temperatures and pressures, which may be attributed to superconductivity.

¹This work was partly supported by the Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

3:42PM T22.00007 ABSTRACT WITHDRAWN —

3:54PM T22.00008 Magnetism, superconductivity, and the volume collapse transition in $(\text{Ca}_{0.67}\text{Sr}_{0.33})\text{Fe}_2\text{As}_2$ under pressure¹, JASON JEFFRIES, N.P. BUTCH, Lawrence Livermore National Laboratory, S.R. SAHA, K. KIRSHENBAUM, University of Maryland, S.T. WEIR, Lawrence Livermore National Laboratory, Y.K. VOHRA, University of Alabama, Birmingham, J. PAGLIONE, University of Maryland — The alkaline earth site of CaFe_2As_2 can be chemically substituted with Sr, forming a homogeneous solid solution series ending with SrFe_2As_2 . It is found that $(\text{Ca}_{0.67}\text{Sr}_{0.33})\text{Fe}_2\text{As}_2$ exhibits a pressure-temperature phase diagram intermediate between the two end members of the series, shifting the phase lines for the suppression of magnetism, the development of superconductivity, and the occurrence of a volume collapse transition to higher pressures. The overall shift in the pressure-temperature phase diagram permits the study of each phase field, yielding valuable information about the correlations between local atomic structure, magnetism, superconductivity, and the volume collapse transition. Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344.

¹This work was performed under LDRD (11-LW-003)

4:06PM T22.00009 Inducing structural collapse and superconductivity in CaFe_2As_2 by systematic substitutions of rare earths, SHANTA SAHA, TYLER DRYE, NICHOLAS BUTCH, RONGWEI HU, KEVIN KIRSHENBAUM, STEVEN ZIEMAK, JOHNPierre PAGLIONE, Center for Nanophysics and Advanced Materials, Dept. of Physics, University of Maryland, College Park, MD 20742, PETER ZAVALIJ, Dept. of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742, JEFFREY LYNN, NIST Center for Neutron Research, Gaithersburg, MD 20899 — Recently, we have reported structural collapse and 47 K superconductivity in CaFe_2As_2 by aliovalent rare earth substitutions for Ca atoms [1]. We will present the evolution of structural and superconducting properties in single crystals of CaFe_2As_2 by systematic substitutions of R (=La, Ce, Pr, and Nd) for Ca, causing electron doping that is indirect to FeAs layer. Effect of annealing, growth method, etching, and pressure on $\text{Ca}_{1-x}\text{R}_x\text{Fe}_2\text{As}_2$, indicating the intrinsic nature of this high T_c superconductivity, the highest in 122 Fe-based materials, will be discussed. Ref. [1] S. R. Saha *et al.* arXiv:1105.4798.

4:18PM T22.00010 Defect-Associated Superconductivity in $(\text{Pr,Ca})\text{Fe}_2\text{As}_2$, FENGYAN WEI, BING LV, LIANGZI DENG, YANYI SUN, YUYI XUE, Texas Center for superconductivity at University of Houston Department of Physics, CHINGWU CHU, Texas Center for superconductivity at University of Houston Department of Physics, Lawrence Berkeley National Laboratory — The superconductivity in rare earth doped CaFe_2As_2 remains puzzled. As reported before, there are two distinguishable superconductive transitions at 20 K and 49 K, respectively, and the 49 K superconductivity can be better modeled as Josephson-Junction-Arrays (JJA). The H- and T-dependencies of the ac/dc magnetization are further explored here. The data suggest that the effective lower-critical-fields at both *c*- and *ab*-directions are below 1 Oe down to 5 K, in agreement with previous JJA assumption. The ac susceptibility below the critical field is highly anisotropy, suggesting a thin-disk-like morphology of the JJA's. The associated weak-links, however, appear to be broken above 20 K by a *dc* bias as small as 10 Oe. The ac response at higher bias fields, therefore, will be dominated by the isolated superconducting islands of JJA. It is interesting to note, therefore, that the ac susceptibility remains highly anisotropic at high fields, but is much weaker than that expected from the field-cooled magnetization. We interpret this as the result of sub-micron size, thin-disk-like local superconductivity, *i.e.* Defect-associated superconductivity.

4:30PM T22.00011 Rare Earth Doping in the $(\text{Sr,Ca})\text{Fe}_2\text{As}_2$ System, TYLER DRYE, SHANTA SAHA, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland-College Park, PETER ZAVALIJ, Department of Chemistry, University of Maryland-College Park, JOHNPierre PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland-College Park — The $(\text{Sr,Ca})\text{Fe}_2\text{As}_2$ system shows an unusual persistence of the Neel ordering temperature of ~ 200 K up to a concentration of 70% calcium. We present electrical transport, magnetic susceptibility and structural characterization data as a function of rare earth substitution into $\text{Sr}_{0.3}\text{Ca}_{0.7}\text{Fe}_2\text{As}_2$ single crystals, focusing on the resultant phase diagram and the comparisons of solubility limit of rare earth substitution as compared to end members SrFe_2As_2 and CaFe_2As_2 .

4:42PM T22.00012 Microstructure and the non-bulk superconductivity up to 49K in electron-doped Rare-earth $(\text{Ca, R})\text{Fe}_2\text{As}_2$ (R=La, Ce, Pr and Nd) Single Crystals, BING LV, FENGYAN WEI, LIANGZI DENG, YANYI SUN, YU-YI XUE, MELISSA GOOCH, TCSUH and Department of Physics, University of Houston, JAMES MEEN, TCSUH and Department of Chemistry, University of Houston, CHING-WU CHU¹, TCSUH and Department of Physics, University of Houston — In an attempt to raise the T_c in the 122 family, we have carried out electron-doping and observed an onset T_c up to 49K in the single crystalline $(\text{Ca, R})\text{Fe}_2\text{As}_2$ (R=La, Ce, Pr and Nd). The single crystals up to 5 × 5 mm size are grown from self-flux technique and the optimal doping parameters for different rare-earth elements will be reported. Magnetic and resistivity data suggest possible existence of two superconducting transitions in all the rare-earth electron doped $(\text{Ca, R})\text{Fe}_2\text{As}_2$ samples: one starts at ~ 40 s K, and the other at ~ 20 K, with drastically different response to the field. Detailed single crystals diffraction analysis show that there are no significant difference in terms of atomic position, bond distances, angles and lattice parameters upon different rare earth doping; the defect-related local structure might be responsible for the observed high T_c in this system. The unusual superconducting phase appears to be filamentary or interfacial in nature, and the possible mechanism will be discussed.

¹Also at Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720

4:54PM T22.00013 Codoping – A way to enhance the upper critical field in iron-arsenic superconductors¹, M. NICKLAS, MPI for Chemical Physics of Solids, Dresden, Germany, F. WEICKERT, LANL, MPA-CMMS, Los Alamos, NM, USA, J. WOSNITZA, HLD, HZDR, Dresden, Germany, A. LEITHE-JASPER, W. SCHNELLE, H. ROSNER, MPI for Chemical Physics of Solids, Dresden, Germany — Technological key features of iron-based superconductors are the high critical temperature T_c of up to 55 K and the high tolerance against magnetic fields, which led so far to upper critical fields in the range of 75 T. Furthermore, the small H_{c2} -anisotropy between field applied along the *c*-direction and in the *ab*-plane, in particular for the FeSe and AEFe_2As_2 ($\text{AE} = \text{Ca, Sr, Ba}$) materials, is a prerequisite for several technical applications. Currently, different approaches (chemical substitutions, processing) are discussed how to increase H_{c2} further. Here, we show a feasibility study for codoping of polycrystalline Sr- or BaFe_2As_2 samples, namely the simultaneous substitution of K on the Sr/Ba layer and of Co on the FeAs layer. The upper critical field was investigated by magnetoresistance in high pulsed magnetic fields up to 64 T. We find, that the extrapolated critical field $H_{c2}(T \rightarrow 0)$ is enhanced by 15% for $\text{Ba}_{0.55}\text{K}_{0.45}\text{Fe}_{1.95}\text{Co}_{0.05}\text{As}_2$ in comparison to $\text{Ba}_{0.55}\text{K}_{0.45}\text{Fe}_2\text{As}_2$, although T_c is almost identical in both materials. These results suggest that codoping is a promising route for the systematic optimization of iron-arsenic based superconductors for high-magnetic field and high-current applications.

¹Supported by the MPG Research Initiative: Materials Science and Condensed Matter Research at the HLD, EuroMagNET II under the EC contract 228043, and DFG through SPP 1458

5:06PM T22.00014 Influence of random point defects introduced by proton irradiation on the vortex pinning and dynamics of superconducting 122 iron arsenides¹, LEONARDO CIVALE, NESTOR HABERKORN, IGOR USOV, JEEHOON KIM, BORIS MAIOROV, MARCUS WEINGARD, Los Alamos National Laboratory, G.F. CHEN, W. YU, Department of Physics, Renmin University of China, Beijing, China, W. HIRATA, S. MIYASAKA, S. TAJIMA, N. CHIKUMOTO, K. TANABE, Superconductivity Research Laboratory-ISTEC, 1-10-13 Shinonome, Koto-ku, Tokyo 135-0062, Japan — Vortex matter in iron-arsenide superconductors exhibits a rich phenomenology that is still largely unexplored. One way to understand and manipulate the pinning mechanisms and the vortex dynamics in superconductors is by the artificial introduction of additional defects. In this work we explore the influence of the random point defects introduced by proton irradiation on the vortex dynamics and critical currents of 122 iron arsenide superconductors. Our comparison includes $\text{Ca}_{1-x}\text{Na}_x\text{Fe}_2\text{As}_2$ and Co-doped BaFe_2As_2 single crystals. We find that the influence of random point defects on the creep rate (S) and the elastic to plastic crossover of the vortex dynamics show a strong dependence with intrinsic superconductor parameters such as the coherence length. We analyze the magnetic field – temperature (H - T) vortex phase diagrams for the as-grown single crystals and the changes produced by the random point defects.

¹Work supported by the US DOE, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

5:18PM T22.00015 Upper critical and irreversible fields of polycrystalline $\text{CeFeAsO}_{1-x}\text{F}_x$ superconductors, SHEN V. CHONG, JEFFERY L. TALLON, Industrial Research Limited, New Zealand, GRANT V.M. WILLIAMS, The MacDiarmid Institute, Victoria University of Wellington, New Zealand — We have investigated the upper critical (H_{c2}) and irreversible (H_{irr}) fields of polycrystalline samples of Ce oxypnictide at different doping levels. H_{c2} was obtained from temperature dependent resistivity measurements with increasing applied magnetic field. Critical field values as high as 150 Tesla were observed with a decreasing trend as the doping level shifts from a slightly under-doped state to the highly over-doped region. The irreversible fields were lower in this superconductor compared with other rare-earth oxypnictides, with values below 3 Tesla at 20 K. However, H_{irr} was found to increase with increasing doping, opposite to that of H_{c2} . The origin of H_{irr} was studied by determining the exponent 'n' extracted from plots of $\log_{10}(H_{irr})$ versus $\log_{10}(1-T/T_c)^n$. We found that H_{irr} follows a 3D vortex lattice-melting model similar to the other low anisotropic iron-based superconductors.

Wednesday, February 29, 2012 2:30PM - 5:30PM – Session T23 DCMP: Actinides and Transport Magnetism in Metals 255

2:30PM T23.00001 A quantum Monte Carlo study of thorium halide molecules, SHI GUO, MINYI ZHU, North Carolina State University, ENRIQUE BATISTA, RICHARD MARTIN, Los Alamos National Lab, LUBOS MITAS, North Carolina State University — We present electronic structure calculations of thorium halide molecules, namely, a series of ThCl_n and ThBr_n ($n=1,2,3,4$) systems. We calculate the bond dissociation energies for the sequence of the following dissociation reactions: $\text{ThCl}_n \rightarrow \text{ThCl}_{n-1} + \text{Cl}$ and $\text{ThBr}_n \rightarrow \text{ThBr}_{n-1} + \text{Br}$. We apply both large core and small core energy-consistent pseudopotentials for thorium atom and we employ DFT GGA and hybrid functionals for energies and geometry calculations. For high accuracy energies we use the fixed-node diffusion Monte Carlo (DMC) method. In DMC calculations we employ both single- and multi-reference trial wave functions in order to test the quality of the nodal surfaces. We study the dissociation energies with regard to different multiplicities of the ThX_n molecules and the different behavior of the bromides with respect to chlorides. We compare our results with hybrid DFT methods and experimental values. Supported by DOE and NSF.

2:42PM T23.00002 Electron binding energy of uranium-ligand and uranyl-ligand anions¹, LEI WANG, STEVEN HOROWITZ, BRAD MARSTON, Brown University — Electron binding energies of the early actinide element uranium in gas-phase anion complexes are calculated by relativistic density functional theory (DFT) with two different exchange-correlation functions (RPBE and B3LYP) and also in the Hartree-Fock (HF) approximation². Scalar and spin-orbit calculations are performed, and the calculated energies are compared to available experimental measurements and shown to disagree by energies of order 1 eV. Strong correlations that are poorly treated in DFT and HF can be included by a hybrid approach in which a generalized Anderson impurity model is numerically diagonalized. Reduction-oxidation (redox) potentials of aqueous actinide ions show improved agreement with measured values in the hybrid approach³. We test whether or not similar improvements are found in the gas-phase.

¹Supported in part by NSF DMR-0605619.

²ADF2010.02, SCM.com

³S. E. Horowitz and J. B. Marston, J. Chem. Phys **134** 064510 (2011).

2:54PM T23.00003 Electronic structure of Pu metal and intermetallics as determined by ARPES and XPS¹, MILES BEAUX, TOMASZ DURAKIEWICZ, KEVIN GRAHAM, JEREMY MITCHELL, SCOTT RICHMOND, ERIC BAUER, DAVID MOORE, FRANZ FREIBERT, PAUL TOBASH, JOHN KENNISON, JOHN JOYCE, Los Alamos National Laboratory — We exploit our unique capability in angle resolved photoemission (ARPES) measurement for plutonium materials to compare the electronic structure of delta Pu, PuCoIn_5 and PuCoGa_5 . We present a systematic study for polycrystalline delta Pu metal as well as the first photoemission measurements on single crystals of the superconductor PuCoIn_5 . These first results for PuCoIn_5 are compared to results for PuCoGa_5 and variations in the electronic structure are attributed to differences in 5f hybridization with conduction states based on differences in lattice values. Laser ablation was used to clean the surface of Pu materials and cleanliness was monitored through O 1s and Pu 4f core levels as well as valence band features. Observation of these spectra provides better insight into the differentiation of contaminant features versus the strong correlation effects within Pu metal.

¹Work supported by the US DOE, BES, Division of Materials Science, and the G.T. Seaborg Institute for Transactinium Science

3:06PM T23.00004 Elastic moduli of nearly pure polycrystalline plutonium, ALBERT MIGLIORI, ARKADY SHEKHTER, JON B. BETTS, VICTOR FANELLI, NHMFL, Pulsed Field facility, LANL, Los Alamos, NM — We measure elastic moduli of microalloyed polycrystalline cylindrical specimen of Pu-239. We observe $\alpha \rightarrow \beta \rightarrow \gamma \rightarrow \delta$ phase transitions and find that the elastic moduli of nearly pure plutonium are the same as those of Ga-stabilized plutonium.

3:18PM T23.00005 Magnetization at 1 Mbar Near the Tricritical Point in the Ce(0.9- x)La(x)Th(0.10) System¹, J.L. SMITH, K. GOFRYK, R.D. TAYLOR, J.C. LASHLEY, Los Alamos National Lab, M.P. PASTERNAK, Tel Aviv University, D.J. POLANCIC, Quantum Design, Inc. — The gamma to alpha isostructural transition in the Ce(0.9- x)La(x)Th(0.10) system is measured as a function of La alloying and external pressure up to 1 Mbar using magnetic susceptibility. We probe a line of discontinuous transitions, as indicated by the change in volume, decreasing exponentially from 118 K to close to 0 K with increasing La doping, and the transition changes from being first order to continuous at a critical concentration close to $x = 0.14$. At the tricritical point, the magnetic susceptibility increase rapidly near the critical concentration and approaches large values at $x = 0.35$ signifying that a heavy Fermi-liquid state evolves at large doping near the critical concentration. The Wilson ratio reaches a value above two for a narrow range of concentrations where the specific heat and susceptibility vary most rapidly with the doping concentration.

¹Work performed under the auspices of the U.S.D.O.E.

3:30PM T23.00006 ABSTRACT WITHDRAWN —

3:42PM T23.00007 Actinide oxides under pressure, LEON PETIT, Daresbury Laboratory, MALCOLM STOCKS, Oak Ridge National Laboratory, MARTIN LUEDERS, ZDZISLAWA SZOTEK, WALTER TEMMERMAN, Daresbury Laboratory, AXEL SVANE, Aarhus University — We use the self-interaction corrected local spin density approximation to investigate the oxidation of actinide dioxides under pressure. The methodology enables us to determine the ground state valency configuration of the actinide 5f electrons and to study the localization/delocalization transition that occurs under pressure. We argue that this delocalization facilitates the oxidation of the actinide dioxides and present results for the estimated transition pressures.

3:54PM T23.00008 Dephasing due to electron interactions in inhomogeneous systems, MAXIMILIAN TREIBER, OLEG YEVTUSHENKO, JAN VON DELFT, Ludwig-Maximilians-University, Physics Department, ASC, CeNS, Theresienstrasse 37, D-80333 Munich, Germany — At sufficiently low temperatures, the dephasing time τ_φ of mesoscopic samples is governed by so-called Johnson-Nyquist (electronic) noise. We study the spatial dependence of the corresponding noise correlation function (NCF) in inhomogeneous systems. Using the fluctuation-dissipation theorem and the random-phase approximation, we derive a real-space integro-differential equation for the NCF and show that it reduces to a diffusion equation in the case of strong screening. In particular, using a method based on the spectral determinant, we evaluate the NCF for arbitrary networks of quasi-1D disordered wires with boundary conditions. As an application, we construct a realistic quantum dot model via a set of parallel wires connected at contacts to leads, and calculate the temperature dependence of τ_φ as well as the quantum corrections to the conductance. Furthermore, we analyze the observability of the elusive 0D regime (reached at $T < E_{\text{Thouless}}$ with the characteristic $\tau_\varphi \propto T^{-2}$ behavior) in such systems, and discuss alternative scenarios of its observation.

4:06PM T23.00009 Does aluminum conduct better than copper at the nanoscale? A first-principles study of metallic nanowires¹, ADAM SIMBECK, NICK LANZILLO, NEERAV KHARCHI, SAROJ NAYAK, Rensselaer Polytechnic Institute — From first-principles, we present a theoretical and comparative investigation of the role of quantum confinement in altering the electronic, transport, and phonon properties of linear, single-atom thick chains, i.e. nanowires, of metallic (Au, Ag, Cu, and Al) atoms. Our results for the ballistic quantum transport properties and electronic structure are in perfect agreement with those previously published. Motivated by this, we also consider electron-phonon interactions in such devices, where we report an order of magnitude reduction in the electron-phonon coupling constant for Al, whereas an enhancement is predicted for Au, Ag, and Cu.

¹Work supported by Interconnect Focus Center (MARCO program), State of New York, and the National Science Foundation's Integrative Graduate Education and Research Traineeship program, Grant No. 0333314

4:18PM T23.00010 Quantum oscillations and low-T resistivity of the 5s delafossite PdCoO₂¹, CLIFFORD HICKS, ALEXANDRA GIBBS, ANDREW MACKENZIE, University of St Andrews, U.K., HIROSHI TAKATSU, Tokyo Metropolitan University, Japan, YOSHITERU MAENO, Kyoto University, Japan, EDWARD YELLAND, University of St Andrews, U.K. — We report dHvA torque and resistivity data on the highly conductive delafossite PdCoO₂. Quantum oscillations confirm electronic structure calculations in showing a single, highly 2D Fermi surface with almost exactly half filling. However the cyclotron masses and the details of the warping are consistent with PdCoO₂ being a 5s metal, rather than the 4d metal indicated in most electronic structure papers. The room temperature resistivity is $\rho_{ab} = 2.6 \pm 0.2 \mu\Omega\text{-cm}$, lower than all elemental metals apart from the noble metals. The low-T residual resistivity of our samples is $0.008 \mu\Omega\text{-cm}$, corresponding to an extremely long mean free path of $20 \mu\text{m}$, surprising for a flux-grown material. The temperature dependence of the electron-phonon contribution to the resistivity is exponential rather than T^5 , indicating phonon drag, and the only observation of phonon drag in resistivity outside the alkali metals.

¹Engineering and Physical Sciences Research Council; Scottish Universities Physics Alliance

4:30PM T23.00011 Dielectric function of Ni-Pt alloys from 0.6 to 6.6 eV by spectroscopic ellipsometry¹, LINA ABDALLAH, STEFAN ZOLLNER, TAREK TAWALBEH, IGOR VASILIEV, NMSU, CHRISTIAN LAVOIE, AHMET OZCAN, IBM, MARK RAYMOND, GLOBALFOUNDRIES — The complex dielectric function of different Ni-Pt alloys (10% to 25% Pt concentration, 10nm thickness) was determined using spectroscopic ellipsometry over a broad photon energy range from 0.6 to 6.6eV. The films were deposited on a thick SiO₂ layers using Si as a substrate. The data were fitted using previously determined optical constants for Si and SiO₂. Optical constants of the Ni-Pt alloys were described using a Drude model (free carrier term), a pole due to d-intraband transition, and 2 to 3 Lorentz oscillators due to interband transitions. Data were compared with the calculated band structure of Nickel and Platinum. Results showed only small changes with the variation of Pt concentration or with annealing at 500 °C for 30s.

¹NSF DMR-1104934

4:42PM T23.00012 The Role of d -Orbitals in the Rashba Splitting on Au(111) and Ag(111), HYUNJUN LEE, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — We investigate the Rashba-type spin splitting in sp -derived Shockley surface states on (111) surfaces of noble metals, such as Au(111) and Ag(111), based on first-principles calculations including the spin-orbit interaction. By turning on and off l -dependent spin-orbit coupling one by one, we find that although the surface states on Au(111) have predominantly p -orbital character, the spin splitting in energy originates mainly from d -orbital character of the surface states. We also demonstrate that the spin splitting in surface states of both metallic surfaces of Au(111) and Ag(111) can be controlled by varying the sizes of d -orbital parts of the surface-state wave functions. These results show that in addition to difference in the atomic spin-orbit strength in Au and Ag, difference in d -orbital contributions to the surface states makes substantial difference in the sizes of the Rashba-type spin splitting in their surface electronic structures. This work was supported by the NRF of Korea (Grant Nos. 2009-0081204 and 2011-0018306) and KISTI Supercomputing Center (Project No. KSC-2011-C2-04).

4:54PM T23.00013 Effects of Co doping on the metamagnetic states in fcc $\text{Fe}_{1-x}\text{Co}_x$ ¹, ROMEO DE COSS, FILIBERTO ORTIZ-CHI, Departamento de Física Aplicada, Cinvestav-Merida, Yucatán, Mexico — It is well known that fcc-Fe have shows meta-magnetism, with a low-spin state (LS) at small volume and a high-spin state (HS) at large volume in the total-energy vs volume curve. In this work, we have studied the evolution of the metamagnetic states in the $\text{Fe}_{1-x}\text{Co}_x$ alloy as a function of Co concentration by means of first principles calculations. The ground state properties were obtained using the Full-Potential Linear Augmented Plane Waves method and the Generalized Gradient Approximation for the exchange-correlation functional. The alloying was modeled using the self-consistent virtual crystal approximation. The magnetic states are obtained from the total-energy as a function of the spin moment calculations, obtained using the Fixed Spin Moment methodology. For fcc-Fe, we found that the ground state corresponds to the LS state. Increasing the Co concentration the HS state decrease in energy. Thus, for $x = 0.05$ the energy of the LS and HS states is practically the same, corresponding to a spin-glass state. The LS state is substituted by a paramagnetic state for $x > 0.3$ of Co concentration. Interestingly, for the alloy with $x \sim 0.35$ the total-energy vs volume curve shows “effective symmetry,” which is expected to exhibit invar behavior.

¹This research was supported by Conacyt-Mexico under Grant No. 83604.

5:06PM T23.00014 Investigation of Possible Phase Separation in Rapidly Quenched $\text{Fe}_{1-x}\text{Co}_x$ Alloys with Cluster Expansion Model, XIN ZHAO, MANH CUONG NGUYEN, MIN JI, IVER E. ANDERSON, M.J. KRAMER, R. WILLIAM MCCALLUM, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory, US DOE and Department of Physics and Astronomy, Iowa State University — Recently, experiments observed phase separation in rapidly quenched $\text{Fe}_{1-x}\text{Co}_x$ alloy in the ordered α' phase [J. Alloys Compd. 424, 145 (2006)]. It is also believed that this is not an equilibrium result because of phase rule violation in the published phase diagram. To clarify this situation, we calculate the phase diagram of the system using cluster expansion in combination with a genetic algorithm. We calculated free energy of the system using super-cells up to 32 atoms with compositions ranging from 35 to 100 at. % Fe. Possible explanations for the experimental observations will be discussed.

5:18PM T23.00015 Atomic Structures and Magnetic Properties of Fe-rich $\text{Fe}_{1-x}\text{Co}_x$ Alloys: A Genetic Algorithm Search, MANH CUONG NGUYEN, XIN ZHAO, MIN JI, BRUCE HARMON, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory, US DOE and Department of Physics and Astronomy, Iowa State University — Using genetic algorithm with first-principles calculations, we performed a broad global search for low-energy crystal structures of Fe-rich $\text{Fe}_{1-x}\text{Co}_x$ alloys. We found that Fe-rich $\text{Fe}_{1-x}\text{Co}_x$ alloys are highly configurationally degenerate and there are many additional off-stoichiometric stable structures to the well-known stoichiometric FeCo - B_2 structure, giving a possibility for atomistic manipulation of the alloys. The Co-Co nearest-neighbor pair is strongly unfavorable in Fe-rich $\text{Fe}_{1-x}\text{Co}_x$ alloys. The magnetic moment of Fe atom is increasing with Co concentration while that of Co atom is almost constant, inducing a Slater-Pauling curve for magnetic moment per atom. The magnetic moment of Fe atom is strongly dependent on the number of Co nearest-neighbors and it increases with this number.

Wednesday, February 29, 2012 2:30PM - 5:42PM – Session T24 FIAP: Fractional Quantum Hall Effect III 256

2:30PM T24.00001 Evolution of 7/2 fractional quantum Hall state in two subband systems¹, YANG LIU, JAVAD SHABANI, D. KAMBUROV, M. SHAYEGAN, L.N. PFEIFFER, K.W. WEST, K.W. BALDWIN, Electrical engineering, Princeton University — We report the evolution of the fractional quantum Hall state (FQHS) at total Landau level (LL) filling factor $\nu = 7/2$ in wide GaAs quantum wells in which electrons occupy two electric subbands. The data reveal subtle and distinct evolutions as a function of density, magnetic field tilt-angle, or symmetry of the charge distribution. At intermediate tilt angles, for example, we observe a strengthening of the $\nu = 7/2$ FQHS. Moreover, in a well with asymmetric charge distribution, there is a developing FQHS when the LL filling factor of the symmetric subband ν_S equals 5/2 while the antisymmetric subband has filling $1 < \nu_A < 2$.

¹We acknowledge support through DOE BES (DEFG0200-ER45841) for measurements, and the Moore Foundation and the NSF (DMR-0904117 and MRSEC DMR-0819860) for sample fabrication and characterization.

2:42PM T24.00002 Observation of reentrant quantum Hall states in the lowest Landau level¹, M. SHAYEGAN, YANG LIU, C.G. PAPPAS, L.N. PFEIFFER, K.W. WEST, K.W. BALDWIN, Electrical engineering, Princeton university — Measurements in very low disorder two-dimensional electrons confined to relatively wide GaAs quantum well samples with tunable density reveal reentrant $\nu = 1$ integer quantum Hall states in the lowest Landau level near filling factors $\nu = 4/5$ and $6/5$. These states are not seen at low densities and become more prominent with increasing density and in wider wells. Our data suggest that these reentrant phases are (bubble) Wigner crystal states, stabilized here in the lowest Landau level thanks to the large electron layer thickness.

¹We acknowledge support through the Moore Foundation and the NSF (DMR-0904117 and MRSEC DMR-0819860) for sample fabrication and characterization, and the DOE BES (DE-FG0200-ER45841) for measurements.

2:54PM T24.00003 Spin waves in the second Landau level: Probing the spin-polarization enigma¹, URSULA WURSTBAUER, TREVOR DAVID RHONE, ARON PINCZUK, Columbia University, KEN W. WEST, LOREN N. PFEIFFER, Princeton University — The physics in the second Landau level (SLL) is governed by competing phases resulting in striking phenomena. We use resonant inelastic light scattering experiments to explore collective excitation modes with the focus on low lying spin excitation modes in the SLL. The intensity of the small momentum spin-wave at the bare Zeeman energy (E_Z) collapses for filling factors away from integer filling factor $\nu < 3$ and are dominated by a continuum of modes. We find that at the fractional filling factors $14/5$, $8/3$, $5/2$, $7/3$, $11/5$ the continuum coexists with a weak but distinct signal at E_Z , a long wavelength spin-wave that suggests a degree of spin polarization. In addition, at $5/2$ an intriguing well developed sharp mode is observable below E_Z , which is unique for the even-denominator filling factor. Modes at energies larger than E_Z merge additionally at odd-denominator states in ILS spectra, most pronounced for $7/3$, in a manner that is similar to that of the $1/3$ state. This observation could be evidence that the CF framework could be applicable to these states.

¹Supported by NSF and AvH

3:06PM T24.00004 Ballistic transport of (001) GaAs two-dimensional holes and hole-flux composite fermions through a lateral strain-induced superlattice¹, DOBROMIR KAMBUROV, HASSAN SHAPOURIAN, MANSOUR SHAYEGAN, LOREN PFEIFFER, KEN WEST, KIRK BALDWIN, Princeton University — The addition of a unidirectional superlattice on the surface of high-mobility two-dimensional carrier systems leads to a potential modulation signaled by the observation of magnetoresistance commensurability oscillations. We present measurements in high-mobility, two-dimensional (001) GaAs systems patterned with strain-induced surface superlattices of periodicity 100 to 250 nm. The data exhibit pronounced commensurability oscillations of holes near zero magnetic field and of hole-flux composite fermions near filling factor $\nu = 1/2$, allowing us to probe the Fermi contours of these quasi-particles.

¹We acknowledge support through the NSF (ECCS-1001719 and MRSEC DMR-0819860) for sample fabrication and characterization, and the DOE BES (DE-FG0200-ER45841) for measurements.

3:18PM T24.00005 Microscopic Disorder-Based model for non-Abelian Quasi-Particles in $\nu = 5/2$ FQH states¹, GILAD BEN-SHACH, CHRIS R. LAUMANN, AMIR YACOBY, BERTRAND I. HALPERIN, Harvard University — The detection of non-Abelian quasiparticles remains an outstanding experimental problem in the $\nu = \frac{5}{2}$ fractional quantum Hall (FQH) state. The presence of non-Abelian statistics would lead to additional low energy states in the system, and hence an additional low-temperature entropy. One approach to test for non-Abelian quasiparticle statistics uses thermodynamic measurements to detect this entropy contribution [1,2]. We present a microscopic model for quasiparticles in the $\nu = \frac{5}{2}$ FQH state with a disorder potential that fluctuates on the order of several magnetic lengths, and attempt to determine the feasibility of the experiments proposed in [1], based on local probe measurements of incompressibility [3].

[1] Cooper, N.R., Stern, A. PRL. **102**, 176807 (2009).

[2] Yang, K., Halperin, B.I. PRB **79**, 115317 (2009).

[3] Venkatachalam, V., Yacoby, A., Pfeiffer, L., West, K. Nature **469**, 185 (2011).

¹This work is partially supported by Microsoft Station Q, NSF, ITAMP, the Lawrence Golub Fellowship, NSERC, and FQRNT.

3:30PM T24.00006 Correlating scattering times with the strength of the $\nu=5/2$ fractional quantum Hall state, SUMIT MONDAL, Department of Physics, Purdue University, JOHN WATSON, Birck Nanotechnology Center and Department of Physics, Purdue University, GEOFFREY GARDNER, Birck Nanotechnology Center and School of Materials Engineering, Purdue University, NODAR SAMKHARADZE, GABOR CSATHY, Department of Physics, Purdue University, MICHAEL MANFRA, Department of Physics, Birck Nanotechnology Center and Schools of Materials and Electrical and Computer Engineering, Purdue University — There is widespread interest in the fractional quantum Hall effect at $\nu=5/2$. Theory predicts that the state at $\nu=5/2$ may possess non-Abelian braiding statistics. Experimental interrogation remains difficult due to the fragility of the excitation gaps requiring both high quality samples and examination at low temperatures. Mounting evidence suggests that the strength of the most fragile fractional quantum Hall states in the 2nd Landau level including $\nu=5/2$ are poorly correlated with the scattering time extracted from zero-field mobility measurements at higher temperatures. It is also unclear if the quantum scattering time derived from analysis of the low-field Shubnikov de-Haas oscillations provides any additional information relevant to prediction of the strengths of the observed fractional states. We report on a systematic attempt to correlate the T=0.3K behavior of the mobility lifetime, quantum scattering time, and an effective high field mobility lifetime evaluated at $\nu=5/2$ with the measured activation gap. We will present results from a number of heterostructure designs over a wide span of zero-field mobility ranging from $\sim 10 \times 10^6 \text{ cm}^2/\text{Vs}$ to greater than $20 \times 10^6 \text{ cm}^2/\text{Vs}$.

3:42PM T24.00007 “Perfect” Coulomb Drag in a Bilayer Quantum Hall System¹, D. NANDI, A.D.K. FINCK, J.P. EISENSTEIN, California Institute of Technology, L.N. PFEIFFER, K.W. WEST, Princeton University — We report Coulomb drag measurements in Corbino geometry which reveal that equal but oppositely directed electrical currents can freely propagate across the insulating bulk of the bilayer quantized Hall state at $\nu_T = 1$ even when the two 2D layers are electrically isolated and interlayer tunneling has been heavily suppressed by an in-plane magnetic field. This effect, which we dub “perfect” Coulomb drag, reflects the transport of charge neutral excitons across the bulk of the 2D system. The equal magnitude of the drive and drag currents is lost at high current and when either the temperature or effective separation between the two 2D layers is increased. In each of these cases, ordinary quasiparticle charge transport across the annulus has grown to dominate over exciton transport.

¹This work was supported by the NSF via grant DMR-1003080.

3:54PM T24.00008 Topological order, quasi-particle statistics and braiding from ground state entanglement, YI ZHANG, TARUN GROVER, University of California, Berkeley, ARI TURNER, University of Amsterdam, MASAKI OSHIKAWA, Institute for Solid State Physics, University of Tokyo, ASHVIN VISHWANATH, University of California, Berkeley — Topologically ordered phases are gapped states, defined by the properties of excitations when taken around each other. By calculating Topological Entanglement Entropy (TEE) of a disc shaped partition using a Monte Carlo technique, we establish the existence of topological order in $SU(2)$ symmetric gapped spin liquids and lattice Laughlin states obtained by the Gutzwiller projection technique. On the other hand, the TEE of partitioning the torus into two cylinders is generally different and depends on the chosen ground state. We demonstrate a method to extract the statistics and braiding of excitations, given just the set of ground state wave-functions on a torus. Central to our scheme is the identification of groundstates with minimum entanglement entropy, which reflect the quasi-particle excitations. We demonstrate our method by extracting the modular S matrix of an $SU(2)$ symmetric chiral spin liquid, and prove that its quasi-particles obey semionic statistics. This method offers a route to a nearly complete determination of the topological order in several cases.

4:06PM T24.00009 Paired Quantum Hall States at Weak Coupling: Phenomenology¹, S.A. PARAMESWARAN, University of California, Berkeley, S.A. KIVELSON, Stanford University, S.L. SONDHIL, Princeton University, B.Z. SPIVAK, University of Washington — Paired quantum Hall states such as the Pfaffian exhibit a weak-coupling regime much like that of BCS superconductivity. In this regime their lowest energy excitations are neutral fermions – Bogoliubov quasiparticles constructed from the composite fermions – and not the charged vortices which generally govern the behavior of quantum Hall states. We discuss a rich set of phenomena which follow from this observation. At finite temperatures of order the pairing scale these include (i) an almost sharp phase transition (ii) a new finite-temperature length scale for the penetration of longitudinal electric fields, and (iii) the existence of a new collective excitation in paired QH states which is a cousin to the well known Artemenko-Volkov-Carlson-Goldman-Schmid-Schon mode in conventional superconductors. At lower temperatures, we find (i) a proximity effect between the paired states and their ancestor metals, which in turn mediates (ii) ‘Josephson’ couplings between paired QH droplets separated by metallic regions and leads to (iii) a distinctive response of such states to disorder; and finally, we also comment on (iv) an analog of Andreev reflection in these systems.

¹S.A.P. is supported by a Simons Postdoctoral Fellowship at UC Berkeley.

4:18PM T24.00010 From Luttinger liquid to non-Abelian quantum Hall states¹, JEFFREY C.Y. TEO, University of Illinois at Urbana-Champaign, C.L. KANE, University of Pennsylvania — We formulate a theory of non-Abelian fractional quantum Hall states by considering an array of coupled interacting one dimensional wires, each described by a Luttinger liquid theory. This coupled wire construction provides a solvable Hamiltonian formulated in terms of electronic degrees of freedom, and provides a direct route to characterizing the quasiparticles and edge states in terms of conformal field theory. It also leads to a simple interpretation of the coset construction of conformal field theory, which is a powerful method for describing non-Abelian states. The level- k Read-Rezayi state at filling $\nu = k/(2+qk)$ is constructed by an uneven but periodic magnetic field configuration that organizes the wires into bundles. Gapless degrees of freedom in each bundle are decomposed into conformal sectors, which acquire energy gaps independently by intra-bundle and time reversal breaking inter-bundle interactions.

¹NSF grant DMR-0906175

4:30PM T24.00011 A comparative study of the reentrant integer quantum Hall states in the second and third Landau levels, NIANPEI DENG, JOHN WATSON, MICHAEL MANFRA, GABOR CSATHY, Purdue University — In the two-dimensional electron gas competing electron-electron interactions and disorder effects give rise to many-body ground states such as the fractional quantum Hall and the reentrant integer quantum Hall states (RIQHS). The latter are not yet well understood, but they are believed to be Wigner crystal-like electron solids with one or more electrons at each lattice nodes. We have recently shown that for the RIQHS in the second Landau level one can extract their onset temperature from the temperature-dependent magnetoresistance. We report similar studies of the RIQHS in the third Landau level. To our surprise, the onset temperatures of the RIQHSs in the third Landau level are about a factor of 3 larger than those in the second Landau level. This result clearly shows that the RIQHSs in the second and third Landau level have vastly different cohesion energies and may indicate different internal symmetries for these states. This work was supported by the DOE grant DE-SC0006671.

4:42PM T24.00012 Pomeranchuk Instability driven by Coulomb interaction in half-filled Landau levels, JUNPING SHAO, Cornell University, EDWARD REZAYI, Cal State LA, EUN-AH KIM, Cornell University — We study the Coulomb interaction driven Pomeranchuk instability as a mechanism for observed electronic nematic phases at high Landau levels. Such a mechanism will be signaled by the instability of the Fermi surface to quadrupolar deformations: $F_2 < -1$, where F_2 is the Fermi liquid parameter for the angular momentum $L = 2$ channel. We compare the Fermi Liquid parameters for the lowest three half-filled Landau levels ($\nu = 1/2, 5/2, 9/2$). We calculate the Fermi liquid parameters by evaluating energies of eight independent particle-hole pair excitation configurations using a quantum Monte Carlo algorithm through correlated sampling. We used composite fermion many-body wave functions for 37 electrons on a toroidal geometry that are interacting through the Coulomb potential. We find F_2 to become increasingly negative as we go to higher Landau levels. This is consistent with experimental observations.

4:54PM T24.00013 Bulk-edge correspondence and entanglement spectra of quantum Hall trial wave functions, JEROME DUBAIL, NICHOLAS READ, Yale University, EDWARD REZAYI, California State University — We construct edge states wave functions for quantum Hall trial states built out of conformal blocks (e.g. Laughlin, Moore-Read or Read-Rezayi wave functions). We then compute the overlaps between these edge states in the thermodynamic limit. The result is that the Hilbert space of the edge theory is isomorphic to the one of the conformal field theory (CFT) which defines the quantum Hall state. This is a microscopic derivation of the bulk/edge correspondence for trial states given by conformal blocks. Our result definitely rules out the use of non-unitary theories for the construction of quantum Hall states. We obtain this result by analysing the quantum Hall droplet in the thermodynamic limit, under the assumption that all correlations are short-range inside the droplet. We argue that one is then left with a CFT in the domain outside the droplet, with a perturbed conformal boundary condition along the edge. We show that the entanglement spectra of these states can be tackled analytically with the same techniques.

5:06PM T24.00014 Finite-size studies of the $\nu = 5/2$ quantum Hall state in wide quantum wells: the effect of subband mixing and breaking of particle-hole symmetry¹, Z. PAPIĆ, F.D.M. HALDANE, Princeton University, E.H. REZAYI, California State University, Los Angeles — A number of theoretical studies have argued that the quantized plateau at half filling of the second Landau level is described by the Pfaffian wavefunction of Moore and Read, or by its particle-hole conjugate, the anti-Pfaffian. The two wavefunctions are difficult to compare in finite-size systems due to their different shifts in the spherical geometry, or because of their high mutual overlap on the torus. Here we propose a way to circumvent these problems by envisioning systems with periodic boundary conditions, for which the Pfaffian and anti-Pfaffian become orthogonal to each other due to their different symmetry properties under discrete rotations. Furthermore, we show that periodic boundary conditions can be used to study the Moore-Read ground state, as well as the collective excitation spectrum, in finite systems in a “quartered” Brillouin zone scheme. To demonstrate the utility of this method, we provide a realistic, two-component model of a wide quantum well that can unambiguously distinguish between the Pfaffian and anti-Pfaffian state in finite-sized systems. These results describe the recent experiments that probed the stability of the $\nu = 5/2$ state by tuning the mixing between electronic subbands and Landau levels in a wide quantum well.

¹This work was supported by DOE grant DE-SC0002140.

5:18PM T24.00015 Quantitative analysis of the disorder broadening and the intrinsic gap for the $\nu=5/2$ fractional quantum Hall state, NODAR SAMKHARADZE, JOHN WATSON, GEOFF GARDNER, MICHAEL MANFRA, Purdue University, LOREN PFEIFFER, KEN WEST, Princeton University, GABOR CSATHY, Purdue University — We analyze several different methods of extracting intrinsic gaps of fractional quantum Hall states (FQHS) of the second Landau level from experimental data. Because of the discrepancy between these methods, we introduce a new way of estimating the disorder broadening in the second Landau level based on scaling of the gaps of the major odd denominator states. The results of our technique are in good agreement with a previously used method utilizing only the gaps of the even denominator states. We successfully apply this technique to several samples of high quality and find an excellent agreement between the estimated intrinsic gap and results of numerical simulations. We also report, for the first time, the dependence of the intrinsic gap of $\nu=5/2$ FQHS on Landau level mixing. This work was supported by the NSF grant DMR- 0907172.

5:30PM T24.00016 Quantum Topology of Lattice Dislocations in Fractional Chern Insulators, MAISSAM BARKESHLI, XIAOLIANG QI, Stanford University — An exciting prospect in condensed matter physics is the possibility of realizing fractional quantum Hall (FQH) states in simple lattice models without a large external magnetic field. Here we find a remarkable consequence of the interplay between the lattice translation symmetry and topological properties of these fractional Chern insulators. When the partially filled flat band has a Chern number N , it can be mapped to an N -layer quantum Hall system. We find that lattice dislocations can act as wormholes connecting the different layers and effectively change the topology of the space. Lattice dislocations become defects with non-trivial quantum dimension, topological degeneracy, and non-Abelian statistics, even when the FQH state being realized is a conventional Abelian FQH state.

Wednesday, February 29, 2012 2:30PM - 5:30PM –
Session T25 DCOMP DCMP: High Pressure: Theory 257A

2:30PM T25.00001 Nanoshells as a high-pressure gauge, JACQUES TEMPERE, NICK VAN DEN BROECK, KATRIJN PUTTENEERS, Universiteit Antwerpen, ISAAC SILVERA, Harvard University — Nanoshells, consisting of multiple spherical layers, have an extensive list of applications, usually performing the function of a probe. We add a new application to this list in the form of a high-pressure gauge in a Diamond Anvil Cell (DAC). In a DAC, where high pressures are reached by pressing two diamonds together, existing gauges fail at higher pressures because of calibration difficulties and obscuring effects in the diamonds. The nanoshell gauge does not face this issue since its optical spectrum can be engineered by altering the thickness of its layers. Furthermore their properties are measured by broad band optical transmission spectroscopy leading to a very large signal-to-noise ratio even in the multi-megabar pressure regime where ruby measurements become challenging. Theoretical calculations based on the Maxwell equations in a spherical geometry combined with the Vinet equation of state show that a three-layer geometry ($\text{SiO}_2\text{-Au-SiO}_2$) indeed has a measurable pressure-dependent optical response desirable for gauges.

2:42PM T25.00002 Pressure-induced phase transitions and superconductivity in platinum hydride¹, CHAO ZHANG, Beijing Computational Science Research Center, XIAOJIA CHEN, Department of Physics, South China University of Technology, HAIQING LIN, Beijing Computational Science Research Center — The transition metal hydrides have attracted much attention from the scientific community due to their promising properties from both fundamental and practical points of view. Here we present our recent work about platinum hydride under pressure. Structural phase transitions and superconducting properties of platinum hydride under pressure are explored through the first-principles calculations based on the density functional theory. Three new low-pressure phases (Pm-3m, Cmmm, and P4/nmm) are predicted, and all of them are metallic and stable relative to decomposed cases. Two high-pressure phases are close-packed structure with hydrogen atoms occupying the octahedral interstices. The superconducting critical temperature of two high-pressure phases correlates with the electron-phonon coupling. The presence of soft modes induced by Kohn anomalies and the hybridization between H and Pt atoms result in the strong electron-phonon coupling. Our results have great implications for other transition metal hydrides under pressure.

¹This work was supported by the HKRGC (402108) and NSFC (10874046).

2:54PM T25.00003 ABSTRACT MOVED TO Y26.00015 —

3:06PM T25.00004 The hard-disk melting transition, ETIENNE BERNARD, Condensed Matter Theory, Massachusetts Institute of Technology, WERNER KRAUTH, Laboratoire de Physique Statistique, Ecole Normale Supérieure, France — Melting in two spatial dimensions, as realized in thin films or at interfaces, represents one of the most fascinating phase transitions in nature, but it remains poorly understood. Even for the fundamental hard-disk model, the melting mechanism has not been agreed upon after 50 years of studies. A recent Monte Carlo algorithm [1] allows us to thermalize systems large enough to access the thermodynamic regime. I will show that melting in hard disks proceeds in two steps with a liquid phase, a hexatic phase, and a solid. The hexatic-solid transition is continuous while, surprisingly, the liquid-hexatic transition is of first order [2]. This melting scenario solves one of the fundamental statistical-physics models, which is at the root of a large body of theoretical, computational, and experimental research. 1. Bernard, E. P.; Krauth, W. & Wilson, D. B. *Phys. Rev. E*, **2009**, 80, 056704 2. Bernard, E. P. & Krauth, W. *Phys. Rev. Lett.*, **2011**, 107, 155704

3:18PM T25.00005 Electric Field Induced Phase Transitions, MARCO NARDONE, Bowling Green State University, Bowling Green, Ohio, VICTOR KARPOV, University of Toledo, Toledo, Ohio — A novel theory of phase transitions that are driven by strong, symmetry-breaking electric fields is presented. The underlying mechanism is based on the formation of needle-shaped, metallic embryos that acquire strong dipole moments in the applied field. It is shown that the electrostatic contribution to the free energy can be so significant that it dominates the nucleation process and elongated metallic particles can form even in cases where they would be otherwise unstable in the bulk. As such, the theory predicts that any insulator will eventually form metallic inclusions when immersed in a sufficient electric field. Materials can thus be synthesized by the controlled application of a dc or laser field. In this work, the general mechanism is described and closed form expressions are presented for the field-dependent nucleation barrier and the effective field range as functions of material parameters. Overall, the theory presents a new parameter space to explore phase transitions and opens the venue of Field Induced Materials Synthesis (FIMS). As a provocative example, the potential for FIMS of metallic hydrogen at standard pressure is discussed; the effective field range is estimated to be $10^7 < E \ll 10^9$ V/cm (laser intensity $10^{12} < I \ll 10^{16}$ W/cm²).

3:30PM T25.00006 Consistent first-principles pressure scales for diffraction experiments under extreme conditions, ALBERTO OTERO-DE-LA-ROZA, School of Natural Sciences, University of California, Merced, 5200 North Lake Road, Merced, California 95343, USA, VICTOR LUNA CABAL, Departamento de Química Física y Analítica, Facultad de Química, Universidad de Oviedo, ES-33006 Oviedo, Spain — Diamond anvil cell (DAC) diffraction experiments are fundamental in geophysics and materials science to explore the behavior of solids under very high pressures and temperatures. A factor limiting the accuracy of DAC experiments is the lack of an accurate pressure scale for the calibration materials that extends to the ever-increasing pressure and temperature limits of the technique. In this communication, we address this problem by applying a newly developed technique that allows the calculation of accurate thermodynamic properties from first-principles calculations [Phys. Rev. B 84 (2011) 024109, 84 (2011) 184103]. Three elements are key in this method: i) the quasi-harmonic approximation (QHA) and the static energies and phonon frequencies obtained from an electronic structure calculation ii) the appropriate representation of the equation of state by using averages of strain polynomials and iii) the correction of the systematic errors caused by the exchange-correlation functional approximation. As a result, we propose accurate equations of state for typical pressure calibrants that can be used in the whole experimental range of pressures and temperatures. The internal consistency and the agreement with the ruby scale based on experimental data is examined.

3:42PM T25.00007 Low-temperature phases of dense hydrogen and deuterium by first-principles path-integral molecular dynamics, MARC TORRENT, GREGORY GENESTE, CEA, DAM, DIF, F-91297 Arpajon, France — The low-temperature phases of dense hydrogen and deuterium have been investigated using first-principles path-integral molecular dynamics, a technique that we have recently implemented in the ABINIT code and that allows to account for the quantum fluctuations of atomic nuclei. A massively parallelized scheme is applied to produce trajectories of several tens of thousands of steps using a 64-atom supercell and a Trotter number of 64. The so-called phases I, II and III are studied and compared to the structures proposed in the literature. The quantum fluctuations produce configurational disorder and are shown to systematically enhance the symmetry of the system: a continuous gain of symmetry in the angular density of probability of the molecules is found from classical particles to quantum D2 and finally to quantum H2. Particular emphasis is made on the “broken-symmetry” phase (phase II).

3:54PM T25.00008 Predictive equation of state method for heavy materials based on the Dirac equation and density functional theory, JOHN M. WILLIS, Los Alamos National Laboratory, ANN E. MATTSSON, Sandia National Laboratories — Density functional theory (DFT) provides a formally predictive base for equation of state properties. Available approximations to the exchange/correlation functional provide accurate predictions for many materials in the periodic table. For heavy materials however, DFT calculations, using available functionals, fail to provide quantitative predictions, and often fail to be even qualitative. This deficiency is due both to the lack of the appropriate confinement physics in the exchange/correlation functional and to approximations used to evaluate the underlying equations. In order to assess and develop accurate functionals, it is essential to eliminate all other sources of error. In this talk we describe an efficient first-principles electronic structure method based on the Dirac equation and compare the results obtained with this method with other methods generally used. Implications for high-pressure equation of state of relativistic materials are demonstrated in application to Ce and the light actinides. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

4:06PM T25.00009 Requirements for Predictive Density Functional Theory Methods for Heavy Materials Equation of State, ANN E. MATTSSON, Sandia National Laboratories, JOHN M. WILLIS, Los Alamos National Laboratory — The difficulties in experimentally determining the Equation of State of actinide and lanthanide materials has driven the development of many computational approaches with varying degree of empiricism and predictive power. While Density Functional Theory (DFT) based on the Schrödinger Equation (possibly with relativistic corrections including the scalar relativistic approach) combined with local and semi-local functionals has proven to be a successful and predictive approach for many materials, it is not giving enough accuracy, or even is a complete failure, for the actinides. To remedy this failure both an improved fundamental description based on the Dirac Equation (DE) and improved functionals are needed. Based on results obtained using the appropriate fundamental approach of DFT based on the DE we discuss the performance of available semi-local functionals, the requirements for improved functionals for actinide/lanthanide materials, and the similarities in how functionals behave in transition metal oxides. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

4:18PM T25.00010 ABSTRACT WITHDRAWN —

4:30PM T25.00011 High pressure/temperature equation of state of gold silver alloys¹, ZSOLT JENEI, MAGNUS J. LIPP, JAE-HYUN P. KLEPEIS, HYUNCHAE CYNN, WILLIAM J. EVANS, Lawrence Livermore National Laboratory, CHANGYONG PARK, HPCAT, Advanced Photon Source, Argonne National Laboratory — Gold-silver alloys crystallize in face centered cubic structures, like their constituent pure elements [McKeehan – Phys.Rev. 20, 424 (1922)]. The cell parameter of the alloys does not scale linearly with the ratio of Ag/Au. In this work we investigate the high-pressure/temperature behavior of gold-silver alloys with different Au/Ag ratios. Powder x-ray diffraction experiments performed at HPCAT/Advanced Photon Source confirm the stability of the alloy's fcc structure to pressures/temperatures exceeding 100 GPa/1000 K. We will present isothermal EOS of the alloys from ambient temperature up to 1000 K, discuss the thermal expansion and its variation with pressure.

¹This work performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344. HPCAT use is supported by DOE-BES, DOE-NNSA, NSF, and the W.M. Keck Foundation. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.

4:42PM T25.00012 Persistence of Covalent Bonding in Liquid Silicon Probed by Inelastic X-ray Scattering, JUNPEI OKADA, Japan Aerospace Exploration Agency (ISAS/JAXA), P. SIT, Princeton U., Y.J. WANG, B. BARBIELLINI, Northeastern U., Y. WATANABE, U. Tokyo (JAPAN), A. BANSIL, Northeastern U., Y. SAKURAI, JASRI/SPRing-8 (JAPAN), M. ITOU, JASRI/SPRing-8, T. ISHIKAWA, ISAS/JAXA, K. KIMURA, U. Tokyo, P. PARADIS, ISAS/JAXA, S. NANAŌ, U. Tokyo — Metallic liquid silicon at 1787K is investigated using x-ray Compton scattering. An excellent agreement is found between the measurements and the corresponding Car-Parrinello molecular dynamics simulations. Our results show persistence of covalent bonding in liquid silicon and provide support for the occurrence of theoretically predicted liquid-liquid phase transition in supercooled liquid states. The population of covalent bond pairs in liquid silicon is estimated to be 17% via a maximally-localized Wannier function analysis. Compton scattering is shown to be a sensitive probe of bonding effects in the liquid state.

4:54PM T25.00013 Effects of the Structure of the Confinement Matrix on Liquid-Liquid Phase Transition and Density Anomaly, ELENA STREKALOVA, JIAYUAN LUO, GENE STANLEY, Boston University, GIAN-CARLO FRANZESE, Universitat de Barcelona, SERGEY BULDYREV, Yeshiva University — We investigate using molecular dynamics the effect of geometrical order in nanoconfinement of liquids with water-like anomalies that display liquid-liquid coexistence at low pressure and low temperature. Our studies using both a ramp and a shoulder interaction potentials show that regularly structured confinement matrices preserve the anomalies, while the phase diagram is shifted to lower temperatures, higher pressures and higher densities with respect to bulk. On the contrary, if the confinement matrices have no geometrical order, we find a drastically different phase diagram: the liquid-liquid coexistence region shrinks significantly and the anomalies are washed out. To understand this effect we calculate the changes in the system at the microscopic level. In the vicinity of the confining nanoparticles we observe that the liquid has a dramatic increase of density that we interpret as an entropic effect. We explain the macroscopic effect of confinement as a consequence of the amount of disorder that is introduced through the configuration of the confining nanoparticles.

5:06PM T25.00014 First-principles calculations for pressure-induced transition of Sr₂CuO₃, MITSURU KODERA, TAMIO OGUCHI, ISIR, Osaka University — One-dimensional cuprate, Sr₂CuO₃ has attracted much attention from the theoretical and material research. Recently, it is found that Sr₂CuO₃ exhibits the pressure-induced structural transition with the space group change. In this work, we perform the first-principles calculations in order to investigate the mechanism for the pressure-induced structural transition of Sr₂CuO₃. The calculation results are in good accordance with the experimental ones. The structural transition of Sr₂CuO₃ are related with the ionic interaction between strontium and oxygen atoms. We also discuss the electronic and magnetic structure of Sr₂CuO₃.

5:18PM T25.00015 Magnetic Phase Transition in Rare Earth Metal Holmium at Low Temperatures and High Pressures, SARAH THOMAS, WALTER UHOYA, LOWELL WENGER, YOGESH VOHRA, University of Alabama at Birmingham — The heavy rare earth metal Holmium has been studied under high pressures and low temperatures using a designer diamond anvil cell and neutron diffraction using a Paris-Edinburgh Cell at the Spallation Neutrons and Pressure (SNAP) Diffractometer. The electrical resistance measurement using designer diamond shows a change in slope at the Neel temperature as the temperature is lowered at high pressures. At atmospheric pressure TN=120 K and decreases with a slope of -4.7 K/GPa as pressure is increased, until reaching 9 GPa, at which pressure the magnetic ordering is lost. This correlates to the pressure at which there is a structural change from an hcp phase to an α -Sm structure. Neutron diffraction measurements made above and below the Neel temperature at increasing pressures show the reversibility of the change between the paramagnetic and antiferromagnetic states. The parameters of the low temperature incommensurate magnetic phase will be reported at various pressures.

Wednesday, February 29, 2012 2:30PM - 5:30PM –

Session T26 DCOMP: Focus Session: Computational Frontiers in Quantum Spin Systems II

257B

2:30PM T26.00001 Cubic Interactions and Quantum Criticality in Dimerized Antiferromagnets, S. WESSEL, RWTH Aachen University, Germany, L. FRITZ, Universitaet zu Koeln, Germany, R.L. DORETTO, Universidade Estadual Paulista, Brazil, S. WENZEL, EPFL, Switzerland, S. BURDIN, Universite de Bordeaux, France, M. VOJTA, TU Dresden, Germany — Dimerized quantum antiferromagnets can be driven through a quantum phase transition from a dimerized phase into a magnetically ordered state upon tuning the exchange parameters. In recent years, the critical properties in such dimerized antiferromagnets were examined in detail, based on large-scale quantum Monte Carlo simulations, which reported deviations from O(3) universality for specific two-dimensional geometries, in particular for the staggered-dimer antiferromagnet. Symmetry arguments and microscopic calculations exhibit that a nontrivial cubic term arises in the relevant order-parameter quantum field theory, related to three-particle interactions among the triplet excitations within the paramagnetic phase of this model. The consequences of such cubic terms are explored using a combination of analytical and numerical methods. Complemented by finite-temperature quantum Monte Carlo simulations, these results lead to the conclusion that critical exponents in dimerized antiferromagnets are identical to that of the standard O(3) universality class, but with anomalously large corrections to scaling for these specific dimerization geometries.

2:42PM T26.00002 Computational Studies of $T = 0$ Neel-Valence bond solid transitions in two dimensional quantum antiferromagnets, KEDAR DAMLE, Tata Institute, FABIEN ALET, SUMIRAN PUJARI, Univ. Paul Sabatier, Toulouse, ARGHA BANERJEE, Institute for Mathematical Sciences, India, ARUN PARAMAKANTI, University of Toronto — We use Quantum Monte Carlo techniques to study a direct quantum phase transition in two dimensional quantum antiferromagnets between a collinear Neel ordered state and a valence bond solid ordered singlet state. We contrast the strongly first order behavior of the transition in cases where the valence bond solid order is of a “staggered” type with the deconfined critical behavior seen in cases where the valence-bond solid order is of a columnar type. In the deconfined case, we find evidence for weak, apparently logarithmic violations of scaling. [References: preprint; Phys. Rev. B 83, 235111 (2011); Phys. Rev. B 83, 134419 (2011); Phys. Rev. B 82, 155139 (2010)]

2:54PM T26.00003 Velocities of Goldstone and critical modes in SU(2) symmetric quantum spin systems¹, ARNAB SEN, Max-Planck-Institute, Dresden, ANDERS SANDVIK, Boston University — The low-energy excitations of many interesting quantum spin systems are gapless and linearly dispersing. Examples include Goldstone modes in the Néel phase and critical modes at a $z=1$ quantum critical point. We calculate the velocities of such modes for a variety of SU(2) symmetric $S=1/2$ systems using quantum Monte Carlo (QMC) methods. We use two complementary approaches: a) The lowest triplet gap from the singlet ground state is calculated using $T=0$ projector QMC by measuring appropriate imaginary-time correlation functions. The velocity is obtained from extracted momentum dependent gaps. b) We use a method based on tuning the system to the cubic regime by varying its temperature to equate the variance of spatial and temporal winding numbers, which was recently used by Jiang [1] for a system with Goldstone modes. We find that this method can also be applied to a $z=1$ critical point (the critical point of an $S=1/2$ Heisenberg bilayer) and to the 1D Heisenberg spin chain, where there are no Goldstone modes. We also extract the velocity of the critical modes of the J-Q model. It agrees very well with the velocity obtained from a phenomenological approach [2] based on a spinon gas picture. [1] Jiang, Phys. Rev B 83, 024419 (2011) [2] Sandvik et al., Phys. Rev. Lett. 106, 207203 (2011)

¹Funding from NSF DMR-1104708

3:06PM T26.00004 Unconventional versus conventional destruction of square lattice SU(N) magnetism¹, RIBHU KAUL, University of Kentucky — Recently we have found SU(N) symmetric square lattice spin models of quantum antiferromagnets, which have quantum phase transitions between magnetic and non-magnetic phases for arbitrary N , and which are nonetheless free of the “sign-problem” of quantum Monte Carlo. The absence of the notorious sign-problem allows detailed unbiased numerical simulations of two-dimensional magnetic quantum phase transitions on lattices containing in excess of 10^4 spins. Depending on the absence or presence of uncompensated Berry phases in our microscopic models we find evidence for both conventional first order phase transitions and unconventional continuous quantum phase transitions at which both Néel- and valence bond solid-order (VBS) are *simultaneously* quantum critical. A detailed quantitative study of the Néel and VBS scaling dimensions as a function of N provides compelling evidence that the long-wavelength description of these quantum critical points may be found in the CP^{N-1} gauge theory, as predicted by the deconfined quantum criticality scenario. R. K. Kaul and A. W. Sandvik, <http://arxiv.org/abs/1110.4130>. R. K. Kaul (forthcoming).

¹Supported in part by NSF Grant No. DMR-1056536

3:42PM T26.00005 Neel to valence-bond solid transitions in generalized amplitude-product states with correlated weights¹, YU-CHENG LIN, Graduate Institute of Applied Physics, National Chengchi University, Taiwan, JIE LOU, Institute for Solid State Physics, ISSP, University of Tokyo, Japan, YING TANG, ANDERS SANDVIK, Department of Physics, Boston University, USA — An amplitude-product state is a superposition of valence-bond states with the expansion coefficients being products of individual bond amplitudes that depend only on the bond shape. In two dimensions, these states have Neel order or are spin liquids, but they never have any valence-bond solid order. We construct generalized amplitude-product states on the square lattice which include correlated weights for short-range bonds. Using these states, we explore phase transitions between Neel phase, valence-bond solid phases, and spin liquid. We also study the Neel-VBS transition in the standard amplitude-product states in one dimension.

¹NSC (Taiwan): 98-2112-M-004-002-MY3, NSF: DMR- 0803510

3:54PM T26.00006 Emergent U(1) Symmetry in Square Lattice Quantum Dimer Models, SYLVAIN CAPPONI, DAVID SCHWANDT, Laboratoire de Physique Théorique, CNRS & Université de Toulouse, F-31062 Toulouse, France, SERGEI ISAKOV, Institut für Theoretische Physik, ETH Zürich, CH-8093 Zürich, Switzerland, RODERICH MOESSNER, Max Planck Institut für komplexe Systeme, Nöthnitzer Straße 38, D-01187 Dresden, Germany, ANDREAS LÄUCHLI, Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck, Austria — We report an exact diagonalization study of Rokhsar-Kivelson quantum dimer models on square lattice. Using a finite-size scaling analysis of excited energy levels, we are able to identify a regime of length scales where the quantum dimer model exhibits a $U(1)$ symmetry. Dimer order parameter histograms confirm this remarkable symmetry. Beyond this crossover length, columnar dimer order emerges at least for $v/t \lesssim 0.6$. Our interpretation is supplemented with field-theory analysis as well as large-scale quantum Monte-Carlo simulations.

4:06PM T26.00007 A round-trip from spin to quantum dimer models, MATTHIEU MAMBRINI, FABIEN ALET, CNRS, Université de Toulouse, F-31062 France, SYLVAIN CAPPONI, Université de Toulouse, F-31062 France — Short-range valence bonds wave-functions are often used as a paradigm for non-magnetic states (such as spin liquids or valence bond crystals). Recently, two local $S=1/2$ spin Hamiltonians which admits nearest neighbor valence bond wave-function(s) as ground-state(s) on the square lattice have been proposed by Cano and Fendley [Phys. Rev. Lett. **105**, 067205 (2010)]. We present a numerical study, by means of exact diagonalizations and diagonalizations restricted in the subspace spanned by nearest neighbor valence bond states, of the ground state and excitations of these models. We show that it corresponds to a new type of spin liquid state, with gapped spin but gapless non-magnetic excitations. Mixing the two models is shown to stabilize valence bond crystal ground states that are very reminiscent of the phases present in the Rokhsar-Kivelson quantum dimer model phase diagram. Using a generic mapping scheme [Phys. Rev. B **81**, 214413 (2010)] of spin hamiltonians to generalized quantum dimer models we show how this correspondence between the phase diagram of a local $S=1/2$ spin hamiltonian and the Rokhsar-Kivelson quantum dimer model can be understood.

4:18PM T26.00008 Phase Diagram of a Frustrated Quantum Antiferromagnet on the Honeycomb Lattice: Magnetic Order versus Valence-Bond Crystal Formation, DAVID SCHWANDT, FABRICIO ALBUQUERQUE, Laboratoire de Physique Théorique, Université de Toulouse, UPS (IRSAMC), CNRS, F-31062 Toulouse, France, BALAZS HETÉNYI, Department of Physics, Bilkent University, Ankara, Turkey, SYLVAIN CAPPONI, MATTHIEU MAMBRINI, Laboratoire de Physique Théorique, Université de Toulouse, UPS (IRSAMC), CNRS, F-31062 Toulouse, France, ANDREAS LÄUCHLI, Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck, Austria — We present a comprehensive computational study of the phase diagram of the frustrated $S = 1/2$ Heisenberg antiferromagnet on the honeycomb lattice, with second-nearest (J_2) and third-neighbor (J_3) couplings. Using a combination of exact diagonalizations of the original spin model, of the Hamiltonian projected into the nearest neighbor short range valence bond basis, and of an effective quantum dimer model, we determine the boundaries of several magnetically ordered phases in the region $J_2, J_3 \in [0, 1]$, and find a sizable magnetically disordered region in between. We characterize part of this magnetically disordered phase as a *plaquette* valence bond crystal phase.

4:30PM T26.00009 Plaquette order and deconfined quantum critical point in the spin-1 bilinear-biquadratic Heisenberg model on the honeycomb lattice¹, HUI-HAI ZHAO, Institute of Physics, Chinese Academy of Sciences, Beijing, CENKE XU, Department of Physics, University of California, Santa Barbara, Q.N. CHEN, Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing, Z.C. WEI, M.P. QIN, Institute of Physics, Chinese Academy of Sciences, Beijing, G.M. ZHANG, State Key Laboratory of Low-Dimensional Quantum Physics and Department of Physics, Tsinghua University, Beijing, T. XIANG, Institute of Physics and Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing — We have precisely determined the ground state phase diagram of the quantum spin-1 bilinear-biquadratic Heisenberg model on the honeycomb lattice using the tensor renormalization group method. We find that the ferromagnetic, ferroquadrupolar, and a large part of the antiferromagnetic phases are stable against quantum fluctuations. However, around the phase where the ground state is antiferro-quadrupolar ordered in the classical limit, quantum fluctuations suppress completely all magnetic orders, leading to a plaquette order phase which breaks the lattice symmetry but preserves the spin $SU(2)$ symmetry. The quantum phase transition between the antiferromagnetic phase and the plaquette phase is found to be a direct second order transition, being the first candidate of the deconfined quantum critical point for the spin-1 quantum systems.

¹This work is supported by NSFC and the grants of National Program for Basic Research of MOST of China. Cenke Xu is supported by the Sloan Research Fellowship.

4:42PM T26.00010 Three-sublattice order in the $SU(3)$ Heisenberg model on the square and triangular lattice, BELA BAUER, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland and Station Q, Microsoft Research, Santa Barbara, CA 93106, PHILIPPE CORBOZ, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland and Institut de theorie des phenomenes physiques, Ecole Polytechnique Federale de Lausanne, ANDREAS M. LAEUCHLI, Institut fuer Theoretische Physik, Universitaet Innsbruck, Austria and Max-Planck-Institut fuer Physik komplexer Systeme, Dresden, Germany, LAURA MESSIO, Institut de theorie des phenomenes physiques, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland, KARLO PENC, Research Institute for Solid State Physics and Optics, H-1525 Budapest, P.O. Box 49, Hungary, MATTHIAS TROYER, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland, FREDERIC MILA, Institut de theorie des phenomenes physiques, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland — We present a numerical study of the $SU(3)$ Heisenberg model on the triangular and square lattice by means of the density-matrix renormalization group (DMRG) and infinite projected entangled-pair states (iPEPS). For the triangular lattice we confirm that the ground state has a three-sublattice order with a finite ordered moment which is compatible with the result from linear flavor wave theory (LFWT). The same type of order has recently been predicted also for the square lattice. However, for this case the ordered moment cannot be computed with LFWT due to divergent fluctuations. Our numerical study clearly supports this three-sublattice order, with an ordered moment of $m=0.2-0.4$ in the thermodynamic limit.

4:54PM T26.00011 Zero- vs. finite-field transition in $S=1$ Heisenberg antiferromagnet with single-ion anisotropy, PINAKI SENGUPTA, IAN YAP, ZHIFENG ZHANG, Nanyang Technological University, Singapore — We use large scale quantum Monte Carlo simulation on finite size lattices to study the ground state and finite temperature transitions in a $S = 1$ Heisenberg antiferromagnet (HAFM) with single-ion anisotropy (D) in the presence of an external magnetic field (h_z). The ground state phase diagram (in the $h_z - D$ plane) is characterized by a quantum paramagnetic phase (QPM) at large D and small h_z and an XY-AFM phase at small D and/or large h_z separated by a continuous transition. We show that the QPM to XY-AFM transition belongs to the XY universality class at $h_z = 0$ (driven by varying D) whereas it belongs to the BEC universality class at $h_z \neq 0$ (driven by either varying D at constant h_z or varying h_z at constant D). This has important implication in the behavior of the specific heat at the transition point which can be verified experimentally. Finally, we discuss the experimental relevance of our results in the case of DTN.

5:06PM T26.00012 Ferronematic order in a spin-1 Heisenberg antiferromagnet, KEOLA WIERSCHEM, PINAKI SENGUPTA, Nanyang Technological University, Singapore, CRISTIAN BATISTA, Theoretical Division, Los Alamos National Lab — We study the field-induced ground-state phase transition of a spin-1 Heisenberg antiferromagnet with large easy-axis single-ion anisotropy D . Direct spin-wave treatment predicts a single first-order phase transition from an antiferromagnetic Néel phase at low magnetic fields to a fully polarized state at high magnetic fields. Mean field arguments, based on an effective spin-1/2 model that is exact in the $D \rightarrow \infty$ limit, show that this transition is preempted by an intermediate phase with double-spin-flip correlations. We call this phase the *ferronematic* phase, as the effective spin model for large (negative) D is a spin-1/2 XXZ model with *ferromagnetic* transverse exchange. Using exact diagonalization and quantum Monte Carlo, we confirm the presence of the ferronematic phase. Long range order is observed in the equal-time Green's function $\langle S_i^+ S_i^+ S_j^- S_j^- + H.c. \rangle$, which is the correlation function for ferronematic order. We also show the rapid convergence to the effective model for large values of D .

5:18PM T26.00013 Monte Carlo study of a $U(1) \times U(1)$ system with π -statistical interaction, SCOTT GERAEDTS, OLEXEI MOTRUNICH, California Institute of Technology — We study a $U(1) \times U(1)$ system with two species of loops with mutual π -statistics in (2+1) dimensions. We are able to reformulate the model in a way that can be studied by Monte Carlo and we determine the phase diagram. In addition to a phase with no loops, we find two phases with only one species of loop proliferated. The model has a self-dual line, a segment of which separates these two phases. Everywhere on the segment, we find the transition to be first-order, signifying that the two loop systems behave as immiscible fluids when they are both trying to condense. Moving further along the self-dual line, we find a phase where both loops proliferate, but they are only of even strength, and therefore avoid the statistical interactions. We study another model which does not have this phase, and also find first-order behavior on the self-dual segment.

**Wednesday, February 29, 2012 2:30PM - 5:30PM –
Session T28 FIAP: Semiconductors 258C**

2:30PM T28.00001 Interaction-driven versus disorder-driven transport in ultra-dilute GaAs two-dimensional hole systems¹, JIAN HUANG, Wayne State University, L.N. PFEIFFER, K.W. WEST, Princeton University — It is well-known that the insulating behavior in the two-dimensional metal-to-insulator transition demonstrates a finite temperature conduction via hopping. Recently, however, some very strongly interacting higher purity two-dimensional electron systems at temperatures $T \rightarrow 0$ demonstrate certain nonactivated insulating behaviors that are absent in more disordered systems. Through measuring in dark the T -dependence of the conductivity of ultra-high quality 2D holes with charge densities down to $7 \times 10^8 \text{ cm}^{-2}$, an approximate power-law behavior is identified. Moreover, for the lowest charge densities, the exponent exhibits a linearly decreasing density-dependence which suggests an interaction-driven nature. Such an electron state is fragile to even a slight increase of disorder which causes a crossover from nonactivated to activated conduction. The non-activated conduction may well be an universal interaction-driven signature of an electron state of strongly correlated (semiquantum) liquid.

¹Supported by NSF

2:42PM T28.00002 Abruptness improvement of the interfaces of AlGa_N/Ga_N superlattice by cancelling asymmetric diffusion, DUANJUN CAI, XIAOHONG CHEN, NA LIN, FUCHUN XU, HANGYANG CHEN, Department of Physics, Xiamen University, Xiamen, 361005, China, SHANSHAN CHEN, University of Texas at Austin — Interface abruptness has been an important issue in the construction of quantum wells as active layer in optoelectronic devices, which is extremely crucial in achieving stronger quantum confinement and consequently higher emission efficiency. The interfacial sharpness is highly associated with the crystal structure as well as the elemental transition. However, few studies have been done focusing on the elemental diffusion effect at the interface. In this work, the accurate determination was approached to the elemental inter-diffusion depth across the Ga_N/Al_{0.5}Ga_{0.5}N interfaces by using transmission electron microscopy, Auger electron microscopy, and X-ray diffraction. The Ga_N/Al_{0.5}Ga_{0.5}N superlattice was grown by metalorganic chemical vapor deposition (MOCVD) at high growth temperature (1070 °C). The results showed that the Al diffusion at the upper and lower interfaces of Al_{0.5}Ga_{0.5}N barrier appears an asymmetric behavior, which is 0.62 and 0.99 nm, respectively. Such will lead to the gradient interfacial region and asymmetric quantum well, affecting the carrier quantum confinement. To improve the abruptness of the interface and to modify the asymmetric diffusion, self-compensation pair technique was proposed and introduced to the growth of the lower Al_{0.5}Ga_{0.5}N/Ga_N interface, blocking the Al downward diffusion. First-principles simulations also showed that the structural relaxation at the strained heterointerface influences the electronic structure as well as elemental diffusion.

2:54PM T28.00003 Local Structure of Amorphous GaN_{As} Alloys Across the Composition Range, ALEJANDRO LEVANDER, University of California, Berkeley, KIN YU, Lawrence Berkeley National Laboratory, SERGEI NOVIKOV, University of Nottingham, ZUZANNA LILIENTAL-WEBER, Lawrence Berkeley National Laboratory, OSCAR DUBON, University of California, Berkeley, TOM FOXON, University of Nottingham, JUNQIAO WU, University of California, Berkeley, WLADEK WALUKIEWICZ, Lawrence Berkeley National Laboratory — Typically only dilute (up to ~10%) highly mismatched alloys (HMAs) can be grown due to the large differences in atomic size and electronegativity of the host and the alloying elements. Recently, we overcame the miscibility gap of the Ga_{N_{1-x}As_x} system using low temperature molecular beam epitaxy (LT-MBE) and successfully synthesized alloys over a wide composition range. In the intermediate composition range ($0.10 < x < 0.75$) the resulting alloys are amorphous. To gain a better understanding of the amorphous structure, the local environment of the As and Ga atoms was investigated using extended x-ray absorption fine structure (EXAFS). The EXAFS analysis shows a high concentration of dangling bonds compared to the crystalline binary endpoint compounds of the alloy system. The disorder parameter was larger for amorphous films compared to crystalline references, but comparable with other amorphous semiconductors. By examining the Ga local environment, the dangling bond density and disorder associated with As-related and N-related bonds could be decoupled. The N-related bonds had a lower dangling bond density and lower disorder. The significant dangling bond density may help explain the difficulty of doping the material.

3:06PM T28.00004 Characterization of GaN grown on Si substrate with sputtering AlN buffer layer by molecular beam epitaxy¹, WEN-YUAN PANG, IKAI LO, Y.C. HSU, C.H. SHIH, C.H. HU, Y.C. WANG, Department of Physics, National Sun Yat-sen University, Kaohsiung, Taiwan, SEAN WU, Department of Electrical Engineering, Far East College, Tainan, Taiwan — This study reports the characterization of GaN grown on Si substrate with sputtering AlN buffer layer by plasma-assisted molecular beam epitaxy. Structural properties were measured by X-ray diffraction measurement and transmission electron microscopy. XRD spectrum showed the sputtering buffer layer which was mainly (100)_{AlN} and followed by the GaN epilayer which contained poly M-plane GaN and other structural planes such as (002)_{GaN} (c-plane), and (101)_{GaN}. In TEM analysis, we demonstrated GaN of c- and A-plane grains. The pure M-plane GaN was also found in the form of grain and the high-resolution images showed clear atomic arrangement. Besides, the diffraction pattern with multi M-plane GaN was attributed to several M-plane GaN crystals which were grown in different orientations on in-plane surface. In addition, optical properties measured by photoluminescence and cathodoluminescence measurement both showed two main peaks at 3.2 eV and 3.4 eV, indicated that zinc-blende and wurtzite structure exist in the GaN layer at the same time.

¹The project is supported by National Research Council of Taiwan (grant No. NRC 98-2112-M-110-003-MY3).

3:18PM T28.00005 Characterization of InGa_N/Ga_N Quantum Well grown on Ga_N microdisk using γ -LiAlO₂ substrate by Plasma-assisted Molecular Beam Epitaxy¹, YU-CHI HSU, IKAI LO, W. Y. PANG, C.H. SHIH, C.H. HU, Y.C. WANG, C.C. YANG, Y.C. LIN, S.T. YOU, Department of Physics, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan, MITCH M.C. CHOU, Department of Materials and Optoelectronic Science, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan — The InGa_N/Ga_N quantum wells grown on Ga_N microdisks by plasma-assisted molecular beam epitaxy (PAMBE) have been investigated. The optical properties and micro-structure of InGa_N/Ga_N quantum wells were studied by Cathodoluminescence (CL) and transmission electron microscope (TEM). According to the observation of high-resolution TEM, we obtained the high quality of InGa_N/Ga_N quantum wells grown on Ga_N micro-disk. The In-ratio (x) of In_xGa_{1-x}N is ~8% determined by the measurement of energy-dispersive X-ray spectroscopy (EDX). The optical gap of In_{0.08}Ga_{0.92}N was measured to be ~3eV determined by CL measurement, which is consistent with the calculation of bowing parameters and the measurement of EDX.

¹The project is supported by National Research Council of Taiwan (NRC 98-2112-M-110-003-MY3)

3:30PM T28.00006 Unraveling the Atomic Structure of GaN(0001) Pseudo-1×1: Surface-Electron-Gas Mediated Dimer Ordering¹, TIANJIAO CHEN, Ohio University Nanoscale and Quantum Phenomena Institute, NOBORU TAKEUCHI, Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, KANGKANG WANG, DANDA ARCHAYA, YINGHAO LIU, SAW-WAI HLA, ARTHUR SMITH, Ohio University Nanoscale and Quantum Phenomena Institute — Gallium nitride based light emitting devices have seen a steep rise of attention in recent years because of their potential in revolutionizing the current lighting industry. Of great importance in advancing the material technology is the understanding of the GaN(0001) surface, onto which most of the commercial devices are grown. We report a novel dimer-based model for Ga-rich GaN(0001), which exhibits an intriguing reconstruction known as the pseudo-1×1. To unravel its atomic structure, we have cooled the surface to cryogenic temperatures while monitoring the reconstruction by reflection high-energy electron diffraction and scanning tunneling microscopy. Upon cooling, the pseudo-1×1 phase transforms into a new phase consisting of buckled Ga-dimers on the surface. This observation then strongly suggests the existence of Ga dimers also at the room-temperature surface, although only partially ordered compared to the low temperature case. Combined with first-principles calculations, we propose a new model for the pseudo-1×1 consisting of dimers that are spaced ~1.9 nm (6a) apart along <1120> azimuths, while being randomly distributed along other directions. The mechanism of this partial ordering is identified to be through the surface electron gas residing within the bulk band-gap.

¹Authors gratefully acknowledge support from the U.S. DOE and the NSF.

3:42PM T28.00007 The electrical properties of epitaxial p-type ZnO films grown on GaAs (001), WEI-REIN LIU, Research Group, National Synchrotron Radiation Research Center, C.Y. LIN, B.H. LIN, S.T. HSU, Department of Photonics and Institute of Electro-Optical Engineering, National Chiao Tung University, F.S.-S. CHIEN, Department of Physics, Tunghai University, CHEN-SHIUNG CHANG, Department of Photonics and Institute of Electro-Optical Engineering, National Chiao Tung University, CHIA-HUNG HSU, Research Group, National Synchrotron Radiation Research Center, WEN-FENG HSIEH, Department of Photonics and Institute of Electro-Optical Engineering, National Chiao Tung University — Wurtzite ZnO epitaxial layers with both p-type and n-type characteristics are grown on n-type GaAs(001) substrates by pulsed laser deposition (PLD). The local electrical properties of the ZnO layers were investigated by electrostatic force microscope (EFM), Kelvin force microscopy (KFM), and conducting atomic force microscopy (CAFM). Local work function difference of ~125.5 meV was observed on p-type ZnO layer from KFM and EFM measurements due to the un-uniform diffusion of As atoms from the GaAs substrate upon thermal annealing. We also found the work function of p-type ZnO is larger than that of n-type ZnO layer, in which the difference varied from 368.4 to 493 meV. The rectifying junction under p-ZnO/n-GaAs configuration and Ohmic contact under metal probe (Ti)/p-ZnO configuration were both observed by CAFM.

3:54PM T28.00008 Mapping the band profile across the Gd₂O₃/GaAs(100) hetero-interface by using scanning tunneling microscopy, B.C. HUANG, Y.P. CHIU, M.C. SHIH, Department of Physics, National Sun Yat-Sen University, Kaohsiung, 80424, Taiwan, J.Y. SHEN, P. CHANG, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, 30013, Taiwan, C.S. CHANG, Institute of Physics, Academia Sinica, Taipei, 10617, Taiwan, M.L. HUANG, Department of Physics, National Tsing Hua University, Hsinchu, 30013, Taiwan, M.H. TSAI, Department of Physics, National Sun Yat-Sen University, Kaohsiung, 80424, Taiwan, M. HONG, Department of Physics and Graduate Institute of Applied Physics, National Taiwan University, Taipei, 10617, Taiwan, J. KWO¹, Center for Condensed Matter Sciences, National Taiwan University, Taipei, 10617, Taiwan — Direct measurements of atomic-scale electronic structure at nm-thick epitaxial Gd₂O₃ gate oxides on GaAs have been performed using cross-sectional scanning tunneling microscopy and spectroscopy. Both scanning tunneling spectroscopy and analysis of the local electronic states across the gate oxides suggest the Ga-O terminated hetero-interface. In addition, along with the theoretical modeling, the band offsets for both conduction and valence states are identified. A unique combination of STM and STS successfully provides direct information on the interfacial band profile and band offsets across the model high- κ /III-V system in the work.

¹Affiliation2:Department of Physics, National Tsing Hua University, Hsinchu, 30013, Taiwan

4:06PM T28.00009 Phase-dependence and manipulation of coherent oscillations of a single-electron wavefunction in a dynamic quantum dot, MATTHEW BENESH, ADAM THORN, MASAYA KATAOKA¹, MICHAEL ASTLEY, CHRIS FORD, CRISPIN BARNES, JONATHAN GRIFFITHS, GEB JONES, IAN FARRER, DAVE RITCHIE, University of Cambridge, UK — Surface acoustic waves (SAWs) in a GaAs heterostructure generate dynamic quantum dots, each capable of carrying a single electron through a gated potential landscape. At the SAW velocity (2800 m/s), the change in potential due to a 100nm surface gate will occur in a period of 40ps in the rest frame of the dot. This high-speed modulation of the potential, far beyond the experimental limit of fast gate-switching, allows for the observation of coherent single-electron dynamics. Previous work has shown that an abrupt shift in dot confinement will cause an electron to oscillate unitarily from side to side. This excitation was measured non-invasively via a tunnel barrier, and good agreement was found between measurements and simulations of the dot dynamics. We present here the results of further work in which we examine the coherence length and phase-dependence of the single-electron oscillations. Through the use of a time-dependent model we also study surface-gate arrangements which may be used to manipulate the electron dynamics mid-stream.

¹Now at NPL Teddington

4:18PM T28.00010 Equi-spin-splitting distribution near the minimum-spin-splitting surface under biaxial strains in bulk wurtzite materials, HSIU-FEN KAO, IKAI LO, JIH-CHEN CHIANG, C.L. WU, W.T. WANG, Department of Physics, Center for Nanoscience and Nanotechnology, National Sun Yat-sen University, Kaohsiung 80424, Taiwan, MENG-EN LEE, Department of Physics, National Kaohsiung Normal University, Yanchao, Kaohsiung 82444, Taiwan, CHUN-NAN CHEN, Department of Physics, Tamkang University, Tamsui, New Taipei City 25137, Taiwan, Y.C. HSU, Department of Physics, Center for Nanoscience and Nanotechnology, National Sun Yat-sen University, Kaohsiung 80424, Taiwan — The spin-splitting energies in biaxially strained bulk wurtzite materials are calculated using the linear combination of atomic orbital method, and the equi-spin-splitting distributions in k -space near the minimum-spin-splitting (MSS) surfaces are illustrated. These data are compared with those derived analytically using the two-band $\mathbf{k} \cdot \mathbf{Dp}$ (2KP) model. It is found the results from these two methods are in good agreement for small k . However, the ellipsoidal MSS surface under compressively biaxial strain predicted by the 2KP model does not exist, due to the data points are far from the Γ point in this case. As a result, from compressively to tensilely biaxial strain, only three types of shapes of the MSS surface exist in the wurtzite Brillouin zone; that is, a hyperboloid of two sheets, a hexagonal cone and a hyperboloid of one sheet.

4:30PM T28.00011 How Hydrogen Terminated Diamond Acquires a Negative Electron Affinity Surface, JONATHAN RAMEAU, JOHN SMEDLEY, ERIK MULLER, Brookhaven National Lab, TIM KIDD, University of Northern Iowa, PETER JOHNSON, Brookhaven National Lab — Electron emission from the negative electron affinity (NEA) surface of hydrogen terminated, boron doped diamond in the [100] orientation is investigated using angle resolved photoemission spectroscopy (ARPES). ARPES measurements using 16 eV synchrotron and 6 eV laser light are compared and found to show a catastrophic failure of the sudden approximation. While the high energy photoemission is found to yield little information regarding the NEA, low energy laser ARPES reveals for the first time that the NEA results from a novel Franck-Condon mechanism coupling electrons in the conduction band to the vacuum. The result opens the door to the development of a new class of NEA electron emitter based on this effect.

4:42PM T28.00012 Laser Phase Separation of Si Rich Oxides: The Role of Composition, EMEL SUNGUR OZEN, ATILLA AYDINLI, SINAN GUNDOGDU, Bilkent University, Department of Physics, Ankara, 06800 — Continuous-wave laser annealing of Si-rich oxide thin films with varying Si content were performed in order to obtain Si nanocrystals (Si_{nc}) embedded in silica. The composition, irradiation times and power densities were investigated as well as the role of hydrogen in phase separation. Si_{nc} in SiO_2 appear to be very promising for the realization of optical function as light emission or optical memory. Nanocrystalline Si finds also important utility in photovoltaics thanks to quantum confinement in the nanostructures offering a wider bandgap material which, in a tandem configuration, can allow a better use of the solar spectrum. Conventional techniques utilize high-temperature processing to obtain Si- SiO_2 phase separation. These processes are not compatible with mass production methods. An alternative approach capable of avoiding high temperature processing is the laser annealing of SiO_x films. The structural effect due to annealing were investigated by Raman and photoluminescence spectroscopy. It has been shown that the size and amount of Si_{nc} depends both on the oxygen content and on the laser power density. PECVD grown hydrogenated SiO_x films were compared with sputtered films without hydrogen to identify its role for the phase separation.

4:54PM T28.00013 A Novel Technique for Detecting Trace Residues of Contamination on GaAs Surfaces before MBE Growth¹, JERRY LEE, KEN WEST, KIRK BALDWIN, LOREN PFEIFFER, Princeton University — To prepare a GaAs substrate for molecular beam epitaxial (MBE) growth, the nominal ~ 3 nm native oxide is typically thermally desorbed in vacuum. To test the completeness of this desorption, we describe a technique, which combines MBE, thermal desorption, atomic force microscopy (AFM), reflection high-energy electron diffraction (RHEED), and secondary ion mass spectroscopy (SIMS), for detecting trace residues of contamination on (100) GaAs surfaces before MBE growth. At all desorption temperatures in the range 600 °C to 665 °C, our RHEED measurements show that the native oxide is largely desorbed within 2 min. However, the SIMS and AFM data indicate that a residue of sub-monolayer oxide invariably remains on the GaAs (100) surface, and tenaciously resists all further attempts at its removal by thermal desorption. Since thermal desorption of the native oxide has long been the standard technique before MBE growth, we suggest that all MBE growth of GaAs heterostructures has been through a partial monolayer of native oxide. We believe that this is the likely reason for the failure of high quality attempts at MBE growth of GaAs after lithographic patterning on a previously grown MBE structure.

¹Funded by the Gordon and Betty Moore Foundation and the NSF MRSEC Program through the Princeton Center for Complex Materials (DMR-0819860).

5:06PM T28.00014 High-performance substrate-emitting quantum cascade ring lasers, TARIQ MANZUR, Naval Undersea Warfare Center (NUWC, DIVNPT) Newport, RI-02841 — An InP based mid-infrared quantum cascade laser with a ring-shaped cavity is demonstrated in room temperature continuous wave operation. The light is coupled out with a second order distributed feedback grating buried inside the cavity. The device is epilayer-down bonded to a heat spreader and the light is emitted through the substrate. The emission wavelength is around 4.85 μ m with a high power output of 0.51 W. Single mode operation persists up to 0.4 W. Far field exhibits concentric ring features. Modal behavior is analyzed using the coupled mode theory, which suggests that the device operates in an extremely high order mode. Polarization measurement indicates that the beam is azimuthally polarized. This unique polarization state with high power output may find applications in tight focusing, optical tweezers, and material processing.

5:18PM T28.00015 3D Simulation of the Growth of Alloy Semiconductor Quantum Dots Considering Morphological and Compositional Coupling, JUNYAN GUO, YONG-WEI ZHANG, SRIDHAR NARAYANASWAMY, IHPC, Singapore — Fabrication of quantum dots (QDs) with high density may be realized by self-assembly via heteroepitaxial growth of thin films. Since the electronic and optoelectronic properties of QDs are sensitive to size, morphology, strain and especially composition, it is of great importance to control their composition profiles and morphology, and engineer the strain in them. Since the growth is a dynamic process, which carries out via surface diffusion driven primarily by strain relaxation and entropy change due to chemical intermixing, a strong coupling between morphological and composition evolutions during this process leads to a rather complex dynamics, which has not been fully understood. In this work, a 3-D finite element model is developed, which is capable of modeling the formation, self-assembly and coarsening of hetero-epitaxial alloy islands by considering the coupling of morphological and compositional evolution. Several interesting experimental observations, such as fast coarsening kinetics; asymmetries in composition profile and island shape; lateral motion of alloy islands have been observed in our simulations. Our model predictions have painted a rather complete picture for the entire dynamic evolution during the growth of nanoscale heteroepitaxial islands.

Wednesday, February 29, 2012 2:30PM - 5:30PM —
Session T29 GQI: Focus Session: Semiconductor Qubits - Coherent Control, Decoherence, and Relaxation 259A

2:30PM T29.00001 Electrical control of single spin dynamics¹, JASON PETTA, Princeton University — Over ten years ago, Daniel Loss and David DiVincenzo proposed using the spin of a single electron as a quantum bit. At the time of the proposal, it was not possible to trap a single electron in a device and measure its spin, let alone demonstrate control of quantum coherence. In this talk I will describe recent progress in the field, focusing on two new methods for single spin control that have been developed by my group at Princeton. The first method is based on quantum interference and implements spin-interferometry on a chip. The second method utilizes the strong spin-orbit coupling of InAs. By shifting the orbital position of the electronic wavefunction at gigahertz frequencies, we can control the orientation of a single electron spin and measure the full g-tensor, which exhibits a large anisotropy due to spin-orbit interactions. Both methods for single spin control are orders of magnitude faster than conventional electron spin resonance and allow investigations of single spin coherence in the presence of fluctuating nuclear and spin-orbit fields. I will also describe recent efforts to transfer these methods to silicon quantum dots, where the effects of fluctuating nuclear fields are much smaller.

¹Research performed in collaboration with Michael Schroer, Karl Petersson, Minkyung Jung, George Stehlik, Hong Lu, and Art Gossard. We acknowledge support from the Sloan and Packard Foundations, ARO, DARPA, and NSF.

3:06PM T29.00002 Harmonic Generation in InAs Nanowire Double Quantum Dots, M.D. SCHROER, M. JUNG, K.D. PETERSSON, J.R. PETTA, Princeton University — InAs nanowires provide a useful platform for investigating the physics of confined electrons subjected to strong spin-orbit coupling. Using tunable, bottom-gated double quantum dots, we demonstrate electrical driving of single spin resonance.^{1,2} We observe a standard spin response when the applied microwave frequency equals the Larmor frequency f_0 . However, we also observe an anomalous signal at frequencies $f_n = f_0/n$ for integer n up to $n \sim 5$. This is equivalent to generation of harmonics of the spin resonance field. While a $f_0/2$ signal has been observed,³ we believe this is the first observation of higher harmonics in spin resonance. Possible mechanisms will be discussed.⁴ Acknowledgements: Research supported by the Sloan and Packard Foundations, the NSF, and Army Research Office.

¹S. Nadj-Perge *et al.*, Nature **468**, 1084 (2010)

²M.D. Schroer *et al.*, Phys. Rev. Lett. **107**, 176811 (2011)

³E.A. Laird *et al.*, Phys. Rev. Lett. **99**, 246601 (2007)

⁴E.I. Rashba, arXiv:1110.6569 (2011)

3:18PM T29.00003 Composite pulse sequences for Z-rotations robust against small magnetic field gradient in singlet-triplet qubits¹, XIN WANG, EDWIN BARNES, LEV S. BISHOP, JASON P. KESTNER, KAI SUN, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park — We design piecewise composite pulse sequences of the exchange interaction in singlet-triplet qubits, suitable for achieving a Z-rotation along the Bloch sphere of arbitrary angle under the influence of a small stray magnetic field gradient. We explicitly show that upon appropriately choosing the pulse parameters, the error arising from the magnetic field gradient can be canceled at least to the third order. Examining the error as a function of the magnetic field gradient, we estimate the magnitude of fluctuation in the magnetic field gradient that can be tolerated under certain quantum error correction threshold.

¹This work is supported by IARPA, LPS-CMTC and CNAM.

3:30PM T29.00004 Composite pulse sequences for robust universal control of singlet-triplet qubits¹, LEV S. BISHOP, Joint Quantum Institute and Condensed Matter Theory Center, University of Maryland, College Park, XIN WANG, EDWIN BARNES, JASON P. KESTNER, KAI SUN, SANKAR DAS SARMA, Condensed Matter Theory Center, University of Maryland, College Park — We consider composite pulse sequences for the exchange interaction in singlet-triplet qubits, in the presence of a finite magnetic field gradient (producing a term in the Hamiltonian similar in magnitude to the exchange interaction). We find pulse sequences achieving arbitrary rotations on the Bloch sphere, for which there is no first-order term in the error arising from fluctuations of the magnetic field gradient. We quantify the range of experimental parameters where our composite sequences can outperform naive uncorrected sequences.

¹Support from JQI, IARPA, LPS-CMTC, CNAM

3:42PM T29.00005 Analytically solvable pulses for spin qubit rotations, SOPHIA ECONOMOU, Naval Research Lab — The hyperbolic secant pulse is a well known pulse shape for which the time dependent Schrodinger equation of a two-level system is analytically solvable. It has in the past been proposed [1] for optical spin rotations in quantum dots, and used experimentally to that end [2]. In this talk, a family of pulses will be introduced which can be viewed as the generalization of the sech pulse. These pulses may have skewed temporal profiles and frequency modulation (“chirping”). I will present results for the fidelity of spin rotations using some of these pulses and show that in the case of “Raman-type” control, where an auxiliary excited state is used, it can be advantageous to replace the usual 2π sech pulse.

[1] Economou et al., Phys. Rev. B **74**, 205415 (2006), Economou and Reinecke, Phys. Rev. Lett. **99**, 217401 (2007)

[2] Greilich et al., Nature Physics **5**, 262 (2009)

3:54PM T29.00006 Universal set of single-qubit gates based on geometric phase of electron spin in a quantum dot, VLADIMIR MALINOVSKY, SERGEY RUDIN, Army Research Laboratory, 2800 Powder Mill Road, Adelphi, MD 20783 — The electron spin in a single quantum dot is one of the perspective realizations of a qubit for the implementation of a quantum computer. During last decade several control schemes to perform single gate operations on a single quantum dot spin have been reported. We propose a scheme that allows performing ultrafast arbitrary unitary operations on a single qubit. We demonstrate how to use the geometric phase, which the Bloch vector gains along the cyclic path, to prepare an arbitrary state of a single qubit. It is shown that, the geometrical phase is fully controllable by the relative phase between the external fields. Using the analytic expression of the evolution operator for the electron spin in a quantum dot, we propose a scheme to design a universal set of single-qubit gates based solely on the geometrical phase that the qubit state acquires after a cyclic evolution in the parameter space. The scheme is utilizing ultrafast linearly-chirped pulses providing adiabatic excitation of the qubit states and the geometric phase is fully controlled by the relative phase between pulses.

4:06PM T29.00007 A fast “hybrid” silicon double quantum dot qubit¹, TECK SENG KOH, ZHAN SHI, C.B. SIMMONS, J.R. PRANCE, JOHN KING GAMBLE, YUN-PIL SHIM, University of Wisconsin-Madison, XUEDONG HU, University at Buffalo, SUNY, D.E. SAVAGE, M.G. LAGALLY, M.A. ERIKSSON, MARK FRIESEN, S.N. COPPERSMITH, University of Wisconsin-Madison — We propose a quantum dot qubit architecture that has an attractive combination of speed and fabrication simplicity. It consists of a double quantum dot with one electron in one dot and two electrons in the other. The qubit itself is a set of two states with total spin quantum numbers $S^2 = 3/4$ ($S = 1/2$) and $S_z = -1/2$, with the two different states being singlet and triplet in the doubly occupied dot. The architecture is relatively simple to fabricate, a universal set of fast operations can be implemented electrically, and the system has potentially long decoherence times. These are all extremely attractive properties for use in quantum information processing devices.

¹Work done was supported in part by ARO and LPS (W911NF-08-1-0482), by NSF (DMR-0805045, PHY-1104660, and a graduate fellowship to JKG), and by United States Department of Defense.

4:18PM T29.00008 Theory of Spin Relaxation in Two-Electron Lateral Coupled Quantum Dots¹, MARTIN RAITH, Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany, PETER STANO, Institute of Physics, Slovak Academy of Sciences, 845 11 Bratislava, Slovakia, FABIO BARUFFA, German Research School for Simulation Sciences, Forschungszentrum Juelich, D-52425 Juelich, Germany, JAROSLAV FABIAN, Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany — We present a global picture of the phonon-induced spin relaxation of two-electron lateral double quantum dots. The analysis covers a wide range of tuning parameters, such as the magnetic field, the exchange coupling, and the electric field (detuning). Our examples cover experimentally important scenarios. Quantitative results were obtained with a highly accurate numerical technique for the two most relevant host materials—GaAs and silicon. We find that in the presence of spin-orbit coupling, the rate becomes anisotropic and its maxima and minima are generated with an in-plane magnetic field parallel or perpendicular to the dots’ alignment dependent on specifics, such as spectral (anti-)crossings (spin hot spots), or the detuning strength. For all regimes, we give qualitative explanations of our observations. By understanding the spin lifetimes (T_1), this work marks a crucial step to the realization of two-electron semiconductor qubits.

¹This work was supported by DFG under grant SPP 1285 and SFB 689, ERDF OP R&D “QUTE”, and CE SAS QUTE.

4:30PM T29.00009 Dephasing in lateral double quantum dot systems due to evanescent-wave Johnson noise¹, ROBERT JOYNT, MAXIM VAVILOV, LUKE LANGSJOEN, AMRIT POUDEL, University of Wisconsin-Madison — Lateral double quantum dots suffer decoherence due to coupling to the environment. Previous theoretical calculations of dephasing time based on the phonon bath model (Vorojtsov et al. PRB **71**, 2005) and gate-voltage fluctuations (Valente et al. PRB **82**, 2010) are insufficient to explain the short dephasing time observed in experiment with a charge-based double quantum dot system (Petta et al. PRL **93**, 2004). Here we analyze the effect of fluctuating electromagnetic fields in the vicinity of conducting gates on the dephasing rate of charge-based double quantum dot systems.

¹This work was supported by ARO and DOD (W911NF-11-1-0030)

4:42PM T29.00010 Spin relaxation times and spin-dependent transport of silicon 2DEG and donors in high magnetic fields¹, CHEUK CHI LO, C.D. WEIS, J. BOKOR, T. SCHENKEL, Lawrence Berkeley National Laboratory, V. LANG, R.E. GEORGE, J.J.L. MORTON, University of Oxford, A.M. TYRSHKIN, S.A. LYON, Princeton University, J. VAN TOL, National High Magnetic Field Laboratory — We measured the spin-lattice relaxation (T_1) and spin coherence (T_2) times of the two-dimensional electron gas (2DEG) and neutral donors in a silicon field-effect transistor by pulsed electrically detected magnetic resonance at ≈ 3.4 T. The 2DEG T_1 varies between $\approx 200 - 800$ ns depending on the carrier density with an in-plane magnetic field configuration, but remains constant at ≈ 400 ns with an out-of-plane field configuration. On the other hand, $T_2 \approx 50 - 150$ ns for all carrier densities and both field orientations. The neutral donor T_1 and T_2 are found to be similar to that of the 2DEG. At even higher out-of-plane magnetic fields of $8 - 12$ T, Landau levels are clearly resolved in transport measurements and both the 2DEG and donor EDMR signals show corresponding oscillatory behavior as the carrier density is varied. We attribute this behavior to the alignment of the Fermi level with spin-split and different indexed Landau levels.

¹This work was supported by NSA (100000080295) and DOE (DE-AC02-05CH11231).

4:54PM T29.00011 Two-electron dephasing in a single silicon quantum dot¹, JOHN KING GAMBLE, MARK FRIESEN, S.N. COPPERSMITH, Department of Physics, University of Wisconsin-Madison, Madison, WI 53706, USA, XUEDONG HU, Department of Physics, University at Buffalo, SUNY, Buffalo, NY 14260, USA — We study the dephasing of two-electron states in a single silicon quantum dot. Specifically, we consider dephasing due to the electron-phonon coupling and charge noise, treating orbital, valley, and mixed valley-orbit excitations. For phonon-induced dephasing, the intervalley processes are most important and lead to a dephasing rate of about 1 MHz. In an ideal system, dephasing due to charge noise is strongly suppressed due to a vanishing dipole moment. However, introduction of disorder or anharmonicity leads to large effective dipole moments, and hence possibly strong dephasing.

¹This work was supported in part by ARO and LPS (W911NF-08-1- 0482) and by NSF (PHY-1104660).

5:06PM T29.00012 Long Spin Relaxation and Coherence Times of Electrons In Gated Si/SiGe Quantum Dots¹, JIANHUA HE, A.M. TYRSHKIN, S.A. LYON, Princeton University, C.-H. LEE, S.-H. HUANG, C. W. LIU, National Taiwan University — Single electron spin states in semiconductor quantum dots are promising candidate qubits. We report the measurement of $250 \mu\text{s}$ relaxation (T_1) and coherence (T_2) times of electron spins in gated Si/SiGe quantum dots at 350 mK. The experiments used conventional X-band (10 GHz) pulsed electron spin resonance (pESR), on a large area ($3.5 \times 20 \text{ mm}^2$) dual-gate undoped high mobility Si/SiGe heterostructure sample, which was patterned with 2×10^8 quantum dots using e-beam lithography. Dots having 150 nm radii with a 700 nm period are induced in a natural Si quantum well by the gates. The measured T_1 and T_2 at 350 mK are much longer than those of free 2D electrons, for which we measured T_1 to be $10 \mu\text{s}$ and T_2 to be $6.5 \mu\text{s}$ in this gated sample. The results provide direct proof that the effects of a fluctuating Rashba field have been greatly suppressed by confining the electrons in quantum dots. From 0.35 K to 0.8 K, T_1 of the electron spins in the quantum dots shows little temperature dependence, while their T_2 decreased to about $150 \mu\text{s}$ at 0.8 K. The measured 350 mK spin coherence time is 10 times longer than previously reported for any silicon 2D electron-based structures, including electron spins confined in “natural quantum dots” formed by potential disorder at the Si/SiO₂² or Si/SiGe interface, where the decoherence appears to be controlled by spin exchange.

¹supported by NSA/LPS and the ARO (W911NF-04-1-0389)

²S. Shankar *et al.*, Phys. Rev. B 82, 195323 (2010)

5:18PM T29.00013 Creation of entangled exciton states in coupled quantum dots¹, CELESTINO CREATORE, RICHARD T. BRIERLEY, RICHARD T. PHILLIPS, PETER B. LITTLEWOOD², Cavendish Laboratory, University of Cambridge, JJ Thomson Avenus, CB3 0HE, Cambridge, UK, PAUL R. EASTHAM, School of Physics, Trinity College, Dublin 2, Ireland — Quantum state preparation through external control is fundamental to established methods in quantum information processing and in studies of dynamics. In this respect, systems such as excitons in semiconductor quantum dots (QDs) are of particular interest since they can be easily driven to a particular state through the coherent interaction with a tuned optical field such as an external laser pulse. Here we propose to use adiabatic rapid passage (ARP) to excite entangled states in an ensemble of coupled quantum systems. The ARP protocol makes use of optical pulses with both frequency and temporal modulation and it is an efficient method to achieve population inversion in quantum dot ensembles as it is robust with respect to fluctuations in coupling and detuning. We explore this problem using a generalized t-J Hamiltonian to model an interacting many-dot system described in terms of hard-core bosons. Our quantitative analysis shows that ARP can be successfully implemented to create entangled states in a realistic ensemble of inhomogeneously distributed QDs.

¹This work is supported by EPSRC grant EP/F040075/1

²Argonne National Laboratory, Argonne IL 60439, USA, James Franck Inst., University of Chicago, Chicago IL 60637, USA

Wednesday, February 29, 2012 2:30PM - 5:30PM – Session T30 GQI: Quantum Algorithms 259B

2:30PM T30.00001 Adiabatic Surface Code Quantum Computing, CHRIS CESARE, CQILC, University of New Mexico, DAVE BACON, Department of Computer Science & Engineering, University of Washington, STEVE FLAMMIA, Perimeter Institute for Theoretical Physics, ANDREW LANDAHL, Sandia National Laboratories, ALICE NEELS, Department of Computer Science & Engineering, University of Washington — There are many approaches to constructing a quantum computer. In addition to the numerous different physical substrates available, there are a plethora of different underlying computational architectures from which to choose. Two major classes of architectures can be distinguished: those requiring a substantial external active control system to suppress errors, and those whose underlying physical construction eliminates much, if not all, of the need for such a control system. Here we focus on the latter class of architectures and address the question: “How does one fault-tolerantly quantum compute on a system protected from decoherence by a static Hamiltonian?” We present a solution that adiabatically interpolates between static Hamiltonians, each of which protects the quantum information stored in its ground space. Since each of these ground spaces can be described as a quantum error-correcting codespace, we call this process adiabatic code deformation. After describing a particular surface code (the toric code) and the way to encode information in code defects, we give explicit adiabatic interpolations that effect braids between defects, allowing for a CNOT gate between encoded qubits. We finish by describing how to extend our procedures to allow for universality.

2:42PM T30.00002 Quantum Random Walks and the Graph Isomorphism Problem¹ , KENNETH RUDINGER, JOHN KING GAMBLE, MARK WELLONS, MARK FRIESEN, ERIC BACH, ROBERT JOYNT, S.N. COPPERSMITH, University of Wisconsin-Madison — We investigate the quantum dynamics of particles on graphs (“quantum walk”), with the aim of developing quantum algorithms for determining whether or not two graphs are isomorphic. We investigate such walks on strongly regular graphs (SRGs), a class of graphs with high symmetry. We explore the effects of particle number and interaction range on a walk’s ability to distinguish non-isomorphic graphs. We numerically find that both non-interacting three-boson and three-fermion continuous time walks have the same distinguishing power on a dataset of 70,712 pairs of SRGs, each distinguishing over 99.6% of the pairs. We also find that increasing to four non-interacting particles further increases distinguishing power on this dataset. While increasing particle number increases distinguishing power, we prove that any walk of a fixed number of non-interacting particles cannot distinguish all SRGs. We numerically find that increasing particle number and increasing interaction range both result in increased distinguishing power of non-SRGs that are designed to be indistinguishable to the hard-core two-boson walk.

¹This work was supported by ARO and DOD (W911NF-09-1-0439) and NSF (CCF-0635355). J.K.G. acknowledges support from the NSF.

2:54PM T30.00003 Hamiltonian Simulation Using Linear Combinations of Unitary Operations , NATHAN WIEBE, ANDREW CHILDS, University of Waterloo — We present a new approach to simulating Hamiltonian dynamics based on implementing linear combinations of unitary operations rather than products of unitary operations. The resulting algorithm has superior performance to existing simulation algorithms based on product formulas and, most notably, scales better with the simulation error than any known Hamiltonian simulation technique. Our main tool is a general method to nearly deterministically implement linear combinations of similar unitary operations, which we show is optimal among a large class of methods.

3:06PM T30.00004 Measurement-Based Quantum Computation with Thermal States and Always-on Interactions , YING LI, Centre for Quantum Technologies, National University of Singapore, DANIEL BROWNE, Department of Physics and Astronomy, University College London, LEONG CHUAN KWEK, Centre for Quantum Technologies, National University of Singapore and Nanyang Technological University, ROBERT RAUSSENDORF, Department of Physics and Astronomy, University of British Columbia, TZU-CHIEH WEI, CN Yang Institute for Theoretical Physics, Stony Brook University — Quantum computation can be achieved by single-qubit measurements on an initial entangled state. It is often implicitly assumed that the interactions between spins can be switched off so that the dynamics of the measured spins does not affect the computation. We propose a model spin Hamiltonian so that measurement-based quantum computation can be accomplished on a thermal state with always-on interactions. Moreover, computational errors induced by thermal fluctuations can be corrected and thus the computation can be executed fault tolerantly if the temperature is below a threshold value.

3:18PM T30.00005 Quantum Computational Universality of the 2D Cai-Miyake-Dür-Briegel Quantum State , TZU-CHIEH WEI, CN Yang Institute for Theoretical Physics, Stony Brook University, ROBERT RAUSSENDORF, Department of Physics and Astronomy, University of British Columbia, LEONG CHUAN KWEK, Centre for Quantum Technologies, National University of Singapore and Nanyang Technological University — Universal quantum computation can be achieved by simply performing single-qubit measurements on a highly entangled resource state, such as cluster states. Cai, Miyake, Dür, and Briegel recently constructed a ground state of a two-dimensional quantum magnet by combining multiple Affleck-Kennedy-Lieb-Tasaki quasichains of mixed spin-3/2 and spin-1/2 entities and by mapping pairs of neighboring spin-1/2 particles to individual spin-3/2 particles [Phys. Rev. A **82**, 052309 (2010)]. They showed that this state enables universal quantum computation by constructing single- and two-qubit universal gates. Here, we give an alternative understanding of how this state gives rise to universal measurement-based quantum computation: by local operations, each quasichain can be converted to a one-dimensional cluster state and entangling gates between two neighboring logical qubits can be implemented by single-spin measurements. Furthermore, a two-dimensional cluster state can be distilled from the Cai-Miyake-Dür-Briegel state.

3:30PM T30.00006 Algorithmic Quantum Cooling , MAN HONG YUNG, SERGIO BOIXO, ALAN ASPURU-GUZIK, Harvard University, HARVARD TEAM — Efficient methods of cooling are essential for exploring the fundamental properties of low temperature physics. A remarkable cooling method is known as the evaporative cooling (or “coffee” cooling), where energetic particles are filtered away so as to lower the mean energy of the rest of the system. Inspired by the idea of evaporative cooling, we developed a method called algorithmic quantum cooling (AQC) for achieving the goal of cooling for any physical system which is simulable by a quantum computer. The novel feature of AQC is that the evolution of the state of the system is modeled as the movement of a one-dimensional classical random walk; the walker plays the role of the motion of the gas particles in an ordinary evaporative cooling. The implementation of this method is analogous to the setting of Maxwell’s demon, where the experimentalist can monitor the heat-up or cool-down of the system, and apply feedback control to the resulting states. Here we cover the results of the connection of AQC with quantum non-demolition measurement, a scaling analysis of AQC, and the application of amplitude amplification to achieve quantum speedup. Experimental realization of AQC can be accomplished with currently available technologies.

3:42PM T30.00007 Progress on exploring practical applications of quantum annealing and D-Wave One , SERGIO BOIXO, USC- ISI, FEDERICO SPEDALIERI, USC - ISI — A D-Wave One quantum optimizer is currently being installed at the newly created USC-Lockheed Martin Quantum Computing Center. This chip implements quantum annealing at finite temperature as a computational resource, with 90 working qubits. Quantum annealing is a particularly simple branch of adiabatic quantum computation. We report work in progress on exploring practical applications of quantum annealing in general, and this chip in particular. Some of this work is done in collaboration with Aspuru-Guzik’s group at Harvard.

3:54PM T30.00008 Adiabatic Quantum Anomaly Detection and Machine Learning¹ , KRISTEN PUDENZ, DANIEL LIDAR, University of Southern California — We present methods of anomaly detection and machine learning using adiabatic quantum computing. The machine learning algorithm is a boosting approach which seeks to optimally combine somewhat accurate classification functions to create a unified classifier which is much more accurate than its components. This algorithm then becomes the first part of the larger anomaly detection algorithm. In the anomaly detection routine, we first use adiabatic quantum computing to train two classifiers which detect two sets, the overlap of which forms the anomaly class. We call this the learning phase. Then, in the testing phase, the two learned classification functions are combined to form the final Hamiltonian for an adiabatic quantum computation, the low energy states of which represent the anomalies in a binary vector space.

¹Research supported by the Lockheed Martin Corporation, the NSF, and NASA Ames Research Center

4:06PM T30.00009 Universal Blind Quantum Computation, JOSEPH FITZSIMONS, National University of Singapore, ELHAM KASHEFI, University of Edinburgh — Blind Quantum Computing (BQC) allows a client to have a server carry out a quantum computation for them such that the client's inputs, outputs and computation remain private. Recently we proposed a universal unconditionally secure BQC scheme, based on the conceptual framework of the measurement-based quantum computing model, where the client only needs to be able to prepare single qubits in separable states randomly chosen from a finite set and send them to the server, who has the balance of the required quantum computational resources. Here we present a refinement of the scheme which vastly expands the class of quantum circuits which can be directly implemented as a blind computation, by introducing a new class of resource states which we term *dotted-complete graph states* and expanding the set of single qubit states the client is required to prepare. These two modifications significantly simplify the overall protocol and remove the previously present restriction that only nearest-neighbor circuits could be implemented as blind computations directly. As an added benefit, the refined protocol admits a substantially more intuitive and simplified verification mechanism, allowing the correctness of a blind computation to be verified with arbitrarily small probability of error.

4:18PM T30.00010 Experimental demonstration of blind quantum computing, STEFANIE BARZ, VCQ, University of Vienna; IQOQI, Austrian Academy of Sciences, Austria, ELHAM KASHEFI, School of Informatics, University of Edinburgh, UK, ANNE BROADBENT, Institute for Quantum Computing, University of Waterloo; Department of Combinatorics & Optimization, University of Waterloo, Canada, JOE FITZSIMONS, Centre for Quantum Technologies, National University of Singapore, Singapore; School of Physics, University College Dublin, Ireland, ANTON ZEILINGER, PHILIP WALTHER, VCQ, University of Vienna; IQOQI, Austrian Academy of Sciences, Austria — Quantum computers are among the most promising applications of quantum-enhanced technologies. Quantum effects such as superposition and entanglement enable computational speed-ups that are unattainable using classical computers. The challenges in realising quantum computers suggest that in the near future, only a few facilities worldwide will be capable of operating such devices. In order to exploit these computers, users would seemingly have to give up their privacy. It was recently shown that this is not the case and that, via the universal blind quantum computation protocol, quantum mechanics provides a way to guarantee that the user's data remain private. Here, we demonstrate the first experimental version of this protocol using polarisation-entangled photonic qubits. We demonstrate various blind one- and two-qubit gate operations as well as blind versions of the Deutsch's and Grover's algorithms. When the technology to build quantum computers becomes available, this will become an important privacy-preserving feature of quantum information processing.

4:30PM T30.00011 Classical Ising Models Realised on Optical Lattices, MAURO CIRIO, G.K. BRENNEN, J. TWAMLEY, S. IBLISDIR, O. BOADA, Macquarie University — We describe a simple quantum algorithm acting on a register of qubits in d spatial dimensions which computes statistical properties of $d + 1$ dimensional classical Ising models. The algorithm works by measuring scattering matrix elements for quantum processes and Wick rotating to provide estimates for real partition functions of classical systems. This method can be implemented in a straightforward way in ensembles of qubits, e.g. three dimensional optical lattices with only nearest neighbor Ising like interactions. By measuring noise in the estimate useful information regarding location of critical points and scaling laws can be extracted for classical Ising models, possibly with inhomogeneity. Unlike the case of quantum simulation of quantum hamiltonians, this algorithm does not require Trotter expansion of the evolution operator and thus has the advantage of being amenable to fault tolerant gate design in a straightforward manner. Through this setting it is possible to study the quantum computational complexity of the estimation of a classical partition function for a 2D Ising model with non uniform couplings and magnetic fields. We provide examples for the 2 dimensional case.

4:42PM T30.00012 Initialization and Readout of Spin Chains for Quantum Information Transport, GURNEET KAUR, PAOLA CAPPELLARO, Massachusetts Institute of Technology, MIT — Linear chains of spins acting as quantum wires are a promising approach to achieve scalable quantum information processors. Nuclear spins in apatite crystals closely emulate a one-dimensional spin chain, thus providing an ideal test-bed for the experimental study of quantum information transport by means of Nuclear Magnetic Resonance techniques. The natural dipolar interaction among the spins can be manipulated via the available collective NMR control to simulate the Hamiltonian capable of driving quantum transport. We present control protocols for initialization and readout of ^{19}F spin chains in Fluorapatite, even in the absence of single-spin addressability. We experimentally prepare and read out desired initial states for transport tasks, such as the simulation of single-spin excitation transport and a two-spin encoded state for quantum information transfer. Our control schemes enable experimental characterization of quantum transport in spin chains and will allow further studies of protocols for perfect fidelity transfer.

4:54PM T30.00013 Dynamical decoupling and quantum error suppression in adiabatic quantum computation, KEVIN YOUNG, Sandia National Laboratories — Adiabatic quantum information processing, like other quantum computing paradigms, is susceptible to noise which can potentially spoil a computation. This talk will address two proposed methods to utilize stabilizer codes to combat such noise: dynamical decoupling and quantum error suppression. A combination of numerical and analytical techniques will illustrate the connections between these two approaches. The talk will conclude with a discussion of the practical advantages of dynamical decoupling over quantum error suppression.

5:06PM T30.00014 Complexity of the Quantum Adiabatic Algorithm, ITAY HEN, A.P. YOUNG, University of California Santa Cruz — The Quantum Adiabatic Algorithm (QAA) has been proposed as a mechanism for efficiently solving optimization problems on a quantum computer. Here, we determine its efficiency by considering several constraint satisfaction (SAT) problems. We do this by studying the size dependence of their typical minimum energy gap using quantum Monte Carlo methods. We find that for most problems this gap decreases exponentially with the size of the problem, indicating that the QAA is not more efficient than existing classical search algorithms. However, for one specific problem, namely, MAX-2-XORSAT, there is evidence to suggest that the gap may be polynomial near the phase transition.

5:18PM T30.00015 Discrete-time quantum walks on the symmetric group (quantum card shuffling), ZLATKO DIMCOVIC, YEVGENIY KOVCHegov, Oregon State University — The next stage in uses of classical stochastic approaches, going beyond Markov chains (random walks on graphs), are walks on algebraic structures. The prime and classic example of such a problem is "card shuffling," a walk on the permutation (symmetric) group. The richness of this non-Abelian group lends itself to modeling of complex phenomena, while it also quickly leads to rather complicated problems. The challenge of studying such quantum processes is no lesser, but the benefits can be expected to even outweigh the classical uses. We study a quantum analog of the classical "top-to-random" shuffle, where the top card is placed at random in the deck. We construct a "coined" DTQW on the permutation group: based on the action of a (unitary) "coin" operator in an additional ("coin") space, (unitary) steps in the group space are taken, resulting in a (quantum) walk over group elements. We use general techniques for the eigenvalue problem of the combined coin and permutation operators, utilizing regularities in the block structure. We have reached preliminary solutions for low-dimensional cases. Currently we are integrating them into a more general solution, which will yield the first step in this deep and far-reaching, while challenging problem.

Wednesday, February 29, 2012 2:30PM - 5:30PM —
Session T31 DMP: Focus Session: Topological Insulators: Synthesis and Characterization - Spin Transport and Superconductivity 260

2:30PM T31.00001 Towards spin injection from silicon into topological insulators¹, CLAUDIA OJEDA-ARISTIZABAL, MICHAEL S. FUHRER, IAN APPELBAUM, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742, USA, IAN APPELBAUM TEAM — Attempts to uncover evidence of spin-momentum coupling in a topological insulator (TI) using transport measurements are hampered by many challenges. Most importantly, injection of a spin polarized current from a ferromagnet that is in contact or close proximity to a topological insulator can easily give rise to anisotropic magnetoresistance signals or planar Hall effect from stray fields, which have the same symmetry and hence are indistinguishable from any signal coming from the spin-momentum-locked surface states. Here we propose a scheme to remove this difficulty by injecting spin-polarized electrons from undoped silicon into the TI surface states. In addition to providing a long-distance transport region to separate the ferromagnetic spin source from the TI by several hundred microns or even millimeters, this approach will also allow spin precession measurements (necessary for unambiguous identification of spin signals) whereas direct injection does not. Detection is provided by differential measurement from two ballistic current contacts on the topological insulator. We will describe our progress in fabrication and measurement of devices with exfoliated crystals of TI Bi₂Se₃, including the determination of the silicon-Bi₂Se₃ Schottky barrier height of 0.34 eV

¹This work is supported by the University of Maryland NSF-MRSEC under Grant No. DMR 05-20471 and the ONR.

2:42PM T31.00002 Spin-momentum helical locking induced spin-valve effects in topological insulator/ferromagnet heterostructures¹, LAN WANG, BIN XIA, CHANG KE, PENG REN, PENG LIU, HAIBIN SU, ALFRED HUAN, Nanyang Technological University — Topological insulator is composed of an insulating bulk state and an odd number of massless spin-helical Dirac cone formed two dimensional surface state. Here we report a novel spin-valve effect in Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}/CoFe heterostructures. This effect indicates the spin-momentum helical locking on the Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2} topological surface state. It is also indicated that the characteristics of helical surface can be preserved at topological insulator/ferromagnet interface although the ferromagnetism can break the time reversal symmetry and therefore generate an energy gap at the topological Dirac cone.

¹Supports for this work came from Singapore National Research Foundation (RCA-08/018) and MOE Tier 2 (MOE2010-T2-2-059).

2:54PM T31.00003 Spin Transport Experiments in Topological Insulator Bi₂Se₃ Thin Films, JIFA TIAN, ISAAC CHILDRES, HELIN CAO, Department of Physics and Birck Nanotechnology Center, Purdue University, West Lafayette, IN, 47907, IREK MITKOWSKI, Department of Physics, Purdue University, West Lafayette, IN, 47907, YONG P. CHEN, Department of Physics and Birck Nanotechnology Center, Purdue University, West Lafayette, IN, 47907 — Topological insulators are an unusual phase of quantum matter with an insulating bulk gap and gapless spin-momentum locked Dirac surface states. Such a spin-helical surface state provides rich opportunities for potential applications in spintronics. We performed spin valve experiments on exfoliated Bi₂Se₃ thin films (~10 nm thick) with ferromagnetic electrodes using a DC driving current in an in-plane magnetic field. We observed the two-terminal resistances are asymmetric between the large positive (> 0.5 T) and negative (<-0.5 T) in-plane magnetic fields. The high and low resistance states can be reversed by changing the direction of the driving DC current. Furthermore, the measured resistance asymmetry decreases as temperature increases. One interpretation of our observation is related to the spin-momentum helical locking of topological surface states producing a spin-polarized surface current. We also performed the non-local spin valve measurements, and observed an asymmetry in the measured signal between opposite large magnetic fields.

3:06PM T31.00004 Josephson supercurrent through a topological insulator surface state, MENNO VELDHORST, MARIEKE SNELDER, MARCEL HOEK, TIAN GANG, MESA+ Institute for Nanotechnology, University of Twente, The Netherlands, XIAO-LIN WANG, Institute for Superconducting and Electronic Materials, University of Wollongong, Australia, VEERENDRA GUDURU, ULI ZEITLER, High Field Magnet Laboratory, Radboud University Nijmegen, The Netherlands, WILFRED WIEL, MESA+ Institute for Nanotechnology, University of Twente, The Netherlands, ALEXANDER GOLUBOV, HANS HILGENKAMP, ALEXANDER BRINKMAN, MESA+ Institute for Nanotechnology, University of Twente, The Netherlands — The long-sought yet elusive Majorana fermion is predicted to arise from a combination of a superconductor and a topological insulator. An essential step in the hunt for this emergent particle is the unequivocal observation of supercurrent in a topological phase. Here, we present direct evidence for a Josephson supercurrent in superconductor (Nb) - topological insulator (Bi₂Te₃) - superconductor e-beam fabricated junctions by the observation of clear Shapiro steps under microwave irradiation, and a Fraunhofer-type dependence of the critical current on magnetic field. The dependence of the critical current on temperature and electrode spacing shows that the junctions are in the ballistic limit. Shubnikov-de Haas oscillations in magnetic fields up to 30 T reveal a topologically non-trivial two-dimensional surface state. We argue that the ballistic Josephson current is hosted by this surface state despite the fact that the normal state transport is dominated by diffusive bulk conductivity. The lateral Nb-Bi₂Te₃-Nb junctions hence provide prospects for the realization of devices supporting Majorana fermions.

3:18PM T31.00005 Hybrid Superconducting Junctions of Bi₂Se₃ Topological Insulator Nanoribbons, YONG-JOO DOH, Korea University Sejong Campus, HYUNHO NOH, Korea Research Institute of Standards and Science, LEE-SEUL PARK, Sookmyung Women's University, EUN-KYOUNG JEON, Korea Research Institute of Chemical Technology, HONG-SEOK KIM, Korea University Sejong Campus, JEONG-O LEE, Korea Research Institute of Chemical Technology, JIN SEOK LEE, Sookmyung Women's University, JINHEE KIM, Korea Research Institute of Standards and Science — Topological insulators are exotic materials with bulk band gap and metallic edge states which are protected on their own boundary topologically. Here, we report on the fabrication and measurement results of the superconducting proximity junctions of topological insulator nanoribbons of Bi₂Se₃. Single-crystalline Bi₂Se₃ nanoribbons are synthesized using the vapor-liquid-solid method, while the superconducting Al electrodes are formed on top of the nanowire. When a magnetic field (H) is applied along the axial direction, the magneto-resistance data exhibit quasi-periodic oscillations with an average periodicity of $H^* \sim 0.4$ T, which is consistent with the Aharonov-Bohm oscillations. In the superconducting state, the supercurrent branch with a critical current of $I_c \sim 90$ nA is clearly observed in the current-voltage curve as a result of the superconducting proximity effect in Bi₂Se₃ nanoribbon. Quantized voltage steps of the Bi₂Se₃ nanoribbon Josephson junction under the microwave irradiation satisfy the ac Josephson relation.

3:30PM T31.00006 Signature of Majorana Fermions in Josephson Junctions of Bi₂Se₃¹, JAMES WILLIAMS, ANDREW BESTWICK, Stanford University, PATRICK GALLAGHER, Harvard University, JAMES ANALYTIS, IAN FISHER, DAVID GOLDBERGER, Stanford University — At the surface of a three-dimensional topological insulator lie Dirac fermions. Placing a superconductor in proximity to these surface fermions has been theoretically shown to produce Majorana fermions, an as-yet unobserved elementary particle. We report on the fabrication and low-temperature transport of a topological insulator in proximity to two superconductors – a device forming a Josephson Junction with a topological insulator (Bi₂Se₃) as a weak link. Several departures from conventional Josephson Junctions are observed and evaluated in the context of the presence of a one-dimensional wire of Majorana fermions induced in the device.

¹This work is supported in part by the Keck Foundation

3:42PM T31.00007 Superconductivity in the topological semimetal YPtBi, NICHOLAS BUTCH, Lawrence Livermore National Laboratory — Superconductivity was recently discovered in the half Heusler compound YPtBi. Electrical resistivity and Hall data provide compelling evidence that supports the idea that band structure calculations are correct and that YPtBi is indeed a semimetal with nontrivial topology. The low-temperature superconductivity emerges from a remarkable normal state with an extremely low carrier density, no crystalline inversion symmetry, and strong band inversion. I will discuss the normal state properties of YPtBi and details of its superconducting state, and compare them to the characteristics of other potential topological superconductors. This research was performed at the University of Maryland, College Park in collaboration with Paul Syers, Kevin Kirshenbaum, Andrew P. Hope, and Johnpierre Paglione.

4:18PM T31.00008 Superconductivity in Bi₂Te₃ type three dimensional topological compounds induced via pressure, CHANGQING JIN, J. ZHU, P.P. KONG, S.J. ZHANG, J.L. ZHANG, S.M. FENG, H.M. WENG, Q.Q. LIU, X.C. WANG, J.L. ZHU, X.H. YU, L.X. YANG, R.C. YU, Institute of Physics, Chinese Academy of Sciences, L. WANG, W.G. YANG, HPCAT, Geophysical Laboratory, Carnegie Institute of Washington, S.C. ZHANG, Stanford University, X. DAI, Z. FANG, Institute of Physics, Chinese Academy of Sciences — We report experimental updates on pressure induced superconductivity in Bi₂Te₃ type topological compounds. The topological nature of the superconductivity observed will be discussed in conjunction with on site high pressure structure investigations & first principles calculations. A phase diagram of superconductivity as function of pressure will be provided.

4:30PM T31.00009 Proximity-Induced High-Temperature Superconductivity in a Topological Insulator, PARISA ZAREAPOUR, ALEX HAYAT, SHU YANG FRANK ZHAO, ANJAN REIJNDERS, MIKHAIL KRESHCHUK, ACHINT JAIN, Department of Physics and Institute for Optical Sciences, University of Toronto, DANIEL KWOK, NARA LEE, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, ZHIJUN XU, ALINA YANG, G.D. GU, CMP&MS Department, Brookhaven National Laboratory, KENNETH BURCH, Department of Physics and Institute for Optical Sciences, University of Toronto — New topological phases of matter have been proposed to exist at the surface of some materials with spin-orbit coupling called topological insulators. Among the different exotic features of topological insulators, the interface between a topological insulator and a superconductor is of great interest. It is predicted that combining these two materials would lead to the emergence of Majorana fermion excitations which enable several applications in spintronics and quantum computing. Towards this goal, we have investigated Bi₂Sr₂CaCu₂O_{8+δ}(Bi-2212)-Bi₂Se₃ interface junctions made by a new mechanical-bonding technique. Current vs. voltage and differential conductance measurements have been performed in various temperatures ranging from room temperature to 5K. Several anomalies were observed in the Andreev spectra including a zero bias conductance peak appearing below the critical temperature of the superconductor Bi-2212 (85K), a reduced gap in Bi-2212 as well as the intrinsic gap of Bi-2212. These features suggest the induction of high-temperature superconductivity in the Bi₂Se₃ due to proximity to Bi-2212.

4:42PM T31.00010 Point-contact Andreev Reflection Spectroscopy on Bi₂Se₃ Single Crystal, XUNCHI CHEN, CHAO HUAN, Georgia Inst of Tech, IREK MITKOWSKI, YONG CHEN, Purdue University, ZHIGANG JIANG, Georgia Inst of Tech — Point-contact spectroscopy measurement is carried out on Bi₂Se₃ single crystals via approaching a superconducting niobium tip ($T_c=9.5$ K) to the crystal surface. The tip-sample junction conductance is studied as a function of DC bias voltage, temperature, and magnetic field. The resulting spectra show a conductance dip at zero bias, indicative of ballistic transport. A homebuilt positioning stage enables us to approach the superconducting tip in nanometer accuracy, to precisely control the inter-facial barrier strength. We find that our experimental results cannot be simply described by the standard Blonder, Tinkham and Klapwijk (BTK) model even when the inelastic scattering at the interface is considered. An improved model taking into account the spin-orbit coupling effect is needed to fit our data.

4:54PM T31.00011 Crystal growth and physical property of Bi-Sb-Te-Se topological insulator and CuxBi2Se3 topological superconductor materials¹, GENDA GU, ALINA YANG, JOHN SCHNEELOCH, ZHIJUN XU, JOHN TRANQUADA, J.G. ZHÖA, Z.H. PAN, H.B. YANG, W.D. SI, T. VALLA, CMP&MS, Brookhaven National Laboratory — The discovery of 3D topological insulator and topological superconductor materials opens up a new research field in the condensed matter physics. In order to exploit the novel surface properties of these topological insulators, it is crucial to achieve a bulk-insulating state in these topological insulator crystals. Unfortunately, all available topological insulator crystals are not bulk-insulating. We have grown a number of Bi-Se, Bi-Te, Sb-Te-Se, Bi-Sb-Se, Bi-Sb-Te-Se and Bi-Sb-Te-Se-S topological insulator single crystals by using 5N and 6N pure elements. We have measured the physical properties on these single crystals. We have studied the effect of growth condition and impurity on the bulk electrical conductivity of these single crystals. We try to answer two questions if it is possible to grow the bulk-insulating topological insulator single crystals and which maximum resistivity of these topological insulator single crystals we can grow. We have also grown a number of CuxBi2Se3 topological superconductor single crystals.

¹The work was supported by DOE under contract No. DE-AC02-98CH10886.

5:06PM T31.00012 Crystal structure and superconducting properties in Cu_xBi₂Se₃, YUSUKE SUZUKI, PRADIP DAS, University of Tsukuba, TAKASHI MOCHIKU, NIMS, TAKANARI KASHIWAGI, MASASHI TACHIKI, KAZUO KADOWAKI, University of Tsukuba — The recent discovery of the anomalous superconductivity in Cu_xBi₂Se₃ (0.10<x<0.25) has attracted much attention because of the relation between superconducting state and topological surface state. In order to understand the role of Cu doping in superconducting Bi₂Se₃, we study the doping dependence of the magnetic properties and the characteristics of crystal structures. We made high quality of Cu_xBi₂Se₃ single crystals with several doping level of x by using melt growth technique. We confirmed the superconducting transition from Cu_xBi₂Se₃ for several doping levels and determined the phase diagram of a function of x. The lattice constant increases with increasing Cu doping level, however it saturated around x=0.25 which corresponds to the saturation of T_c as well. We analyzed the crystal structure in detail in explaining the occurrence of superconductivity. Details of the structural and magnetization study will be discussed in the conference.

5:18PM T31.00013 Electrical Transport Properties of Bi₂Te₃ Nanotubes and Nanowires, REN-ZHONG DU, JIAN WANG, QI LI, Department of Physics, The Pennsylvania State University, University Park, PA, USA, YUEWEI YIN, SINING DONG, XIAO GUANG LI, Hefei National Laboratory for Physical Sciences at Microscale, Department of Physics, University of Science and Technology of China, Hefei, China — Electrical transport properties of promising topological insulator, Bi₂Te₃ nanowires and nanotubes are measured at different temperatures and magnetic field and the results are compared with the Bi₂Se₃ thin films. The nanotube and nanowire samples are synthesized by galvanostatic electrodeposition and solution phase methods, with diameters of 70nm (ex) and 50nm (in) for nanotubes and 80~100nm for nanowires, respectively. The contact leads (Pt) are fabricated by using Focusing Ion Beam (FIB). The magnetoresistance of Bi₂Te₃ nanotubes shows linear dependence as a function of magnetic field, with a notable peak around zero field. This is different from Bi₂Se₃ thin films which show quadratic behavior, with a significant dip near zero field. The results will be discussed based on the possible weak localization effect in the nanotubes in comparison with the weak anti-localization effect in the films.

Wednesday, February 29, 2012 2:30PM - 5:30PM —
Session T32 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides - Manganites 261

2:30PM T32.00001 Colossal magnetodielectric effect in DyMn2O5: Electromagnons or rare earth?¹, ANDREI SUSHKOV, DENNIS DREW, MRSEC and CNAM, Department of Physics, University of Maryland, CHRISTIAN KANT, ALEXEY SHUVAEV, ANDREI PIMENOV, ISSP, Vienna University of Technology, Austria, SERGEI ZVYAGIN, Dresden High Magnetic Field Laboratory, Germany, BERND LORENZ, University of Houston, SANG-WOOK CHEONG, Rutgers University — We report on the results of spectroscopic studies of the excitations responsible for the colossal magnetodielectric effect in DyMn2O5 [1]. On one hand, many RMn2O5 compounds have electromagnons capable of inducing large steps in the dielectric constant. On the other hand, rare earth ions can possess electric dipole moments and also can produce dielectric anomalies. Both types of excitations are expected in the experimentally difficult low energy range 0.1-1 meV. We use high frequency dielectric, Fourier transform and back-wave oscillator spectroscopies in combination with low temperature and magnetic field up to 9 T to clarify the origin of the dielectric anomaly in DyMn2O5. [1] N. Hur, S. Park, P. A. Sharma, S. Guha, and S-W. Cheong, Colossal Magnetodielectric Effects in DyMn2O5, PRL 93, 107207 (2004).

¹Work supported in part by NSF-MRSEC under grant DMR-0520471

2:42PM T32.00002 Magnetism-Driven Ferroelectricity in GdMn2O5, NARA LEE, Rutgers University, YOUNG JAI CHOI, Yonsei University, C. VECCHINI, Diamond Light Source Ltd, L. C. CHAPON, ISIS Facility, Rutherford Appleton Laboratory, P. G. RADAELLI, Oxford Physics, A. BOMBARDI, Diamond Light Source Ltd, S-W. CHEONG, Rutgers University — REMn2O5 (RE=rare-earth) is one of the well-studied multiferroics which exhibits the reversible switching of ferroelectric polarization under the application of external magnetic fields. It is known that the ferroelectricity in REMn2O5 originates from the symmetric exchange interaction between Mn ions. However, the role of the rare-earth elements has never been elucidated. In order to reveal the full magnetic structure and the contribution of rare-earth magnetism to the ferroelectricity, we have studied the detailed magnetic and structural properties of high-quality single-crystalline GdMn2O5 (space group, Pbam). We have performed the resonant x-ray scattering experiment, and comprehensive measurements of physical properties of the system, including magnetic susceptibility, dielectric constant and ferroelectric polarization with the variation of temperature and magnetic fields.

2:54PM T32.00003 Raman and Infrared studies of the multiferroics TbMn2O5 and YMn2O5, SABEUR MANSOURI, SERGE JANDL, Université de Sherbrooke, 2500 Boulevard University, Sherbrooke, Quebec J1K 2R1, Canada, P. ORLITA, COLLABORATION¹, M. M. GOSPODINOV, COLLABORATION² — Orthorhombic manganites of the RMnO3 and RMn2O5 families develop an electric polarization induced, flipped and flopped by application of a magnetic field. The Tb(Y)Mn2O5 Anti-ferromagnetic order is incommensurate between $T_N = 42K$ (44K) and $T_C = 38K$ and becomes commensurate between $T_C = 38K$ and $T = 24K$ (18K); at this temperature ferroelectricity appears and remains incommensurate below 24K (18K)[1,2]. We have studied the TbMn2O5 and YMn2O5 Raman active phonons as a function of temperature and compared their behavior to similar multiferroic compounds Bi(Dy)Mn2O5 phonons where the A_g high frequencies modes soften between $T^* \sim 70K$ and T_N and harden below $T_N \sim 42K$ [3]. The over-hardening of the phonon frequencies above anharmonicity at low temperatures confirm that the spin-lattice interaction plays an important role in the magnetoelectric properties. The TbMn2O5 infrared active phonon frequencies are also studied as a function of temperature and under applied magnetic field (up to 10 Tesla). As predicted theoretically the TbMn2O5 infrared-active phonon frequencies soften below T_N . Evolutions of the phonon frequencies under the applied magnetic field are reported and analyzed.

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²Institute of Solid State Physics, Bulgarian Academy of Sciences, 1784 Sofia, Bulgaria

3:06PM T32.00004 Absence of ferroelectricity in hexagonal InMnO3, MARTIN LILIENBLUM, YU KUMAGAI, Department of Materials, ETH Zurich, ALEXEI A. BELIK, International Center for Materials Nanoarchitectonics, NIMS, NAËMI LEO, NICOLA A. SPALDIN, MANFRED FIEBIG, Department of Materials, ETH Zurich — So far, it was believed that hexagonal (h-) InMnO3 exhibit the same type of multiferroic order as the other compounds from the h-RMnO3 family (R = Sc, Y, Dy - Lu), including, in particular, a unit-cell-tripling improper ferroelectric order. Here we present experimental evidence for the absence of ferroelectricity in hexagonal InMnO3 based on three different techniques: x-ray diffraction (XRD), piezoresponse force microscopy (PFM) and optical second harmonic generation (SHG). XRD data are ambiguous because they can be described likewise by the non-ferroelectric $P\bar{3}c$ structure and by the ferroelectric $P6_3cm$ structure present in the other h-RMnO3 compounds. However, PFM at room temperature and SHG measurements at low temperature uniquely reveal the absence of ferroelectric order in InMnO3. We therefore propose that InMnO3 exhibits antiferrodistortive, but non-ferroelectric order according to the $P\bar{3}c$ symmetry. Density functional calculations show that the relative energy between the $P\bar{3}c$ and $P6_3cm$ structures is determined by a competition between electrostatic and covalency effects, with an absence of covalency favoring the ferroelectric structure.

3:18PM T32.00005 Long range order beyond vortices in h-REMnO3, SEUNG CHUL CHAE, NARA LEE, YOICHI HORIBE, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — Fascinating vortices were discovered recently in ferroelectric domain patterns in hexagonal (h-)YMnO3. One of the important ingredients for these vortex domain patterns is mutual interlocking of ferroelectric and structural antiphase domain walls. In contrast to expected vortex domain patterns, we have found intriguing stripe domain patterns in other h-REMnO3 (RE=Ho, Er, Tm, Yb, Lu). These stripe domain patterns appear to indicate the presence of long-range-ordered state as the true ground state in h-REMnO3. On the other hand, vortex domain patterns suggest the presence of a Kosterlitz-Thouless-like transition. We argue that this significant difference stems from very slow kinetics associated the ordering of six possible degrees of freedom.

3:30PM T32.00006 Electronic and Structural Properties Near the Ferroelectric Transition in Multiferroic Hexagonal RMnO3, HAIYAN CHEN, TREVOR TYSON, TAO WU, New Jersey Institute of Technology, JIANMING BAI, Oak Ridge National Laboratory, KEN AHN, New Jersey Institute of Technology, KUMI PANDYA, Brookhaven National Laboratory, S.B. KIM, SANG-WOOK CHEONG, Rutgers University — Combined local and long range structural measurements were conducted on RMnO3 for temperatures extending significantly above the ferroelectric transition temperature, (T_{FE}). We find in hexagonal RMnO3 no large atomic (bond distance or thermal factors) or electronic structure changes on crossing T_{FE} . The born effective charge tensor is found to be highly anisotropic at the O sites indicating very strong hybridization of the charge. The tensor does not change significantly above T_{FE} revealing no charge redistribution and suggests an unusual transition. Molecular dynamic simulations on large supercells are used to provide a general picture of the transition. This work is supported by DOE Grants DE-FG02-07ER46402 (NJIT) and DE-FG02-07ER46382 (Rutgers University).

3:42PM T32.00007 Role of the apical oxygen in RMnO₃ (R = Ho and Lu) low temperature magneto-electric effect , JONATHAN VERMETTE, SERGE JANDL, Département de Physique, Université de Sherbrooke, M. ORLITA COLLABORATION, M. M. GOSPODINOV COLLABORATION — Multiferroic materials are promising candidates for new innovative devices, particularly in the field of memory storage. The strong coupling between magnetic ordering and ferroelectricity characterizing these compounds allows the modulation of the electric polarization (magnetic moment) with an external magnetic (electric) field. Hexagonal RMnO₃ (Ho to Lu) compounds are type-I multiferroics in which ferroelectricity and magnetism have different sources giving a relative weak magneto-electric coupling with a large polarization. In this case ferroelectricity is induced at a relative high temperature ($T_C \sim 800\text{K}$) following a structural transition, while magnetic ordering of Mn³⁺ and R³⁺ occurs at lower temperatures ($T < 100\text{K}$). In order to determine which atoms play a major role in the giant low temperature magneto-electric effect, we study the evolutions of infrared active phonon frequencies in HoMnO₃ and LuMnO₃ under applied magnetic field below $T_{Ho} = 5\text{K}$. By comparing the renormalized force constants and the Born-effective charges, apical oxygen role in Ho³⁺-Mn³⁺ superexchange interaction is particularly underlined.

3:54PM T32.00008 Piezoelectric-response of charged 180° ferroelectric domain walls¹ , EDWARD LOCHOCKI, Department of Physics and Astronomy and Rutgers Center for Emergent Materials, Rutgers University, Piscataway, New Jersey 08854, USA, SOONYONG PARK, Department of Physics, Chung-Ang University, Seoul 156, Republic of Korea, NARA LEE, S-W. CHEONG, WEIDA WU, Department of Physics and Astronomy and Rutgers Center for Emergent Materials, Rutgers University, Piscataway, New Jersey 08854, USA — We report ambient piezoresponse force microscopy (PFM) studies of the multiferroic hexagonal manganite HoMnO₃ performed on the cleaved (110) surface of a single crystal specimen. By changing the sample orientation with respect to the cantilever, we observed an unexpected out-of-plane PFM signal at domain walls which depends on domain wall orientation, in addition to the expected in-plane PFM signal in domains. Further studies confirmed that the domain wall PFM signal results from an out-of-plane displacement, which can be explained by a simple model of local elastic response with conservation of unit cell volume at head-on domain walls.

¹NSF-DMR-0844807 and NSF-DMR-1104484

4:06PM T32.00009 A First Principle exploration of A site ordered Ho_{0.5}A_{0.5}MnO₃ (A=Ge, Sn, Pb, As, Sb, Bi, Se, Te) , SATHYA SHEELA SUBRAMANIAN, National Institute of Technology, Trichy, India, Japan Advanced Institute of Science and Technology, Japan, TAISUKE OZAKI, Japan Advanced Institute of Science and Technology, Japan, KUNHIKO YAMAUCHI, ISIR-SANKEN, Osaka University, Japan, NATESAN BASKARAN, National Institute of Technology, Trichy, India, TAMIO OGUCHI, ISIR-SANKEN, Osaka University, Japan — In this work a first principle attempt has been made to study the structure and properties of doping lone pair cations to ortho-HoMnO₃. Electronic structure calculations were carried out to study Ho_{0.5}A_{0.5}MnO₃ (A=Ge, Sn, Pb, As, Sb, Bi, Se, Te) under the Generalized Gradient Approximation of Density Functional Theory in an attempt to analyze the effect of lone pair cations towards electric polarization and to predict new multiferroics. Under the first principle calculations, Ho_{0.5}A_{0.5}MnO₃ (A=Ge, Sn, As, Sb, Bi, Se, Te) is found to be multiferroic. Doping 50% of Se and Sn to HoMnO₃ is found to highly enhance the electric polarization compared to parent ortho-HoMnO₃. O2p- A valence p orbital hybridization is expected to be the cause of this polarization. Thus Ho_{0.5}Se_{0.5}MnO₃ and Ho_{0.5}Sn_{0.5}MnO₃ are expected to be good candidate multiferroics. A first principle attempt has thus been made to perform an extensive search for new multiferroics in which p-p hybridization is found to have a strong role in causing electric polarization predicting new multiferroics providing a pathway for experimentalists to synthesis new promising multiferroic compounds.

4:18PM T32.00010 Synthesis of Perovskite ScMnO₃ under High Temperature and Pressure¹ , TIAN YU, PENG GAO, Department of Physics, New Jersey Institute of Technology, TREVOR A. TYSON, Dept of Physics, New Jersey Institute of Technology; Dept of Physics and Astronomy & Rutgers Center for Emergent Materials, Rutgers University, H. CHEN, Department of Physics, New Jersey Institute of Technology, J. BAI, Oak Ridge National Laboratory — Perovskite type ScMnO₃ was synthesized under high temperature and pressure starting with hexagonal ScMnO₃. The detail of the structure is examined by synchrotron x-ray diffraction and IR spectroscopy at room temperature. A highly distorted perovskite phase which is similar to the structure of LaMnO₃ is identified by XRD Rietveld Refinement. Due to the small Sc ion radius, each Mn site has a distorted MnO₆ polyhedron. This work is supported by DOE Grant DE-FG02-07ER46402.

¹DOE Grant DE-FG02-07ER46402

4:30PM T32.00011 Low Temperature Structural of ScMnO₃ , PENG GAO, TIAN YU, TREVOR A. TYSON, Department of Physics, New Jersey Institute of Technology, XINGUO HONG, ZHIQIANG CHEN, Mineral Physics Institute, Stony Brook University, SANJIT GHOSE, National Synchrotron Light Source II, Brookhaven National Laboratory, LARS EHM, Mineral Physics Institute, Stony Brook University, ZHENXIAN LIU, Geophysical Laboratory, Carnegie Institution of Washington — We present the temperature dependent structural changes of hexagonal ScMnO₃ probed on multiple length scales. These measurements are compared by IR results. These results are used to assess the structural changes across the Néel temperature which may coincide and couple with the ferroelectric behavior. This work is supported by DOE Grants DE-FG02-07ER46402 (NJIT), by COMPRES, the Consortium for Materials Properties Research in Earth Sciences under NSF Cooperative Agreement EAR 10-43050 (X17B3) and EAR 01-35554 (U2A), and by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886 (for use of the National Synchrotron Light Source at Brook Haven National Laboratory).

4:42PM T32.00012 Time-resolved imaging of magnetoelectric switching in MnWO₄¹ , TIM HOFFMANN, PHILIP THIELEN, HISKP, University Bonn, Germany, PETRA BECKER, LADISLAV BOHATY, Institute of Crystallography, University of Cologne, Germany, MANFRED FIEBIG, Department of Materials, ETH Zurich, Switzerland — The interaction of magnetic and ferroelectric order is intrinsically strong in spin-spiral multiferroics. Here the complex magnetic long range order breaks inversion symmetry and induces a spontaneous electric polarization. The interaction allows to switch the magnetic order by an electric field and is thus of great interest for applications. Although such magnetoelectric switching is a major goal in multiferroics, hardly any work was devoted to the dynamic aspects of the actual switching process. Here we report time-resolved optical second harmonic generation measurements of the electric-field-induced reversal of the spin-spiral domains in multiferroic MnWO₄. Ferroelectric and magnetic orders appear to remain rigidly coupled even during the non-equilibrium state of the transition. The switching is governed by domain wall motion on the millisecond time scale. Even though, locally domains can disappear within nanoseconds. The slow global response can be explained by an energy estimate: As the dipole energy in the electric field is much weaker than the magnetic anisotropy energy, the electric field is only a weak lever for manipulating the magnetic system. Therefore magnetoelectric switching in this compound is inherently slow.

¹The authors thank DFG for financial support via SFB 608.

4:54PM T32.00013 Displacement-type ferroelectric transition with magnetic Mn ions in perovskite $\text{Sr}_{1-x}\text{Ba}_x\text{MnO}_3$, HIDEAKI SAKAI, University of St Andrews, JUN FUJIOKA, University of Tokyo, TATSUO FUKUDA, JAEA/SPring8, DAISUKE OKUYAMA, CMRG/CERG, RIKEN, DAISUKE HASHIZUME, RIKEN, FUMITAKA KAGAWA, University of Tokyo, HIRONORI NAKAO, YOUICHI MURAKAMI, CMRC-PF, KEK, TAKAHISA ARIMA, University of Tokyo, ALFRED Q.R. BARON, RIKEN/SPring8, YASUJIRO TAGUCHI, CMRG/CERG, RIKEN, YOSHINORI TOKURA, University of Tokyo — Almost all the proper ferroelectrics with a perovskite structure discovered so far have no *d*-electrons in the off-center transition metal site, as exemplified by BaTiO_3 and $\text{Pb}(\text{Zr,Ti})\text{O}_3$. This empirical *d*⁰ rule is incompatible with the emergence of magnetism and has significantly restricted the variety of multiferroic materials. In this work, we have discovered a displacement-type ferroelectric transition originating from off-center Mn^{4+} ions in antiferromagnetic Mott insulators $\text{Sr}_{1-x}\text{Ba}_x\text{MnO}_3$. As Ba concentration increases, the perovskite lattice shows the typical soft mode dynamics, and the ferroelectricity shows up for $x \geq 0.45$. In addition to the large polarization and high transition temperature comparable to BaTiO_3 , we demonstrate that the magnetic order suppresses the ferroelectric lattice dilation by $\sim 70\%$ and increases the soft-phonon energy by $\sim 50\%$, indicating gigantic magnetoelectric effects [1]. This work was supported by the FIRST program on “Quantum Science on Strong Correlation”.

[1] H. Sakai *et al.*, Phys. Rev. Lett. **107**, 137601 (2011).

5:06PM T32.00014 Antiferromagnetic pinning of a phase-like mode below T_N in NdMnO_3 , NESTOR MASSA, LANAIS EFO-CEQUINOR, UNLP, La Plata, Argentina, LEIRE DEL CAMPO, DOMINGOS DE SOUSA MENESES, PATRICK ECHEGUT, CNRS-CEMHTI, Orléans, France, MARIA JESUS MARTÍNEZ-LOPE, JOSE ANTONIO ALONSO, ICMM-CSIC, Madrid, Spain — We report on reflectivity and emission far infrared spectra of NdMnO_3 between 4K and its dissociation temperature. Phonon bands at 300K are in agreement with orthorhombic Pbnm space group assignments. In addition, a broad strong band, reminiscent to a phase-mode in quasi-one dimension metals, is found at very low frequencies that it is understood originating in charge fluctuations in d-orbitals. There is no distinctive behaviors between 1073 K and 1173 K, where orthorhombic O and O' coexist. Beyond ~ 700 K a mid-infrared polaron band turns into a Drude tail suggesting hopping conductivity double exchange due to air heating oxidation $\text{Mn}^{3+} \rightarrow \text{Mn}^{4+} + 1e^-$. Below 300 K phonons are better defined and the low frequency giant dipole acquires strength. Few degrees above the antiferromagnetic transition it broadens as electrons loosing coherence. At $T_N \sim 76$ K we find strong phonon magnetostriction while the band turns asymmetric locking-in to the underlying magnetic order. Preliminary measurements of hexagonal TmMnO_3 , show that asymmetry split due to lower symmetry and the triangular magnetic lattice two exchange integrals J_1 and J_2 in the a-b plane. Similar to a soft mode those two bands and a lower frequency resonance undergo strong hardening down to 4 K.

5:18PM T32.00015 Low temperature Electrical and Magnetic studies of Nsutite, JOHN DISTIN, PAUL YENO, PETER LEMAIRE, Department of Physics and Earth Sciences, Central Connecticut State University, New Britain CT 06050, MELINDA MCNALLY, KELSEY COOLAHAN, Department of Chemistry and BioChemistry, Rowan University, Glassboro NJ 08028 — Nsutite is a naturally occurring Manganese Oxide of the composition $\text{Mn}_{1-x}^{4+}\text{Mn}_x^{2+}\text{O}_{2-2x}(\text{OH})_{2x}$ where $x = 0.06 - 0.07$. D.C. electrical transport measurements were carried out on samples from Nsuta, Ghana between 40 K and 400 K. Non-linear I-V curves were observed below 140 K even at very low currents. The resistivity vs. temperature data suggests electron transport is by the variable range hopping mechanism between 140 K and 400 K. Magnetic moment vs. temperature data were obtained between 5K and 300K at high field (10,000 Oe) and low field (1,000 Oe). Both high and low field data suggest paramagnetic behavior with a possible Neel temperature at about 15K, below which the materials exhibits antiferromagnetic behavior. The electrical and magnetic properties as well as high temperature thermal analysis (DSC) data will be discussed.

Wednesday, February 29, 2012 2:30PM - 4:18PM – Session T35 DCP: Focus Session: Plyler Award Symposium 107B

2:30PM T35.00001 Earle K. Plyler Prize for Molecular Spectroscopy and Dynamics Lecture: 2D IR Spectroscopy of Peptide Conformation, ANDREI TOKMAKOFF, MIT Department of Chemistry — Descriptions of protein and peptide conformation are colored by the methods we use to study them. Protein x-ray and NMR structures often lead to impressions of rigid or well-defined conformations, even though these are dynamic molecules. The conformational fluctuations and disorder of proteins and peptides is more difficult to quantify. This presentation will describe an approach toward characterizing and quantifying structural heterogeneity and disorder in peptides using 2D IR spectroscopy. Using amide I vibrational spectroscopy, isotope labeling strategies, and computational modeling based on molecular dynamics simulations and Markov state models allows us to characterize distinct peptide conformers and conformational variation. The examples illustrated include the beta-hairpin tripp2 and elastin-like peptides.

3:06PM T35.00002 Vibrational spectroscopy of interacting water molecules, JAMES SKINNER, University of Wisconsin — I will discuss a new simulation model for water that includes three-body interactions explicitly, and describe our theoretical approach for calculating OH-stretch spectroscopic observables. I will present illustrative examples, involving pump-probe energy-transfer-induced anisotropy decay in liquid water, IR and Raman line shapes in ice Ih, phase-sensitive SFG spectra of the liquid/vapor interface, and energetics and IR spectra for the different conformations of the water hexamer.

3:42PM T35.00003 Two-dimensional Fourier transform electronic spectroscopy, DAVID JONAS, University of Colorado — Sensitive interference detection of the electric field of femtosecond four-wave mixing signals (stimulated photon echoes) at their point of origin in the sample can be used to record two-dimensional (2D) Fourier transform electronic spectra. In direct analogy to 2D nuclear magnetic resonance, 2D Fourier transform spectra have nearly homogeneous linewidths in each frequency dimension and sort the signal spectrum according to the initial excitation frequency. The initial excitation frequency information is stored in a robust population grating, so 2D spectra can be used to study both coherent and incoherent processes, and have revealed coherent aspects of energy transfer processes. Femtosecond 2D spectra also have the advantage of “freezing out” vibrational motions as inhomogeneities, raising interesting questions about what kinds of broadening can be rephased in 2D spectra recorded with stimulated photon echo pulse sequences. This talk will focus on coherent aspects of non-adiabatic electronic curve crossing and their manifestation in 2D electronic spectra.

Wednesday, February 29, 2012 2:30PM - 4:42PM – Session T37 FEd: Physics Education Research and Resources 108

2:30PM T37.00001 Strength of Student Models of Force and Motion¹ , CECILIA T. MARKES, University of Nebraska at Kearney — With a three-year FIPSE grant, it has been possible to develop and implement activity-based algebra level introductory physics. The Force and Motion Conceptual Evaluation (FMCE) has been given as a pretest and a posttest to both the traditional lecture/lab classes and the activity-based classes. The responses are analyzed to determine the models that students use. The questions are separated into eight groups. Responses are divided into expert model, student model, and null model. Students are categorized as being in an expert state, a mixed state, or a student state. Previous work assumed a particular model if the answers to 70 percent (or more) of the questions in a group fit that model. To determine the strength of the models, the analysis is repeated assuming 85 percent and then 100 percent. The results are analyzed to determine if there is a significant difference from 70 percent to 85 percent to 100 percent. This will indicate the strength of the models in each group of questions.

¹This work was supported by the US DOE's FIPSE Grant No. P116B51449.

2:42PM T37.00002 Project-Based Learning Courses: The Relationship Between Faculty-Intended Course Implementation and Students' Perceptions¹ , JENNIFER A. SIMONOVICH, EMILY TOWERS, YEVGENIYA V. ZASTAVKER, F. W. Olin College of Engineering — Project-based learning (PjBL) has been shown to improve students' performance and satisfaction with their coursework, particularly in science and engineering courses. Specific aspects of PjBL that contribute to this improvement are student autonomy, course scaffolding, and instructor support. This study investigates two PjBL courses required for engineering majors at a small technical school, *Introductory Mechanics Laboratory* and *Introductory Engineering Design*. The three data sources used in this work are classroom observations (one laboratory and four design sessions) and semi-structured in-depth interviews with twelve students and six faculty. Grounded theory approach is used in a two-step fashion by (1) analyzing each data set individually and (2) performing full triangulation of all three data sets. In this talk, we demonstrate the relationship between faculty intentions and student perceptions regarding the three PjBL aspects – student autonomy, course scaffolding, and instructor support – within the context of these two courses. We further discuss implications for the course design and professional development of faculty.

¹NSF HRD #0624738

2:54PM T37.00003 Combining Wikis and JiTT to enhance critical thinking abilities , HASHINI MOHOTTALA, University of Hartford, West Hartford, CT 06117 — I report the combine use of Just in Time Teaching (JiTT) and Wikispaces (Wikis) in introductory level, calculus based, physics classes. Over the years, JiTT had been effectively used in teaching physics and some uses on Wikis were also reported in the recent years.¹ Wiki helps students, instructors and technology to interact with one another and JiTT boosts the self-confidence of students to tackle physics problems. Thus, the combine use of Wiki-JiTT is going to be a new experience for both instructors and students. In this experiment, I used Wikis as a platform for JiTT, and conventional JiTT was slightly altered to best fit the combination and to focus on enhancing critical thinking abilities in my students.

¹H. Mohottala The Physics Teacher – September 2011 – Vol. 49, Issue 6

3:06PM T37.00004 Student Self-Efficacy in Introductory Project-Based Learning Courses¹ , GEOFFREY PLEISS, YEVGENIYA V. ZASTAVKER, F. W. Olin College of Engineering — This study investigates first-year engineering students' self-efficacy in two introductory Project-Based Learning (PjBL) courses – *Physics (Mechanics) Laboratory* and *Engineering Design* – taught at a small technical institution. Twelve students participated in semi-structured open-ended interviews about their experiences in both courses. Analysis was performed using grounded theory. Results indicate that students had lower self-efficacy in *Physics Lab* than in *Engineering Design*. In *Physics Lab*, students reported high levels of faculty-supported scaffolding related to final project deliverables, which in turn established perceptions of an outcome-based course emphasis. Conversely, in *Engineering Design*, students observed high levels of scaffolding related to the intermediate project deliverables, highlighting process-centered aspects of the course. Our analyses indicate that this difference in student perceptions of course emphases – resulting from the differences in scaffolding – is a primary factor for the discrepancy in self-efficacy between *Physics Lab* and *Engineering Design*. Future work will examine how other variables (e.g., academic background, perception of community, gender) affect students' self-efficacy and perception of scaffolding in these PjBL courses.

¹NSF HRD #0624738

3:18PM T37.00005 ABSTRACT WITHDRAWN —

3:30PM T37.00006 The IPAD as a Pedagogical Tool in an Algebra-Based Introductory Physics Class¹ , ANGELA GARRIOTT, LEAH BUSH, ROBERTO RAMOS, Indiana Wesleyan University — We report our experience in using the IPAD as a pedagogical tool for enhancing physics learning in an introductory algebra-based physics laboratory course for primarily pre-med students. We used several applications including (1) video analysis for experiments in accelerated motion (2) virtual oscilloscope for studying wave motion and circuit response to low frequency driving voltages; (3) applications for visualization of electric fields and magnetic fields. We compare student responses to this platform versus more traditional experiments. Using student surveys and polls. We also evaluate the IPAD as a new and familiar interface versus traditional interfaces like the standard oscilloscope. We report on the advantages and disadvantages of using this mobile, popular platform in delivering experimental physics content and promoting student engagement.

¹We acknowledge Indiana Wesleyan University for awarding an IPAD mini-grant to Prof. R. Ramos.

3:42PM T37.00007 Physics: A student's guide through the great texts¹ , KERRY KUEHN, Wisconsin Lutheran College — Although memorizing formulae and learning how to perform calculations is crucial for acquiring a working knowledge of physical theories, the standard pedagogical method employed by many textbooks does not prepare the student to become a practicing scientist precisely because it tends to mask the actual scientific method: the science is presented as an accomplished fact; the prescribed questions revolve largely around technological applications of accepted laws. In this talk, I will describe a two-year general physics curriculum which I have developed and taught for the past decade to undergraduate students at Wisconsin Lutheran College. The curriculum is unique in that it provides students of the natural and mathematical sciences with a comprehensive introduction to physics based on the careful reading and analysis of selections from foundational texts in physics and astronomy. The curriculum is designed to encourage a critical and circumspect approach to the study of natural science, while at the same time developing a suitable foundation for advanced coursework in physics. Through the careful reading and analysis of foundational scientific texts, students learn skills which are essential when considering the practical and philosophical implications of scientific theories.

¹I would like to acknowledge Springer Science+Business Media, LLC for collaborating with me on this project.

3:54PM T37.00008 A student's guide to searching the literature using online databases¹, CASEY W. MILLER, DUSTIN BELYEA, MICHELLE CHABOT, University of South Florida, TROY MESSINA, Centenary College of Louisiana — A method is described to empower students to efficiently perform general and specific literature searches using online resources [Miller et al., Am. J. Phys. 77, 1112 (2009)]. The method was tested on multiple groups, including undergraduate and graduate students with varying backgrounds in scientific literature searches. Students involved in this study showed marked improvement in their awareness of how and where to find scientific information. Repeated exposure to literature searching methods appears worthwhile, starting early in the undergraduate career, and even in graduate school orientation.

¹Supported by NSF-CAREER and the Mattie Allen Broyles and Gus S. Wortham Endowments.

4:06PM T37.00009 A jumping cylinder in an incline, RAUL W. GOMEZ, JORGE HERNANDEZ, VIVIANNE MARQUINA, Facultad de Ciencias, UNAM — The problem of a cylinder of mass m and radius r , with its center of mass out of the cylinder axis, rolling in an incline that makes an angle α respect to the horizontal is analyzed. The equation of motion is solved to obtain the site where the cylinder loses contact with the incline (jumps). Several simplifications are made: the analyzed system consists of an homogeneous disc with a one dimensional straight line of mass parallel to the disc axis at a distance $d < r$ of the center of the cylinder. To compare our results with experimental data, we use a Styrofoam cylinder of radius $r = 10.0 \pm 0.05$ cm, high $h = 5.55 \pm 0.05$ cm and a mass $m_1 = 24.45 \pm 0.05$ g, to which a 9.50 ± 0.01 mm diameter and 5.10 ± 0.001 cm long brass rod of mass $m_2 = 30.75 \pm 0.05$ g was imbedded parallel to the disc axis at a distance of 5.40 ± 0.05 cm from it. Then the disc rolls on a 3.20 m long wooden ramp inclined at 30° and 45° respect to the horizontal. To determine the jumping site, the movements were recorded with a high-speed video camera (Casio EX ZR100) at 400 frames per second. The experimental results agree well with the theoretical predictions.

4:18PM T37.00010 Design and operation of an inexpensive far-field laser scanning microscope suitable for use in an undergraduate laboratory course, ARTHUR PALLONE, Northern Kentucky University, ERIC HAWK, None — Scanning microscope applications span the science disciplines yet their costs limit their use at educational institutions. The basic concepts of scanning microscopy are simple. The microscope probe - whether it produces a photon, electron or ion beam - moves relative to the surface of the sample object. The beam interacts with the sample to produce a detected signal that depends on the desired property to be measured at the probe location on the sample. The microscope transforms the signal for output in a form desired by the user. Undergraduate students can easily construct a far-field laser scanning microscope that illustrates each of these principles from parts available at local electronics and hardware stores and use the microscope to explore properties of devices such as light dependent resistors and biological samples such as leaves. Students can record, analyze and interpret results using a computer and free software.

4:30PM T37.00011 Variational Calculations for Hydrogen in Introductory Solid State, JAVIER HASBUN, University of West Georgia — Molecular hydrogen is very important in the introductory solid state physics course because it is used as one of the simplest molecular realistic models where bonding and anti-bonding takes place. This system is one of the first examples in which interactions among the ions and the electrons is incorporated realistically. To this end, we approach the system starting from the hydrogen atom. Here we introduce a numerical approach that reproduces the known analytic result for the ground state. The idea is to expand the hydrogenic wavefunction in terms of Gaussians (four of them) with variational parameters. As the parameters are varied the numerical approach stops when the energy is a minimum. The scheme is consistently extended through the ionized hydrogen molecule and the reproduction of its analytically known ground state energy result. We finally culminate with the hydrogen molecule using a variational wavefunction, a la Hartree, and proceed to repeat the process with a particular flavor of a Hartree-Fock wavefunction [1] and finally obtaining a hydrogen molecule total ground state energy of -31.10 eV with a bond length of 1.37 Bohr radius.

[1] "Atomic and Electronic Structure of Solids," Efthimios Kaxiras (Cambridge UP, Cambridge UK, 2003).

Wednesday, February 29, 2012 2:30PM - 5:30PM –

Session T40 DBIO DPOLY: Focus Session: Cytoskeleton and Biomechanics - Forced Dynamics

156A

2:30PM T40.00001 Dynamics of focal adhesions modulates active cellular response¹, MOUMITA DAS, SHILADITYA BANERJEE, M. CRISTINA MARCHETTI, Department of Physics, Syracuse University — The cytoskeleton of living cells connects to and senses the extracellular mechanical environment through protein clusters called focal adhesions. We study how the mechanics and dynamics of focal adhesions influence the distribution of mechanical stresses and deformations in a cell which is modeled as an active elastic gel. We carry out our investigations for two types of bond dynamics of focal contacts (a) slip bond dynamics where the bonds are weakened by a tensile mechanical force and (b) catch bond dynamics where they are initially strengthened upon application of a tensile mechanical force, and undergo failure at very large forces. We comment on the effect of different types of focal adhesions on the transmission and regulation of cell traction forces and on cellular mechanosensing.

¹This work was supported in part by the NSF through grant DMR-1004789.

2:42PM T40.00002 3D Neutrophil Tractions in Changing Microenvironments, JENNET TOYJANOVA, Graduate Student, School of Engineering, Brown University, Providence, RI, ESTEFANY FLORES, Research Assistant, Department of Surgery, Rhode Island Hospital, Providence, RI, JONATHAN REICHNER, Department of Surgery, Rhode Island Hospital and the Warren Alpert Medical School of Brown University, Providence, CHRISTIAN FRANCK, School of Engineering, Brown University, Providence, RI — Neutrophils are well-known as first responders to defend the body against life threatening bacterial diseases, infections and inflammation. The mechanical properties and the local topography of the surrounding microenvironment play a significant role in the regulating neutrophil behavior including cell adhesion, migration and generation of tractions. In navigating to the site of infection, neutrophils are exposed to changing microenvironments that differ in their composition, structure and mechanical properties. Our goal is to investigate neutrophil behavior, specifically migration and cellular tractions in a well-controlled 3D in vitro system. By utilizing an interchangeable 2D-3D sandwich gel structure system with tunable mechanical properties neutrophil migration and cell tractions can be computed as a function of gel stiffness and geometric dimensionality.

2:54PM T40.00003 Force transmission through intercellular fluid transfer, STEVEN ZEHNDER, JOLIE BREAU, ALISON DUNN, GREGORY SAWYER, THOMAS ANGELINI, University of Florida — Cell force generation and transmission play a vital role in controlling cell-to-cell interactions and cell locomotion. Contraction of the cell's cytoskeletal network generates forces that can be transmitted directly to other cells by cell-cell adherens junctions or through a substrate by traction forces. Within monolayers, cytosolic fluid is transferred between cells through gap junctions. The coupling between intercellular fluid movement and contraction can give rise to a different type of cell-cell force transmission. Here we present preliminary results investigating the role of intercellular force transmission through fluid motion across gap junctions.

3:06PM T40.00004 Forcing it on: Cytoskeletal dynamics during lymphocyte activation, ARPITA UPADHYAYA, Department of Physics, University of Maryland, College Park — Formation of the immune synapse during lymphocyte activation involves cell spreading driven by large scale physical rearrangements of the actin cytoskeleton and the cell membrane. Several recent observations suggest that mechanical forces are important for efficient T cell activation. How forces arise from the dynamics of the cytoskeleton and the membrane during contact formation, and their effect on signaling activation is not well understood. We have imaged membrane topography, actin dynamics and the spatiotemporal localization of signaling clusters during the very early stages of spreading. Formation of signaling clusters was closely correlated with the movement and topography of the membrane in contact with the activating surface. Further, we observed membrane waves driven by actin polymerization originating at these signaling clusters. Actin-driven membrane protrusions likely play an important role in force generation at the immune synapse. In order to study cytoskeletal forces during T-cell activation, we studied cell spreading on elastic gels. We found that gel stiffness influences cell morphology, actin dynamics and receptor activation. Efforts to determine the quantitative relationships between cellular forces and signaling are underway. Our results suggest a role for cytoskeleton driven forces during signaling activation in lymphocytes.

3:42PM T40.00005 Aging phenomena in a network model of the cytoskeleton¹, NASRIN AFZAL, MICHEL PLEIMLING, Virginia Tech — Motivated by a series of experiments that study the response of the cytoskeleton in living cells to time dependent mechanical forces, we investigate, through Monte Carlo simulations, a three-dimensional network subjected to perturbations. After having prepared the system in a relaxed state, shear is applied and the relaxation processes are monitored. We measure two-time functions of various quantities such as the Euclidean distance between crosslinks and the energy of the system. We discuss possible implications of our results for relaxation processes taking place in the cytoskeleton.

¹Supported in part by the US National Science Foundation through Grant DMR-0904999.

3:54PM T40.00006 Mechanical interactions may explain synchronized growth of cytoskeletal actin networks in motile cells, ANTONIO DESIMONE, LUCA CARDAMONE, ALESSANDRO LAIO, SISSA-International School for Advanced Studies, SISSA TEAM — Growing networks of actin fibers are able to organize into compact, stiff two-dimensional structures inside lamellipodia of crawling cells. We examine critically the hypothesis that the growing actin network is a critically self-organized system, in which long-range mechanical stresses arising from the interaction with the plasma membrane provide the selective pressure leading to organization. We show that a simple model based only on this principle leads to stochastic protrusion of lamellipodia (growth periods alternating with fast retractions) and several of the features observed in experiments: a growth velocity initially insensitive to the external force; the capability of the network to organize its orientation; a load-history-dependent growth velocity. Our model predicts that the spectrum of the time series of the height of a growing lamellipodium decays with the inverse of the frequency. This behavior is confirmed by optical tweezer measurements performed in vivo on neuronal growth cones. References L. Cardamone et al.: Cytoskeletal actin networks in motile cells are critically self-organized systems synchronized by mechanical interactions. PNAS, vol. 108, no. 34, pp. 13978-13983

4:06PM T40.00007 Investigations of biomechanical activity of macrophages during phagocytosis, DANIEL KOVARI, JENNIFER CURTIS, Georgia Institute of Technology — Phagocytosis has traditionally been investigated in terms of the relevant biochemical signaling pathways that trigger the process and lead to the deformation of the cell as it engulfs a target. Physical changes in the cell include rearrangement and polymerization of actin in the phagocytic cup, large membrane deformations, increased membrane area via exocytosis, and closure of the phagocytic cup through membrane fusion. Hence, phagocytosis is a fine-tuned balance between biophysical cellular events and chemical signaling, which are responsible for driving these materials and mechanical changes. We present a series of assays designed to probe the physical/mechanical parameters that govern a cell during phagocytosis. Custom built micropipette manipulators are used to manipulate individual cells, facilitating high-resolution microscopy of individual phagocytic events. This work has been supported by NSF PoLS #0848797.

4:18PM T40.00008 Collective cell migration during inflammatory response¹, DI WU, KIMBERLY STROKA, HELIM ARANDA-ESPINOZA, Fischell Department of Bioengineering, University of Maryland — Wound scratch healing assays of endothelial cell monolayers is a simple model to study collective cell migration as a function of biological signals. A signal of particular interest is the immune response, which after initial wounding in vivo causes the release of various inflammatory factors such as tumor necrosis alpha (TNF- α). TNF- α is an innate inflammatory cytokine that can induce cell growth, cell necrosis, and change cell morphology. We studied the effects of TNF- α on collective cell migration using the wound healing assays and measured several migration metrics, such as rate of scratch closure, velocities of leading edge and bulk cells, closure index, and velocity correlation functions between migrating cells. We observed that TNF- α alters all migratory metrics as a function of the size of the scratch and TNF- α content. The changes observed in migration correlate with actin reorganization upon TNF- α exposure.

¹Authors acknowledge support from NSF CMMI-0643783

4:30PM T40.00009 Temperature dependence of optically induced cell deformations¹, ANATOL FRITSCH, TOBIAS R. KIESSLING, ROLAND STANGE, JOSEF A. KAES, University of Leipzig, Division of Soft Matter Physics — The mechanical properties of any material change with temperature, hence this must be true for cellular material. In biology many functions are known to undergo modulations with temperature, like myosin motor activity, mechanical properties of actin filament solutions, CO₂ uptake of cultured cells or sex determination of several species. As mechanical properties of living cells are considered to play an important role in many cell functions it is surprising that only little is known on how the rheology of single cells is affected by temperature. We report the systematic temperature dependence of single cell deformations in Optical Stretcher (OS) measurements. The temperature is changed on a scale of about 20 minutes up to hours and compared to defined temperature shocks in the range of milliseconds. Thereby, a strong temperature dependence of the mechanics of single suspended cells is revealed. We conclude that the observable differences arise rather from viscosity changes of the cytosol than from structural changes of the cytoskeleton. These findings have implications for the interpretation of many rheological measurements, especially for laser based approaches in biological studies.

¹Funding from ESF and Graduate School BuildMoNa

4:42PM T40.00010 ABSTRACT WITHDRAWN —

4:54PM T40.00011 Biomechanical changes in endothelial cells result from an inflammatory response¹, JANINA VAITKUS, KIMBERLY STROKA, HELIM ARANDA-ESPINOZA, Fischell Department of Bioengineering, University of Maryland — During periods of infection and disease, the immune system induces the release of TNF- α , an inflammatory cytokine, from a variety of cell types, such as macrophages. TNF- α , while circulating in the vasculature, binds to the apical surface of endothelial cells and causes a wide range of biological and mechanical changes to the endothelium. While the biological changes have been widely studied, the biomechanical aspects have been largely unexplored. Here, we investigated the biomechanical changes of the endothelium as a function of TNF- α treatment. First, we studied the traction forces applied by the endothelium, an effect that is much less studied than others. Through the use of traction force microscopy, we found that TNF- α causes an increase in traction forces applied by the endothelial cells as compared to non-treated cells. Then, we investigated cell morphology, cell mechanics, migration, and cytoskeletal dynamics. We found that in addition to increasing applied traction forces, TNF- α causes an increase in cell area and aspect ratio on average, as well as a shift in the organization of F-actin filaments within the cell. Combining these findings together, our results show that an inflammatory response heavily impacts the morphology, cell mechanics, migration, cytoskeletal dynamics, and applied traction forces of endothelial cells.

¹JV thanks NSF support through a REU award and HAE thanks NSF support through CMMI0643783.

5:06PM T40.00012 Healing of small circular model wounds, OLIVIER COCHET, PHILIPPE MARCQ, JONAS RANFT, Laboratoire Physico-Chimie Curie, UMR168, Institut Curie/CNRS, MYRIAM REFFAY, Laboratoire Matière et Systèmes Complexes, Université Paris Diderot/CNRS, AXEL BUGUIN, PASCAL SILBERZAN, Laboratoire Physico-Chimie Curie, UMR168, Institut Curie/CNRS, BIOLOGY INSPIRED PHYSICS AT MESOSCALE TEAM¹, PHYSICAL APPROACH OF BIOLOGICAL PROBLEMS TEAM² — We develop a new method to produce numerous circular wounds in an epithelial tissue of MDCK cells in a non-traumatic fashion. The reproducibility of the wounds allows for a quantitative study of the dynamics of healing and for a better understanding of the key processes involved in those collective morphogenetic movements. First, we show different mechanisms of closing depending on the initial size of the wound. We then focus on the healing of the smallest wounds from an experimental and theoretical point of view. At the onset of closure, an actomyosin ring is formed around the wound and small protrusions appear and invade the free surface. Using inhibition and laser ablation experiments, we show the relative contribution of both processes to the dynamics of closing. Finally, we develop a theoretical model of the tissue as a whole, combined with the observed forces, in order to better understand the underlying mechanics of this process. We hope that this qualitative and quantitative description will prove useful in the future for the study of epithelial architecture, collective mechanisms in migrating tissues and, on a broader context, cellular invasion in cancerous tissues.

¹Olivier Cochet, Myriam Reffay, Axel Buguin, Pascal Silberzan

²Philippe Marcq, Jonas Ranft

5:18PM T40.00013 Mechanical coupling of smooth muscle cells using local and global stimulations¹, CRAIG COPELAND, Johns Hopkins University, CHRISTOPHER CHEN, University of Pennsylvania, DANIEL REICH, Johns Hopkins University — Mechanical stresses can directly alter many cellular processes, including signal transduction, growth, differentiation, and survival. These stresses, generated primarily by myosin activity within the cytoskeleton, regulate both cell-substrate and cell-cell interactions. We report studies of mechanical cell-cell and cell-substrate interactions using patterned arrays of flexible poly(dimethylsiloxane) (PDMS) microposts combined with application of global stretch or local chemical stimulation. Bovine pulmonary artery smooth muscle cells are patterned onto micropost arrays to create multicellular structures to probe intercellular coupling. Global stimulation is applied by building the micropost arrays on a flexible membrane that can be stretched while allowing simultaneous observation of cell traction forces. Results for triangle wave stretches of single cells show increasing traction forces with increasing strain, and immediate weakening of traction forces as strain is decreased. "Spritzing," a laminar flow technique, is used to expose a single cell within a construct to a drug treatment while cell traction forces are recorded via the microposts. Results will be described showing the response of cells to external stimulation both directly and through intercellular coupling.

¹Supported in part by NIH grant HL090747

Wednesday, February 29, 2012 2:30PM - 5:42PM – Session T41 DFD: Swimming, Motility and Locomotion 156B

2:30PM T41.00001 Undulatory swimming on a free surface¹, RAMIRO GODOY-DIANA, SOPHIE RAMANANARIVO, OLIVIA GANN, BENJAMIN THIRIA, PMMH UMR7636 CNRS; ESPCI ParisTech; UPMC; U. Diderot Paris 7 — A wide variety of swimmers in nature use body undulations to generate a propulsive force, in part owing to the relative insensitivity of the principle of undulatory swimming to the value of the Reynolds number $Re = UL/\nu$, which measures the relative importance of viscous and inertial forces in the flow considered (U and L being the typical speed and length of the animal, and ν the kinematic viscosity of the surrounding fluid). Here we study a flexible filament forced to oscillate by imposing a harmonic motion to one of its extremities (using magnetic interactions) and propelling itself at the surface of a water tank. This experiment serves as a canonical model for studying the interactions between an elastic structure undergoing complex deformations and the surrounding fluid.

¹We acknowledge support from the French National Research Agency through project No. ANR-08-BLAN-0099 and of EADS Foundation through project "Fluids and elasticity in biomimetic propulsion"

2:42PM T41.00002 Geometry, Curvature, and Locomotion, ROSS HATTON, HOWIE CHOSET, Carnegie Mellon University — Many animals and robots locomote by undulating their bodies in traveling waves. Together with the generally inextensible nature of such systems, the large deformations involved in these motions introduce significant nonlinearities into their analysis. As a result, the equations of motion for these systems are often treated as black boxes – the displacement resulting from a given input (e.g., wave amplitude) can be calculated, but the relationship between the inputs and the net displacement over a period of the wave is hidden inside the nonlinearities. Drawing on results from the geometric mechanics community, we have developed an analysis framework for high-deformation locomotion that looks inside this black box, based on three core principles: (1) Working in terms of body curvature provides a linear basis for describing nonlinear high-deformation shapes. (2) Lie bracket analysis (the exploitation of system nonlinearities through oscillatory inputs) captures the nonlinearity of the system interaction with the world. (3) Systematically optimizing the coordinate choice transforms the system nonlinearity into a form that can be geometrically analyzed over the space of body curvatures to characterize the system's ultimate locomotory capabilities.

2:54PM T41.00003 Optimizing turning for locomotion, LISA BURTON, Massachusetts Institute of Technology, ROSS HATTON, HOWIE CHOSET, Carnegie Mellon University, A.E. HOSOI, Massachusetts Institute of Technology — Speed and efficiency are common and often adequate metrics to compare locomoting systems. These metrics, however, fail to account for a system's ability to turn, a key component in a system's ability to move a confined environment and an important factor in optimal motion planning. To explore turning strokes for a locomoting system, we develop a kinematic model to relate a system's shape configuration to its external velocity. We exploit this model to visualize the dynamics of the system and determine optimal strokes for multiple systems, including low Reynolds number swimmers and biological systems dominated by inertia. Understanding how shape configurations are related to external velocities enables a better understanding of biological and man made systems. Using these tools, we can justify biological system motion and determine optimal shape configurations for robots to maneuver through difficult environments.

3:06PM T41.00004 Effect of confinements: Bending in Paramecium, AJA EDDINS, Engineering Science and Mechanics - Virginia Tech, SUNG YANG, Department of Nano-bio Materials and Electronics, GIST, Republic of Korea, CORRIE SPOON, SUNGHWAN JUNG, Engineering Science and Mechanics - Virginia Tech — Paramecium is a unicellular eukaryote which by coordinated beating of cilia, generates metachronal waves which causes it to execute a helical trajectory. We investigate the swimming parameters of the organism in rectangular PDMS channels and try to quantify its behavior. Surprisingly a swimming Paramecium in certain width of channels executes a bend of its flexible body (and changes its direction of swimming) by generating forces using the cilia. Considering a simple model of beam constrained between two walls, we predict the bent shapes of the organism and the forces it exerts on the walls. Finally we try to explain how bending (by sensing) can occur in channels by conducting experiments in thin film of fluid and drawing analogy to swimming behavior observed in different cases.

3:18PM T41.00005 ABSTRACT WITHDRAWN —

3:30PM T41.00006 Enhanced swimming motion of nematode in a non-Newtonian fluid, JIN-SUNG PARK, Department of Physics and School of Engineering and Applied Sciences, Harvard University, DAEYEON KIM, JENNIFER SHIN, School of Mechanical, Aerospace and Systems Engineering, Division of Mechanical Engineering, Korea Advanced Institute of Science and Technology, DAVID WEITZ, Department of Physics and School of Engineering and Applied Sciences, Harvard University — Small organisms navigate their complex terrestrial substrates, which have the property of non-Newtonian complex fluids. Although a large body of literature exists on the locomotion of these organisms, the previous studies are mostly limited in simple Newtonian systems. Here we present experimental results on the locomotion of *Caenorhabditis elegans* (*C. elegans*), especially investigated in colloidal suspensions that exhibit the behavior of shear thinning fluid in the range of shear rate of undulating nematode. Interestingly, we observed that the swimming speed of nematodes was gradually increased with an increase of particle volume fraction in suspensions, and this enhanced motion of nematode is closely related to the shear thinning in the fluid viscosity.

3:42PM T41.00007 Hydrodynamic Optimality in the Bacterial Flagellum, SAVERIO SPAGNOLIE, Brown University, ERIC LAUGA, University of California, San Diego — Most bacteria swim through fluids by rotating helical flagella which can take one of 12 distinct polymorphic shapes, the most common of which is the normal form used during forward swimming runs. To shed light on the prevalence of the normal form in locomotion, we have gathered all available experimental measurements of the various polymorphic forms and computed their intrinsic hydrodynamic efficiencies. The normal helical form is found to be the most efficient of the 12 polymorphic forms by a significant margin—a conclusion valid for both the peritrichous and polar flagellar families, and robust to a change in the effective flagellum diameter or length. Hence, although energetic costs of locomotion are small for bacteria, fluid mechanical forces may have played a significant role in the evolution of the flagellum.

3:54PM T41.00008 Characterisation of metachronal waves on the surface of the spherical colonial alga *Volvox carteri*, DOUGLAS BRUMLEY, MARCO POLIN, CONSTANT MOREZ, RAYMOND GOLDSTEIN, TIMOTHY PEDLEY, University of Cambridge — *Volvox carteri* is a spherical colonial alga, consisting of thousands of biflagellate cells. The somatic cells embedded on the surface of the colony beat their flagella in a coordinated fashion, producing a net fluid motion. Using high-speed imaging and particle image velocimetry (PIV) we have been able to accurately analyse the time-dependent flow fields around such colonies. The somatic cells on the colony surface may beat their flagella in a perfectly synchronised fashion, or may exhibit metachronal waves travelling on the surface. We analyse the dependence of this synchronisation on fundamental parameters in the system such as colony radius, characterise the speed and wavelength of the observed metachronal waves, and investigate possible models to account for the exhibited behaviour.

4:06PM T41.00009 Collective dynamics of active suspensions in confined geometries, DENIS BARTOLO, ESPCI-Paris Diderot University, ERIC LAUGA, UCSD, JEAN-BAPTISTE CAUSSIN, ENS Lyon — We discuss the collective dynamics of suspensions of self-propelled particles confined in confined geometries. First, we revisit the conventional description of the hydrodynamic couplings between swimmers living in thin films or in shallow channels. We show that these hydrodynamic interactions are chiefly set by the particle size and shape irrespective of the microscopic propulsion mechanism. Second, we use kinetic theory to study the phase behavior of dilute suspensions. Finally, we exploit these results to show that the hydrodynamic interactions destabilize isotropic suspensions of polar particles, thereby yielding spontaneous collective motion at large scales. In contrast, suspensions of apolar particles only display weakly cooperative motion at small scales. We also investigate the case of aligned suspensions. Their behavior is very similar to the bulk phase of dipolar swimmer. They display generic instabilities at all scales. Comparisons of our theoretical findings with experiments on artificial swimmers will be shown.

4:18PM T41.00010 Giant number fluctuations in self-propelled particles without alignment¹, YAOUEN FILY, SILKE HENKES, Syracuse University, M. CRISTINA MARCHETTI, Syracuse University and Syracuse Biomaterials Institute — Giant number fluctuations are a ubiquitous property of active systems. They were predicted using a generic continuum description of active nematics, and have been observed in simulations of Vicsek-type models and in experiments on vibrated granular layers and swimming bacteria. In all of these systems, there is an alignment interaction among the self-propelled units, either imposed as a rule, or arising from hydrodynamic or other medium-mediated couplings. Here we report numerical evidence of giant number fluctuations in a minimal model of self-propelled disks in two dimensions in the absence of any alignment mechanism. The direction of self-propulsion evolves via rotational diffusion and the particles interact solely via a finite range repulsive soft potential. It can be shown that in this system self propulsion is equivalent to a non Markovian noise whose correlation time is controlled by the amplitude of the orientational noise.

¹Supported by the NSF through grants DMR-0806511 and DMR-1004789. The computations were carried out on SUGAR, a cluster supported by NSF-PHY-1040231.

4:30PM T41.00011 Chemotactic Self-Organization of Bacteria in Three-Dimensions, YEVGENIY KALININ, DAVID GRACIAS, Chemical and Biomolecular Engineering, Johns Hopkins University — Self-assembly with cellular building blocks represents an important yet relatively unexplored area of research. In this talk, we describe the self-assembly of motile cells using three-dimensional (3D) patterns of chemical (such as chemoattractants) that guide cellular and organization. These 3D chemical patterns are created when chemicals are released via diffusion from lithographically patterned self-assembled polyhedral containers. We show that a number of conceptually different strategies can be utilized for chemical patterns creation. In one such strategy, the overall shape of the container can be chosen to closely match the desired 3D spatial profile. As a part of a different strategy, we discuss how the chemical patterns can be engineered by specific placement of pores on the polyhedral containers. Combining these two strategies allows chemicals to be released in a variety of spatial patterns. To demonstrate applicability of our concept to in vitro organization of living cells in specific 3D geometries, we describe chemotactic self-organization of *E. coli* bacteria in a variety of well-defined shapes and space curves. We link the parameters that characterize the patterns of cells and the patterns of chemicals and describe how one can engineer the spatial shape of the multicellular constructs.

4:42PM T41.00012 Collective Dynamics of a Laboratory Insect Swarm, NICHOLAS OUELLETTE, DOUGLAS KELLEY, NIDHI KHURANA, Dept. of Mech. Eng., Yale University — Self-organized collective animal behavior is ubiquitous throughout the entire biological size spectrum. But despite broad interest in the dynamics of animal aggregations, little empirical data exists, and modelers have been forced to make many assumptions. In an attempt to bridge this gap, we report results from a laboratory study of swarms of the non-biting midge *Chironomus riparius*. Using multicamera stereoimaging and particle tracking, we measure the three-dimensional trajectories and kinematics of each individual insect, and study their statistics and interactions.

4:54PM T41.00013 Dimensional transitions for coupled rotational/translational diffusion in powered nanorotors¹, AMIR NOURHANI, Chem. Eng. Dpt., Penn State Univ, PAUL LAMMERT, Phys. Dpt., Penn State Univ, ALI BORHAN, Chem. Eng. Dpt., Penn State Univ, VINCENT CRESPI, Phys. Dpt., Penn State Univ — Small colloidal particles in fluids are well-known to engage in rotational and translational Brownian motion. Over the past several years, experimentalists have developed a new class of colloidal particles which exhibit autonomous powered motion due to consumption of chemical fuels. Two such classes of nanomotor that have been developed are linear and rotary motors. Nanorotors engage in cyclical motions due to asymmetries in the distribution of force on the surface of the particles. We have analyzed the diffusion of powered rotary motors, considering how the addition of a powered component to their motion affects their diffusional properties.

¹Supported by MRSEC at Penn State

5:06PM T41.00014 Swimming of bio-inspired micro robots in circular channels, SERHAT YESILYURT, FATMA ZEYNEP TEMEL, Sabanci University — In recent years, bio-inspired micro swimming robots have been attracting attention for use in biomedical tasks such as opening clogged arteries, carrying out minimally invasive surgical operations, and carrying out diagnostic tasks. There have been a number of experimental and modeling studies that address swimming characteristics of micro swimmers with helical tails attached to magnetic heads that rotate and move forward in rotating external magnetic fields. We carried out experimental studies with millimeter long helical swimmers in glass tubes placed in between Helmholtz coils, and demonstrated that swimming speed increases linearly with the frequency of the external field up to the step-out frequency. In order to study interaction of the swimmer with the circular boundary we used a computational fluid dynamics model. In simulations we compared swimming speeds of robots with respect to the frequency of the external magnetic field, wavelength and amplitude of the helical tail, and distance to the channel wall. According to simulation results, as the swimmer gets closer to the boundary swimming speed and efficiency improve. However step-out frequency decreases near the wall due to increased torque to rotate the swimmer.

5:18PM T41.00015 ABSTRACT WITHDRAWN —

5:30PM T41.00016 Bristle-Bots: a model system for locomotion and swarming, LUCA GIOMI, NICO HAWLEY-WELD, L. MAHADEVAN, Harvard University — The term *swarming* describes the ability of a group of similarly sized organisms to move coherently in space and time. This behavior is ubiquitous among living systems: it occurs in sub-cellular systems, bacteria, insects, fish, birds, pedestrians and in general in nearly any group of individuals endowed with the ability to move and sense. Here we address the problem of the origin of collective behavior in systems of self-propelled agents whose only social capability is given by aligning contact interactions. Our model system consists of a collection of Bristle-Bots, simple automata made from a toothbrush and the vibrating device of a cellular phone. When Bristle-Bots are confined in a limited space, increasing their number drives a transition from a disordered and uncoordinated motion to an organized collective behavior. This can occur through the formation of a swirling cluster of robots or a collective dynamical arrest, according to the type of locomotion implemented in the single devices. It is possible to move between these two major regimes by adjusting a single construction parameter.

Wednesday, February 29, 2012 2:30PM - 5:06PM —
Session T42 DBIO GSNP: Focus Session: Evolutionary Systems Biology III - Evolutionary Games 156C

2:30PM T42.00001 Bacterial tower of Babel –How cheating and lying diversify bacterial communication, AVIGDOR ELDAR, Tel-Aviv University, Department of molecular microbiology and biotechnology — In microbial “quorum sensing” (QS) communication systems, microbes produce and respond to a signaling molecule, enabling a cooperative response at high cell densities. Many species of bacteria show fast, intraspecific, evolutionary divergence of their QS pathway specificity—signaling molecules activate cognate receptors in the same strain but fail to activate, and sometimes inhibit, those of other strains. Despite many molecular studies, it has remained unclear how a signaling molecule and receptor can coevolve, what maintains diversity, and what drives the evolution of cross-inhibition. Here I use mathematical analysis to show that when QS controls the production of extracellular enzymes —“public goods”—diversification can readily evolve. Coevolution is positively selected by cycles of alternating “cheating” receptor mutations and “cheating immunity” signaling mutations. The maintenance of diversity and the evolution of cross-inhibition between strains are facilitated by facultative cheating between the competing strains. My results suggest a role for complex social strategies in the long-term evolution of QS systems. More generally, my model of QS divergence suggests a form of kin recognition where different kin types coexist in unstructured populations.

3:06PM T42.00002 Coupling between evolutionary and population dynamics in experimental microbial populations, ALVARO SANCHEZ, JEFF GORE, Department of Physics, Massachusetts Institute of Technology — It has been often been assumed that population dynamics and evolutionary dynamics occur at such different timescales that they are effectively de-coupled. This view has been challenged recently, due to observations of evolutionary changes occurring in short timescales. This has led to a growing interest in understanding eco-evolutionary dynamics of populations. In this context, recent theoretical models have predicted that coupling between population dynamics and evolutionary dynamics can have important effects for the evolution and stability of cooperation, and lead to extremely rich and varied dynamics. Here, we report our investigation of the eco-evolutionary dynamics of a cooperative social behavior, sucrose metabolism, in experimental yeast populations. We have devised an experimental strategy to visualize trajectories in the phase space formed by the population size (N) and the fraction of cooperator cells in the population (f). Our measurements confirm a strong coupling between evolutionary and population dynamics, and allowed us to characterize the bifurcation plots. We used this approach to investigate how sudden environmental changes affect the stability and recovery of populations, and therefore the stability of cooperation.

3:18PM T42.00003 Competition between species can drive public goods cooperation within a species, HASAN CELIKER, EECS department, MIT, JEFF GORE, Physics department, MIT — Costly cooperative strategies are vulnerable to exploitation by cheats. Microbial studies have suggested that cooperation can be maintained in nature by mechanisms such as reciprocity, spatial structure and multi-level selection. So far, however, almost all laboratory experiments aimed at understanding cooperation have relied on studying a single species in isolation. In contrast, species in the wild live within complex communities where they interact with other species. Little effort has focused on understanding the effect of interspecies competition on the evolution of cooperation within a species. We test this relationship by using sucrose metabolism of budding yeast as a model cooperative system. We find that when co-cultured with a bacterial competitor, yeast populations become more cooperative compared to isolated populations. We show that this increase in cooperation within yeast is mainly driven by resource competition imposed by the bacterial competitor. A similar increase in cooperation is observed in a pure yeast culture when essential nutrients in the media are limited experimentally.

3:30PM T42.00004 The emergence of cooperation from a single cooperative mutant, JONAS CREMER, University of California, San Diego, ANNA MELBINGER, ERWIN FREY, Ludwig-Maximilians University Munich, Germany — Population structure is one central condition which promotes the stability of cooperation: If cooperators more likely interact with other cooperators (positive assortment), they keep most of their benefit for themselves and are less exploited by non-cooperators. However, positive assortment can only act successfully if cooperation is already well established in the population such that cooperative individuals can successfully assort. But how can cooperation emerge when starting with a single cooperative mutant? Here we study this issue for a generic situation of microbial systems where microbes regularly form new colonies and show strong population growth. We show how and when the dynamical interplay between colony formation, population growth and evolution within colonies can provoke the emergence of cooperation. In particular, the probability for a single cooperative mutant to succeed is robustly large when colony-formation is fast or comparable to the time-scale of growth within colonies; growth supports cooperation.

[1] A. Melbinger, J. Cremer, and E. Frey, Evolutionary game theory in growing populations, *Phys. Rev. Lett.* **105**, 178101 (2010)

[2] J. Cremer, A. Melbinger, and E. Frey, Evolutionary and population dynamics: a coupled approach, arXiv:1108.2604

3:42PM T42.00005 Coping with stress in a synthetic world, LINGCHONG YOU, Duke University — A major focus of synthetic biology is the engineering of gene circuits to perform user-defined functions. In addition to generating systems of practical applications, such efforts have led to the identification and evaluation of design strategies that enable robust control of dynamics in single cells and in cell populations. On the other hand, there is an increasing emphasis on using engineered systems programmed by simple circuits to explore fundamental biological questions of broad significance. In this talk, I will discuss our efforts along this line of research, whereby we have used engineered gene circuits to examine the evolutionary dynamics of two common bacterial survival strategies in stress response: programmed death and cell-cell communication.

4:18PM T42.00006 Bacterial cheating limits antibiotic resistance, HUI XIAO CHAO, EUGENE YURTSEV, Gore Lab, Department of Physics, Massachusetts Institute of Technology, MANOSHI DATTA, Computational Systems Biology, Massachusetts Institute of Technology, TANYA ARTEMOVA, JEFF GORE, Gore Lab, Department of Physics, Massachusetts Institute of Technology — The widespread use of antibiotics has led to the evolution of resistance in bacteria. Bacteria can gain resistance to the antibiotic ampicillin by acquiring a plasmid carrying the gene beta-lactamase, which inactivates the antibiotic. This inactivation may represent a cooperative behavior, as the entire bacterial population benefits from removing the antibiotic. The cooperative nature of this growth suggests that a cheater strain—which does not contribute to breaking down the antibiotic—may be able to take advantage of cells cooperatively inactivating the antibiotic. Here we find experimentally that a “sensitive” bacterial strain lacking the plasmid conferring resistance can invade a population of resistant bacteria, even in antibiotic concentrations that should kill the sensitive strain. We observe stable coexistence between the two strains and find that a simple model successfully explains the behavior as a function of antibiotic concentration and cell density. We anticipate that our results will provide insight into the evolutionary origin of phenotypic diversity and cooperative behaviors.

4:30PM T42.00007 Bacterial Transformation and Competition Under Antibiotic Stress, JONAS PEDERSON, Danish Technical University, ANDREW BERGMAN, None, CHRIS CLEVELAND, Princeton University, TOLGA CAGATAY, UT Southwestern, ROBERT AUSTIN, Princeton University, GABOR BALASZI, M.D. Anderson Medical Center — Transformation, the process by which bacteria uptake DNA directly from their environment and incorporate it as their own genetic material, is a form of Horizontal Gene Transfer that occurs throughout nature as an important mechanism for spurring on bacterial evolution. We examine the capacity of bacteria to undergo transformation and will discuss work that has been done by the Austin group using Micro-Habitat Patches (MHPs) to examine the emergence of phenotypes due to horizontal gene transfer.

4:42PM T42.00008 Rapid Antibiotic Resistance Evolution of GASP Mutants, QIUCEN ZHANG, Princeton University, HYUNSUNG KIM, NADER POURMAND, UC Santa Cruz, ROBERT AUSTIN, Princeton University — The GASP phenotype in bacteria is due to a mutation which enables the bacteria to grow under high stress conditions where other bacteria stop growing. We probe using our Death Galaxy microenvironment how rapidly the GASP mutant can evolve resistance to mutagenic antibiotics compared to wild-type bacteria, and explore the genomic landscape changes due to the evolution of resistance.

4:54PM T42.00009 Spatial vs. individual variability with inheritance in a stochastic Lotka-Volterra system, ULRICH DOBRAMYSL, UWE C. TAUBER, Department of Physics, Virginia Tech — We investigate a stochastic spatial Lotka-Volterra predator-prey model with randomized interaction rates that are either affixed to the lattice sites and quenched, and / or specific to individuals in either population. In the latter situation, we include rate inheritance with mutations from the particles' progenitors. Thus we arrive at a simple model for competitive evolution with environmental variability and selection pressure. We employ Monte Carlo simulations in zero and two dimensions to study the time evolution of both species' densities and their interaction rate distributions. The predator and prey concentrations in the ensuing steady states depend crucially on the environmental variability, whereas the temporal evolution of the individualized rate distributions leads to largely neutral optimization. Contrary to, e.g., linear gene expression models, this system does not experience fixation at extreme values. An approximate description of the resulting data is achieved by means of an effective master equation approach for the interaction rate distribution.

Wednesday, February 29, 2012 2:30PM - 5:30PM –

Session T44 DPOLY: Focus Session: Interparticle Interactions in Polymer Nanocomposites - Grafted Chains 157C

2:30PM T44.00001 Colloidal assembly on soft substrates, JURE DOBNIKAR, TINE CURK, FRANCISCO MARTINEZ VERACOECHEA, DAAN FRENKEL, University of Cambridge, UK — We studied – by Monte Carlo computer simulations - ordering of hard sphere colloidal particles subject to gravity and soft interactions induced by polymer-coated substrates. The polymers are randomly anchored to a flat surface with an average density ranging from very dilute values to a situation where a dense polymer brush with the average height h forms. Studying a single colloid subject to such substrate and the gravity we observed a transition from a regime where it is confined to the hard surface at $z=0$, via a bimodal regime where it is equally likely to find it at the bottom or at the top, to the regime where it lies on top of the brush at $z=h$. In a system of many colloids the polymers induce an effective colloid-colloid interaction of entropic origin. We have performed Grand canonical Monte Carlo simulations and explored the structure formation as a function of the anchoring density and the effective gravity of the colloids. Colloids are initially attracted and grow into elongated assemblies with a well-defined lateral width. At low grafting densities such assemblies form percolated networks, while at high enough grafting densities finite clusters are observed. We discuss the relevance of our results to applications like particle sorting, reactions catalysis and passive diffusion.

2:42PM T44.00002 Molecular Dynamics Simulations on the Thermal and Mechanical Properties of Blend of Polymer and Polymer Grafted Nanoparticles, SANAT KUMAR, DONG MENG, Department of Chemical Engineering, Columbia University, GARY GREST, Sandia National Laboratories — Grafting polymers onto the surface of NPs has become one of the most effective approaches to integrate NPs into polymer melts. It then becomes crucial to be able to understand how the presence of grafted chains affects the effective interactions between NPs as well as the mechanical properties of the resulting composites. Using molecular dynamics simulations we first measure the potential of mean force between grafted NPs from two-particle simulations. Simulations of systems containing many grafted NPs are then performed to determine the phase behavior and structure of grafted NPs in explicit polymer matrices. Finally, we cool the nanocomposites to temperatures below their glass transition and stress the systems to investigate how the presence of grafted NPs changes their mechanical properties.

2:54PM T44.00003 Self Assembly of Tethered Nanoparticle Telechelics, RYAN MARSON, Materials Science and Engineering, University of Michigan, CAROLYN PHILLIPS, Applied Physics, University of Michigan, JOSHUA ANDERSON, SHARON GLOTZER, Chemical Engineering, University of Michigan — Simulations, theory, and experiment predict that aggregating nanoparticles functionalized with polymer tethers can self-assemble to form phases seen in block copolymer and surfactant systems, but with additional nanoparticle ordering and mesophase complexity. Here we consider a novel class of “telechelic” tethered nanoparticle building blocks, where two nanoparticles are connected together by a polymer tether. The architecture is similar to a triblock copolymer, but with additional geometric constraints imposed by the rigid particle end groups. Using Brownian dynamics simulations, we explore the phase diagrams of several examples of this class of nano-building-block, and present predictions of novel phases and their dependence on particle size, tether length, and thermodynamic parameters. We compare our results with recent simulations of di-tethered nanospheres [1, 2] and mono-tethered nanospheres [2, 3].

1. Iacovella, C. R.; Glotzer, S. C.; *Soft Matter* **2009**, 5, 4492-4498.
2. Iacovella, C. R.; Keys, A.S.; Glotzer, S. C. *PNAS*, in press. arXiv:1102.5589.
3. Phillips, C. L.; Iacovella, C. R.; Glotzer, S. C.; *Soft Matter* **2010**, 6, 1693-1703.

3:06PM T44.00004 Controlling the Phase Behavior of Gold Nanoparticles within Polymer Matrix by Varying Composition and Length of Ligands, SEYONG KIM, MISANG YOO, Korea University, BUMJOON KIM, Korea Advanced Institute of Science and Technology, JOONA BANG, Korea University — Nanocomposites have been investigated for many years due to their fascinating features. In spite of the captivative properties, compatibility problem has been an obstacle for manufacturing the nanocomposites. To achieve the compatibility between NPs and polymer matrix, thiol-terminated polymeric ligands have been used for tuning the surface property of the NPs. However, in case of Au NPs, Au-thiol bond is unstable above 60 °C. In our recent work, we designed thermally stable Au NPs by using thiol terminated photo crosslinkable block copolymer, PS-b-PSN3-SH. With the thermally stable Au NPs, we demonstrated that Au NPs are stable at high temperature and can serve as compatibilizers for PS/PMMA blends. Herein, we prepared Au NPs using photo crosslinkable polymeric ligands which have various ligand composition and lengths. As the ligands characteristics were changed, the phase behaviors of Au NPs in both homopolymer and block copolymer bulk sample were significantly different. For example, the NPs become more dispersed within the polymer matrix with longer polymer ligands, while they are aggregates when shorter ligands were used. In this work, morphologies of Au NPs within polymer matrix were systematically investigated using the cross-sectional transmission electron microscopy.

3:18PM T44.00005 ABSTRACT WITHDRAWN —

3:30PM T44.00006 Molecular Weight Distribution Effects on the Structure of Strongly Adsorbed Polymers by Monte Carlo Simulation, VIKRAM KUPPA, University of Cincinnati — Monte Carlo simulations are used to investigate the adsorption of polymers from solution onto strongly attractive, perfectly smooth substrates. Using a coarse-grained united atom model for freely rotating polymer chains, three systems with different polydispersities are studied. The structure of the adsorbed layers, exemplified by density profiles, bond orientation order parameters, radii of gyration, and distribution of the adsorbed chain fractions, is shown to be highly dependent on the molecular weight distribution of the polymer phase. The results for the more monodisperse polymer systems are qualitatively similar to experimental and theoretical investigations, but devolve from very different chain conformations and statistics. For the first time ever, equilibrium polymer adsorption on highly attractive surface is studied, with all molecules in the adsorbed layers demonstrated to be indistinguishable from each other. The ergodicity of states explored by the polymer chains is in contrast to the kinetically constrained viewpoint of irreversible adsorption, and the observed behavior is explained in the context of the competition between polymers to make contact with the surface.

3:42PM T44.00007 Role of Stretchable Arms, Grafting Density and Parallel Reformable Bonds in the Self-Healing of Cross-Linked Star Nanogel Particles, BALAJI IYER VAIDYANATHAN SHANTHA, ISAAC SALIB, VICTOR YASHIN, GERMAN KOLMAKOV, University of Pittsburgh, KRZYSZTOF MATYJASZEWSKI, Carnegie Mellon University, ANNA BALAZS, University of Pittsburgh — We investigate the role of stretchable and reformable bonds in the self-healing of a network formed by star-like nanogel particles. The individual particles of the network are composed of a cross-linked gel core and a corona of grafted polymeric arms with sticky end groups. The sticky groups in the coronas of adjacent particles interact to form multiple labile bonds (up to N) that lead to the formation of the nanogel network. Interaction between soft colloids with polymeric arms is combined with the Bell model for rupture and formation of bonds to model the interaction of array of particles. While the stretch of the bonds is captured through the bond spring constant (k) and cutoff radius for bond breaking (rc), the equilibrium distance (req) at which the labile bonds reform is obtained from the corona thickness. We show that the presence of stretchable arms allows for rearrangements leading to either increase or decrease of the strength and ductility of the nanogel network depending on the grafting density. We also show that while the force required to rupture the nanogel network is proportional to the number of parallel bonds (N), the ductility is a more complex function of N.

3:54PM T44.00008 Poly(ethylene-oxide)/clay/silica nanocomposites: Morphology and thermomechanical properties, ENGIN BURGAZ, Materials Sci. and Eng., Ondokuz Mayıs Univ. Samsun, Turkey — Poly(ethylene oxide) PEO/clay/silica nanocomposites were prepared via solution intercalation by exploiting phase separation based on the bridging of particles by polymer chains. The intercalated morphology of nanocomposites was confirmed by XRD. Vibrational modes of the ether oxygen of PEO in the hybrids are shifted due to the coordination of the ether oxygen with the sodium cations of clay and the H-bonding interactions of the ether oxygen with the surface silanols of hydrophilic fumed silica. Based on SEM, the overall density of nanoparticle aggregates in the interspherulitic region was observed to be higher compared to that inside spherulites. PEO/clay/silica hybrids show significant property improvements compared to PEO/clay hybrids and pure PEO. The system containing 10 wt.% clay and 5 wt.% silica has substantially higher modulus and much lower crystallinity compared to the 15 wt.% clay system. The physics behind the reinforcement effect and the reduction of crystallinity as a function of fumed silica loading is discussed based on the morphological characterization of the hybrids. Lastly, PEO/clay/silica hybrids display good thermal stability and are much stiffer compared to pure PEO and PEO/clay nanocomposites.

4:06PM T44.00009 Copolymer mediated interactions in dense nanocomposites: role of chemical heterogeneity and sequence, DEBAPRIYA BANERJEE, KENNETH S. SCHWEIZER, UIUC — Microscopic PRISM integral equation theory is applied to study the structure and dispersion of nanospheres in AB copolymer melts as a function of architecture and chemical heterogeneity of the interfacial attractions spanning the depletion, stabilization and bridging regimes. For a random copolymer (RCP) with coexisting weak and strong monomer-particle attractions, the nanoparticle potential-of-mean-force (PMF) at intermediate copolymer compositions varies non-monotonically between the two homopolymer limits. Non-adsorbing monomers are generically found to be crucial for achieving good filler dispersion in RCP melts. For 50/50 multiblock melts the role of block length, R , has been studied over a wide range ($R=1,2,5,10,25,50$). Filler miscibility dramatically increases when one of the monomers is weakly adsorbing (depletion). Dispersion is also improved for some block lengths when one of the monomers strongly adsorbs (bridging) due to the emergence of a long-ranged repulsive barrier in the PMF just beyond a local non-contact minimum, resulting in a positive second virial coefficient. Strikingly, better stability is predicted as the particle-to-monomer diameter ratio increases from 2 to 10, contrary to the behavior in homopolymer or RCP melts.

4:18PM T44.00010 Effect of bidispersity in grafted chain length on potential of mean force between polymer grafted nanoparticles in a homopolymer matrix, ARTHI JAYARAMAN, NITISH NAIR, University of Colorado at Boulder — In polymer nanocomposites consisting of polymer grafted nanoparticles in a polymer matrix the molecular weight of the grafted polymers plays a key role in dictating the effective inter-particle interactions. Despite the importance of graft molecular weight on effective inter-particle interactions in monodisperse polymer grafted nanoparticles, and evidence of non-trivial polydispersity effects in systems containing polymers grafted on flat surfaces, not much work has been done to explore polydispersity effects in polymer grafted nanoparticles. In this talk we will present self-consistent PRISM theory-Monte Carlo simulation studies showing how bidispersity in grafted chain lengths affects the grafted chain conformations and inter-particle interactions in a dense homopolymer polymer matrix. The value of the potential of mean force (PMF) between bidisperse grafted particles at contact is governed by the short grafts and values at large inter-particle distances are governed by the longer grafts. Our results suggest that by introducing bidispersity in grafted chains one can change the rules seen in monodisperse polymer grafted particles for wetting/dewetting of grafted polymers by matrix polymer.

4:30PM T44.00011 Concentration, Interaction and Temperature Dependent Chain Dynamics in Polybutadiene / Clay Nanocomposites Characterized by Solid State ^1H Double Quantum NMR Spectroscopy, XIAOLIANG WANG, Nanjing University, PINGCHUAN SUN, Nankai University, H. HENNING WINTER, University of Massachusetts, Department of Chemical Engineering, GI XUE, Nanjing University — A concentration, interaction and temperature dependent multimode segmental chain dynamics of carboxy terminated polybutadiene (CTPB) in CTPB/organo-clay (C18-clay) nanocomposite was investigated by solid state ^1H double quantum (DQ) NMR spectroscopy. Here, the measurements were performed on a series of samples of CTPB physically attached to the surface of C18-clay. NMR results showed that the nanocomposite exhibit discrete dynamic component with stepwise increase in their motional freedom with decreasing clay content. A remarkable change of CTPB chain dynamics at organo-clay concentration of 40 wt% was found, indicating a saturation effect of the polymer adsorbed on the clay surface. The transverse magnetization relaxation experiment help us quantitatively analysis the rigid, intermediate, and mobile components. Removal of either the end-group of CTPB or of the modifier on the clay changed the polymer-clay interaction profoundly, and thus changed polymer chain dynamics, especially for chains in proximity to the clay surface. The measurement confirmed our earlier hypothesis that the strong polymer-clay interaction was the key to the synergy effect in polymer/clay nanocomposites.

4:42PM T44.00012 Structural Transitions of Polymer Grafted Magnetic Nanoparticles¹, YANG JIAO, PINAR AKCORA, Stevens Institute of Technology — We decorate iron oxide nanoparticles with polymers to investigate the various interactions between particles and particle-polymer on the formation of different morphologies. We show that very low to intermediate grafting densities (2-20 chains/particle) can be achieved by controlling the concentration of free polymer chains in solution by grafting-to method. Nanostructural transitions of poly(styrene) grafted Fe_3O_4 nanoparticles are investigated upon varying the grafting densities and brush lengths. The roles of these parameters as well as dipolar force in the formation of various aggregates, such as star-like shape and chains, are discussed. This morphological transition is found to be sensitive to small grafting density change in very low to intermediate regime (0.01-0.04 chains/nm²). Interestingly, the matrix shows reverse effects on nanostructures with increment of brush lengths.

¹NSF-CAREER Award (DMR-0955170)

4:54PM T44.00013 ABSTRACT WITHDRAWN —

Wednesday, February 29, 2012 2:30PM - 5:30PM —
Session T45 DPOLY: Polymeric Glasses 159

2:30PM T45.00001 Formation of Polymer Glasses Under Stress and Its Influence on Physical Aging, LAURA GRAY, PAUL YOON, CONNIE ROTH, Department of Physics, Emory University — Understanding and controlling the stability and physical aging of polymer glasses is important for many technological applications from gas separation membranes to optical coatings. We investigate the stability of polymer glasses when thermally quenched under different stress conditions. Ellipsometry is used to measure the physical aging rate of polystyrene films supported or transferred onto silicon wafers. We quantify the time-dependent decrease in film thickness that results from the increase in average film density during aging to obtain a physical aging rate. We have observed significant differences between films quenched in a free-standing versus supported state, even though all films were aged in a supported state. Films quenched in a free-standing state exhibit a strong thickness dependence to their physical aging rate at micron length scales, an order of magnitude or two larger than thicknesses where nanoconfinement effects on the glass transition and modulus are typically observed. In contrast, supported films do not display any film thickness dependence to their aging rate at this large length scale. All available evidence suggests that different stress conditions are the underlying cause of this effect. In order to investigate the role of stress during the vitrification of polymer glasses, we have constructed a unique jig to apply a known stress to free-standing films during the thermal quench.

2:42PM T45.00002 Deformation-induced molecular mobility allows polystyrene glasses to flow, MARK EDIGER, BEN BENDING, KELLY CHRISTISON, University of Wisconsin-Madison — Experiments on colloidal glasses show that local rearrangements occur more rapidly during deformation. For polymeric glasses, similar features are expected but cannot be directly imaged. Dye reorientation has been used to measure segmental mobility in polymer glasses during active deformation. In creep deformations, we see a hundred-fold enhancement of mobility occurring in polystyrene glasses lightly cross-linked with 2 and 4 weight percent of divinylbenzene. Qualitatively similar mobility enhancement has been previously reported for lightly cross-linked poly(methyl methacrylate). Data from all three systems superpose on a master plot of the mobility as a function of the local strain rate during creep. Additionally, in the flow regime we see a significant narrowing of the distribution of relaxation times for both the polystyrene and poly(methyl methacrylate) glasses, similar to what has been reported for colloidal systems. Because polystyrene lacks the prominent beta relaxation of poly(methyl methacrylate), we conclude that the changes in mobility during creep deformation are a result of changes in the alpha segmental relaxation time.

2:54PM T45.00003 Temperature Divergence of the Dynamics of a PVAc glass: Dielectric vs. Mechanical Behaviors¹, GREGORY MCKENNA, JING ZHAO, Texas Tech University — The dynamics of glass forming liquids as the glass transition is traversed has become of special interest because of the continuing question as to whether or not these dynamics diverge towards an ideal glass transition/Kauzmann temperature or if the apparent Vogel-Fulcher divergence is lost as one goes below the conventional T_g but remains in equilibrium. Here we examine the response of a PVAc polymer glass-former using both dielectric and mechanical methods in the vicinity of T_g . Isothermal measurements were performed to study the aging behavior of PVAc and to assure that the equilibrium state was achieved and for temperatures to as much as 15 °C below the T_g . Surprisingly, we found that the mechanical response took much longer to age into equilibrium than did the dielectric response. Also, although the dielectric and mechanical responses seem to probe the glassy dispersion, the temperature dependence of the time-temperature shift factors obtained from the two methods are different and the dielectric measurement response shows a turnover to Arrhenius behavior rather than a continuation of the VFT divergence at the lowest temperatures tested.

¹The authors thank the National Science Foundation under grant DMR-0804438 for support of this project.

3:06PM T45.00004 Determination of effective correlation length in a glassy polymer using electrostatic force microscopy, BRANT RUMBERGER, NATHAN ISRAELOFF, Northeastern University — Various fourth-order correlation functions have been used to study the size of dynamically correlated regions in colloidal glasses and simulated glass forming liquids or polymers. However, measuring these correlation functions in molecular glasses has been limited by the small length scales on which the dynamics occur. Electrostatic force microscopy techniques are employed here to probe dielectric noise in polyvinyl acetate. We analyze fourth-order statistical fluctuations in order to determine spatio-temporal correlation lengths and their temperature dependence near the sample's glass transition. The first harmonic response of an applied AC voltage between the conducting AFM tip and the conducting substrate beneath the thin film polymer sample is proportional to the local electric polarization. Noise in this signal is examined and many hours are recorded at various temperatures in order to improve statistical precision. We employ a variety of statistical analysis techniques ranging from power spectrum analysis to variance of autocorrelation functions in order to find deviations from Gaussian statistics. Super-sharp carbon nanotube EFM tips (nominal radius of 10 nm) are employed to probe smaller effective volumes and thus more easily detect these fluctuations.

3:18PM T45.00005 Stable Nanostructured Polymer Films Formed Via Matrix Assisted Pulsed Laser Evaporation, YUNLONG GUO, KIMBERLY SHEPARD, RODNEY PRIESTLEY, Princeton University — Via typical routes to the vitreous state, the ability to significantly alter the properties of amorphous solids is restricted due to the kinetic nature of the glass transition. In this talk, we show that matrix assisted pulsed laser evaporation (MAPLE) can be used to form ultra-stable and nanostructured glassy polymers with significantly reduced densities, enhanced glass transition temperatures, and superior kinetic stability at high temperatures. Relative to the standard poly(methyl methacrylate) glass formed on cooling at standard rates, glasses prepared by MAPLE can be 40 percent less dense and have 40 K higher glass transition temperatures. Furthermore, the kinetic stability in the glassy-state can be enhanced by 2-orders-of-magnitude. The unique combination of properties is a result of the glass morphology, i.e., the glassy films are formed by the assembly of nearly spherical-like polymer nanoglobules.

3:30PM T45.00006 A Scattering Model for Amorphous, Intrinsically Microporous Polymers¹, AMANDA G. MCDERMOTT, Penn State University, PETER M. BUDD, University of Manchester, NEIL B. MCKEOWN, Cardiff University, CORAY M. COLINA, JAMES RUNT, Penn State University — We discuss the development of a scattering model for glassy, porous polymers in which porosity is equivalent to free volume, deriving significant insight from molecular dynamics simulations. Polymers of intrinsic microporosity (PIMs) exhibit high gas permeability and a large concentration of pores smaller than 1 nm; their porosity arises from an unusual chain structure combining rigid segments with sites of contortion, rather than from any templating effect. Although for many porous materials, useful information such as pore sizes and specific surface areas can be extracted from scattering patterns, a successful scattering model for PIMs must account for several unusual features. Simulated structures that reproduce characteristic scattering features are used to test model assumptions, with the ultimate goal of increasing the utility of scattering for studying microporous polymeric membrane processing and physical aging.

¹Supported by NSF (Materials World Network and Graduate Research Fellowship Program).

3:42PM T45.00007 Non-Equilibrium Water-Glassy Polymer Dynamics, ERIC DAVIS, Drexel University, MATTEO MINELLI, MARCO BASCHETTI, GIULIO SARTI, Università di Bologna, YOSSEF ELABD, Drexel University — For many applications (e.g., medical implants, packaging), an accurate assessment and fundamental understanding of the dynamics of water-glassy polymer interactions is of great interest. In this study, sorption and diffusion of pure water in several glassy polymers films, such as poly(styrene) (PS), poly(methyl methacrylate) (PMMA), poly(lactide) (PLA), were measured over a wide range of vapor activities and temperatures using several experimental techniques, including quartz spring microbalance (QSM), quartz crystal microbalance (QCM), and time-resolved Fourier transform infrared-attenuated total reflectance (FTIR-ATR) spectroscopy. Non-Fickian behavior (diffusion-relaxation phenomena) was observed by all three techniques, while FTIR-ATR spectroscopy also provides information about the distribution of the states of water and water transport mechanisms on a molecular-level. Specifically, the states of water are significantly different in PS compared to PMMA and PLA. Additionally, a purely predictive non-equilibrium lattice fluid (NELF) model was applied to predict the sorption isotherms of water in these glassy polymers.

3:54PM T45.00008 Self-consistent Mixing Rule for the Viscoelasticity of Heterogeneous Systems, FRANCOIS LEQUEUX, ESPCI/SIMM Paris France, PEILUO SHI, HELENE MONTES, None — Heterogeneous systems –like glasses mixtures - can exhibit huge local fluctuations of their viscoelastic modulus. The average viscoelastic modulus is often approximated either as the average modulus, or as the inverse of the average of the inverse of the modulus. Here we test a self-consistent method based on the Olroyd Palierne model for blend viscoelasticity [1]. We test this method on polymer miscible blends, with a very different glass transition temperature. We first deduce from Differential Scanning Calorimetric measurements the distribution of glass transition and thus of local viscoelastic modulus. From that we predict quantitatively the viscoelastic modulus of the polymer blends. It appears thus that the self-consistent averaging for disordered systems is extremely efficient, describing quantitatively systems where the modulus varies locally by at least 3 decades. [1] F. Lequeux, A. Ajdari, "Averaging rheological quantities in descriptions of soft glassy materials" Phys. Rev E 63 R030502 (2001)

4:06PM T45.00009 Understanding failure behavior of polymer glasses: a molecular viewpoint, GREGORY ZARTMAN, SHIWANG CHENG, SHI-QING WANG, The University of Akron — In surveying the vast literature we note that a unified simple picture appears to be lacking to account for all the known facts on failure behavior of polymer glasses. In this work, we first apply the fresh insight we have gained from studying nonlinear extensional rheology of entangled melt to show why a melt-stretched polystyrene turns ductile. We further show that the ductile polycarbonate can also turn brittle upon pre-melt-stretching. Finally, blending oligomeric PC into an originally ductile PC also causes the mixture to become brittle. All these old and new phenomena point to the fact that the strength of the load bearing chain network dictates at a given temperature whether the polymer glass would undergo ductile failure through shear yielding or brittle fracture via crazing. This presentation will provide a description of how the entanglement structure can be altered by melt deformation or the choice of different chemical specificity (that influences the packing length) to affect the strength of polymer glasses. It is this network strength relative to the yield strength associated with the inter-segmental van der Waals interactions that determines how strain localization (shear yielding – necking vs. crazing) takes place.

4:18PM T45.00010 Heterogeneous Dynamics During Creep of Rod Containing Polymer Nanocomposites, GREGORY TOEPPERWEIN, University of Wisconsin, ROBERT RIGGLEMAN, University of Pennsylvania, JUAN DE PABLO, University of Wisconsin — Polymer glasses exhibit regions of locally higher or lower mobility leading to heterogeneous dynamics. While heterogeneous dynamics have been examined in some detail in pure polymers, less is known about polymer nanocomposites (PNCs). We have previously studied PNCs, providing descriptions of how particles alter the network of entanglements, measuring local mechanical heterogeneity, demonstrating strain response under uniaxial deformation, and examining crazing and failure under multiaxial deformation. In the present work, we examine dynamic heterogeneity in rod-containing PNCs by performing creep deformation simulations and monitoring several measures of mobility. We are able to directly probe how dynamic heterogeneity evolves during deformation, and explore the origins of molecular mobility in polymer glasses. Examination of the segmental motion of a PNC undergoing creep reveals that the glassy heterogeneity of these systems decreases significantly following the onset of flow. It is found that the more heterogeneous distribution of relaxation times characteristic of PNCs in the bulk remains unaltered regardless of deformation state. It is found that the mobility and heterogeneity of PNCs are less susceptible to change upon deformation than those for the pure polymer.

4:30PM T45.00011 Molecular dynamics simulations of highly cross-linked polymer networks: prediction of thermal and mechanical properties, NATALIA SHENOGINA, Wright State University, Dayton, OH, MESFIN TSIGE, University of Akron, Akron, OH, SHARMILA MUKHOPADHYAY, Wright State University, Dayton, OH, SOUMYA PATNAIK, Wright-Patterson Air Force Base, Dayton, OH — We use all-atom molecular dynamics (MD) simulations to predict the mechanical and thermal properties of thermosetting polymers. Atomistic simulation is a promising tool which can provide detailed structure-property relationships of densely cross-linked polymer networks. In this work we study the thermo-mechanical properties of thermosetting polymers based on amine curing agents and epoxy resins and have focused on the DGEBA/DETDA epoxy system. At first we describe the modeling approach to construction of realistic all-atom models of densely cross-linked polymer matrices. Subsequently, a series of atomistic simulations was carried out to examine the simulation cell size effect as well as the role of cross-linking density and chain length of the resin strands on thermo-mechanical properties at different temperatures. Two different methods were used to deform the polymer networks. Both static and dynamic approaches to calculating the mechanical properties were considered and the thermo-mechanical properties obtained from our simulations were found in reasonable agreement with experimental values.

4:42PM T45.00012 Heterogeneity: A Solution to the Mysteries of the Glass transition?¹, XIAOJUN DI, GREGORY MCKENNA, Department of Chemical Engineering, Texas Tech Univ — For most phase transitions, dynamic slowdown is accompanied by static structure change. However, in supercooled liquids there is a pronounced dynamic slowdown, i.e. diffusion coefficient, relaxation time and viscosity change 14 orders of magnitude within a small temperature range, without any static structure change. Over the past several decades, extensive research has been performed to understand this dramatic dynamical slowing, i.e., why the glass transition occurs? What exactly is the glass transition? And how molecules move near the glass transition? In the present work, the idea that the large decrease in mobility in supercooled liquids during cooling from above T_g occurs due to the increasing length scale of heterogeneous sub-regions, or the Cooperative Rearranging Regions (CRR) proposed by Adam and Gibbs, is evaluated by analyzing both experiment and computer simulation results. Although the existence of microscopic heterogeneous regions is confirmed, the values of the fitting parameters obtained from both VFT and power law fits of the temperature dependent heterogeneity data suggest that the heterogeneity, itself, might not play in the key role in the T_g and/or tightly connect with the CRRs.

¹The authors acknowledge the Office of Naval Research under grant N00014-11-1-0424 and the National Science Foundation under grant CBET-1133279 for partial support of this work.

4:54PM T45.00013 The effect of polar interactions on the dynamics in vitreous liquids, ALEXANDER AGAPOV, YANGYANG WANG, PHILIP GRIFFIN, ALEXEI SOKOLOV, Department of Chemistry, University of Tennessee — It is known that in small molecule and polymeric systems the long-range process like diffusion and chain relaxation decouple from the local structural relaxation temperature dependence as system approaches its T_g . Recently, it was shown by Sokolov and Schweizer (*Phys. Rev. Lett.* **2009**, 102, 248301) that these decoupling phenomena seem to have similar underlying mechanism irrespective whether system is a polymeric or a molecular liquid. The degree of decoupling for both polymers and small molecule systems show very similar trend with respect to the fragility of the material. More fragile systems show higher degree of decoupling. However, such behavior was shown only on the example of dynamics in weakly interacting van der Waals systems. On the example of three polymers and one room temperature ionic liquid (RTIL) it is demonstrated that the presence of polar interactions leads to rather steep temperature dependence of large length scale dynamic processes, like chain relaxation and self-diffusion. As a result, the degree of decoupling between large length scale and local dynamic processes in such polar materials is significantly lower than in weakly interacting liquids with comparable fragilities. The microscopic mechanism behind an unusual dynamic behavior seen in polar polymers and RTILs remains unclear. Nevertheless, knowledge of such structure-property relationship can significantly aid in the development of novel materials. Authors are thankful to NSF and (U.S.) DOE, Office of Basic Energy Sciences for the financial support.

5:06PM T45.00014 The Twinkling Fractal Theory of the Glass Transition: Applications to Soft Matter, RICHARD WOOL, Chemical Engineering, University of Delaware — The Twinkling Fractal Theory (TFT) of the glass transition has recently been demonstrated experimentally [J.F. Stanzione et al., *J. Non Cryst. Sol.*, (2011), 357,311]. The hard to-soft matter transition is characterized by the presence of solid fractal clusters with liquid-like pools that are dynamically interchanging via their anharmonic intermolecular potentials with Boltzmann energy populations with a characteristic temperature dependent vibrational density of states $g(\omega) \sim \omega^{d_f}$. The twinkling fractal frequencies ω cover a range of 10^{12} Hz to 10^{-10} Hz and the fractal solid clusters of size R have a lifetime $\tau \sim R^{d_f/d_f}$, where the fractal dimension $D_f \approx 2.4$ and the fracton dimension $d_f = 4/3$. Here we explore its application to a number of soft matter issues. These include (a) Confinement effects on T_g reduction in thin films of thickness h , where by virtue of large cluster exclusion, $\Delta T_g \sim 1/h^{D_f/d_f}$; (b) T_g gradients near bulk surfaces, where the smaller clusters on the surface have a faster relaxation time; (c) Effect of twinkling surfaces on cell growth, where at $T \approx T_g + 20$ C, there exists a twinkling fractal range that leads to bell-shaped enhancement of cell growth and chemical up-regulation via the twinkling surfaces “communicating” with the cells through their vibrations; and (d) adhesion above and below T_g where topological fluctuations associated with $g(\omega)$ promotes the development of nano-nails at the interface.

5:18PM T45.00015 Nano-indentation of Polycarbonate and Diamine Blends, SURESH AHUJA, Retired — Nanoindentation of complex surfaces is of great interest from academic and industrial point of view. There are unique properties such as indentation effects resulting in strain softening and strain hardening. There is a differentiation in structure with the depth exhibited with variation of T_g . Hertzian and non-linear deformation models including usage of FEM offer opportunity in analyzing nano-indentation. In polycarbonate, the effective elastic modulus and the hardness decreases as the applied load is increased. As the hold time was increased, the effective elastic modulus and the hardness also decreased. The contact stress increases as the contact strain rate is increased. Presence of diamine(MTBD) in polycarbonate results in making the surface and bulk brittle and acts as an anti-plasticizer by increasing its modulus and reducing yield stress (hardness) and strain to break. Data on modulus and hardness of polycarbonate and blends of diamine as function of depth (strain) and strain rate are presented and compared with those of composites with silica.

Wednesday, February 29, 2012 2:30PM - 5:30PM –
Session T46 GIMS: Invited Session: Keithley Award Session: Photoacoustic and Photothermal Measurement Science 160AB

2:30PM T46.00001 Joseph F. Keithley Award For Advances in Measurement Science Lecture: Thermophotonic and Photoacoustic Radar Imaging Methods for Biomedical and Dental Imaging¹

, ANDREAS MANDELIS, Center for Advanced Diffusion-Wave Technologies, MIE, Univ. of Toronto — In the first part of this presentation I will introduce thermophotonic radar imaging principles and techniques using chirped or binary-phase-coded modulation, methods which can break through the maximum detection depth/depth resolution limitations of conventional photothermal waves. Using matched-filter principles, a methodology enabling parabolic diffusion-wave energy fields to exhibit energy localization akin to propagating hyperbolic wave-fields has been developed. It allows for deconvolution of individual responses of superposed axially discrete sources, opening a new field: depth-resolved thermal coherence tomography. Several examples from dental enamel caries diagnostic imaging to metal subsurface defect thermographic imaging will be discussed. The second part will introduce the field of photoacoustic radar (or sonar) biomedical imaging. I will report the development of a novel biomedical imaging system that utilizes a continuous-wave laser source with a custom intensity modulation pattern, ultrasonic phased array for signal detection and processing coupled with a beamforming algorithm for reconstruction of photoacoustic correlation images. Utilization of specific chirped modulation waveforms (“waveform engineering”) achieves dramatic signal-to-noise-ratio increase and improved axial resolution over pulsed laser photoacoustics. The talk will conclude with aspects of instrumental sensitivity of the PA Radar to optical contrast using cancerous breast tissue-mimicking phantoms, super paramagnetic iron oxide nanoparticles as contrast enhancement agents and in-vivo tissue samples.

¹With N. Tabatabaei, S. Telenkov, and R. Alwi

3:06PM T46.00002 Photoacoustics and Photothermal instrumentation in the study of thermal properties of liquids and semisolids

, JUAN JOSE ALVARADO-GIL, Applied Physics Department, Cinvestav-Unidad Merida, Carretera antigua a Progreso Km. 6, Merida, Yucatan, Mexico, 97217 — The fundamentals of the measurements of the thermal properties of solids and semisolids using photoacoustics and photothermal techniques are presented. It is shown that photoacoustics is a high stability technique which allows the monitoring of complex process in which the physical properties of the liquid can evolve. Additionally, it is shown that the methodology known as thermal wave cavity can be used successfully in high accuracy measurements for a wide variety of materials. In particular the case of magnetic fluids in which the viscosity can be varied, using an external magnetic fluid, is presented. It is also shown that the thermal wave cavity permits the study of magnetic fluids in which high aspect ratio particles are introduced in the fluid matrix. The effect of the orientation of non-magnetic particles inside the magnetic fluid generated by external magnetic field is also investigated. The possible applications and consequences in the development of windows of controlled thermal conductivity are discussed.

3:42PM T46.00003 Photoacoustic and Photothermal Effects in Periodic Structures and Acoustic Resonators

, GERALD DIEBOLD, Brown University — Laser excited photoacoustic and photothermal waves can be generated in one-dimensional structures whose acoustic or thermal properties vary sinusoidally in space. The wave equations describing the pressure or the temperature in such structures can be shown to reduce to inhomogeneous Mathieu equations. Solutions of the Mathieu equation are obtained based on both the method of variation of parameters and expansion of the pressure or temperature in a summation over eigenfunctions. The solutions for the photoacoustic effect show the space equivalent of subharmonic generation where resonances occur at one half of the period of the structure. The positions of the band gaps and the dispersion relations for any modulation depth of the acoustic properties of the structure can be found directly from the Mathieu characteristic exponent. Since the photoacoustic effect is governed by an inhomogeneous differential equation, excitation within forbidden gaps is possible. For excitation within a finite region of the structure, the Mathieu equation equivalent of Hankel functions are defined. From these functions the properties of the photoacoustic waves excited within or outside of the band gaps are found. For thermal waves, the character of the waves and the dispersion relation can be found as well, however no band gaps result from the periodicity of the thermal properties of the structure. The generation of sound by continuous, unmodulated irradiation of an absorbing gas in a resonant cavity is discussed. A longitudinal resonance of the cavity is predicted to be excited since any pressure increase from optical absorption is accompanied by a density increase, the latter resulting in additional energy deposition by the laser beam. Thus, on each return of the pressure pulse to the window of the resonator where laser beam enters the acoustic signal is amplified. Calculations show that for a strongly absorbing gas, the acoustic modes of the resonator become mode locked.

4:18PM T46.00004 Linear and Nonlinear Laser-Based Guided Acoustic Waves Propagating at Surfaces (2D) and Edges (1D)

, PETER HESS, University of Heidelberg — In recent years photoacoustics opened the door to many new applications of 2D linear surface acoustic waves (SAWs), e.g., nondestructive evaluation (NDE) of surface-breaking cracks. Real partially-closed cracks of micrometer size have been analyzed. More recently also pulsed laser excitation of solitary elastic surface pulses and their detection with a continuouswave probe laser has been achieved, by generating dispersion with a thin film coating that introduces a length scale. In addition, such laser-based pump-probe experiments allow the excitation of short nonlinear SAW pulses developing steep shock fronts that fracture brittle materials such as silica or silicon. With this method it is possible to measure the fracture strength of materials and compare the critical failure stress with ab initio calculations of the ideal strength of the corresponding perfect single crystal. The excitation and detection of 1D edge or wedge waves propagating along a wedge formed by two planar surfaces that meet at the apex of the wedge or wedge tip has been performed by laser irradiation. The characteristic features of the non-dispersive linear wedge waves such as their small phase velocity below the Rayleigh velocity, the very high degree of localization of the displacement field at the wedge tip, and their existence for certain geometries in anisotropic media such as silicon could be verified by photoacoustic experiments. Despite the strong nonlinearity of certain edge-localized modes, as expected from theoretical considerations, 1D solitary waves and nonlinear wedge waves with steep pulse profiles could not be detected up to now. The latest progress will be discussed.

4:54PM T46.00005 Understanding climate: the role of photoacoustic spectroscopy at NIST¹

, KEITH GILLIS, National Institute of Standards and Technology — Sophisticated climate models predict that soot aerosols have a significant impact on Earth's energy budget; however, the uncertainty of these predictions is large, in part, because soot in the atmosphere and in the laboratory is poorly characterized. In the atmosphere, soot's optical and physical properties change as it combines with water vapor and sulfuric acid. We will describe a novel photoacoustic spectrometer system that measures the optical absorption cross section of various soots as they age in diverse environments. We also measure the albedo (optical scattering) of aerosols ranging from black-carbon-like to brown-carbon-like using simultaneous photoacoustic spectroscopy and cavity ring-down spectroscopy. Lastly, we developed a photoacoustic spectrometer system that measures the concentration of carbon dioxide in atmospheric air with sub-ppm uncertainty. We will report results of field tests of this spectrometer.

¹This work is supported by NIST's Greenhouse Gas Measurements Program

**Wednesday, February 29, 2012 2:30PM - 5:30PM –
Session T47 DPOLY: Focus Session: Heterogeneous Colloids I 160C**

2:30PM T47.00001 Janus and Multiblock Colloids¹, STEVE GRANICK, University of Illinois — This talk surveys emerging areas opened up by the directional interactions presented by the specially-designed spheres known as Janus. The “diblock” motif, mutually attractive on one domain and repulsive on another, makes this a prototypical system for elucidating, on a mechanistic level, how concepts of chemical reaction kinetics explain the development of stable and highly ordered nonequilibrium structures. With the “triblock” motif, spheres that attract one another on two polar regions but repel at the middle band, we go beyond this to demonstrate the self-assembly of a useful low-density lattice of spheres, the colloidal Kagome lattice, and visualize its aqueous assembly dynamics on the single-particle level. A newer area of opportunity is “dynamic self-assembly,” in which energy fed into the system as a control variable generates big surprises. The generalization of these design rules will be discussed.

¹Work performed with Erik Luijten, Qian Chen, Jing Yan, Nobuhiro Yanai, Jie Zhang, Jonathan K. Whitmer, and Sung Chul Bae.

3:06PM T47.00002 Synchronized Dancing of Magnetic Janus Particles, JING YAN, Department of Materials Science and Engineering at University of Illinois at Urbana-Champaign, MOSES BLOOM, Department of Materials Science and Engineering at Northwestern University, SUNGCHUL BAE, Department of Materials Science and Engineering at University of Illinois at Urbana-Champaign, ERIK LUIJTEN, Department of Materials Science and Engineering at Northwestern University, STEVE GRANICK, Department of Materials Science and Engineering at University of Illinois at Urbana-Champaign — With Janus particle coated with magnetic material on one side, we demonstrate here first a complicated dance of single particle under external field. Then we show various quasi-one dimensional and two dimensional assembly from synchronized motion of a collection of these microspheres. With combination of experiment and simulation, we show how they are phase-locked in motion and self-organize into unexpected structures. By exploring a range of parameters, we also demonstrate fine control of the phase behavior of such dynamic self-assembled materials. We provide an vivid example here how synchronization in both time and space could lead to a new class of responsive materials.

3:18PM T47.00003 Hierarchical assemblies and cluster growth regimes of bipolar Janus nanoparticles: effect of particle characteristics, MAHDY MALEKZADEH MOGHANI, Materials Research and Innovative Laboratory (MRIL), Department of Chemical and Biomolecular Engineering, University of Tennessee, BAMIN KHOMAMI, Department of Chemical and Biomolecular Engineering, University of Tennessee — Numerous current and potential applications have motivated fundamental understanding of self assembly of colloidal Janus particles (JP). Experimental studies on nano and micron sized JPs have demonstrated a plethora of simple and complex structures. However, computational approaches to date have lacked the sophistication required to capture the rich free energy landscape of suspension of JPs especially for nanoscale particles and hence have been unable to elucidate the underlying principles that govern their complex self assembly. In this study, molecular dynamic simulation of a restricted primitive model, which also includes long range coulombic interaction, has been performed in order to elucidate the underlying physics in the self assembly of bipolar JP at different surface charge density ($0.2\sim 1.3$ e/nm²), salt concentration ($0\sim 3$ mM) and particle sizes. Our results clearly indicate formation of two distinct sub structures in very low JP concentration, namely: strings and rings. As the concentration of JP increases these sub structures joins and/or hierarchically assemble into larger clusters. Furthermore, the interconnection between the ionic cloud around a single JP and sequential cluster growth in JPS as a function of surface charge density, particle size and steric hindrance of surface ions has been elucidated.

3:30PM T47.00004 Stability of helical Janus clusters, CONNOR L. ECK, Northwestern University, JONATHAN K. WHITMER, University of Wisconsin–Madison, QIAN CHEN, STEVE GRANICK, University of Illinois at Urbana–Champaign, ERIK LUIJTEN, Northwestern University — Recent experimental and computational work has elucidated the importance of kinetic pathways in the formation of helical structures by hydrophobic-charged Janus particles.¹ Motivated by these findings, we perform free-energy calculations to investigate the equilibrium structure and relative stability of helical aggregates as a function of cluster size and Janus balance. These results simultaneously aid in the interpretation of experimental observations and in the design of building blocks for specific structures.

¹Q. Chen, J.K. Whitmer, *et al.*, *Science* **331**, 199 (2011).

3:42PM T47.00005 Hierarchical Self-assembly of Triblock Janus Spheres, QIAN CHEN, SUNG CHUL BAE, STEVE GRANICK, University of Illinois at Urbana-Champaign — We show how monodisperse triblock Janus spheres in aqueous suspension, whose poles are attractive and middle band repulsive, self-assemble into hierarchical supracolloidal structures, on two sequential levels. Based upon the delicate dependence of interactions on ionic strength, we first activate attraction between larger patches, obtaining finite-sized 3D clusters. These clusters, now concrete objects themselves, are triggered later to be linked through topologically determined orientations. A family of unprecedented, complex structures is produced, with order over multiple length scales.

3:54PM T47.00006 Janus particles at fluid-fluid interfaces: the third face of Janus particles, DAEYEON LEE, TERESA BRUGAROLAS, BUM JUN PARK, MYUNG HAN LEE, University of Pennsylvania — Janus spheres are asymmetric particles with polar and apolar hemispheres. In this work, we study the interactions and assembly of Janus spheres – bubbles and solid particles – at fluid-fluid interfaces. Both the Janus bubbles and the Janus particles have strikingly different interfacial behaviour compared to their homogeneous counterparts. Janus spheres at a fluid-fluid interface interact with each other via long-ranged attractions. We show that the attractive interactions between interface-trapped Janus spheres are induced by the presence of diffuse boundary between the two hemispheres. Three phase contact line anchored around the rugged Janus boundary deforms that the fluid interface leading to attractive interactions between the spheres. The orientation and fluid deformation caused by Janus spheres are directly observed using a gel trapping method. We also show that the surface chemistry of Janus spheres plays a critical role in determining their interfacial behaviour. Potential implications of the observed long-range attractions will be discussed.

4:06PM T47.00007 Self Assembly of Hard, Space-Filling Polytopes¹, BENJAMIN SCHULTZ, University of Michigan, Dept. of Physics, PABLO DAMASCENO, University of Michigan, Dept. of Applied Physics, MICHAEL ENGEL, SHARON GLOTZER, University of Michigan, Dept. of Chemical Engineering — The thermodynamic behavior of systems of hard particles in the limit of infinite pressure is known to yield the densest possible packing [1,2]. Hard polytopes that tile or fill space in two or three spatial dimensions are guaranteed to obtain packing fractions of unity in the infinite pressure limit. Away from this limit, however, other structures may be possible [3]. We present the results of a simulation study of the thermodynamic self-assembly of hard, space-filling particles from disordered initial conditions. We show that for many polytopes, the infinite pressure structure readily assembles at intermediate pressures and packing fractions significantly less than one; in others, assembly of the infinite pressure structure is foiled by mesophases, jamming and phase separation. Common features of these latter systems are identified and strategies for enhancing assembly of the infinite pressure structure at intermediate pressures through building block modification are discussed.

[1] P. F. Damasceno, M. Engel, S.C. Glotzer arXiv:1109.1323v1 [cond-mat.soft]

[2] A. Haji-Akbari, M. Engel, S.C. Glotzer arXiv:1106.4765v2 [cond-mat.soft]

[3] U. Agarwal, F.A. Escobedo, *Nature Materials* **10**, 230–235 (2011)

¹Supported by the DOD/DDRE under Award No. N00244-09-1-0062 and by the U.S. ARO under Grant Award No. W911NF-10-1-0518

4:18PM T47.00008 Self Assembly of Colloids¹, STEFANO SACANNA, New York University — We are exploring the self assembly of colloidal matter using building blocks with complex shapes and functionalities. Our toolbox includes particles with tunable cavities and protrusions, particles with flexible ball-and-socket joints, colloidal cubes and particles with magnetic patches. Using these building blocks and a variety of interactions, including chemical, steric, magnetic and lock-and-key shape recognition, we aim to develop new assembly schemes to build structures with a reconfigurable structural arrangement.

¹This work was supported by a MURI grant (W911NF-10-1-0518).

4:54PM T47.00009 Surface Roughness directed Self-Assembly of Patchy Particles into Colloidal Micelles, DANIELA KRAFT, Center for Soft Matter Research, New York University, RAN NI, FRANK SMALLENBURG, MICHEL HERMES, Soft Condensed Matter, Utrecht University, KISUN YOON, DAVID WEITZ, Experimental Soft Condensed Matter Group, Harvard University, ALFONS VAN BLAADEREN, Soft Condensed Matter, Utrecht University, JAN GROENEWOLD, Van 't Hoff Laboratory for Physical and Colloid Chemistry, Utrecht University, MARJOLEIN DIJKSTRA, Soft Condensed Matter, Utrecht University, WILLEM KEGEL, Van 't Hoff Laboratory for Physical and Colloid Chemistry, Utrecht University — Self-assembly of colloidal particles into larger structures bears potential for creating materials with unprecedented properties, such as full photonic band gaps in the visible spectrum. Colloidal particles with site-specific directional interactions, so called “patchy particles,” are promising candidates for bottom-up assembly routes towards such complex structures with rationally designed properties. Here we present an experimental realization of patchy colloidal particles based on material independent surface roughness specific depletion interactions. Smooth patches on rough colloids are shown to be exclusively attractive due to their different overlap volumes. We discuss in detail the case of colloids with one patch that serves as a model for molecular surfactants both with respect to their geometry and their interactions. These one-patch particles assemble into clusters that resemble surfactant micelles. We term these clusters “colloidal micelles.” Similarities as well as differences between the colloidal model system and molecular surfactants are discussed and quantified by employing computational and theoretical models.

5:06PM T47.00010 Entropic selection of patchy particle assemblies¹, XIAOMING MAO, University of Pennsylvania, QIAN CHEN, STEVE GRANICK, University of Illinois at Urbana-Champaign — We explore the statistical physics of triblock patchy colloids with degenerate valency, i.e., particles with excessively large attractive areas on two opposite sides, via analytic theory, which has the advantage of revealing fundamental laws of self-assembly more easily compared to the usual “trial-and-error” approach taken in experiments and simulations. From calculations of the free energy of multiple possible ground states, we conclude that the rotational entropy of individual particles favors certain bond angles, whereas vibrational entropy favors open rather than close-packed structures. Our analytic calculation is readily generalizable to other types of patchy particles and provides guidelines for new designs. We conclude that whereas the seemingly unfavorable degenerate valency of patchy colloids can lead to multiple energetic ground states and difficulties in selecting a unique ordered state, it also opens doors to surprising ordering phenomena. This shares pleasing commonalities with the “order-from-disorder” effect in frustrated magnets.

¹We acknowledge supports from NSF-DMR-0804900 (X.M.) and DOE DE-FG02-07ER46471 (Q.C. and S.G.)

5:18PM T47.00011 Assembling Colloidal Clusters from Spherical Codes¹, CAROLYN PHILLIPS, ERIC JANKOWSKI, MICHELLE MARVAL, SHARON GLOTZER, University of Michigan — Anisotropic building blocks assembled from colloidal particles are attractive building blocks for self-assembled materials because their complex interactions can be exploited to drive self-assembly. In this work we consider the thermodynamically driven self-assembly of terminal clusters of particles. We predict that clusters related to spherical codes, a mathematical sequence of points, can be synthesized via self-assembly. These anisotropic clusters, which derive from packing solutions of spheres around a sphere, can be tuned to different anisotropies via the ratio of sphere diameters and temperature. Structural and dynamical analysis of these tiny systems reveal rich and sometimes surprising properties.

¹Supported by DOE-BES, under award DE-FG02-02ER46000

Wednesday, February 29, 2012 2:30PM - 5:30PM —
Session T48 DPOLY DBIO: Focus Session: Advanced Optical Probes of Soft Matter - Microrheology, Microbiography 161

2:30PM T48.00001 Colloidal Diffusion and Hydrodynamic Interactions near Boundaries, BHASKAR JYOTI KRISHNATREYA, DAVID G. GRIER, Department of Physics and Center for Soft Matter Research, New York University, New York, NY 10003, CENTER FOR SOFT MATTER RESEARCH, NEW YORK UNIVERSITY TEAM — Holographic optical tweezers allow trapping of colloidal spheres in fluid in three dimensions. In-line digital holographic microscopy yields time-resolved information on the three dimensional distribution of material in a sample. Analysis of in-line holographic images of diffusing colloidal spheres provides their three dimensional positions with nanometer resolution. We studied diffusion of colloidal spheres in three dimensions as a function of distance from boundary by analyzing particle trajectories generated by blinking optical tweezers and digital holographic microscopy. From the trajectories we calculated the particle-particle and particle-wall hydrodynamic interactions as a function of distance from the boundary. The results will help in understanding interactions between micron-sized colloidal particles near a boundary.

2:42PM T48.00002 Non-contact microrheology at the air-water interface¹, THOMAS BOATWRIGHT, University of California, Irvine, ROIE SHLOMOVITZ, ALEX LEVINE, University of California, Los Angeles, MICHAEL DENNIN, University of California, Irvine — Mechanical properties of biological interfaces, such as cell membranes, have the potential to be measured with optical tweezers. We report on an approach to measure air-water interfacial properties through microrheology of particles near, but not contacting, the surface. An inverted optical tweezer traps beads of micron size or greater in the bulk, and can then translate them perpendicular to the interface. Through the measurement of thermally driven fluctuations, the mobility of the particle is found to vary as a function of submerged depth and the boundary conditions at the interface. Near a rigid wall, the mobility is confirmed to decrease in a way consistent with Faxén's law. Very close to the free air-water interface, the mobility changes with the opposite sign, increasing by about 30% at the surface, consistent with recent calculations by Shlomovitz and Levine. In addition, the presence of a Langmuir monolayer at the interface is found to significantly change the mobility of the particle close to the interface. With an accurate theory, it should be possible to infer the shear modulus of a monolayer from the fluctuations of the particle beneath the interface. Since particles are not embedded in the monolayer, this technique avoids impacting the system of study.

¹We acknowledge the support of NSF-DMR-0907212 and Research Corporation.

2:54PM T48.00003 Competing effects of inertia in passive microrheology¹, TSUTOMU INDEI, JAY

SCHIEBER, ANDRÉS CÓRDOBA, Department of Chemical and Biological Engineering, Illinois Institute of Technology — Single-point passive microrheology is generalized to account for both bead and medium inertia, and to incorporate a nonlinear optical trap or elastic trap. We first show that inertial motion of the bead couples with the elasticity of the viscoelastic material, resulting in a resonant oscillation of the mean-square displacement (MSD) of the bead well beyond the time scales of bead inertia. However, this prediction is rather different from both the original result of GSER and what is typically observed for viscoelastic materials. We next show that medium inertia tends to attenuate the oscillations because it dissipates bead energy by radiation of transverse sound waves through the Basset force. Thus, bead inertia competes with medium inertia for the MSD's oscillation. We find that it is sufficient to damp bead oscillations via Basset forces when the bead density is $> 4/7$ of the fluid density, independent of most other details in the system. We also show that the non-conservative forces that exist in an optical trap [Roichman et al., PRL, **101**, 128301 (2008)] also result in circulation in a viscoelastic medium. However, the rates are not sufficiently rapid to excite elastic modes.

¹Army Research Office (grants W911NF-08-2-0058 and W911NF-09-1-0378)

3:06PM T48.00004 High bandwidth linear viscoelastic properties of complex fluids from the measurement of their free surface fluctuations, BASILE POTTIER, LAURENCE TALINI, CHRISTIAN FRÉTIGNY, PPM-D-SIMM

— We present a new optical method to measure the linear viscoelastic properties of materials, ranging from complex fluids to soft solids, within a large frequency range (about $0.1\text{--}10^4$ Hz). The surface fluctuation specular reflection technique is based on the measurement of the thermal fluctuations of the free surfaces of materials at which a laser beam is specularly reflected. The propagation of the thermal surface waves depends on the surface tension, density, and complex viscoelastic modulus of the material. For known surface tension and density, we show that the frequency dependent elastic and loss moduli can be deduced from the fluctuation spectrum. Using a viscoelastic solid (a cross-linked PDMS), which linear viscoelastic properties are known in a large frequency range from rheometric measurements and the time-temperature superposition principle, we show that there is a good agreement between the rheological characterization provided by rheometric and fluctuation measurements. We also present measurements conducted with complex fluids that are supramolecular polymer solutions. The agreement with other low frequency and high frequency rheological measurements is again very good, and we discuss the sensitivity of the technique to surface viscoelasticity.

3:18PM T48.00005 Holographic microrefractometer, HAGAY SHPAISMAN, BHASKAR J. KRISHNATREYA, DAVID G.

GRIER, Department of Physics and Center for Soft Matter Research, New York University, New York, NY 10003 — In-line holographic microscopy of micrometer-scale colloidal spheres yields heterodyne scattering patterns that may be interpreted with Lorenz-Mie theory to obtain precise time-resolved information on the refractive index of the suspending medium. We demonstrate this method's efficacy with measurements on calibrated refractive index standards, and apply it to measurements of varying Sucrose concentration in a microfluidic channel. Using commercial colloidal spheres as probe particles and a standard video camera for detection yields volumetric refractive index measurements with a resolution approaching 10^{-3} RIU for each probe particle in each holographic snapshot. The combination of spatial resolution, temporal resolution, multi-point *in situ* access and technical simplicity favor this approach for cost-effective lab-on-a-chip applications.

3:30PM T48.00006 Studying colloidal particles on an emulsion droplet with digital holographic microscopy, JEROME FUNG, Harvard University, Dept. of Physics, REBECCA W. PERRY, Harvard University, School of Engineering and Applied Sciences, THOMAS G. DIMIDUK, Harvard University, Dept. of Physics, VINOTHAN N. MANOHARAN, Harvard University, Dept. of Physics and School of Engineering and Applied Sciences

— Interactions between colloidal particles at a curved liquid-liquid interface remain poorly understood. We study how the interactions between micron-sized polymethyl methacrylate (PMMA) particles bound to the surface of $\sim 5\text{ }\mu\text{m}$ decane droplets dispersed in an aqueous continuous phase influence the particle dynamics. We track the 3D position of up to 6 particles moving on a droplet by imaging particle-laden droplets with digital holographic microscopy and fitting the recorded holograms with Lorenz-Mie scattering calculations. We demonstrate particle tracking with ~ 10 nm precision in all directions at up to millisecond frame rates, which allows the study of rapid particle motions. In addition, we use negative dielectrophoresis to keep the droplets far away from the walls of our sample holders during imaging. Our measurements probe the interparticle interactions and allow us to determine particle contact angles *in situ*.

3:42PM T48.00007 Brownian motion goes ballistic¹, ERNST-LUDWIG FLORIN, University of Texas at Austin

— It is the randomness that is considered the hallmark of Brownian motion, but already in Einstein's seminal 1905 paper on Brownian motion it is implied that this randomness must break down at short time scales when the inertia of the particle kicks in. As a result, the particle's trajectories should lose its randomness and become smooth. The characteristic time scale for this transition is given by the ratio of the particle's mass to its viscous drag coefficient. For a $1\text{ }\mu\text{m}$ glass particle in water and at room temperature, this timescale is on the order of 100 ns. Early calculations, however, neglected the inertia of the liquid surrounding the particle which induces a transition from random diffusive to non-diffusive Brownian motion already at much larger timescales. In this first non-diffusive regime, particles of the same size but with different densities still move at almost the same rate as a result of hydrodynamic correlations. To observe Brownian motion that is dominated by the inertia of the particle, i.e. ballistic motion, one has to observe the particle at significantly shorter time scales on the order of nanoseconds. Due to the lack of sufficiently fast and precise detectors, such experiments were so far not possible on individual particles. I will describe how we were able to observe the transition from hydrodynamically dominated Brownian motion to ballistic Brownian motion in a liquid. I will compare our data with current theories for Brownian motion on fast timescales that take into account the inertia of both the liquid and the particle. The newly gained ability to measure the fast Brownian motion of an individual particle paves the way for detailed studies of confined Brownian motion and Brownian motion in heterogeneous media.

[1] Einstein, A. Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen. Ann. Phys. 322, 549–560 (1905).

[2] Lukic, B., S. Jeney, C. Tischer, A. J. Kulik, L. Forro, and E.-L. Florin, 2005, Direct observation of nondiffusive motion of a Brownian particle, Physical Review Letters 95, 160601 (2005).

[3] Huang, R., Lukic, B., Jeney, S., and E.-L. Florin, Direct observation of ballistic Brownian motion on a single particle, arXiv:1003.1980v1 (2010).

[4] Huang, R., I. Chavez, K.M. Taute, B. Lukic, S. Jeney, M.G. Raizen, and E.-L. Florin, 2011, Direct observation of the full transition from ballistic to diffusive Brownian motion in a liquid, Nature Physics 7, 576–580 (2011).

¹This research was supported by NSF grants PHY-0647144 and DBI-0552094

4:18PM T48.00008 Imaging dynamics and transitions in colloidal clusters¹, REBECCA W. PERRY, Harvard

University, School of Engineering and Applied Sciences, THOMAS G. DIMIDUK, Harvard University, Dept. of Physics, JESSE W. COLLINS, Harvard University, School of Engineering and Applied Sciences, JEROME FUNG, GUANGNAN MENG, Harvard University, Dept. of Physics, VINOTHAN N. MANOHARAN, Harvard University, Dept. of Physics and School of Engineering and Applied Sciences — We use digital holographic microscopy to measure the relative motions of particles in colloidal clusters containing micron-sized spherical particles interacting through short-range attractions. These clusters explore many configurations as they approach their equilibrium states. Furthermore, clusters formed with weak interactions continue to transition between equal-energy configurations. We solve the challenge of tracking closely-packed, thermally-driven colloidal spheres in three dimensions by fitting the holograms using an exact solution for the scattering from multiple spheres. The method allows us to track each sphere with 10 nm precision in all three dimensions with millisecond time resolution.

¹We acknowledge support from the NSF through grant no. CBET-0747625, the Harvard MRSEC, and the NSF graduate research fellowship program.

4:30PM T48.00009 Holography of Cells fitted to DDA scattering solutions, THOMAS DIMIDUK, JEROME FUNG, REBECCA PERRY, Harvard, RYAN MCGORTY, UCSF, VINOTHAN MANOHARAN, Harvard — Understanding the dynamics of cells is important to many areas of biophysics. Digital Holography offers a way to observe these dynamics at high speed, in 3D, in relatively native conditions. I will present work studying single cell dynamics through in-line digital holography. To quantify the motion of subcellular components, we fit our holograms to models of scattering based on the Discrete Dipole Approximation. In particular, we apply the technique to determine the fluctuations of the cell membrane. The technique allows us to interrogate the cells over a broad range of time scales, from 10^{-3} s up to the time scale for cell division.

4:42PM T48.00010 Holographic deconvolution microscopy for high resolution particle tracking¹, LISA DIXON, FOOK CHIONG CHEONG, DAVID GRIER, New York University — Rayleigh-Sommerfeld back-propagation can be used to generate a volumetric reconstruction of the light field responsible for the recorded intensity in an in-line hologram. Deconvolving the three dimensional light intensity with an optimal kernel derived from the Rayleigh-Sommerfeld propagator itself emphasizes the objects responsible for the scattering pattern while suppressing undesired artifacts. Bright features in the deconvolved volume may be identified with such objects as colloidal spheres and nanorods. Tracking their thermally-driven Brownian motion through multiple holographic video images provides estimates of the tracking resolution, which approaches 1 nm in all three dimensions.

¹QORS Program of DARPA and NSF grant DMR-0922680

4:54PM T48.00011 Measuring Nanoparticle Dynamics with Real-Time, 3D Tracking, KAN DU, Center for Nanoscale Science and Technology at National Institute of Standard and Technology, University of Maryland, ANDREW BERGLUND, Center for Nanoscale Science and Technology at National Institute of Standard and Technology — Nanoparticles in liquids are an important platform for nanofabrication and nanomanufacturing processes. Few *in situ* methods are available for measuring the time-resolved dynamics of individual nanoparticles at nanoscale spatial resolution. Drawing on recent advances in real-time single-particle feedback control, we have developed an apparatus that enables us to measure the 3D motion and dynamics of individual fluorescent nanoparticles in liquid environments. Real-time feedback control methods enable us to monitor the dynamics of individual nanoparticles by locking them in focus in an optical microscope, which enhances both the temporal and spatial resolution of our instrument. We applied the technique to study diffusion dynamics of polystyrene nanoparticles adsorbed at liquid-liquid interfaces. This tool can also be applied to study nanoparticle binding, self-assembly processes, and single-molecule biophysics.

5:06PM T48.00012 Nano-domains of high viscosity and stiffness mapped in the cell membrane by thermal noise imaging, YUNHSIANG HSU, ARND PRALLE, University at Buffalo, SUNY — The cell membrane is thought to contain spatial domains, created by cholesterol-lipid clusters and by interactions with the membrane cytoskeleton. The influence of these domains on membrane protein mobility and cell signaling has clearly been demonstrated. Yet, due to their small size and transient nature, the cholesterol stabilized domains cannot be visualized directly. We show here that thermal noise imaging (TNI) which tracks the diffusion of a colloid labeled membrane protein with microsecond and nanometer precision, can visualize cholesterol stabilized domains, also known as lipid rafts, in intact cells. Using TNI to confine a single membrane protein to diffuse for seconds in an area of 300nm x 300nm provides sufficient data for high resolution maps of the local diffusion, local attraction potentials and membrane stiffness. Using a GPI-anchored GFP molecule to probe the membrane of PtK2 cells we detect domains of increased membrane stiffness, which also show increased viscosity and are the preferred location for the GPI-anchored protein. These domains are further stabilized by addition of ganglioside cross linking toxins and disappear after removal of the cholesterol.

5:18PM T48.00013 Fluorescence correlation spectroscopy enumerate the number of nanoparticles in optical confinement, YI HU, XUANHONG CHENG, H. DANIEL OU-YANG, Lehigh University — In the presence of an optical trap, both the concentration and diffusion dynamics of the nanoparticles near the center of the laser focus are affected. This phenomenon could affect the interpretation of the result from fluorescence correlation spectroscopy (FCS) where highly focused laser is often used. A recent Monte Carlo simulation study shows, for non-interacting particles under trapping energy up to 2 kT, the zero-time autocorrelation function $G(0)$ can be used to enumerate the mean number of particles N in the trap. It is not clear, however, how particle interactions or higher trapping will affect this prediction. To address these issues, we conducted FCS experiments to examine $G(0)$ as a function of trapping energy and particle interaction strength. We discovered that $G(0) = 1/N$ is true up to 6 kT as long as the particle interactions are negligible. As the particle interaction is increased, the validity of the above relation quickly breaks down. We interpret our experimental finding based on the consideration of Poisson statistics.

Wednesday, February 29, 2012 2:30PM - 5:30PM –

Session T49 DMP DPOLY: Focus Session: Organic Electronics and Photonics: Structure - Property Correlations 162A

2:30PM T49.00001 Correlating the efficiency and nanomorphology of polymer blend solar cells utilizing resonant soft x-ray scattering, HONGPING YAN, BRIAN COLLINS, ELIOT GANN, NCSU, CHENG WANG, ALS, HARALD ADE, NCSU, CHRISTOPHER MCNEILL, Monash Univ — Enhanced scattering contrast afforded by resonant soft x-ray scattering (R-SoXS) is used to probe the nanomorphology of all-polymer solar cells based on blends of the donor poly(3-hexylthiophene) (P3HT) with the acceptor either poly((9,9-dioctylfluorene)-2,7-diyl-alt-[4,7-bis(3-hexylthien-5-yl)-2,1,3-benzothiadiazole]-2',2''-diyl) (F8TBT) or poly([N,N'-bis(2-octyldodecyl)-11 naphthalene-1,4,5,8-bis(dicarboximide)-2,6-diyl]-alt-5,5'-(2,2'-12 bithiophene)) (P(NDI2OD-T2)). A bimodal distribution of domain sizes is observed for P3HT:P(NDI2OD-T2) blends with small domains of ~ 5 - 10 nm that evolve with annealing and larger domains of ~ 100 nm insensitive to annealing. P3HT:F8TBT blends in contrast show a broader distribution but with the majority structured on 10 nm length scale. For both blends an evolution in device performance is observed, correlated with a coarsening and purification of domains on the 5 - 10 nm length scale. Grazing-Incidence Wide Angle X-ray Scattering (GI-WAXS) reveals 25 - 40 nm thick P(NDI2OD-T2) crystallites embedded in the larger domains observed by R-SoXS. A higher degree of P3HT crystallinity is observed in blends with P(NDI2OD-T2) compared to F8TBT. The propensity of the polymers to crystallize in P3HT:P(NDI2OD-T2) blends is also observed to hinder the morphological development on the sub-10 nm length scale. More broadly, this work also highlights the complementarity of R-SoXS and GI-WAXS.

2:42PM T49.00002 Hierarchical Nanomorphologies Promote Exciton Dissociation in Polymer: Fullerene Bulk Heterojunction Solar Cells¹, WEI CHEN, SETH DARLING, Center for Nanoscale Materials, Argonne National Laboratory — In the last fifteen years, research efforts have led to organic photovoltaic (OPV) devices with power conversion efficiencies (PCEs) up to ~8%, but these values are still insufficient for the devices to become widely marketable. To further improve solar cell performance a thorough understanding of the complex structure-property relationships in the OPV devices is required. In this work, we demonstrated that the OPV active layer of PTB7:fullerene bulk heterojunction (BHJ) solar cells, which set a historic record of PCE (7.4%), involves hierarchical nanomorphologies ranging from several nanometers of crystallites to tens of nanometers of nanocrystallite aggregates in PTB7-rich and fullerene-rich domains, themselves hundreds of nanometers in size. These hierarchical nanomorphologies with optimum crystallinity and intermixing of PTB7 with fullerenes are coupled to significantly enhanced exciton dissociation, which consequently contribute to photocurrent, leading to the superior performance of PTB7:fullerene BHJ solar cells. New insights of performance-related structures afforded by the current study should aid in the rational design of even higher performance polymeric solar cells.

¹W. Chen gratefully acknowledges financial support from Argonne Director's Postdoctoral Fellowship. This work is partially supported by a University of Chicago-Argonne Strategic Collaborative Initiative Seed Grant.

2:54PM T49.00003 Unexpected Morphological Traits of Bulk Heterojunction Organic Solar Cells with Exceptional Power Conversion Efficiencies, JOHN TUMBLESTON, BRIAN COLLINS, North Carolina State University, ANDREW STUART, University of North Carolina, ZHE LI, Monash University, HONGPING YAN, North Carolina State University, CHRISTOPHER MCNEILL, Monash University, WEI YOU, University of North Carolina, HARALD ADE, North Carolina State University — The synthesis of new polymers for polymer/fullerene bulk heterojunction solar cells has boosted the power conversion efficiency (PCE) of these devices to levels now exceeding 5%. Even with these advancements in efficiency, relatively little is known of the morphological characteristics of the active layer including domain size and purity, material crystallinity and orientation, and miscibility of the bulk heterojunction components. Herein, we employ a suite of soft and hard x-ray scattering and microscopy techniques to probe defining traits of the morphology for the high-performing polymers, poly[4,8-(3-butylthiophenyl)benzo[1,2-b:4,5-b']dithiophene-*alt*-2-(2-butyloctyl)-5,6-difluoro-2H-benzo[d][1,2,3]triazole] (BnDT-FTAZ) and thieno[3,4-b]thiophene-*alt*-benzodithiophene (PTB7) blended with phenyl-C61-butyric acid methyl ester (PC₆₁BM) and PC₇₁BM, respectively. PCEs of 7.4% for BnDT-FTAZ and 5.3% for PTB7 based solar cells are achieved when processing methods result in smaller, more mixed polymer/fullerene phases where non-zero miscibility is measured for each system. Furthermore, the polymers do not strongly crystallize in the active layer and average domain sizes larger than 50 nm are noted for both systems.

3:06PM T49.00004 Correlating Free-Carrier production in P3HT with Solid-State Microstructure using Time-Resolved Microwave Conductivity¹, GARRY RUMBLES, NREL — The nature of the primary photoexcitation in conjugated polymers has been a subject of interest for a number of years, and two models have emerged: neutral excitons and free charge carriers. While excitons are recognized as the dominant of the two species, there are a small fraction of carriers that appear directly upon photoexcitation that have been detected experimentally either spectroscopically or through conductivity measurements. The fraction of near-instantaneous free charge carriers produced depends both on the chemical structure of the polymer and on the time-scale on which the study is performed. For example, poly(3-hexylthiophene) (P3HT) thin films have been reported to have free carrier yields as high as 15%, when measured on a fast time scale, but as low as 3% when measured on a slow time scale. It is unclear why these numbers are so different, and from where these carriers originate. This presentation will report studies using flash photolysis, time-resolved microwave conductivity (fp-TRMC) to probe carriers produced in a number of thin films of P3HT of differing molecular weights. By correlating the free carrier yield with the solid-state microstructure of the polymer, and the corresponding electronic absorption spectra, we will propose a model that explains the origins of these carriers.

¹Also Department of Chemistry and Biochemistry, University of Colorado, Boulder.

3:42PM T49.00005 Controlling Active Layer Morphology in Polymer/Fullerene Solar Cells, SUCHANUN MOUNGTHAI, NIKHILA MAHADEVAPURAM, GILA STEIN, University of Houston — The active layer in most polymer solar cells is based on the bulk heterojunction (BHJ) design. BHJs are prepared by arresting the phase separation of a polymer/fullerene blend to produce a nanoscale, interpenetrating network. Such non-equilibrium structures are very difficult to control and reproduce, posing a significant challenge for fundamental structure-property investigations. We demonstrate a new approach to control the active layer morphology with a simple two-step process: First, a thin film of poly(3-hexylthiophene) (P3HT) is cross-linked into stable nanostructures or microstructures with electron-beam lithography [1]. Second, a soluble fullerene is spun-cast on top of the patterned polymer to complete the heterojunction. Significantly, irradiated P3HT films retain good optoelectronic properties and bilayer P3HT/fullerene heterojunctions yield power-conversion efficiencies near 0.5%. We have performed preliminary studies with model nanostructured devices and we find that efficiency increases with interfacial area [2]. These model devices are very valuable for fundamental studies because the interfacial area is accurately measured with small-angle X-ray scattering, and the active layer can be “deconstructed” for imaging with atomic force microscopy.

[1] S. Holdcroft, Adv. Mater. 2001, 13, 1753-1765.

[2] He et al., Adv Funct. Mater. 2011, 21, 139-146.

3:54PM T49.00006 The Miscibility of PCBM in Low Band-Gap Conjugated Polymers in Organic Photovoltaics, HUIPENG CHEN, Department of Chemistry, University of Tennessee, WEI YOU, Department of Chemistry, University of North Carolina, JEFF PEET, Konarka Technologies, JASON AZOULAY, GUILLERMO BAZAN, Center for Polymers and Organic Solids The University of California, Santa Barbara, MARK DADMUN, Department of Chemistry, University of Tennessee — Understanding the morphology of the photoactive layer in organic photovoltaics (OPVs) is essential to optimizing conjugated polymer-based solar cells to meet the targeted efficiency of 10%. The miscibility and interdiffusion of components are among the key elements that impact the development of morphology and structure in OPV active layers. This study uses neutron reflectivity to correlate the structure of low band gap polymers to their miscibility with PCBM. Several low band gap polymers that exhibit power conversion efficiencies exceeding 7%, including PBnDT-DTfBT were examined. The intermixing of low band-gap polymer and PCBM bilayers was monitored by neutron reflectivity before and after thermal annealing, providing quantification of the miscibility and interdiffusion of PCBM within the low band gap polymer layer. These results indicate that the miscibility of PCBM ranges from 3% to 26% with the low band-gap polymers studied. The correlation between low band gap polymer structure and miscibility of PCBM will also be discussed.

4:06PM T49.00007 Self-assembly Columnar Structure in Active Layer of Bulk Heterojunction Solar Cell¹, CHENG PAN, JENNIFER SEGUI, YINGJIE YU, HONGFEI LI, Stony Brook University, BULENT AKGUN, SUSHIL K. SATIJA, National Institute of Standards and Technology, DILIP GERSAPPE, Stony Brook University, CHANG-YONG NAM, Brookhaven National Laboratory, MIRIAM RAFAILOVICH, Stony Brook University — Bulk Heterojunction (BHJ) polymer solar cells are an area of intense interest due to their flexibility and relatively low cost. However, due to the disordered inner structure in active layer, the power conversion efficiency of BHJ solar cell is relatively low. Our research provides the method to produce ordered self-assembly columnar structure within active layer of bulk heterojunction (BHJ) solar cell by introducing polystyrene (PS) into the active layer. The blend thin film of polystyrene, poly (3-hexylthiophene-2,5-diyl) (P3HT) and [6,6]-phenyl C₆₁ butyric acid methyl ester (PCBM) at different ratio are spin coated on substrate and annealed in vacuum oven for certain time. Atomic force microscopy (AFM) images show uniform phase segregation on the surface of polymer blend thin film and highly ordered columnar structure is then proven by etching the film with ion sputtering. TEM cross-section technology is also used to investigate the column structure. Neutron reflectometry was taken to establish the confinement of PCBM at the interface of PS and P3HT. The different morphological structures formed via phase segregation will be correlated with the performance of the PEV cells to be fabricated at the BNL-CFN.

¹NSF-DMR-MRSEC

4:18PM T49.00008 Dissipative Particle Dynamics Studies of Rod-Coil Polymer Nanocomposites¹, CHARLES STARBIRD, DONGSHENG ZHANG, ARTHI JAYARAMAN, University of Colorado at Boulder — Organic solar cell efficiency depends strongly on the morphology within the active layer consisting of donor (e.g. conjugated polymer) and acceptor (e.g. fullerene derivative) materials. Higher device efficiency can be obtained if the donor-acceptor morphology has high interfacial area, small domains, and continuous pathways. One way to control donor-acceptor morphology is via copolymerization of the conjugated “rod” polymer and an acceptor “coil” block. Past theory and experimental studies have characterized the phase behavior of pure rod-coil block copolymers. In this talk we will present dissipative particle dynamics simulation studies of composites of symmetric rod-coil block copolymers and nanoscale additives of varying selectivity (rod-, coil- and non-selective). With increasing volume fraction of non- and rod- selective nanoadditives we see a shift in the liquid crystalline and microphase transitions to lower temperatures, and new morphologies (e.g. helical twists in rod block domain and zig-zag lamellae) not seen in pure symmetric rod-coil polymers. These shifts in phase transition are explained by where the nanoadditives reside, which in turn is dictated by where the system can maximize enthalpic gain and minimize loss of nanoadditive translational entropy.

¹DOE Early Career Award DE-SC0003912

4:30PM T49.00009 Model Hamiltonian for predicting the bandgap of conjugated systems, ANDRE LEITAO BOTELHO, YONGWOO SHIN, XI LIN, Division of Materials Science and Engineering, Boston University — We calculate the bandgaps for conjugated systems using the adapted Su-Schrieffer-Heeger Hamiltonian and find good agreement with 130 independent experimental points. The 2D version of the model correctly demonstrates the decrease in bandgap from the addition of vinylene bridges to both poly(*p*-phenylene) and polythiophene indicating that planarization is not a significant effect. Expanding the model to 3D shows that interchain interactions systematically reduces the bandgap. In fused rings sharing dissimilar bonds, such as in isothianaphthene, the bond length dimerization along the carbon backbone decreases leading to a decrease in the bandgap. In contrast, when fusing two of the same rings along equivalent bonds, for example thienoacene, the bandgap change is less than 10% at best when normalized by the number of carbon atoms in the conjugation path. From porphyrin and pyrrole-benzothiadiazole we learn that tautomerization significantly affects the bandgap, as the ϵ value for NH had to be used for both NH and N, indicating that H is being shared by both. In modeling donor-acceptor co-polymers we accurately calculate the reduction in the bandgaps when compared to their parent homopolymers.

4:42PM T49.00010 The Effect of Side-Chain Length on the Solid-State Structure and Optical Properties of F8BT: A DFT Study¹, MOHAMMAD JAVAD ESLAMIBIDGOLI, JOLANTA B. LAGOWSKI, Memorial University of Newfoundland — Using the long-range corrected hybrid density functional theory (DFT/B97D) approach, we have performed bulk solid state calculations to investigate the influence of side-chain length on the molecular packing and optical properties of poly (9,9-di-n-octylfluorene-alt-benzothiadiazole) or F8BT. Two different packing structures, the lamellar and nearly hexagonal, were obtained corresponding to longer and shorter side-chains respectively. This behavior can be attributed to the micro-phase separations between the flexible side-chains and the rigid backbones and is in agreement with previous investigations for other hairy-rod polymers. In addition, as a result of the efficient inter-chain interactions for the lamellar structure, the dihedral angle between the F8 and BT units is reduced providing a more planar configuration for the backbone which leads to the decreased band gap (by 0.2-0.3 eV) in comparison to the hexagonal phase and the gas phase with no side-chain. Time-dependent DFT (TDDFT/B3LYP) was also used to study the excited states of the monomer of F8BT optimized in solid-state structures with different side-chain lengths. It is found that the absorption spectrum is red shifted for the polymers with lamellar structure relative to the polymers in hexagonal and gas phases.

¹Sun Microsystems Canada Inc (Graduate Fellowship administrated by ACEnet at Memorial University)

4:54PM T49.00011 Polymer blend photovoltaics with conjugated block copolymers as surfactants, CHANGHE GUO, MATTHEW WITMAN, KIARASH VAKHSHOURI, Pennsylvania State University, RAFAEL VERDUZCO, Rice University, ENRIQUE GOMEZ, Pennsylvania State University — Conjugated polymer blend photovoltaics are a class of devices where the active layer is composed of a polymer acceptor and a polymer donor. These devices suffer from macrophase separation in the active layer, where it is challenging to kinetically trap domains with characteristic sizes below micron length scales. Thus, for mixtures of poly(3-hexylthiophene) (P3HT) and poly((9,9-dioctylfluorene)-2,7-diyl-alt-[4,7-bis(thiophen-5-yl)-2,1,3-benzothiadiazole]-2',2''-diyl) (PFOTBT), we have synthesized a conjugated block copolymer to act as an A/B surfactant and stabilize a microstructure. The performance of devices where the active layer is composed of P3HT, PFOTBT, and P3HT-PFOTBT block copolymer blends is found to depend on the composition of the mixture and processing conditions. In addition, we have utilized energy-filtered transmission electron microscopy to characterize the morphology of the blends and correlated the microstructure with device performance.

5:06PM T49.00012 ABSTRACT WITHDRAWN —

5:18PM T49.00013 Self-assembly and characterization of two-component films of semiconducting nanoparticles, YIPENG YANG, NAGARJUNA GAVVALAPALLI, HARIHARA VENKATRAMAN, MINA BAGHGAR, MICHAEL BARNES, DHANDAPANI VENKATARAMAN, ANTHONY DINSMORE, University of Massachusetts Amherst — Polymer-based semiconducting materials are promising candidates for large-scale, low-cost photovoltaic devices. To date, the efficiency of these devices has been low in part because of the challenge of optimizing molecular packing while also obtaining a bicontinuous structure with a length scale of approximately 10nm. Here we demonstrate an alternative approach to solving this problem by packing nanoparticles of electron- and hole-transporting semiconductors into a two-component film. We first make nanoparticles of semiconducting materials (P3HT, PCBM, CdSe, etc) suspended in liquid. Then a binary suspension of nanoparticles is dried onto a non-volatile liquid surface to form a solid, two-component film with uniform thickness. The absorbance, photoluminescence, structure, and charge mobility of the films are measured. For a range of stoichiometries, we obtain bicontinuous structures and significant luminescence quenching, indicating charge transfer. This study shows that two-component nanoparticulate films may be an effective route toward bulk heterojunctions with controlled morphology. We acknowledge support from the US Department of Energy, Office of Basic Energy Sciences, through grant DE-SC0001087.

Wednesday, February 29, 2012 2:30PM - 5:30PM –

Session T50 DPOLY: Focus Session: Phase Behavior and Structure in Copolymers 162B

2:30PM T50.00001 Self-assembly of semiflexible-flexible block copolymers, ARUN KUMAR, VENKAT

GANESAN, The University of Texas at Austin — We apply self-consistent Brownian dynamics simulations to study the self-assembly behavior of semiflexible-flexible block copolymers. A Maier-Saupe interaction model was applied for the orientational interactions between the semiflexible polymers, while the enthalpic interactions between semiflexible and flexible polymers were modeled through a standard Flory-Huggins approach. To develop a physical understanding of the phases and their regimes of occurrence as a function of varying persistence length of the semiflexible block, we computed the 2D phase diagram for our model. We quantify the progression of the self-assembly morphologies in transitioning from coil-coil block copolymers on the one hand to rod-coil block copolymers on the other hand. The results obtained are in qualitative agreement with the existing experimental and numerical results.

2:42PM T50.00002 Effect of chain shape on the self-assembly of bioinspired block copolymers

, ADRIANNE M. ROSALES, HANNAH K. MURNEN, University of California, Berkeley, RONALD N. ZUCKERMANN, Lawrence Berkeley National Laboratory, RACHEL A. SEGALMAN, University of California, Berkeley — Polymer chain shape has been shown to affect both polymer properties and block copolymer self-assembly. Polypeptoids, a class of sequence-specific bioinspired polymer, have a chain shape that can be tuned by the introduction of monomers with bulky, chiral side chains, allowing one to change the polymer conformation while preserving the chemical nature of the side chains. Here, it is shown that introducing chiral, aromatic monomers into the polypeptoid chain increases the glass transition by 20 C for a chiral, helical polypeptoid compared to its achiral, non-structured analog. Incorporation of these polypeptoids into block copolymers with poly(methyl acrylate) enables a systematic study of the effect of chain shape while maintaining similar enthalpic interactions. For two otherwise analogous block copolymers, conformational asymmetry is shown to affect both the morphological domain spacing and the order-disorder transition temperature. Future work will focus on interfacial segregation experiments to determine the effect of conformational asymmetry on the Flory-Huggins parameter.

2:54PM T50.00003 Processing-Dependent Self-Assembly of Protein-Polymer Diblock Copolymers

, C.S. THOMAS, L. XU, B.D. OLSEN, MIT — Self-assembly of globular protein-polymer diblock copolymers is a novel method for nanopatterning protein-based materials which maintains a high fraction of protein activity as well as the folded protein structure. By subjecting these copolymers to different processing conditions, long range ordering and the fraction of active protein can be controlled. Here, self-assembly of model mCherry-b-poly(N-isopropyl acrylamide) (PNIPAM) block copolymers is induced by water evaporation from dilute aqueous solutions of conjugate material, and followed by solvent annealing of the resulting nanostructures. Different pathways towards self-assembly are accessed by orthogonally manipulating the solvent quality for each block of the copolymer using temperature and pH. Small-angle scattering and transmission electron microscopy show nanostructure depends heavily on PNIPAM coil fraction and solvent annealing condition, with solution self-assembly reflected in the solid state structure under certain conditions. Protein structure is unaffected by the processing pathway, while protein activity levels in the nanodomains depend strongly on processing conditions and can retain up to 80% of the initial activity.

3:06PM T50.00004 Helical Ordering in Chiral Block Copolymers, WEI ZHAO, SUNG WOO HONG, DIAN CHEN,

GREGORY GRASON, THOMAS RUSSELL, University of Massachusetts Amherst — Introducing molecular chirality into the segments of block copolymers can influence the nature of the resultant morphology. Such an effect was found for poly(styrene-*b*-L-lactide) (PS-*b*-PLLA) diblock copolymers where hexagonally packed PLLA helical microdomains (H* phase) form in a PS matrix. However, molecular ordering of PLLA within the helical microdomains and the transfer of chirality from the segmental level to the mesoscale is still not well understood. We developed a field theoretic model to describe the interactions between segments of chiral blocks, which have the tendency to form a “cholesteric” texture. Based on the model, we calculated the bulk morphologies of chiral AB diblock copolymers using self-consistent field theory (SCFT). Experiments show that the H* phase only forms when microphase separation between PS and PLLA block happens first and crystallization of PLLA block is suppressed or happens within confined microdomain. Hence, crystalline ordering is not necessary for H* phase formation. The SCFT offers the chance to explore the range of thermodynamic stability of helical structures in the phase diagram of chiral block copolymer melts, by tuning parameters not only like the block segregation strength and composition, but also new parameters such as the ratio between preferred helical pitch to the radius of gyration and the Frank elastic constant for inter-segment distortions.

3:18PM T50.00005 Phase Behavior of Binary Blends of AB+AC Block Copolymers with compatible B and C blocks

, VICTOR PRYAMITSYN, VENKAT GANESAN, University of Texas at Austin — Recently the experimental studies of phase behavior of binary blends of PS-*b*-P2VP and PS-*b*-PHS demonstrated an interesting effect: blends of symmetric PS-*b*-P2VP and shorter symmetric (PS-*b*-PHS) formed cylindrical HEX and spherical BCC phases, while each pure component formed lamellas. The miscibility of P2VP and PHS is caused by the hydrogen bonding between P2VP and PHS, which can be described as a negative Flory χ -parameter between P2VP and PHS. We developed a theory of the microphase segregation of AB+AC blends of diblock copolymers based on strong stretching theory. The main result of our theory is that in the copolymer brush-like layer formed by longer B chain and shorter C chains, the attraction between B and shorter C chains causes relative stretching of short C chains and compression of longer B chains. The latter manifests in an excessive bending force towards the grafting surface (BC|AA interface). Such bending force causes a transition from a symmetric lamella phase to a HEX cylinder or BCC spherical phases with the BC phase being a “matrix” component. In a blend of asymmetric BCC sphere forming copolymers (where B and C segments are the minor components), such bending force may unfold BCC spherical phase to a HEX cylinder phase, or even highly uneven lamella phases.

3:30PM T50.00006 Universality in block copolymers: a corresponding states hypothesis

, JENS GLASER, JIAN QIN, PAVANI MEDAPURAM, DAVID MORSE, Dept. of Chemical Engineering and Materials Science, University of Minnesota — Phase behavior and fluctuations of very long block copolymers are well described by self-consistent field theory, and by the random-phase (RPA) approximation for concentration fluctuations. The SCF / RPA predicts behavior that depends on only a few dimensionless parameters. More sophisticated coarse-grained theories instead suggest an extended form of this principle of corresponding states, in which the behavior is predicted to depend on one additional parameter, the independent degree of polymerization $\bar{N}$. We are testing this prediction by comparing extensive computer simulations of several different coarse-grained simulation models of AB diblock copolymer melts. We utilize a novel simulation methodology based on graphical processing unit (GPU) accelerated hybrid molecular dynamics / Monte Carlo replica exchange simulations on a cluster of many GPUs. We present data for off-lattice models with soft- and hard-core non-bonded interactions, and a lattice model, comparing simulations of different models that are designed to have matched values of $\bar{N}$. The results provide extremely strong evidence for the corresponding states hypothesis, which is found to remain accurate even for chains that are much too short to be accurately described by SCFT or the RPA.

3:42PM T50.00007 Manipulating triblock copolymer morphology using tapered block interfaces

, WEI-FAN KUAN, THOMAS H. EPPS, III, University of Delaware — Tapered block copolymers offer the opportunity to manipulate copolymer segregation strengths independently of the molecular weight and chemical constituents. This independent control allows the design of materials with designer interactions and improved mechanical properties, while retaining the desired self-assembled nanostructures. The tapered interfaces between blocks have been shown to significantly decrease the effective interaction parameters between blocks, leading to lower order-to-disorder transition temperatures relative to corresponding non-tapered block copolymers. In this work, we synthesized a series of tapered triblock copolymers using a combination of anionic polymerization, atom transfer radical polymerization, and click chemistry. Comparing the morphologies of our tapered and non-tapered triblock copolymers suggests that the phase behavior of the tapered materials can differ from the non-tapered triblock materials due to the manipulated interfacial profile.

3:54PM T50.00008 Manipulating the morphological behavior of ABA triblock copolymers with block polydispersity, ADAM SCHMITT, MAHESH MAHANTHAPPA, University of Wisconsin-Madison — As an extension of our ongoing efforts to understand the effects of middle B segment polydispersity on the melt-phase behavior of ABA triblock copolymers, we describe the morphological consequences of block polydispersity in the context of poly(lactide-*b*-1,4-butadiene-*b*-lactide) (LBL) triblock copolymers. The complete melt-phase behavior of 52 well-defined LBL triblock copolymers was evaluated using a combination of synchrotron small-angle X-ray scattering (SAXS) and transmission electron microscopy (TEM). Through careful comparisons with monodisperse copolymer control samples, we show that block polydispersity causes large shifts in the composition-dependent phase windows in a manner consistent with previous reports. However, these polydisperse LBL triblocks do not exhibit the substantial domain dilation observed in more weakly segregated SBS triblock copolymers. Based on these observations, we discuss the possibility of using block polydispersity as a new means of tailoring the morphological behavior of microphase separated ABA triblock copolymers.

4:06PM T50.00009 Phase Behavior of Linear ABC Tri Block-Random Copolymers with a Semicrystalline Endblock, BRYAN BECKINGHAM, RICHARD REGISTER, Princeton University — The solid-state structure of semicrystalline block copolymers is set either by block incompatibility or by crystallization of one or more blocks. A variety of solid-state morphologies may be observed depending on the block interaction strength, ranging from spherulitic to confined crystallization within preexisting microphase-separated domains. We aim to explore crystallization from both homogeneous and microphase-separated melts and to characterize the resulting solid-state structure of linear ABC "block-random" copolymers that incorporate a semicrystalline polyethylene endblock. Linear triblock copolymers, poly[butadiene-*b*-isoprene-*b*-(isoprene-*r*-styrene)], are synthesized via anionic polymerization. Two hydrogenation schemes are then applied, either complete saturation of all double bonds or a selective saturation of only diene units. Both schemes yield semicrystalline polyethylene endblocks but dissimilar interblock segregation strengths. In both derivatives of a 30-14-14 kg/mol triblock-random copolymer, small-angle x-ray scattering reveals the formation of a well-ordered three-domain lamellar melt from which crystallization of the polyethylene endblock proceeds. Crystal orientation within the lamellae has been determined by wide-angle x-ray scattering after lamellar orientation in a channel die. We are currently varying relative block and overall molecular weights, and the block sequence to further explore these materials.

4:18PM T50.00010 Discovering Complex Ordered Phases of Block Copolymers, AN-CHANG SHI, McMaster University — Block copolymers with their rich phase behavior and ordering transitions have become a paradigm for the study of structured soft materials. Understanding the structures and phase transitions in block copolymers has been one of the most active research areas in polymer science in the past two decades. One of the achievements is the self-consistent field theory (SCFT), which provides a powerful framework for the study of ordered phase of block copolymers. I will present a generic strategy to discover complex ordered phases of block copolymers within the SCFT framework. Specifically, a combination of real-space and reciprocal-space techniques is used to explore possible ordered phases in multiblock copolymer melts. These candidate phases can then be used to construct phase diagrams. Application of this strategy to linear and star ABC triblock copolymers has led to the discovery of a rich array of ordered phases.

4:54PM T50.00011 Thermodynamic Behavior of Poly(1,4-isoprene-*b*-DL-lactide) Diblock Copolymers, TIMOTHY M. GILLARD, SANGWOO LEE, FRANK S. BATES, University of Minnesota — The phase behavior of a series of poly(1,4-isoprene-*b*-DL-lactide) (IL) diblock copolymers near the order-disorder transition temperature (T_{ODT}) was investigated using a combination of dynamic mechanical spectroscopy (DMS), small angle x-ray scattering (SAXS) and differential scanning calorimetry (DSC). IL copolymers of relatively low molecular weight ($\sim 2.5 - 6$ kg/mol) formed ordered phases with experimentally accessible T_{ODTs} due to the large segment-segment interaction parameter (χ_{IL}). The order-disorder transitions were accompanied by distinct signatures in the DSC traces, where the magnitude of the latent heat of the ODT (ΔH_{ODT}) depends strongly on the ordered phase morphology. Symmetric compounds exhibited almost no hysteresis in the onset temperature for ordering and disordering, indicative of an absence of a nucleation barrier, while asymmetric IL diblocks displayed considerable hysteresis. These findings will be discussed in the context of composition fluctuation effects in the disordered melt near T_{ODT} .

5:06PM T50.00012 Direct Comparisons among Fast Off-Lattice Monte Carlo Simulations, Integral Equation Theories, and Gaussian Fluctuation Theory for Disordered Symmetric Diblock Copolymers, DELIAN YANG, JING ZONG, QIANG WANG, Department of Chemical and Biological Engineering, Colorado State University — Based on the same model system of symmetric diblock copolymers as discrete Gaussian chains with soft, finite-range repulsions as commonly used in dissipative-particle dynamics simulations, we directly compare, without any parameter-fitting, the thermodynamic and structural properties of the disordered phase obtained from fast off-lattice Monte Carlo (FOMC) simulations¹, reference interaction site model (RISM) and polymer reference interaction site model (PRISM) theories, and Gaussian fluctuation theory. The disordered phase ranges from homopolymer melts (i.e., where the Flory-Huggins parameter $\chi = 0$) all the way to the order-disorder transition point determined in FOMC simulations, and the compared quantities include the internal energy, entropy, Helmholtz free energy, excess pressure, constant-volume heat capacity, chain/block dimensions, and various structure factors and correlation functions in the system. Our comparisons unambiguously and quantitatively reveal the consequences of various theoretical approximations and the validity of these theories in describing the fluctuations/correlations in disordered diblock copolymers. [1] Q. Wang and Y. Yin, *J. Chem. Phys.*, **130**, 104903 (2009).

5:18PM T50.00013 The power spectrum of thermal composition fluctuations in a lamellar mesophase, AUGUST BOSSE, Polymers Division, NIST — We derive an analytic expression for the power spectrum of Gaussian thermal composition fluctuations in an ordered lamellar mesophase. We compare this expression to the power spectrum measured in stochastic simulations of a two-dimensional diblock copolymer melt based on the Leibler-Brazovskii Hamiltonian. The analytic expression fits the simulation data with zero adjustable fitting parameters over a relatively wide range of model parameters. This expression will facilitate line-edge roughness (LER) modeling in block copolymer directed self-assembly applications, and it can serve as a model component in a scattering-based LER metrology framework.

Wednesday, February 29, 2012 2:30PM - 5:30PM –
Session T52 GSNP: Non-equilibrium Systems, Especially using Fluctuation Theorems and Fluctuation-Dissipation Relations 153C

2:30PM T52.00001 Transient and steady state behavior of full counting statistics in thermal transport, BIJAY AGARWALLA, BAOWEN LI, JIAN-SHENG WANG, National University of Singapore — We study the statistics of heat transferred in a given time interval t_M , through a finite harmonic system, which is connected with two heat baths, maintained at two different temperatures. We calculate the cumulant generating function (CGF) for heat transfer using non-equilibrium Green's function method. The CGF can be concisely expressed in terms of Green's functions of the system and the self-energy of the lead with shifted arguments, $\Sigma^A(\tau, \tau') = \Sigma_L(\tau + \hbar x(\tau), \tau' + \hbar x(\tau')) - \Sigma_L(\tau, \tau')$, where $\Sigma_L(\tau, \tau')$ is the contour-ordered self-energy of the left lead. The expression of CGF is valid in both transient and steady state regimes. We present a transient result of the first four cumulants of a graphene junction. It is found that measurement causes the energy to flow into the leads. In the steady state we show that the CGF obey “*steady state fluctuation theorem*”. We also study the CGF for the joint probability distribution of left and right lead heat flux $P(Q_L, Q_R)$, which is important to calculate the correlations between Q_L and Q_R , and also the total entropy that flows into the leads. We also discuss the CGF for the total entropy production for two lead system without the center part.

2:42PM T52.00002 Langevin dynamics beyond the weak coupling limit, ALEXANDER PLYUKHIN, Saint Anselm College — Many popular results of non-equilibrium statistical mechanics hold only in leading order in a small parameter λ which controls the strength of the system-environment coupling. In this approximation the equations for the first two moments $\langle v \rangle$ and $\langle v^2 \rangle$ of the Brownian particle's velocity are closed and describe exponential relaxation to thermal equilibrium. To higher orders in λ these equations are not closed but coupled to higher moments $\langle v^n \rangle$. This may result in much richer dynamics (both transient and stationary) and non-trivial ergodic properties. Generalized fluctuation-dissipation relations are derived microscopically and shown to ensure convergence to thermal equilibrium to any order in λ . One exception is the regime of superlinear diffusion, characterized by zero integral friction (vanishing integral of the memory kernel), when the generalized Langevin equation may have non-ergodic solutions that do not relax to equilibrium values. Also, for specific memory kernels the equation may have non-dissipative (non-stationary) solutions even if the integral friction is finite and diffusion is normal.

2:54PM T52.00003 Jarzynski equality for spin glasses and its application, MASAYUKI OHZEKI, Department of Systems Science, Graduate school of Informatics, Kyoto University, KOJI HUKUSHIMA, Department of Basic Science, Graduate School of Arts and Sciences University of Tokyo, HIDETOSHI NISHIMORI, Department of Physics, Tokyo Institute of Technology — We study an application of Jarzynski equality to spin glasses with gauge symmetry. It is shown that the exponentiated free-energy difference appearing in the Jarzynski equality reduces to a simple analytic function written explicitly in terms of the initial and final temperatures if the temperature satisfies a certain condition related to gauge symmetry. This result can be used to derive a lower bound on the performed work during the nonequilibrium process by changing the external magnetic field as well as a pseudo work done during changing temperature. The latter case serves as useful information to implement the population annealing developed in numerical use of the Jarzynski equality to equilibrate the many-body system. We also prove several exact identities that relate equilibrium and nonequilibrium quantities. These identities show possibility of the population annealing to evaluate equilibrium quantities from nonequilibrium computations, which may be useful for avoiding the problem of slow relaxation in spin glasses.

3:06PM T52.00004 Thermodynamic reversibility in feedback processes¹, JORDAN HOROWITZ, JUAN PARRONDO, Universidad Complutense de Madrid — The information acquired during a thermodynamic process with feedback can be converted into useful work. However, the second law of feedback restricts the amount of useful work that can be obtained from this information. In this presentation, I will discuss optimal thermodynamic processes with feedback, where all the information is converted into work. Utilizing the detailed fluctuation theorem for feedback, I will demonstrate that such processes are feedback-reversible: they are indistinguishable from their time-reversal, thereby extending the notion of thermodynamic reversibility to feedback processes.

¹Financial support for this project came from MOSAICO (Spanish Government) and MODELICO (Comunidad de Madrid)

3:18PM T52.00005 Entropy production in non-equilibrium steady states¹, DANIEL BEN-AVRAHAM, Clarkson University, SVEN DOROSZ, University of Luxembourg, MICHEL PLEIMLING, Virginia Tech — We discuss entropy production in non-equilibrium steady states by focusing on paths obtained by sampling at regular (small) intervals, instead of sampling on each change of the system's state. This allows us to directly study entropy production in systems with microscopic irreversibility. The two sampling methods are equivalent otherwise, and the fluctuation theorem also holds for the different paths. We focus on a fully irreversible three-state loop, as a canonical model of microscopic irreversibility, finding its entropy distribution, rate of entropy production, and large deviation function in closed analytical form, and showing that the observed kink in the large deviation function arises solely from microscopic irreversibility [1].

[1] D. ben-Avraham, S. Dorosz, and M. Pleimling, Phys. Rev. E 84, 011115 (2011)

¹Supported in part by the US National Science Foundation through Grant DMR-0904999.

3:30PM T52.00006 Information, entropy, and heat far from equilibrium¹, SEBASTIAN DEFFNER, University of Maryland — For equilibrium states, the Shannon entropy, $H = - \int d\Gamma p(\Gamma) \ln p(\Gamma)$, coincides with the thermodynamic entropy. It has lately been recognized that for systems in nonequilibrium steady states a thermodynamic description based on H becomes feasible, as well. In the present work we derive various generalizations of the second law for nonequilibrium processes with additional information supplied from an external or an internal memory. We will show that the irreversible entropy production is bounded from below by the information transferred from the memory to the system.

¹This work was funded by the DAAD.

3:42PM T52.00007 Effective temperature determines density distribution in a slowly varying external potential beyond linear response, GRZEGORZ SZAMEL, MIN ZHANG, Department of Chemistry, Colorado State University — We consider a sheared colloidal suspension under the influence of an external potential that varies slowly in space in the plane perpendicular to the flow and acts on one selected (tagged) particle of the suspension. Using a Chapman-Enskog type expansion we derive a steady state equation for the tagged particle density distribution. We show that for potentials varying along one direction only, the tagged particle distribution is the same as the equilibrium distribution with the temperature equal to the effective temperature obtained from the violation of the Einstein relation between the self-diffusion and tagged particle mobility coefficients. We thus prove the usefulness of this effective temperature for the description of the tagged particle behavior beyond the realm of linear response. We illustrate our theoretical predictions with Brownian dynamics computer simulations.

3:54PM T52.00008 ABSTRACT WITHDRAWN —

4:06PM T52.00009 Dynamic phase transitions in large work production of linear diffusion systems, HYUNGGYU PARK, Korea Institute for Advanced Study, CHULAN KWON, Myongji University, JAE DONG NOH, University of Seoul — We present the theoretical study on non-equilibrium (NEQ) fluctuations for diffusion dynamics in high dimensions driven by a linear drift force. We find the time-dependent probability distribution function exactly as well as the NEQ work production distribution $P(W)$ in terms of solutions of nonlinear differential equations. In two dimensions, we find analytically a sequence of dynamic phase transitions in the exponential tail shape of $P(W)$. Their implications and origins are discussed.

4:18PM T52.00010 Driven Langevin dynamics: heat, work and pseudo-work, DAVID SIVAK, Lawrence Berkeley National Laboratory, JOHN CHODERA, University of California, Berkeley, GAVIN CROOKS, Lawrence Berkeley National Laboratory — Common algorithms for simulating Langevin dynamics are neither microscopically reversible, nor do they preserve the equilibrium distribution. Instead, even with a time-independent Hamiltonian, finite time step Langevin integrators model a driven, nonequilibrium dynamics that breaks time-reversal symmetry. Herein, we demonstrate that these problems can be resolved with a Langevin integrator that splits the dynamics into separate deterministic and stochastic substeps. This allows the total energy change of a driven system to be divided into heat, work, and pseudo-work – the work induced by the finite time step. The extent of time-symmetry breaking due to the finite time step can be measured and true equilibrium properties recovered. This interpretation of discrete time step Langevin dynamics as a driven process provides new insights into the practical use of stochastic integrators for molecular simulation.

4:30PM T52.00011 Statistical interpretation of heat and work and the adiabatic theorem in irreversible processes, PURU GUJRATI, University of Akron — By generalizing the traditional concept [1] of heat and work to include their irreversible components allows us to express them in statistical terms so that dW is the *isentropic* energy change; this generalizes the equilibrium adiabatic theorem. Then dQ is then nothing but the energy change solely due to the change in the microstate probability. Accordingly $dQ=TdS$ [2] so that *all powerful aspects of the equilibrium formulation are preserved*, a quite remarkable but unexpected result. The traditional formulation of the first law of thermodynamics, which uses the fields (temperature, pressure, etc.) of the medium can be *equivalently* written as $dE=dQ-dW$ using the fields of the system. This makes the two descriptions using the fields of the medium or the system equivalent and settles the long existing dispute in the literature regarding the proper choice of the fields. Moreover, the use of system fields (including affinities) allows us to analyze non-equilibrium processes such as free expansion between non-equilibrium states, which cannot be analyzed in the traditional approach.

[1] P.D. Gujrati, arXiv:1105.5549.

[2] P.D. Gujrati, Phys. Rev. E **81**, 051130 (2010).

4:42PM T52.00012 Application of the generalized fluctuation-dissipation theorem on a sheared suspension¹, EMMANOUELA FILIPPIDI, ALEXANDRE FRANCESCHINI, DAVID PINE, Center for Soft Matter Research, New York University — We explore the validity of the generalized fluctuation-dissipation theorem for steady-state systems (proposed by Prost, Joanny and Parrondo, PRL 103, 090601 2009) in an experimental system: a suspension of non-colloidal spheres under slow periodic strain. The system is out-of-equilibrium and typically undergoes a phase transition from an active fluctuating to an absorbing state as the strain amplitude is decreased. It is a good candidate for applying the proposed theory since it has Markovian dynamics and fluctuating steady states. The control parameters are the applied strain amplitude and its volume fraction and fluctuations of proper observables such as the individual particle locations can be readily measured. Perturbations of the control parameter of strain can lead in new steady states after a transient response, which in turn can be correlated with the fluctuating observable, thus providing a way of verifying the validity of the proposed version of the generalized fluctuation-dissipation theorem.

¹Onassis Foundation

4:54PM T52.00013 Entropy rate of non-equilibrium growing networks, ARDA HALU, KUN ZHAO, Northeastern University, SIMONE SEVERINI, University College London, GINESTRA BIANCONI, Northeastern University — In order to quantify the complexity of networks, new entropy measures have recently been introduced. Most of these entropy measures pertain to static networks or to dynamical processes defined on static complex networks. In this talk, we will discuss the entropy rate of growing network models, which quantifies how many labeled networks are typically generated by those growing network models. We will present an analytical evaluation of the difference between the entropy rate of growing tree network models and the entropy of tree networks that have the same asymptotic degree distribution. We will outline our finding that growing networks with linear preferential attachment generated by dynamical models are exponentially less in number than the static networks with the same degree distribution for a large variety of relevant growing network models. We will also discuss the entropy rate for growing network models that show structural phase transitions, including models with non-linear preferential attachment. We will conclude by presenting numerical simulations showing that the entropy rates above and below the structural phase transitions follow a different scaling with the network size.

5:06PM T52.00014 Persistency and Uncertainty Across the Academic Career, ALEXANDER PETERSEN, MASSIMO RICCABONI, IMT Lucca Institute for Advanced Studies, H. EUGENE STANLEY, Boston University, FABIO PAMMOLLI, IMT Lucca Institute for Advanced Studies — Recent shifts in the business structure of universities and a bottleneck in the supply of tenure track positions are two issues that threaten to change the longstanding patronage system in academia and affect the overall potential of science. We analyze the longitudinal publication rate $n_i(t)$ on the 1-year scale for 300 physicists $i = 1...300$. For most careers analyzed, we observe cumulative production acceleration $N_i(t) \approx A_i t^{\alpha_i}$ with $\alpha_i > 1$, reflecting the benefits of learning and collaboration spillovers which constitute a cumulative advantage. We find that the variance in production scales with collaboration radius size S_i as $\sigma_i^2 \sim S_i^\psi$ with $0.4 < \psi < 0.8$. We develop a preferential growth model to gain insight into the relation between career persistency and career uncertainty. This model shows that emphasis on nonstop production, a consequence of short-term contract systems, results in a significant number of “sudden death” careers that terminate due to unavoidable negative production shocks. Hence, short-term contracts may increase the strength of “rich-get-richer” mechanisms in competitive professions and hinder the upward mobility of young scientists.

5:18PM T52.00015 A Random Walk Picture of Basketball, ALAN GABEL, SIDNEY REDNER, Boston University — We analyze NBA basketball play-by-play data and found that scoring is well described by a weakly-biased, anti-persistent, continuous-time random walk. The time between successive scoring events follows an exponential distribution, with little memory between events. We account for a wide variety of statistical properties of scoring, such as the distribution of the score difference between opponents and the fraction of game time that one team is in the lead.

Wednesday, February 29, 2012 2:30PM - 5:30PM —

Session T53 GSNP: Focus Session: Wave Propagation in Strongly Scattering Media 153B

2:30PM T53.00001 Fluctuations in Intensity in disordered media as a New Sub-wavelength Microscopy Tool , GABRIEL CWILICH, Department of Physics, Yeshiva University, JUAN JOSE SAENZ, Departamento de Física de la Materia Condensada, Universidad Autonoma de Madrid — The intensity-intensity correlations of waves that propagate coherently through a disordered system are discussed, in the mesoscopic scale. Since many of the properties of those correlations are independent of the transport regime (ballistic, diffusive or localized) they can be discussed using the macroscopic approach of random matrix theory [1]. In that framework we have considered the problem of multiple sources emitting simultaneously in a disordered medium, and we will show that the correlations and even the intensity fluctuations at a fixed point outside the turbid system can provide useful information about both the relative position of the sources and their coherence. Moreover, the information obtained is relevant at subwavelength lengths, opening the possibility of new applications to fluorescence studies, communications and image processing in turbid environments, complementary to traditional techniques.

[1] G. Cwilich, L. Froufe, J.J. Saenz, Phys Rev E74, 045603 (R) (2006)

2:42PM T53.00002 Photon localization in a nematic liquid crystal¹ , JIM MCCLYMER, MATT LUDDEN, University of Maine, Dept. of Physics and Astronomy, JESSE WERTHEIM, None — The nematic liquid crystal MBBA, due to director fluctuations, is a highly scattering material with low absorption. We previously² reported that the transmission coefficient for laser light at 633 nm decays exponentially with a decay length of approximately 0.8 mm while the absorption length is over 30 times larger which we interpret as evidence for photon localization. The data does not fit a model of diffusion or diffusion with absorption. We have extended this work by measuring the decay coefficient for incoherent light from 475 to 825 nm. We find that the absorption remains low over this range, with absorption lengths ranging from 8 mm at the blue end of the spectrum to 12 mm in the near IR. The transmission coefficient in the nematic phase shows an exponential decrease with decay constants an order of magnitude smaller than the absorption length, 0.4 mm, in the blue end while increasing to 3 mm in the near IR. The data indicates that photon localization is observed throughout the visible region into the near IR.

¹Maine Space Grant Consortium Grants No. EP-02-09 and No. EP-03-10

² J. P. McClymer and H.M. Shehadeh, Photon Localization in a Nematic Liquid Crystal, Phys. Rev. A 79, 031802(R) (2009)

2:54PM T53.00003 Light Transport in Disordered Media with PT-symmetry¹ , SAMUEL KALISH, ZIN LIN, TSAMPIKOS KOTTOS, Wesleyan University — The localization properties of randomly layered optical media with $\mathcal{PT}$ -symmetric refraction index are studied both theoretically and numerically using the transfer-matrix method. The transmission coefficient decays exponentially as a function of the system size, with a rate $\xi_\gamma(W)^{-1} = \xi_0(W)^{-1} + \xi_\gamma(0)^{-1}$, where $\xi_0(W)$ is the localization length of the equivalent passive disordered system and $\xi_\gamma(0)$ is the attenuation/amplification length of the corresponding perfect system with combined gain/loss refraction index profile. While transmission processes are reciprocal to left and right incident waves, one-sided reflection is found.

¹This research was supported by an AFOSR No. FA 9550-10-1-0433 grant and by a NSF ECCS-1128571 grant.

3:06PM T53.00004 New perspectives on waves in random media: Speckle, modes, transmission eigenchannels, and focusing¹ , AZRIEL GENACK, Queens College of the City University of New York — The understanding of electron localization and conductance fluctuations has been advanced by utilizing notions of speckle, modes, and transmission eigenchannels. These concepts cannot be probed directly for electronic systems but can be explored for classical waves utilizing spectra of field transmission coefficients between arrays of points on the incident and output surfaces of ensembles of random samples. This is illustrated in microwave measurements of transmission through random waveguides in the Anderson localization transition. These experiments supply the link between the statistics of intensity and conductance and show that transmitted wave can be decomposed simultaneously into the underlying quasi-normal modes and transmission eigenchannels of the sample. The power of each of these approaches and the richness of the links between them will be illustrated by examples that reveal new aspects of wave propagation. The delayed onset of transmission following pulse excitation is shown to be the result of destructive interference between highly correlated speckle patterns of neighboring modes, while the falling decay rate at later times reflects the incoherent decay of increasingly prominent long-lived modes. We determine the individual eigenvalues τ_n of the transmission matrix and achieve nearly complete transmission in opaque diffusive samples. We demonstrate that when reflection at the sample interface is taken into account, the spacing between average values of $\ln\tau_n$ is equal to the inverse of the bare conductance, in accord with predictions by Dorokhov [1]. We find that the distribution of total transmission relative to the conductance is determined by the effective number of transmission eigenvalues, $N_{eff} = (\sum_{n=1}^N \tau_n)^2 / \sum_{n=1}^N \tau_n^2$, which provides the link between the statistics of intensity and conductance. For diffusive waves, N_{eff} is the inverse of the degree of intensity correlation. The contrast between the peak and background of maximally focused radiation in the transmitted wave, achieved when the incident is phase conjugated relative to the selected focal point, is equal to $(1 + N_{eff})$.

[1] O. N. Dorokhov, Solid State Commun. **51**, 381 (1984).

¹In collaboration with M. Davy, Z. Shi and J. Wang. I thank the National Science Foundation for support through grant No. DMR-0907285.

3:42PM T53.00005 Experimental Observation of Brachistochrone Wave Dynamics in PT Symmetric Structures¹ , JOSEPH SCHINDLER, HAMIDREZA RAMEZANI, ANG LI, MEI ZHENG, TSAMPIKOS KOTTOS, FRED ELLIS, Wesleyan University, Middletown, CT — Mutually coupled modes of a pair of active LRC circuits, one with amplification and another with an equivalent amount of attenuation, provide an experimental realization of a wide class of systems where gain and loss mechanisms break the Hermiticity while preserving parity-time (PT) symmetry. For a value γ_{PT} of the gain and loss strength parameter the eigenfrequencies undergo a spontaneous phase transition from real to complex values, while the normal modes coalesce, acquiring a definite chirality. A dramatic manifestation of PT symmetry is observed in the brachistochrone wave dynamics. Experimental findings support the theoretical prediction of arbitrarily small energy transfer times between the LRC elements of the circuit. We envision that realization of such design strategies can have applications in telecommunications and metamaterial structures.

¹Wesleyan Project Grant, AFOSR No. FA 9550-10-1-0433

3:54PM T53.00006 Experimental studies of PT-scattering in arrays of active LRC elements¹ , ZIN LIN, JOSEPH SCHINDLER, HAMID RAMEZANI, FRED ELLIS, TSAMPIKOS KOTTOS, Wesleyan University, WAVE TRANSPORT IN COMPLEX SYSTEMS TEAM — One of the fundamental tasks in antenna theory is getting an antenna to radiate by removing mismatch losses between the loaded antenna and the transmission line that delivers the power. We will present experimental data suggesting that $\mathcal{PT}$ -symmetric antenna structures, where active elements associated with the real part of impedance ($\pm R$) are involved, can lead to a broadband, reflectionless behavior. The suggested *optimal matching* strategy can potentially be superior to the existing one which uses active LC elements in order to balance the reactance. Along these lines, we also envision antenna arrangements with unidirectional ultrafast communication capabilities, where the signal will transfer faster (or slower) between the active elements of the $\mathcal{PT}$ -structure depending on the entrance point of the incident wave.

¹We acknowledge AFOSR No. FA 9550-10-1-0433 grant and a NSF ECCS-1128571 grant.

4:06PM T53.00007 Measurement of the Probability Distribution of Optical Transmittance on the Crossover to Anderson localization, ZHOU SHI, JING WANG, AZRIEL GENACK, Department of Physics, Queens College of the City University of New York — We report measurements of spectra of the field transmission matrix t for microwave radiation propagating through waveguide filled with randomly positioned dielectric scattering spheres in the Anderson localization transition. Diagonalizing the matrix product $tt^\dagger$ gives the transmission eigenvalues τ_n , which yields the optical transmittance, $T = \sum_{a,b=1}^N |t_{ba}|^2 = \sum_{n=1}^N \tau_n$. The ensemble average of the transmittance is equal to the dimensionless conductance, $g = \langle T \rangle$. We show the probability distribution of transmittance $P(T)$ changes from Gaussian to log-normal as the value of g decreases. The distribution $P(T)$ is analyzed in terms of the underlying transmission eigenvalues τ_n . For random samples with $g \sim 3.9$, we found $P(T)$ follows a Gaussian distribution. For $g \sim 0.37$, we observe a highly asymmetric distribution for $-\ln T$. The sharp drop for high values of T is attributed to the restriction that $\tau_n < 1$ and the repulsion between transmission eigenvalues even for localized samples. For $g \sim 0.04$, the distribution of transmittance is nearly log-normal. The variance of $-\ln T$, σ^2 , scales linearly with $\langle -\ln T \rangle$ as predicted by single parameter scaling even for weakly localized waves.

4:18PM T53.00008 Mode Statistics in Random Media¹, JING WANG, AZRIEL GENACK, Department of Physics, Queens College, The City University of New York — The nature of transport through a material is determined by the spectrum of modes or energy levels. We have analyzed the frequency variation of the transmitted microwave field speckle pattern for quasi one-dimensional random samples to obtain the central frequencies, linewidths and speckle patterns of the modes for an ensemble of samples at lengths of two and three times the localization length. The number of modes can be determined unambiguously from the spectrum of the goodness of fit. From these results we obtain the statistics of mode spacings and widths. The distribution of spacings between adjacent modes is close to the Wigner surmise predicted for diffusive waves exhibiting strong level repulsion. However, deviations from the Wigner surmise can be seen in the distribution of spacings beyond nearest modes. A weakening in the rigidity of the modal spectrum is observed as the sample length increases because of reduced level repulsion for more strongly localized waves. In contrast to residual diffusive behavior for level spacing statistics, the distribution of level widths are log-normal as predicted for localized waves.

¹The research was supported by the NSF under Grant No. DMR-0907285 and a PSC-CUNY grant.

4:30PM T53.00009 A Random Matrix Approach for Understanding Wave Statistics from Wireless Communications to Quantum Dots¹, JEN-HAO YEH, EDWARD OTT, THOMAS ANTONSEN, STEVEN ANLAGE, University of Maryland — Complexity of a wave propagation environment is advantageous from the perspective of wave chaos theory because, in the semiclassical limit, the corresponding ray trajectories of the wave propagation have chaotic dynamical behavior, and a statistical description is most appropriate. Random matrix theory (RMT) successfully describes universal properties of the system. We combine RMT with our random coupling model that includes non-universal effects, such as the radiation impedance of the ports and the effect of short ray trajectories in the system, and we establish a first-principles model for wave statistical properties such as the fading amplitude in wireless communications, the scattering matrix, the impedance matrix, and the thermopower of quantum dots. We also report experimental tests on two ray-chaotic microwave cavities with different degrees of loss. In the high loss regime the results demonstrate that our RMT model agrees with traditional fading models (Rayleigh fading and Rice fading) and provides a more general understanding of the models and a detailed physical basis for their parameters. Moreover, in the low loss regime the RMT approach describes the data better.

¹This work is funded by the ONR/Maryland AppEl Center Task A2 (contract No. N000140911190), the AFOSR under grant FA95500710049, and Center for Nanophysics and Advanced Materials (CNAM).

4:42PM T53.00010 Quantifying Volume Changing Perturbations to a Wave Chaotic System¹, BINIYAM TADDESE, Department of Electrical & Computer Engineering, University of Maryland, College Park, MD 20742-3285, USA, GABRIELE GRADONI, Department of Physics, University of Maryland, College Park, MD 20742-4111, USA, FRANCO MOGLIE, Dip. di Ingegneria dell'Informazione, Università Politecnica delle Marche, Ancona, Italy, THOMAS ANTONSEN, EDWARD OTT, STEVEN ANLAGE, Department of Physics, University of Maryland, College Park, MD 20742-4111, USA — The Loschmidt Echo and Fidelity decay are used to measure perturbations on a quantum wave chaotic system. We extended these concepts to classical waves to detect perturbations. [1]. In this work, we show that volume changing perturbations to a classical wave chaotic cavity can be quantified with a sub-wavelength sensitivity. This is demonstrated both numerically and experimentally. A wave chaotic quasi-1D star graph model [2], was initially used to show the results. The quantification of electrical-volume changing perturbations to a one cubic meter aluminum box will be demonstrated experimentally; the experimental results are also supported by a finite difference time domain simulation of the box. Finally, the approach to quantify these perturbations will be shown to apply to a generic wave chaotic system by using a time domain version of our Random Coupling Model.

¹Work funded by ONR MURI grant N000140710734, AFOSR grant FA95501010106, and the Maryland CNAM.

4:54PM T53.00011 Nonlinear Time-Reversal in a Wave Chaotic System¹, MATTHEW FRAZIER, BINIYAM TADDESE, EDWARD OTT, THOMAS ANTONSEN, STEVEN ANLAGE, University of Maryland — Time reversal mirrors are particularly simple to implement in wave chaotic systems and form the basis for a new class of sensors [1-3]. These sensors work by applying the quantum mechanical concepts of Loschmidt echo and fidelity decay to classical waves. The sensors make explicit use of time-reversal invariance and spatial reciprocity in a wave chaotic system to remotely measure the presence of small perturbations to the system. The underlying ray chaos increases the sensitivity to small perturbations throughout the volume explored by the waves. We extend our time-reversal mirror to include a discrete element with a nonlinear dynamical response. The initially injected pulse interacts with the nonlinear element, generating new frequency components originating at the element. By selectively filtering for and applying the time-reversal mirror to the new frequency components, we focus a pulse only onto the element, without knowledge of its location. Furthermore, we demonstrate transmission of arbitrary patterns of pulses to the element, creating a targeted communication channel to the exclusion of 'eavesdroppers' at other locations in the system. [1] Appl. Phys. Lett. 95, 114103 (2009) [2] J. Appl. Phys. 108, 1 (2010) [3] Acta Physica Polonica A 112, 569 (2007)

¹Work funded by the Intelligence Community Postdoctoral Research Fellowship Program and the Center for Nanophysics and Advanced Materials.

5:06PM T53.00012 Low-Diffracting Modes in Surface Plasmon Metamaterials, SANDEEP INAMPUDI, Department of Physics and Applied Physics, University of Massachusetts Lowell, IGOR SMOLYNONOV, Department of Electrical and Computer Engineering, University of Maryland, VIKTOR PODOLSKIY, Department of Physics and Applied Physics, University of Massachusetts Lowell — Plasmonic structures, with periodic arrays of thin PMMA ridges on metal substrates have been shown experimentally to overcome the diffraction limit. Here we present a theoretical description of this phenomenon. We use mode matching technique to analyze the dynamics of the electromagnetic waves in the periodic systems, taking into account the extended 3D-geometry and the finite thickness of the PMMA ridges. Specifically, we focus on the behavior of plasmonic mode and its non-trivial coupling to the free space waves and to the other guided modes of the system. The eigen states of the periodic system dominated by the surface waves are identified and their dispersion is analyzed via generalization of mode-matching formalism and Bloch-periodic approach. An analytical approximation, adequately describing the behavior of the system is derived and is used to explain the suppression of diffraction in the system.

5:18PM T53.00013 Nonsymmorphic Phononic Metamaterials: shaping waves over multiple length scales¹, CHEONGYANG KOH, DSO National Laboratories, S118230, Singapore, EDWIN THOMAS, School of Engineering, Rice University, P.O. Box 1892, Houston, Texas 77251, USA — The vector nature of the phonon makes rational design of phononic metamaterials challenging, despite potential in unique wave propagation behavior, such as negative refraction and hyper-lensing. While most designs to date focus on the “meta-atom” (building block) design, their “spatial arrangement” (non-locality) is equally instrumental in dispersion engineering. Here, we present a generalized design framework (DF) for PMM design, utilizing both “global” and “local” symmetry concepts. We demonstrate, utilizing specific properties of nonsymmorphic plane groups, PMMs possessing i) a low-frequency in-plane complete spectral gap (ICSG) of 102% (CSG of 88%), ii) a set of polychromatic ICSGs totaling over 100% in normalized gap size. Within the same DF, we further integrate broken symmetry states (BSS) (edge states, waveguides, etc) with designed polarization, (de)localization and group velocities. In particular, we demonstrate how these BSS may be utilized to elucidate signatures of complex polarization fields through phonon-structure interactions, leading to interesting applications in elastic-wave imaging, as well as information retrieval by probing polarization states of scattering bodies over multiple scales.

¹We gratefully acknowledge funding from NSF, DSO-Singapore.

Wednesday, February 29, 2012 2:30PM - 5:18PM – Session T54 DCMP: Superconductivity: Mostly Spectroscopy and Pairing 152

2:30PM T54.00001 Probing the Photoresponse of Superconducting Materials and Devices by Laser Scanning Microscopy¹, STEVEN ANLAGE², BEHNOOD GHAMSARI, University of Maryland — We present the results of photoresponse experiments on superconducting rf/microwave devices, including Niobium and Cuprate resonators and metamaterials, by means of laser scanning microscopy. The spatially inhomogeneous photoresponse of these devices reveals the distribution of rf/microwave currents. Moreover, it will be discussed that the dependence of the phase of the photoresponse to the exciting microwave frequency may be used to bifurcate the kinetic and resistive parts of the photoresponse mechanism, which, in turn, could be used to probe the evolution of the local order parameter at different temperatures. Furthermore, we will examine the possibility of imaging the anisotropy of superconducting properties, as in the anisotropic Meissner effect, by investigating the photoresponse of a working superconducting resonator to visible light. While most of the aforementioned devices consist of thin films and cast into resonant structures, we will further discuss the techniques through which these measurements can be extended to bulk materials as well as non-resonant structures. These results are particularly useful for identifying the sources of quench and hot spots in a variety of superconducting devices including superconducting RF cavities.

¹This work is, in part, supported by the DOE grant number DESC0004950 and ONR/AppEl, Task D10, through grant number N000140911190.

²The authors would like to acknowledge technical help from Dr. Alexander Zhuravel.

2:42PM T54.00002 Far infrared study of magnetic field induced normal states of $\text{La}_{1.94}\text{Sr}_{0.06}\text{CuO}_4$, THOMAS TIMUSK, Department of Physics and Astronomy, McMaster University, Hamilton ON, Canada, TOOMAS RÖÖM, URMAS NAGEL, DANIEL HÜVONEN, National Institute of Chemical Physics and Biophysics, Tallinn, Estonia, DAVID HAWTHORN, Department of Physics University of Waterloo, Waterloo, ON, Canada, S. WAKIMOTO, H. ZHANG, Department of Physics, University of Toronto, Toronto, ON, Canada, JUNGSEOK HWANG, Department of Physics and Astronomy, McMaster University, Hamilton ON, Canada — We report on the ab-plane optical properties of the magnetic field induced normal state of $\text{La}_{1.94}\text{Sr}_{0.06}\text{CuO}_4$ ($T_c = 5.5\text{K}$), the first such study. We apply strong magnetic fields (4 T and 16 T) along the c-axis. We find that at 4 T fields, which are strong enough to destroy superconductivity, the normal state at 1.4 K is very similar to the normal state at 20 K in zero field. However at higher fields we observed a gap-like depression in the optical conductivity at low frequency along with parallel growth of a broad absorption peak centered at higher frequency. The spectral weight loss in the depression at low frequency is recovered by the spectral weight in the broad peak. We attribute the magnetic field induced gap-like depression and the broad peak to a competing charge order to superconducting order or charge localization in ab-plane of the system.

2:54PM T54.00003 Electron energy loss spectroscopy study of superconducting Nb and its native oxides, RUNZHE TAO, R. TODOROVIC, J. LIU, R. MEYER, A. ARNOLD, University of Illinois at Chicago, W. WALKOSZ, P. ZAPOL, ANL, A. ROMANENKO, L. COOLEY, FNAL, ROBERT KLIE, University of Illinois at Chicago — Niobium has attracted increasing attention in recent years due to its usage in superconducting RF-cavities in next generation particle accelerators. In particular, the possible role of oxidation or the presence of oxygen vacancies on the superconducting properties of niobium metals used in superconducting RF cavities has been the focus on many recent studies. Here, we present a series of electron energy-loss spectroscopy (EELS) studies on niobium (Nb) and its oxides (NbO , NbO_2 , Nb_2O_5) to develop a reliable method for quantifying the oxidation state in mixed niobium oxide thin films. Our approach utilizes a combination of transmission electron microscopy and EELS experiments with density functional theory calculations to distinguish between metallic niobium and the different niobium oxides. Based on these observed changes in the core-loss edges, we propose a linear relationship that correlates the peak positions in the Nb M- and O K-edges with the Nb valence state. The methods developed in this paper will then be applied to ultrathin niobium oxide films to examine the effects of low-temperature baking on the films' oxidation states. In addition to oxides, Niobium hydrides are considered as one of the main reasons for Q-decrease under high field. The different phases of Nb hydride can be identified directly using electron diffraction and EELS, which allows for the local hydrogen concentration to be examined at room temperature as well as 95 K.

3:06PM T54.00004 Strong-Field Pulsed THz Study of Superconductivity Breakdown in NbN ¹, G.L. CARR, Y. SHEN, Y. HIDAKA, J.B. MURPHY, X. YANG, X.-J. WANG, Photon Sciences, Brookhaven National Laboratory — We report the ultra-fast breakdown of the superconducting state in a NbN thin film ($T_c \approx 14\text{K}$) when exposed to an intense single-cycle THz pulse. The THz pulse's transform-limited spectral content was kept below the NbN pair-breaking energy threshold near $2\Delta/\hbar c = 35\text{ cm}^{-1}$ (i.e., $<1\text{ THz}$). Thus, the initial electronic response was dominated by the inductive behavior of the pair condensate. At low THz E-field strength, the NbN film transmitted less for the superconducting state than for the normal state, as expected. As a function of increasing THz E-field strength, the film transmittance remained constant until a threshold range was reached, after which the transmittance changed over to its normal state value. Through this threshold range we also observed a significant non-linear response in the form of THz upconversion to frequencies approaching 3 times the optical gap, corresponding to time scales well below 1 picosecond.

¹Supported by the U.S. Dep't. of Energy under contract DE-AC02-98CH10886 at Brookhaven Nat'l Lab

3:18PM T54.00005 ABSTRACT WITHDRAWN —

3:30PM T54.00006 Spatial Complexity Due to Bulk Electronic Liquid Crystals in Superconducting Dy-Bi2212, ERICA CARLSON, BENJAMIN PHILLABAUM, Purdue University, KARIN DAHMEN, University of Illinois at Urbana-Champaign — Surface probes such as scanning tunneling microscopy (STM) have detected complex electronic patterns at the nanoscale in many high temperature superconductors. In cuprates, the pattern formation is associated with the pseudogap phase, a precursor to the high temperature superconducting state. Rotational symmetry breaking of the host crystal (i.e. from C4 to C2) in the form of electronic nematicity has recently been proposed as a unifying theme of the pseudogap phase [Lawler Nature 2010]. However, the fundamental physics governing the nanoscale pattern formation has not yet been identified. Here we use universal cluster properties extracted from STM studies of cuprate superconductors to identify the fundamental physics controlling the complex pattern formation. We find that due to a delicate balance between disorder, interactions, and material anisotropy, the rotational symmetry breaking is fractal in nature, and that the electronic liquid crystal extends throughout the bulk of the material.

3:42PM T54.00007 Search for order parameter domains in single crystal flakes of chiral p -wave superconductor Sr_2RuO_4 using micrometer size Josephson junctions, YIQUN YING, YING LIU, Department of Physics, The Pennsylvania State University, DAVID FOBES, TIJIANG LIU, ZHIQIANG MAO, Department of Physics, Tulane University — Even though the odd-parity, spin-triplet superconductivity in Sr_2RuO_4 is supported by many experimental studies, the existence of order parameter domains and domain walls remains to be an open question. In addition, how these domains can be controlled experimentally is not understood. We fabricate small Al- Sr_2RuO_4 Josephson junctions using flakes of singlecrystalline Sr_2RuO_4 prepared by mechanical exfoliation, using Ti as an interlayer for adhesion purpose. The $3\text{ }\mu\text{m}$ wide junctions defined by photolithography on a natural ac plane was found to show Josephson coupling. Experiments on the effect of domain walls on Josephson coupling and the control of domain walls are being explored. The work is supported by DOE under Grant No. DE-FG02-04ER46159 and Penn State nanofabrication lab.

3:54PM T54.00008 T-linear resistivity and hot Fermi surface from spin-density wave quantum critical fluctuations¹, DOMINIC BERGERON, A.-M. S. TREMBLAY, Universite de Sherbrooke — The linear dependence in temperature T of the resistivity observed in the normal phase of unconventional superconductors is often attributed to quantum critical behavior. We use the two-particle self-consistent (TPSC) approach to the Hubbard model to study this problem. The quantum critical point is associated with a spin-density wave (SDW) phase transition at zero-temperature on the 2D square lattice at finite doping. Our approach satisfies the Mermin-Wagner theorem, the Pauli principle and conservation laws, and is valid from weak to intermediate coupling. We take into account vertex corrections. For the model with nearest neighbors only and also with t' and t'' , we compute, as a function of T , contributions to the conductivity coming from different directions in the Brillouin zone. Our results show that the low temperature resistivity is linear because the whole Fermi surface is hot down to the lowest temperatures studied. This occurs because the SDW correlation length and the thermal de Broglie wavelength both scale as $1/T$.

¹NSERC, CRC, CIFAR, CFI, MDEIE

4:06PM T54.00009 Controlled Intergrowth of 248 and 247 Phases of Y-Ba-Cu-O in Epitaxial Films and Heterostructures¹, H. ZHANG, University of Toronto, N. GAUQUELIN, G.A. BOTTON, Canadian Centre for Electron Microscopy and McMaster University, J.Y.T. WEI, University of Toronto and Canadian Institute for Advanced Research — Recent studies have shown that superconductivity in the Y-Ba-Cu-O (YBCO) family of cuprates can also be rooted in the quasi-1D Cu-O chains [1], even when the CuO_2 planes are not conducting [2]. The critical temperature (T_c) depends on the phase of YBCO present, such as $\text{Y}_2\text{Ba}_4\text{Cu}_8\text{O}_{16}$ (248) and $\text{Y}_2\text{Ba}_4\text{Cu}_7\text{O}_{15}$ (247). Recent studies have also shown that heterostructuring YBCO with other oxides such as $\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3$ (LCMO) can strongly influence the former's T_c [3]. This talk reports on a reexamination of these issues, by probing and controlling the intergrowth of the various YBCO phases in thin films and heterostructures. The samples were grown epitaxially by pulsed laser-ablated deposition, and characterized by electrical transport, XRD and high-resolution TEM with in-situ EELS. We observed the presence of 248 and 247 phases in YBCO/LCMO heterostructures. We also observed conversion between different phases of YBCO depending on the thermodynamics of the growth and annealing conditions. The implication of our results on the T_c variation in YBCO/LCMO heterostructure is discussed.

[1] J. Ngai *et al.*, PRL. 98, 177003 (2007).

[2] E. Berg *et al.*, PRB. 76, 214505 (2007).

[3] Z. Sefrioui *et al.*, PRB. 67, 21451 (2003)

¹Work supported by NSERC, CFI/OIT and CIFAR.

4:18PM T54.00010 Quantitative measurements of the magnetic field profile in superconductors¹, VLADIMIR KOZHEVNIKOV, Tulsa Community College, ANDREAS SUTER, Paul Scherrer Institute, Switzerland, HELMUT FRITZSCHE, NRC-CNRC Chalk River Laboratories, Canada, KRISTIAAN TEMST, Katholieke Universiteit Leuven, Belgium, THOMAS PROKSCHA, ELVEZIO MORENZONI, Paul Scherrer Institute, Switzerland, MARGRIET VAN BAEI, CHRIS VAN HAESENDONCK, JOSEPH INDEKEU, Katholieke Universiteit Leuven, Belgium — Measurement of the magnetic field profile $B(z)$, z being the distance from the sample surface, in the Meissner state of superconductors is one of the longest standing problems of experimental superconductivity. Importance of $B(z)$ follows, in particular, from the fact, that it provides a direct way to determine the key intrinsic parameters, such as the London penetration depth at zero temperature $\lambda_L(0)$ and the Pippard coherence length ξ_0 . None of these parameters is known with justified uncertainty for *any* superconductor. $B(z)$ can be measured using Low-Energy Muon Spin Rotation spectroscopy (LE- μ SR) and Polarized Neutron Reflectometry (PNR). To verify abilities of these techniques for quantitative measurements of $B(z)$ in unconventional superconductors and to examine the nonlocal electrodynamics effect predicted by Pippard in 1953, we performed an extensive series of cross LE- μ SR and PNR measurements of $B(z)$ with two extreme type-I superconductors, In and Sn. Results obtained at the initial stage of this project were reported last year. Now the project is completed. Results unambiguously validate the nonlocal effect. Conditions which have to be met to use LE- μ SR and/or PNR for measurements of $\lambda_L(0)$ and ξ_0 will be discussed.

¹Supported by NSF, DMR 0904157

4:30PM T54.00011 The critical magnetic field in the intermediate state of a Pippard superconductor¹, VLADIMIR KOZHEVNIKOV, Tulsa Community College, RINKE WIJNGAARDEN, JESSE DE WIT, VU University Amsterdam, The Netherlands, BERT VAN SCHAEYBROECK, Koninklijk Meteorologisch Instituut, Belgium, CHRIS VAN HAESENDONCK, Katholieke Universiteit Leuven, Belgium — One of the fundamental problems of unconventional superconductivity is the magnetic structure of vortices. In order to contribute to the solution of this problem and to address number of unsolved questions of the intermediate state (IS) we undertook an experimental and theoretical study of IS in an extreme type-I superconductor focusing on the critical field of the IS-N (normal) transition. Results shed new light on the structure and evolution of the magnetic flux density in normal domains and may lead to new insights in the structure of vortices in type-II materials. A 2.5 μm thick indium film with mean free path 11 μm was placed in the superconducting vector (3D) magnet. Magneto-optical images were taken simultaneously with measurements of the sample resistance using a small low frequency AC current. The equilibrium domain structure of the IS state was investigated as a function of independently controlled in- and out-of-plane magnetic fields and/or DC transport current applied to the sample. The observed critical field varied in a range from 100% down to 40% of the thermodynamic critical field. A theoretical model based on the classical Landau laminar structure quantitatively accounts for the experimental results for both ordered and disordered domain patterns.

¹Supported by NSF

4:42PM T54.00012 Evidence for s+d wave pairing in copper oxides superconductors from an analysis of NMR and NQR data, ANNETTE BUSSMANN-HOLDER, Max-Planck-Institute for Solid State Research — Knight shift and spin-lattice relaxation rate data of high temperature copper oxide superconductors are analyzed within a two-band model for superconductivity with coupled s+d wave superconducting gaps. The two-gap approach leads to substantial modifications of the coherence factors, which reflects itself in the Knight shift and the relaxation rate $1/T_1T$. From the analysis it is concluded that the data are consistent with 40% s-wave and 60% d-wave gap admixtures in agreement with earlier penetration depth data.

4:54PM T54.00013 Pseudogap studied by optical conductivity spectra of Zn-substituted $\text{YBa}_2\text{Cu}_3\text{O}_y$ ¹, ECE UYKUR, TAKAHIKO MASUI, KIYOHISA TANAKA, SHIGEKI MIYASAKA, SETSUKO TAJIMA, Dept. of Physics, Osaka University, Osaka 560-0043, JAPAN — The pseudogap and the superconducting gap cause a similar suppression of the low energy optical conductivity, but the behaviors of the spectral weight transfers are different, which enables us to distinguish these two gaps. In the c-axis spectra of $\text{YBa}_2\text{Cu}_3\text{O}_y$, however, it is difficult to discuss these spectral weight transfers because of the additional structures due to a transverse Josephson plasma mode [1]. To overcome this problem, we substituted Zn for Cu, which is known to suppress those supplementary structures [2]. In this study, we performed temperature dependent reflectivity measurements in Zn-substituted $\text{YBa}_2\text{Cu}_3\text{O}_y$ system. We have revealed the continuous transfer of the low energy spectral weight to the higher energy region even below T_c , which suggests the coexistence of the pseudogap and the superconducting gap. [1]C. Bernhard et al. Phys. Rev. B, 61 (2000) 618. [2]R. Hauff et al., Phys. Rev. Lett., 77 (1996) 4620.

¹This work was partially supported by a Grant-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

5:06PM T54.00014 Evidence of gate-tunable topological excitations in two-dimensional electron system, R. KOUSHIK, Department of Physics, Indian Institute of Science, Bangalore, MATTHIAS BAENNINGER¹, VIJAY NARAYAN, Cavendish Laboratory, University of Cambridge, J.J.Thomson Avenue, Cambridge; UK, SUBROTO MUKERJEE, Department of Physics, Indian Institute of Science, Bangalore, MICHAEL PEPPER, Department of Electronic and Electrical Engineering, University College London, Torrington Place, London, IAN FARRER, DAVID RITCHIE, Cavendish Laboratory, University of Cambridge, J.J.Thomson Avenue, Cambridge; UK, ARINDAM GHOSH, Department of Physics, Indian Institute of Science, Bangalore — We report experimental observation of a new mechanism of charge transport in two-dimensional electron systems (2DES) in the presence of strong Coulomb interaction and disorder. We show that at low enough temperature the conductivity tends to zero at a non-zero carrier density, which represents the point of essential singularity in a Berezinskii-Kosterlitz-Thouless (BKT)-like transition. Our experiments with many 2DESs in GaAs/AlGaAs heterostructures suggest the charge transport at low carrier densities to be due to the melting of an underlying ordered ground state through proliferation of topological defects. Independent measurement of low-frequency conductivity noise supports this scenario.

[1] R. Koushik *et al.*, Phys. Rev. B **83**, 085302 (2011)

[2] M. Baenninger *et al.*, Phys. Rev. Lett. **100**, 016805 (2008).

¹Present address : Department of Physics, Stanford University, Stanford CA 94305, USA

Wednesday, February 29, 2012 5:45PM - 7:15PM –
Session U18 Meet the NSF-DMR Program Director and Learn About Funding Opportunities at NSF 252B

5:45PM U18.00001 Meet the NSF-DMR Program Director and Learn About Funding Opportunities at NSF, JANICE HICKS, NSF/DMR Deputy Division Director — The session will include a presentation on the mission and programs of the Division of Materials Research (DMR) of the National Science Foundation (NSF), as well as a description of ongoing and forthcoming research funding opportunities. In addition, attendees will have the opportunity to interact “one on one” with NSF Program Directors present.

Wednesday, February 29, 2012 5:45PM - 7:45PM –
Session U20 DCMP: Town Hall Meeting: Mesoscopic Materials and Chemistry 253C

5:45PM U20.00001 Introduction to Mesoscale Science, JOHN SARRAO, Los Alamos National Laboratory, GEORGE CRABTREE, Argonne National Laboratory — BESAC seeks community input for a forthcoming report on Mesoscale Materials and Chemistry, where classical, microscale and nanoscale science meet. The report, to be released in Fall 2012, will identify the most promising research opportunities in two areas:

- new mesoscale materials, phenomena and functionality
- facilities, instruments and tools needed to make, characterize and describe mesoscale materials, phenomena and functionality.

You may contribute to the Town Hall through oral comments or by completing and uploading a Priority Research Direction quad chart through the Meso website, meso2012.com. If you upload a Priority Research Direction quad chart in advance, it can be projected at the Town Hall to illustrate your oral comments. Please see the Mesoscale Materials and Chemistry website for additional background and details: meso2012.com

6:05PM U20.00002 Community Input —

Wednesday, February 29, 2012 7:30PM - 9:00PM —

Session U60 “Trends” in the APS Publication Physics Westin Boston Waterfront Grand Ballroom A/B

7:30PM U60.00001 Spin Caloritronics: spin-dependent thermoelectrics and beyond, GERRIT E.W. BAUER, IMR, Tohoku University and Kavli Institute, TU Delft — Condensed matter physicists hope to alleviate the various energy crises that threaten our way of life through research into the management and recycling of waste heat by solid state structures and devices. In particular, spin caloritronics investigators study the role of the electron's spin in the flow, control, and transformation of heat currents in magnetic materials in order to add new functionalities and increase the efficiency of existing thermoelectric technology. In this talk I will give an overview of spin caloritronics and explain our present understanding of the underlying physics.

8:00PM U60.00002 Animalcules Redux: The fantastic world of microswimmers, RAYMOND GOLDSTEIN, University of Cambridge — Antony van Leeuwenhoek, the master microscopist, discovered many of the microorganisms that are now so familiar to us. His so-called “animalcules” such as bacteria and algae have been central to the study of problems in biological physics ranging from locomotion to evolution. Recent advances in microscopy, micromanipulation, high-speed imaging, and colloidal physics have led to renewed interest in natural, as well as synthetic, swimming microorganisms – microswimmers. In this talk I will give an overview of some fascinating recent developments, including collective behavior and anomalous transport in suspensions of swimmers, synchronization of flagella and colloidal oscillators, and light-driven multicellular locomotion (phototaxis).

8:30PM U60.00003 Metamaterials, Transformation Optics, and the Science of Invisibility, JOHN PENDRY, Imperial College London — Refractive materials give limited control of light: we can fashion lenses, and construct waveguides, but complete control is beyond simple refracting materials. Ideally we might wish to channel and direct light as we please as if diverting the flow of a fluid. Manipulation of Maxwell's equation using transformation optics shows that we can achieve just that, and metamaterials open the door to this new design paradigm for optics, providing the properties required to give almost complete control of light down to sub wavelength scales. One potential application would be to steer light around a hidden region, creating a cloak of invisibility.

Thursday, March 1, 2012 8:00AM - 11:00AM —

Session V1 GIMS: Focus Session: Advances in Scanned Probe Microscopy III: SPM of Single Atoms & Molecules 203

8:00AM V1.00001 Non-contact friction and the relaxational dynamics of surface defects, JIAN-HUANG SHE, ALEXANDER V. BALATSKY, Los Alamos National Lab — When a cantilever oscillates near a sample surface, it experiences a dissipative force. Such non-contact friction is of great practical importance to the ultrasensitive force detection measurements. Previous theories predict the friction coefficient to be six orders of magnitude smaller than the experimental value. Here, inspired by the recent experiments reported in *Phys. Rev. Lett.* 105, 236103 (2010), we propose two new mechanisms to explain the magnitude, as well as the distance, temperature and frequency dependence of the friction. We assume that the surface defects couple to the cantilever tip either in the spin or charge channel, and their relaxational dynamics gives rise to the observed behavior of both the friction coefficient and the induced spring constant. Nice agreement is found with the experiments.

8:12AM V1.00002 Dissecting an organic-metal bond by molecular manipulation, CHRISTIAN WAGNER, NORMAN FOURNIER, CHRISTIAN WEISS, RUSLAN TEMIROV, F. STEFAN TAUTZ, Peter Gruenberg Institut (PGI-3), Forschungszentrum Juelich, Germany

Scanning probe microscopy with a dynamic AFM has been able to answer some fundamental questions of surface science, like the force necessary to move an atom[1]. Recently, we demonstrated the gradual removal of a single 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) molecule from Ag(111) using a dynamic AFM [2]. The continuous force gradient measurement allowed the structural control over the junction. Here, we show how to extract details of the molecule-surface bonding (physisorption, chemisorption, bonding via functional groups) from such an experiment. The importance of a full-fledged simulation of the lifting -including tip oscillation- is emphasized. We point out the necessity of, and fundamental problems related to, a curved tip trajectory. We study PTCDA on Au(111) and Ag(111) and find qualitatively and quantitatively different binding potentials and adsorption energies. The data represents an ideal benchmark for existing and future ab-initio calculations on these systems. Our method should be applicable to various substrate-adsorbate systems and hence has the potential to answer many open questions in the field.

[1] M. Ternes et al., *Science* **319**, 1066 (2008)

[2] N. Fournier et al., *Phys. Rev. B* **84**, 035435 (2011)

8:24AM V1.00003 Multi-frequency amplitude modulated non-contact atomic force microscopy for nanoscale dielectric measurements¹, BHARAT KUMAR, JOSEPH BONVALLET, SCOTT CRITTENDEN, University of South Carolina — Multi-frequency non-contact atomic force microscopy with amplitude feedback in air was used to obtain the dielectric constant of ultra-thin films on metallic substrates. The cantilever was excited at its second bending mode by applying an AC electric field between the substrate and cantilever. The capacitance gradient between the cantilever tip and sample substrate was obtained by measuring the capacitive force driving the cantilever at its second bending mode. An analytic expression relating capacitance and dielectric constant of thin film was then used to fit the experimental data and the dielectric constant was obtained from the fit parameters. The method was validated by obtaining the dielectric constants of self-assembled monolayers of thiol molecules (2.0 ± 0.1) on gold substrate, and sputtered SiO₂ (3.6 ± 0.07) thin film. The high Q-factor of the second bending mode of the cantilever increases the accuracy of capacitive measurements while the low applied potentials minimize the likelihood of variation of dielectric constants at high field strength and of damage from dielectric breakdown of air.

¹Acknowledgements: Army Research Office, grant W911NF-08-1-0387

8:36AM V1.00004 Anomalously large g -factor of single atoms adsorbed on a metal substrate, JENS WIEBE, ALEXANDER A. KHAJETOORIANS, BRUNO CHILIAN, ROLAND WIESENDANGER, Institute of Applied Physics, Hamburg University, Jungiusstrasse 11, D-20355 Hamburg, Germany, SAMIR LOUNIS, Forschungszentrum Jülich, Peter Grünberg Institut and Institute for Advanced Simulation, 52425 Jülich, Germany, ANTONIO T. COSTA, Instituto de Física, Universidade Federal Fluminense, 24210-340 Niterói, Rio de Janeiro, Brazil, DOUGLAS L. MILLS, Department of Physics and Astronomy, University of California Irvine, California, 92697 USA — We performed magnetic field dependent inelastic scanning tunneling spectroscopy (ISTS) on individual Fe atoms adsorbed on different metal surfaces. ISTS reveals a magnetization excitation which is shifting linearly to higher energies in the magnetic field. The data is used to extract the magnetic anisotropies and the g -factors of the Fe atoms, as well as the lifetimes of the excitations. We find lifetimes of hundreds of femtoseconds limited by coupling to electron-hole pairs in the substrate and decreasing linearly upon application of the magnetic field. As expected, the magnetic anisotropy strongly depends on the substrate. Astoundingly, we find that the g -factor is $g \approx 3.1$ for Ag(111) instead of the regular value of 2 which is observed for the Cu(111) substrate [1]. This very large g -shift can be understood when considering the complete electronic structure of both the Ag(111) surface state and the Fe atom, as shown by *ab initio* calculations of the magnetic susceptibility.

[1] A. A. Khajetoorians et al., Phys. Rev. Lett. **106**, 037205 (2011).

8:48AM V1.00005 Spin Parity effects in STM single magnetic atom manipulation, FERNANDO DELGADO, JOAQUÍN FERNÁNDEZ-ROSSIER¹, International Iberian Nanotechnology Laboratory (INL), Av. Mestre José Veiga, 4715-330 Braga, Portugal — Recent experimental work shows that a spin polarized scanning tunneling microscopy tip can be used both to read and write the spin orientation of a single magnetic spin [1]. Inelastic electron tunneling spectroscopy (IETS) shows that spin of the magnetic atom is quantized [2], like the spin of a molecular magnet. Here we discuss two fundamental problems that arise when a bit of classical information is stored on a quantized spin: quantum spin tunneling and back-action of the readout process. Quantum tunneling is responsible of the loss of information due to the relaxation of the spin coupled to the environment, while the detection induced back-action leads to an unwanted modification of the spin state. We find that fundamental differences exist between integer and semi-integer spins when it comes to both, read and write classical information in a quantized spin.

[1] S. Loth et al, Nature Physics 6, 340 (2010).

[2] C. Hirjibehedin et al, Science 317, 1199 (2007).

¹Departamento de Física Aplicada, Universidad de Alicante, 03690 San Vicente del Raspeig, Spain

9:00AM V1.00006 Magnetic Particle Imaging with a Cantilever Detector, JACOB ALLDREDGE, JOHN MORELAND, NIST — We present a novel method for the measurement of the magnetic moment of single micrometer scale particles as a function of the applied field. Our technique is based on magnetic force microscopy (MFM) with a hard magnetic tip in a uniform opposing field. By moving the tip position and using a simple model we can extract the magnetic properties of isolated particles and precisely measure subsurface particle locations in 3D.

9:12AM V1.00007 Scanning Probe Microscopy and Spectroscopy of Molecules on Thin Insulating Films, JASCHA REPP, University Regensburg — Ultrathin insulating films on metal substrates facilitate the use of the scanning tunneling microscope (STM) to study the electronic properties of single atoms and molecules, which are electronically decoupled from the metallic substrate. The ionic relaxations in a polar insulator lead to a charge bi-stability in some adsorbed atoms and molecules. It is shown that control over the charge-state of individual molecules in such systems can be obtained by choosing a substrate system with an appropriate work function. The distribution of the additional charge is studied using difference images. These images show marked intra-molecular contrast [1]. We discuss how atomic-force-microscopy (AFM) in a combined STM/AFM based on the qPlus-sensor [2] reveals additional information that is truly complementary to the STM data set. In the case of a non-planar molecule that shows two different adsorption geometries, only the AFM channel provides reliable information on the conformation of the molecule. In another example of an artificially formed molecule-metal-molecule complex, the AFM channel provides information on the bonding that is important to understand the STM results.

[1] I. Swart, T. Sonleitner, and J. Repp, Nano Letters 11, 1580 (2011).

[2] F. J. Giessibl, Appl. Phys. Lett. 76, 1470 (2000).

9:48AM V1.00008 Tailoring Dirac Fermions in Molecular Graphene, KENJIRO K. GOMES, WARREN MAR, WONHEE KO, CHARLIE D. CAMP, DOMINIK K. RASTAWICKI, Stanford University, FRANCISCO GUINEA, ICMM CSIC Madrid, HARI C. MANOHARAN, Stanford University — The dynamics of electrons in solids is tied to the band structure created by a periodic atomic potential. The design of artificial lattices, assembled through atomic manipulation, opens the door to engineer electronic band structure and to create novel quantum states. We present scanning tunneling spectroscopic measurements of a nanoassembled honeycomb lattice displaying a Dirac fermion band structure. The artificial lattice is created by atomic manipulation of single CO molecules with the scanning tunneling microscope on the surface of Cu(111). The periodic potential generated by the assembled CO molecules reshapes the band structure of the two-dimensional electron gas, present as a surface state of Cu(111), into a “molecular graphene” system. We create local defects in the lattice to observe the quasiparticle interference patterns that unveil the underlying band structure. We present direct comparison between the tunneling data, first-principles calculations of the band structure, and tight-binding models.

10:00AM V1.00009 Synthesizing and Observing Electric and Magnetic Gauge Fields in Molecular Graphene¹ , DOMINIK RASTAWICKI, CHARLIE D. CAMP, KENJIRO K. GOMES, MING RUE D. THIAN, ALEX W. CONTRYMAN, HARI C. MANOHARAN, WONHEE KO, WARREN MAR, Stanford University — Molecular graphene is an artificial analogue of graphene that can be built using a scanning tunneling microscope (STM). It is realized by constraining surface-state electrons to a honeycomb lattice, which we have shown reproduces the Hamiltonian of natural graphene. We experimentally demonstrate that creating strains within the honeycomb lattice modifies the Hamiltonian in the same way that true laboratory-frame electric and magnetic fields do. In our experiments we have created artificial magnetic fields that can reach values as high as 60 T, and which can change their magnitude significantly over a distance as short as 2 nm. Some of the new physical phenomena we have been able to observe include: gauge invariance for lattices with very different real-space strains but the same artificial fields, emergence of Landau levels due to constant artificial magnetic fields, occurrence of a confined state at an interface straddling a sign-inversion of the effective magnetic field, and effective chemical doping and potential changes associated with applied electric gauge fields.

¹Supported by DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under contract DE-AC02-76SF00515.

10:12AM V1.00010 Topologically protected chiral edge state realized on molecular graphene , WONHEE KO, WARREN MAR, KENJIRO K. GOMES, DOMINIK K. RASTAWICKI, CHARLIE D. CAMP, HARI C. MANOHARAN, Stanford University — Graphene has many interesting topological properties arising from the hexagonal lattice shape and sublattice symmetry. Although its edge state is known to be extremely sensitive to the shape of the edge, and is non-topological, it has been shown that graphene with an energy gap produced by broken sublattice symmetry can possess different topologies due to different sign of the carrier mass. By making a junction of two gapped graphene regions with opposite mass, we can realize a topologically protected edge state at the mass domain wall junction, with chirality emerging from the valley degeneracy. Molecular graphene is an artificial honeycomb lattice built by atom manipulation, and due to its extreme tunability, we have realized a topological edge state between gapped molecular graphene regions with opposite signs of Dirac fermion mass. Enhanced density of states restricted only to the junction clearly shows the existence of the edge state. Also, its robustness to the geometrical detail is observed from its persistence over various edge structures, and chirality is revealed by selective scattering at the intersection of edges.

10:24AM V1.00011 Measuring Electronic Properties of Topological Defects in Molecular Graphene , CHARLIE CAMP, DOMINIK RASTAWICKI, KENJIRO GOMES, WONHEE KO, WARREN MAR, MING RUE THIAN, FRANCIS NIESTEMSKI, ALEX CONTRYMAN, CAROLINA GONZALEZ, HARI MANOHARAN, Stanford University — With the development of artificial “molecular” graphene, it is possible to create a two-dimensional electron system very similar to graphene by assembling molecules in the appropriate geometry on surface states using a scanning tunneling microscope (STM) tip. Using this same system, we recreate many lattice defects that occur naturally in graphene. Such defects have a significant effect on the electronic and transport properties of natural graphene, and are thus of notable interest in the development of nanoelectronics. In particular, we study rotational grain boundaries, which are formed by the rotation of a region of graphene with respect to the rest of the lattice. These include the Stone-Wales defect, the simplest with two adjacent carbon sites rotated by 90 degrees, as well as a common larger topological defect recently identified as the flower defect. Using STM, we examine the electronic properties of these defects in molecular graphene, paying particular attention to the emergence of new states close to the Dirac point and the quasiparticle scattering. These geometries are also studied in hole- and electron-doped variants.

10:36AM V1.00012 Scanning Vibronic Spectroscopy of Single Molecules¹ , MING RUE D. THIAN, WARREN MAR, WONHEE KO, KENJIRO K. GOMES, DOMINIK K. RASTAWICKI, CHARLIE D. CAMP, ALEX W. CONTRYMAN, HARI C. MANOHARAN, Stanford University — The dynamics of a single molecule within a quantum point contact or tunnel junction can be quite complex, exhibiting motion over frequency scales ranging from kHz to THz. In this work, we examine in detail the dynamic motion of single molecules by using low-temperature scanning inelastic tunneling, isotopic sorting, and isotopic labeling. Carbon-based molecules such as carbon monoxide, C₆₀, and diamondoids function as prototype homonuclear and heteronuclear molecules. Target structures are assembled on surfaces via atomic manipulation or self-assembly in order to tailor local THz-scale vibrational modes and to control kHz-scale molecular motion. In addition we functionalize a scanning tunneling microscope tip and use its own THz-scale vibrational modes as a probe and a tunable perturbation. These techniques reveal structure not visible in traditional STM data. We compare this data to expected local quantum forces.

¹Ming Rue D. Thian is supported by the Agency for Science, Technology and Research (A*STAR), Singapore.

10:48AM V1.00013 Pitfalls in normalizing scanning tunneling spectroscopy and how to do it “right” (from an experimentalist perspective) , MICHAEL DREYER, RAMI DANA, ANITA ROYCHOWDHURY, University of Maryland — Scanning tunneling spectroscopy is widely used to probe the local density of states (LDOS) by measuring dI/dV typically using a lock in amplifier. According to theory, the data has to be normalized by (I/V) to reveal the true LDOS - of cause still convoluted with the tip density of states. This process can induce its own artifacts and has to be done carefully. In our case the algorithm includes finding the true bias offset (if any), correct any offset in the measured current, rescale the measured dI/dV curves using the calculated version $(\Delta I/\Delta V)$, replacing $I(V)$ around $V_{\text{bias}} = 0$ by a polynomial and finally performing the normalization. The motivation and consequences of each step will be discussed using example data.

Thursday, March 1, 2012 8:00AM - 11:00AM –

Session V2 GMAG: Invited Session: Spin Caloritronics of Magnetic Structures and Devices
204AB

8:00AM V2.00001 Thermal creation of stronger spin-transfer torque in oscillators and memories, JOHN SLONCZEWSKI, formerly with IBM Research Division — Oscillators and magnetic random-access memories (MRAMs) investigated today rely on spin-transfer torque (STT) carried by an electric current flowing through a magnetic tunnel junction (MTJ) having barrier composition MgO.¹ Experiments confirm the theoretical upper bound $\tau_e=1/2$ on the torque yield (defined as dimensionless torque per unit supplied electric current). This bound limits the performance potential of STT-MRAM in which current supplied by one transistor within each cell switches the information bit. Replacement of electric current with heat flow (supplied by a Joule heater) carried by magnons may provide a greater torque yield τ_h .² The essential structure for this *thermagnonic* spin transfer (TMST) comprises a stack of three nano layers: a spontaneously magnetized insulator (*ferrite* for brevity), a non-magnetic metallic spacer, and the free metallic magnet responding to the transferred torque. Phonons carry most of the heat flowing through the ferrite. But spin-1 magnons also carry a portion of it and deposit pure spin polarization into the spacer whose free electrons transport it to the free magnet. Ferrite-metal interfaces also occur in a spin-Seebeck effect.³ Principles of spin relaxation provide estimates of τ_h based on existing data for sd-exchange, superexchange, and non-magnetic interfacial thermal resistance; τ_h may exceed τ_e by one order of magnitude.⁴ Related results of an FMR spin-pumping experiment⁵ and DFT computations⁶ support the potential of TMST-MRAM. In the case of an oscillator, TMST could increase its efficiency and enable largely independent controls of frequency and output voltage.

¹See the STT review by D. Ralph and M. Stiles, J. Magn. Mater. **320**, 1190 (2008).

²J. Slonczewski, Phys. Rev. B **82**, 054403 (2010).

³The talk by E. Saitoh in this Symposium

⁴J. Slonczewski, Phys. Rev. B **82**, 054403 (2010).

⁵B. Heinrich et al, Phys. Rev. Letts. **107**, 066604 (2011).

⁶The talk by K. Xia in this Symposium.

8:36AM V2.00002 Spin pumping and spin Seebeck effect, EIJI SAITOH, Institute for Materials Research, Tohoku University — Utilization of a spin current, a flow of electrons' spins in a solid, is the key technology in spintronics that will allow the achievement of efficient magnetic memories and computing devices. In this technology, generation and detection of spin currents are necessary. Here, we review inverse spin-Hall effect and spin-current-generation phenomena recently discovered both in metals and insulators: inverse spin-Hall effect, spin pumping, and spin Seebeck effect. (1) Spin pumping and spin torque in a Mott insulator system We found that spin pumping and spin torque effects appear also at an interface between Pt and an insulator YIG. This means that we can connect a spin current carried by conduction electrons and a spin-wave spin current flowing in insulators. We demonstrate electric signal transmission by using these effects and interconversion of the spin currents [1]. (2) Spin Seebeck effect We have observed, by using the inverse spin-Hall effect [2], spin voltage generation from a heat current in a NiFe, named the spin-Seebeck effect [3]. Surprisingly, spin-Seebeck effect was found to appear even in insulators [4], a situation completely different from conventional charge Seebeck effect. The result implies an important role of elementary excitation in solids beside charge in the spin Seebeck effect. In the talk, we review the recent progress of the research on this effect. This research is collaboration with K. Ando, K. Uchida, Y. Kajiwara, S. Maekawa, G. E. W. Bauer, S. Takahashi, and J. Ieda.

[1] Y. Kajiwara and E. Saitoh et al. Nature 464 (2010) 262.

[2] E. Saitoh et al., Appl. Phys. Lett. 88 (2006) 182509.

[3] K. Uchida and E. Saitoh et al., Nature 455 (2008) 778.

[4] K. Uchida and E. Saitoh et al., Nature materials 9 (2010) 894 - 897.

9:12AM V2.00003 Computational spin caloritronics, KE XIA, Department of Physics, Beijing Normal University — Recent experimental and theoretical studies focused on spin-mediated heat currents in at interfaces between metals and insulators, where the latter can be either the barrier in a magnetic tunnel junction or a ferromagnetic insulator. A crucial parameter is the efficiency of spin injection and spin-transfer torque. In this talk, we will report realistic electronic structure calculations for two material systems. 1) The pertinent material parameter governing spin transfer and spin Seebeck effect is the spin mixing conductance that we calculate for the Silver-YIG (Yttrium-Iron-Garnett) interface. This turns out to be much larger than expected from the Stoner model. We find mixing conductance comparable to intermetallic interfaces, a surprising result that can be rationalized in terms of magnetic local moments at the interface. These results imply that the spin-mediated energy and information transmissivity of magnetic insulators is potentially much better than has been measured in early experiment, a result that has been experimentally corroborated very recently by several groups. 2). We demonstrate that the thermal spin-transfer torque (TST) in a junction Fe-MgO-Fe tunnel junctions with ultra thin barriers can amount to 10^{-7} J/m²/K at room temperature, which is estimated to cause magnetization reversal for temperature differences over the barrier of the order of 10 K. The large TST for ultrathin barriers can be explained by multiple scattering due to interface states. Direct evidence for the existence of these states can be obtained by comparing shot noise calculations with recent experiments for high-quality junctions [Arakawa et al., Appl. Phys. Lett. 98, 202103(2011)]. *This work was carried out in collaboration with Xingtao Jia, Kai Liu and Gerrit E.W. Bauer.

9:48AM V2.00004 Magneto-Seebeck effect and thermal torques in magnetic tunnel junctions¹, MARKUS MUENZENBERG, I. Phys. Institute, Georg-August-University Goettingen — Creating temperature gradients in magnetic nanostructures has resulted in a new research direction, i.e., the combination of magneto- and thermoelectric effects. Magnetic tunnel devices, known for application as magnetic sensor in hard disc drives or magnetic random access memories (MRAM) show large magnetoresistance. We show that in nanoscale magnetic tunnel junctions, the Seebeck voltage in a heat gradient can be controlled via the magnetization. The Seebeck coefficient changes during the transition from a parallel to an antiparallel magnetic configuration in a tunnel junction – the magneto-Seebeck effect. In that respect, it is the analog to the tunneling magnetoresistance and thus is called tunneling magneto-Seebeck effect (or tunneling magnetothermopower). The change in Seebeck coefficients is in the order of the voltages known from the charge-Seebeck effect in semiconductors (up to 100 μ V/K). Their size and sign can be delicately controlled by the composition of the electrodes' atomic layers adjacent to the barrier and the temperature and we observe a characteristic sign change from positive to negative magneto-Seebeck effects as theoretically predicted. It is known that generally strong electronic asymmetry at around the Fermi level results in a large Seebeck effect. Here the magnetization dependence of the charge-Seebeck coefficients varying up to >100% for the parallel and the antiparallel originates from the half-metallic like transmission of the tunnel junction. Using heating with ultrafast laser pulses, these thermal gradients can be of up to 20 K across the tunnel barrier. We demonstrate that we can achieve the parameters predicted, where by thermal torques magnetization switching is expected. This allows to conceptually think of MRAM's driven by heat gradients only.

[1] M. Walter, et al. Nature Mater. 10, 742 (2011).

¹Work was supported by the German Research Foundation (DFG) via priority program SpinCaT (SPP 1538).

10:24AM V2.00005 Thermomagnonic spin transfer and Peltier effects in insulating magnets¹

ALEXEY A. KOVALEV, University of California at Riverside — The recent discovery of the spin Seebeck effect [1] in metals, insulators and semiconductors stimulated development of spincaloritronics [2]. The possibility of measuring the Onsager reciprocal spin Peltier effect has been investigated recently as well. In our theoretical work [3], we study the fictitious electromagnetic fields induced by magnetic textures which may offer an alternative route for observing the spin Peltier effect. Particularly, in an insulating ferromagnet a moving magnetic texture should effectively drive the spin (wave) current which in turn should lead to the heat current by the spin Peltier effect. We further study the coupled magnon energy transport and collective magnetization dynamics in ferromagnets with magnetic textures. We conclude that the analogy between the fictitious electromagnetic fields and real fields should lead to magnonic counterparts of such effects as the Hall effect, the Ettingshausen effect, the Nernst effect, and the Righi-Leduc effect. By constructing a phenomenological theory based on irreversible thermodynamics, we describe motion of domain walls by thermal gradients and generation of heat flows by magnetization dynamics. From microscopic description based on magnon kinetics, we estimate the transport coefficients and analyze the feasibility of energy-related applications (e.g. nanoscale heat pumps [4]) in insulating ferromagnets, such as yttrium iron garnet and europium oxide. Our estimates show that the viscous coupling effects between magnetization dynamics and magnon flows can be strong in materials with low spin densities (e.g. dilute magnetic systems) and narrow domain walls, which can allow the magnonic manipulation of magnetization dynamics and heat pumping.

[1] K. Uchida et al. Nature 455, 778 (2008).

[2] G. E. W. Bauer, A. H. MacDonald, S. Maekawa, Solid State Commun. 150, 459 (2010).

[3] A. A. Kovalev and Y. Tserkovnyak, arXiv:1106.3135.

[4] A. A. Kovalev and Y. Tserkovnyak, Solid State Commun. 150, 500 (2010).

¹This work was supported in part by the Alfred P. Sloan Foundation, DARPA, and NSF under Grant No. DMR-0840965.

Thursday, March 1, 2012 8:00AM - 11:00AM –

Session V3 DCMP: Invited Session: Spin Fluctuations and Cooper Pairing in Unconventional Superconductors 205AB

8:00AM V3.00001 Linear- T scattering and pairing from spin fluctuations in organic supercon-

ductors, NICOLAS DOIRON-LEYRAUD, Université de Sherbrooke — The (TMTSF)₂X series of organic superconductors, with X=PF₆ or ClO₄, are clean single-band metals that exhibit unconventional superconductivity in the vicinity of a pressure-induced spin-density wave (SDW) quantum critical point. As such, they epitomize the interplay between magnetism and superconductivity observed in heavy fermion, cuprate, and iron-pnictide superconductors. We have recently examined the electrical resistivity $\rho(T)$ of (TMTSF)₂X materials as a function of temperature and pressure. At the SDW quantum critical point, we observed a strictly linear temperature dependence of the resistivity over two decades in temperature [1,2]. Moving away from SDW order with increasing pressure, this linear resistivity was found to decrease in parallel with the weakening superconductivity, such that A , the coefficient of the linear contribution to $\rho(T)$, directly correlates with the superconducting T_c [1,2]. This shows that linear- T scattering and superconducting pairing share a common origin. A similar correlation was also found between A and the spin fluctuations seen by NMR experiments [2]. Owing to the quasi-1D nature of the (TMTSF)₂X system, this connection between spin fluctuations, scattering, and superconductivity is well described theoretically by a model that considers the hitherto overlooked mutual reinforcement of SDW and pairing correlations [3]. In particular, the feedback of pairing correlations on SDW fluctuations appears to be decisive for the strength of the linear resistivity and its extent in temperature and pressure. The fact that the same empirical correlation between linear- T resistivity and T_c is observed in the hole-doped [4,5] and electron-doped [6] cuprates, as well as in iron-pnictides [1,4], shows that the same mechanism is at play in these materials. This points to a common, magnetic origin to the superconducting pairing. Work done in collaboration with S. René de Cotret, P. Auban-Senzier, D. Jérôme, C. Bourbonnais, K. Bechgaard, and L. Taillefer.

[1] N. Doiron-Leyraud et al., Phys. Rev. B 80, 214531 (2009).

[2] N. Doiron-Leyraud et al., Eur. Phys. J. B 78, 23 (2010).

[3] C. Bourbonnais and A. Sedeki, Phys. Rev. B 80, 085105 (2009).

[4] N. Doiron-Leyraud et al., arXiv:0905.0964.

[5] L. Taillefer, Annu. Rev. Condens. Matter Phys. 1, 51 (2010).

[6] K. Jin et al., Nature 476, 73 (2011).

8:36AM V3.00002 Link between spin fluctuations and Cooper pairing in copper oxide superconductors¹

KUI JIN, Center for Nanophysics & Advanced Materials, Department of Physics, University of Maryland, College Park — Although it is generally accepted that superconductivity is unconventional in the high- T_c cuprates, the relative importance of phenomena such as spin and charge (strip) order, superconductivity fluctuations, proximity to Mott insulator, a pseudogap phase and quantum criticality are still a matter of debate. In electron-doped cuprates, the absence of “anomalous” pseudogap phase in the underdoped region of the phase diagram and weaker electron correlations suggest that Mott physics and other unidentified competing orders are less relevant and that antiferromagnetic (AFM) spin fluctuations are the dominant feature. In this talk, I will report results of low temperature magnetotransport experiments in optimal to overdoped (non-superconducting) thin films of the electron-doped cuprate La_{2-x}Ce_xCuO₄ (LCCO). We find that a linear-in- T scattering rate is correlated with the superconductivity (T_c). Our results show that an envelope of such scattering surrounds the superconducting phase, surviving to 20 mK (the limit of our experiments) when superconductivity is suppressed by magnetic fields [1]. Comparison with similar behavior found in organic superconductors [2] strongly suggests that the linear-in- T resistivity in the electron-doped cuprates is caused by spin-fluctuation scattering. Because linear-in- T scattering has also been linked to T_c in some hole-doped cuprates [2], our results suggest a fundamental connection between AFM spin fluctuations and the pairing mechanism of high temperature superconductivity in all cuprates. In addition, I will discuss how quantum criticality plays a significant role in shaping the anomalous properties of the electron-doped cuprate phase diagram. We identify quantum critical scaling in LCCO with a line of quantum critical points that surrounds the superconducting phase as a function of magnetic field and charge doping [3].

[1] K. Jin, N.P. Butch, K. Kirshenbaum, J. Paglione, and R.L. Greene, Nature 476, 73 (2011).

[2] L. Taillefer, Annu. Rev. Cond. Matter Phys. 1, 51 (2010).

[3] N.P. Butch, K. Jin, K. Kirshenbaum, R.L. Greene, and J. Paglione, submitted.

¹This work was supported by the NSF and was done in collaboration with N.P. Butch, K. Kirshenbaum, J. Paglione, and R.L. Greene.

9:12AM V3.00003 Intense paramagnon excitations in a large family of high-temperature superconductors, MATHIEU LE TACON, Max Planck Institute for Solid State Research — Motivated by the search for the mechanism of high-temperature superconductivity, an intense research effort has been focused on the evolution of the spin excitation spectrum upon doping from the antiferromagnetic insulating to the superconducting states of the cuprates. Because of technical limitations, however, the experimental investigation of doped cuprates has been largely focused on excitations with energies ≤ 100 meV in a small range of momentum space [1]. Here we take advantage of the recent developments of high-resolution resonant inelastic x-ray scattering [2,3] to show that a large family of superconductors, encompassing the model compounds $\text{YBa}_2\text{Cu}_4\text{O}_8$ and $\text{YBa}_2\text{Cu}_3\text{O}_7$, exhibits damped spin excitations - or paramagnons - with dispersions and spectral weights closely similar to those of magnons in undoped, antiferromagnetically ordered cuprates over much of the Brillouin zone. The results are in excellent agreement with the spin excitations obtained by exact diagonalization of the $t - J$ Hamiltonian on finite-sized clusters. A numerical solution of the Eliashberg equations based on the experimental spin excitation spectrum of $\text{YBa}_2\text{Cu}_3\text{O}_7$ reproduces its superconducting transition temperature T_c within a factor of two. The discovery of a well-defined, surprisingly simple spin excitation branch over a wide range of doping levels thus strongly supports magnetic Cooper pairing models for the cuprates [4].

- [1] M. Fujita *et al.* arXiv/condmat:1108.4431
- [2] G. Ghiringhelli *et al.*, Review of Scientific Instruments, **77**, (2006).
- [3] L. Braicovich *et al.*, Phys. Rev. Lett., **104**, 077002 (2010).
- [4] M. Le Tacon *et al.*, Nature Physics **7**, 725 (2011).

9:48AM V3.00004 Magnetically driven superconductivity in CeCu_2Si_2 , OLIVER STOCKERT, Max Planck Institute for Chemical Physics of Solids, Dresden — The origin of unconventional superconductivity, including high-temperature and heavy-fermion superconductivity, is still discussed controversially. Spin excitations instead of phonons are thought to be responsible for the formation of Cooper pairs. Unconventional superconductivity is quite often observed in the vicinity of a magnetic quantum critical point (QCP), i.e., a continuous magnetic phase transitions occurring at $T = 0$. Such a QCP can be approached when tuning a continuous finite temperature phase transition to $T = 0$ by means of a non-thermal control parameter like doping, pressure or magnetic field. As a result of the quantum-critical spin fluctuations unusual low-temperature properties are observed. The heavy-fermion compound CeCu_2Si_2 displays unconventional superconductivity and is already at ambient pressure located in the vicinity of a QCP where long-range antiferromagnetism vanishes. Using elastic and inelastic neutron scattering we studied in detail the antiferromagnetic order and the spin excitations spectrum around the QCP. Antiferromagnetism and superconductivity exclude each other on a microscopic scale. While for magnetically ordered samples critical slowing down of the spin fluctuations above T_N is observed, shows the normal state response of superconducting CeCu_2Si_2 an almost critical slowing down for $T \rightarrow 0$. Its temperature dependence and scaling behavior are in line with the expectations for an itinerant spin-density-wave QCP. This interpretation is substantiated by an analysis of specific heat data and the momentum dependence of the magnetic excitation spectrum. The magnetic response in the superconducting state is characterized by a transfer of spectral weight to energies above a spin excitation gap. Compared to the condensation energy there is a larger saving of magnetic exchange energy as the system condenses into a superconducting state. Our results strongly imply that the coupling of Cooper pairs in CeCu_2Si_2 is mediated by overdamped spin fluctuations.

10:24AM V3.00005 2012 IUPAP C10 Young Scientist Prize on the Structure and Dynamics of Condensed Matter Lecture: Spin Fluctuations and Pairing in Fe-based Superconductors, A.D. CHRISTIANSON, Oak Ridge National Laboratory — The origin of superconductivity in the Fe-based superconductors, like that in other unconventional superconductors, remains shrouded in mystery. How the pairing bosons emerge either due to or in spite of the strong magnetic interactions found in the Fe-based superconductors is one of the most thoroughly investigated questions in the field. A prominent example of the interplay of superconductivity and magnetism is the dramatic shift of spectral weight from the low energy spin excitations to an energy which is related to the superconducting gap resulting in a peak in the spin excitation spectrum localized in both momentum and energy which occurs at the onset of superconductivity. The appearance of the new peak in the spin excitation spectrum below the superconducting transition temperature is referred to as s spin resonance and is most commonly interpreted as indicating a sign change of the superconducting order parameter on different portions of the Fermi surface and thus is consistent with an extended s-wave or $s_{\pm}$ pairing symmetry in many Fe-based superconductors. We will review the observations and implications of the spin resonance across the Fe-based superconductors. In particular we will examine the relationship between the resonance energy and the superconducting transition temperature as a function of chemical doping and pressure. While the spin resonance provides important information about pairing symmetry, there does not appear to be sufficient spectral to explain the pairing strength. Thus the remainder of the spin excitation spectrum must be examined to determine if spin fluctuations are ultimately responsible for pairing in the Fe-based materials. Consequently, we will discuss in detail the way in which the spin excitations evolve from the nonsuperconducting compounds to their superconducting relatives as a function of chemical doping.

Thursday, March 1, 2012 8:00AM - 10:36AM – Session V4 DAMOP: Bosons and Fermions in Optical Lattices 205C

8:00AM V4.00001 Doublon production rate by optical lattice modulation for strongly correlated Fermionic atoms, AKIYUKI TOKUNO, DPMC-MaNEP, University of Geneva, EUGENE DEMLER, Harvard University, THIERRY GIAMARCHI, DPMC-MaNEP, University of Geneva — Currently lattice modulation spectroscopy technique is applied to experiments. [1] In this spectroscopy, the number of doubly occupying atom (doublon) produced by amplitude modulation of an optical lattice potential is probed. Theoretically, it allows us to access a kinetic energy correlation function. [2] We discuss doublon excitations of strongly correlated fermionic atoms in a high-temperature regime relevant to current experiments of fermionic atoms in an optical lattice. [3] We employ a slave particle representation, and the self-energy is estimated by using non-crossing approximation based on a spin-incoherent assumption. Furthermore, this formalism is applied to calculation of the doublon production rate as a function of the lattice modulation frequency, chemical potential and temperature. Using parameters given in the experiment [1], a fit to the experimental data is implemented, and quantitatively good agreement is obtained.

- [1] D. Greif, L. Tarruell, T. Uehlinger, R. Jördens, and T. Esslinger, Phys. Rev. Lett. **106**, 145302 (2011).
- [2] C. Kollath, A. Iucci, I. P. McCulloch, and T. Giamarchi, Phys. Rev. A **74**, 041604(R) (2006).
- [3] A. Tokuno, E. Demler, and T. Giamarchi, arXiv:1106.1333.

8:12AM V4.00002 Superfluid to normal phase transition in strongly correlated bosons in two and three dimensions, JUAN CARRASQUILLA, MARCOS RIGOL, Georgetown University — Using quantum Monte Carlo simulations, we investigate the finite temperature phase diagrams of hardcore bosons in two- and three-dimensional lattices. To determine the phase boundaries, we perform a finite-size-scaling analysis of the condensate fraction and/or the superfluid stiffness. We then discuss how these phase diagrams can be measured in experiments with trapped ultracold gases, where the systems are inhomogeneous. For that, we introduce a method based on the measurement of the zero-momentum occupation, which is adequate for experiments dealing with both homogeneous and trapped systems, and compare it with previously proposed approaches.

8:24AM V4.00003 Double occupancy as a universal probe for antiferromagnetic correlations and entropy in cold fermions on optical lattices, NILS BLUEMER, ELENA GORELIK, DANIEL ROST, Institute of Physics, Johannes Gutenberg University, Mainz, Germany, THEREZA PAIVA, Instituto de Física, Universidade Federal do Rio de Janeiro, Brazil, RICHARD SCALETTAR, Department of Physics, UC Davis, USA, ANDREAS KLUEMPER, University of Wuppertal, Wuppertal, Germany — We study antiferromagnetic (AF) order and correlations in the half-filled Hubbard model using dynamical mean-field theory, determinantal quantum Monte Carlo (in dimensions $d = 2, 3$), and Bethe Ansatz (in $d = 1$). We establish a low-temperature enhancement of the double occupancy D at strong coupling as a local probe of strong AF correlations accessible in cold-atom experiments [1]. As a function of entropy $s = S/(Nk_B)$, D is nearly universal with respect to dimensionality, with a minimum in $D(s)$ at $s \approx \log(2)$ [2]. The quantum AF Heisenberg regime at $s \lesssim \log(2)$, driven by an abrupt gain in kinetic energy and with clear signatures also in the next-nearest neighbor correlation function, should be in immediate experimental reach. Long-range order appears hardly relevant for the current search of AF signatures in cold fermions. Thus, experimentalists need not achieve $s < \log(2)/2$ (on a cubic lattice) and should consider lower dimensions, for which the AF effects are larger, or even use dimensionality as a tunable parameter.

[1] E. V. Gorelik, I. Titvinidze, W. Hofstetter, M. Snoek, and N. Blümer, Phys. Rev. Lett. **105**, 065301 (2010).

[2] E. V. Gorelik, T. Paiva, R. Scalettar, A. Klümper, and N. Blümer, arXiv:1105.3356v1.

8:36AM V4.00004 Tunable Phases of Fermionic Cold Atoms Systems in Mixed Dimensions, KYLE IRWIN, SHAN-WEN TSAI, University of California, Riverside — We investigate a system with two species of fermions. One species, f-fermions, moves on a two-dimensional square lattice. Another species, c-fermions, is constrained to move on a one-dimensional lattice embedded in the square lattice of f-fermions. The phases of the effective one-dimensional system whose interactions are mediated by the two-dimensional system can be tuned by manipulating the two-dimensional density. We explore effective theories, quantum phases, correlations, and relevant energy scales for various fillings of the mixed dimensional system using a functional renormalization group approach.

8:48AM V4.00005 Pairing and Density-Wave Phases of Population Imbalanced Fermi-Fermi Mixture on Optical Lattice, CHEN-YEN LAI, CHUNTAI SHI, SHAN-WEN TSAI, University of California Riverside — We study a two species fermion mixture with different populations on a square lattice, which can be modeled by a Hubbard Hamiltonian with on-site inter-species interaction. Such a model can be realized in a cold atom system with fermionic atoms in two different hyperfine states loaded on an optical lattice, and with interaction strength that can be tuned by an external magnetic field. When one of the fermion species is close to half-filling, the system is highly affected by lattice effects. We find several correlated phases for this system, including spin density wave state, d-wave charge density wave state, and p-wave superfluid state for the minority species. We study this system using a functional renormalization group method, determining its phase diagram and providing an estimate for the critical temperature of each phase. These phases emerge from a combination of interaction, population imbalance, and lattice effects. Lattice effects in particular lead to a much richer phase diagram than that of a imbalanced mixture of fermionic gas.

9:00AM V4.00006 ABSTRACT WITHDRAWN —

9:12AM V4.00007 Finite-temperature Properties of the Fermi-Hubbard Model on the Honeycomb Lattice, BAOMING TANG, EHSAN KHATAMI, Georgetown University, THEREZA PAIVA, Universidade Federal do Rio de Janeiro, MARCOS RIGOL, Georgetown University — We study thermodynamic properties of the Fermi-Hubbard model on the honeycomb lattice utilizing the numerical linked-cluster expansion, which is exact in the thermodynamic limit, and quantum Monte Carlo simulations. We obtain the equation of state, double occupancy, entropy and spin correlations for a wide range of temperatures, chemical potentials, and interaction strengths. Employing a local density approximation, we study properties of the system in the presence of a harmonic trapping potential and compare the efficiency of various adiabatic cooling schemes to those obtained for such model on the square lattice.

9:24AM V4.00008 Realizing a fermionic superfluid state from a band insulator in an optical lattice¹, YOGESHWAR P. SARASWAT, AMAL MEDHI, VIJAY B. SHENOY, Indian Institute of Science Bangalore — We propose a route to realizing a fermionic superfluid state in an optical lattice starting from a band insulator. We show that by increasing the strength of attractive interaction between the fermions in the singlet channel, a band insulator can be driven to a superfluid state in an optical lattice. The band structure is suitably designed to avoid other competing states. We estimate the Kosterlitz-Thouless transition temperature of such a superfluid. The proposal could help the realization of a superfluid state of fermions in an optical lattice circumventing the cooling problem.

¹Supported by CSIR, DST and DAE, India

9:36AM V4.00009 A Boson Core Compressibility Measure for Optical Lattices¹, YASAMIN KHORRAMZADEH, FEI LIN, V.W. SCAROLA, Virginia Tech — Trapping in experiments on cold atomic gases in optical lattices leads to inhomogeneity and different phases within the trap. We model a global measure, the boson core compressibility, that can be used to access local properties of a single phase at the center of the trap using observations of double occupancy. We test this measure on the trapped Bose-Hubbard model using mean field theory and quantum Monte Carlo. We find that the boson core compressibility focuses on the core region of the system and eliminates edge effects. We use the core compressibility to identify the transition from Mott insulator to superfluid and show that it is essentially the same as local compressibility in the core region when the system has doubly occupied sites. We generalize the definition of core compressibility to study systems with large densities at the trap center.

¹This work is supported by AFOSR (FA9550-11-1-0313) and DARPA-YFA (N66001-1-1-4122).

9:48AM V4.00010 Numerical studies of exotic paired states in optical lattices¹, SIMONE CHIESA, College William & Mary, SHIWEI ZHANG, College of William & Mary, GEORGE BATROUNI, Institut Non-Linéaire de Nice — Ultracold atoms are a unique tool that allows the exploration of phases of matter not easily accessible in condensed matter systems. Two interesting possibilities are spin-imbalanced systems and spin dependent optical lattices with Fermi surfaces that differ for the two hyperfine species. We use mean-field theory and quantum Monte Carlo simulations of Hubbard-like models with an attractive contact interaction to study the FFLO state and, by rotating the two Fermi surfaces by 90 degrees with respect to each other, a recently proposed exotic paired state [Feiguin and Fisher, 2009].

¹Supported by ARO and NSF.

10:00AM V4.00011 Competing instabilities in a two band Hubbard model on a square lattice, CHUNTAI SHI, SHAN-WEN TSAI, Department of Physics and Astronomy, University of California Riverside — We study a two band Hubbard model on a two dimensional square lattice. In particular, we focus on the cases wherein one band is doped to have a small electron pocket while the other band is doped to have a hole pocket and the Fermi lines of these two pockets are nearly nested. Similar models have been studied extensively in the context related to the Iron-based material where the interactions between electrons are always repulsive. Here we investigate the generalized cases that the interactions between the fermions within the same band U_1 and U_2 and the interactions between electrons in different bands U_{12} can be tuned independently. Such models can potentially be realized in a cold atom system where the manipulation of the interaction is possible by taking advantage of the Feshbach resonance. The freedom of tuning the strength and the sign (repulsive or attractive) of the interactions, combined with the nearly nested Fermi lines, allows both the density wave phases and the pairing phases to be potential candidates for the ground state. We employ the functional renormalization group approach so that we can investigate the competition between these possible instabilities on an equal footing.

10:12AM V4.00012 Condensate Properties for Strongly Repulsive Bosons in a Double Well, JOEL CORBO, UC Berkeley, JONATHAN DUBOIS, LLNL, BIRGITTA WHALEY, UC Berkeley — We present path integral ground state (PIGS) quantum Monte Carlo calculations for the ground state ($T = 0$) properties of repulsively interacting bosons in a three-dimensional external double well potential over a range of interaction strengths and potential parameters. We focus on calculation of ground state number statistics in order to understand the level of squeezing that the system may exhibit as a function of interaction strength. For weak interactions (i.e. where the standard two-mode model of a BEC in a double well is applicable) we produce results consistent with the two-mode model. However, for stronger interactions, we find a novel and somewhat surprising relationship between squeezing and interaction strength. We find that these new features are qualitatively consistent with squeezing calculations carried out using an improved, recently-proposed eight-mode model, although this model is insufficient to quantitatively predict the results of the full quantum Monte Carlo simulation.

10:24AM V4.00013 A Quantum Plasmonic Circuit for Cold Atoms, MICHAEL GULLANS, Harvard University, DARRICK CHANG, California Institute of Technology, JOHANNES FEIST, TOBIAS TIECKE, JEFF THOMPSON, Harvard University, IGNACIO CIRAC, Max-Planck-Institut für Quantenoptik, PETER ZOLLER, Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, MIKHAIL LUKIN, Harvard University — We propose a new architecture for quantum simulation with atoms using a two dimensional lattice of plasmonic nanoparticles to both trap the atoms and mediate interactions between them. This proposal combines existing technologies from ultracold atoms and plasmonics to exploit the unique coherence properties of atoms and the strong light-matter interaction and subwavelength confinement provided by plasmonic systems. We first show that this system allows to increase the energy scales of Hubbard models by two orders of magnitude compared to optical lattices. We then show how this system can realize a dissipative quantum simulator to prepare a wide range of many-body entangled states.

Thursday, March 1, 2012 8:00AM - 11:00AM –
Session V5 DCMP: Surface Electronic & Lattice Properties: Structure, Surface States, & Adsorption 206A

8:00AM V5.00001 Surface energy anisotropy for FCC metals: Functional forms, YAN-JIUN CHEN, MIHIR KHADILKAR, JAMES P. SETHNA, LASSP, Cornell University — The energy of a crystalline surface depends on the angle of the surface normal with respect to the crystalline axes (i.e. the Miller index). We show that the surface energy as a function of angle is surprisingly easy to describe with a simplistic broken bond model including only a few parameters. In particular, this model is successful at capturing the cusps at high symmetry surfaces. We will use our fitted functional form as a characteristic continuum description of material surface energies for FCC metals. The anisotropy of these surface energies can then be utilized in the study of many material properties- equilibrium shapes (Wolff plots) of crystals and voids, fracture mechanics, cleavage and faceting. We calculate the surface energies using ab initio calculations and various interatomic potentials, providing a measure of the fitness of the potentials for studying physical systems with surfaces. Furthermore, we assemble systematic tables of these results, available to the community through the Knowledgebase of Interatomic Models (KIM, <https://openkim.org/>).

8:12AM V5.00002 Explicit consideration of surface structures for work function calculations, SEUNGCHUL KIM, ANDREW M. RAPPE, Department of Chemistry, University of Pennsylvania — We investigate the effects of atomic structure of surfaces on work functions, using density functional theory (DFT) calculations. Despite the well-known orientation dependence of work functions, the effect of geometric structure of surfaces on work functions is rarely considered. To examine whether the atomic structure of a surface is important to the work function, we perform DFT calculations of thick slabs in the periodic supercell. We then extract the energy levels of the occupied states relative to the vacuum level. Surfaces of oxides, such as BaTiO_3 (001), SrTiO_3 (001), and TiO_2 (110), are especially well-tested because of their various reconstructed structures. Our calculations show that, even for the same surface orientation, the difference in stoichiometry and geometry of the surface gives rise to substantially different work functions. This finding strongly implies that the atomic structures of surfaces must be explicitly taken into account in predicting work functions of materials.

8:24AM V5.00003 The role of surface states in inelastic electron tunneling into metal surfaces¹, MINGHU PAN, QING LI, PETER MAKSYMOWYCH, Center of Nanophase Materials Sciences, Oak Ridge National Laboratory, TN, USA 37831 — Inelastic electron tunneling spectroscopy is a highly capable technique to explore dynamic properties of material surfaces, particularly the phonon spectrum. Presently, many of the so-called “propensity” rules that determine the strength of the measured inelastic loss in STM experiments are still unknown or controversial. We have carried out systematic IETS of surface phonons on a Au(111) surface, and spatially-resolved variations in the vibrational spectrum of an adsorbate on the STM tip. In both cases, the IETS intensity markedly dropped at the step edges. At the same time, the IETS intensity exhibits long-range oscillations, the wavelength of which coincided with the Friedel oscillations of the surface state in the vicinity of the defects. All the observations combined, attest to the important role of the surface state in electron-phonon coupling. We will rationalize the observed effects by invoking the symmetry of the tunneling states, with particular emphasis on the effect of the projected band-gap of the gold surface.

¹This research was conducted at the Center for Nanophase Materials Sciences (CNMS), which is sponsored at Oak Ridge National Laboratory by the Office of Basic Energy Sciences, U.S. Department of Energy.

8:36AM V5.00004 Anisotropic Surface State Mediated RKKY Interaction Between Adatoms on a Hexagonal Lattice¹, THEODORE EINSTEIN, University of Maryland, College Park, PAUL PATRONE, University of Maryland, College Park; and NIST Gaithersburg — Motivated by recent numerical studies of Ag on Pt(111), we derive a far-field expression for the RKKY interaction mediated by surface states on a (111) FCC surface, considering the effect of anisotropy in the Fermi edge. The main contribution to the interaction comes from electrons whose Fermi velocity v_F is parallel to the vector $\mathbf{R}$ connecting the interacting adatoms; we show that in general, the corresponding Fermi wave-vector $\mathbf{k}_F$ is not parallel to $\mathbf{R}$. The interaction is oscillatory; the amplitude and wavelength of oscillations have angular dependence arising from the anisotropy of the surface state band structure. The wavelength, in particular, is determined by the component of the aforementioned $\mathbf{k}_F$ that is parallel to $\mathbf{R}$. Our analysis is easily generalized to other systems. For Ag on Pt(111), our results indicate that the RKKY interaction between pairs of adatoms should be nearly isotropic and so cannot account for the anisotropy found in the studies motivating our work.

¹Supported by NSF-MRSEC DMR 05-20471 and NIST-ARRA Grant 70NANB10H026, with ancillary support from CNAM at UMD.

8:48AM V5.00005 Inverse photoemission and LEED investigation of the ion-bombarded Ni(110) surface, BENJAMIN YOUNG, JIM WARNER, DAVID HESKETT, University of Rhode Island — Ion bombardment of the clean Ni(110) surface is investigated by a combination of Inverse Photoemission Spectroscopy (IPES) with a Geiger-Muller detector and Low Energy Electron Diffraction (LEED) with a homebuilt video capture system. Disorder of the surface is induced by argon ion bombardment with various combinations of argon pressure and sputtering time. The intensity of the unoccupied surface state at $\sim 2\text{eV}$ above the Fermi level at the $\bar{Y}$ point of the surface Brillouin zone decreases with increasing surface bombardment. Simultaneously, intensity profiles of diffraction spots in LEED exhibit broadening and a rising background level for increasing surface disorder. Multiple attempts at correlation between the results of the two techniques are presented.

9:00AM V5.00006 Electronic structure of the indium-adsorbed Au/Si(111)- $\sqrt{3} \times \sqrt{3}$ surface: a first-principles study, FENG-CHUAN CHUANG, CHIA-HSIU HSU, WEN-HUAN LIN, Department of Physics, National Sun Yat-sen University, Taiwan, VIDVUDS OZOLINS, Department of Materials Science and Engineering, University of California, Los Angeles, Los Angeles, CA 90095-1595, USA — Electronic structures of the indium-adsorbed Au/Si(111)- $\sqrt{3} \times \sqrt{3}$ surface were examined using first-principles calculations at In coverages range from 0.15 ML to 1 ML. The band structures of the various proposed models were analyzed in detail. Our results show that the calculated bands for the identified atomic models for indium-adsorbed on conjugate honeycomb-chained-trimer model at In coverages of 1/3 ML and 2/3 ML are in agreement with the identified bands in the angle-resolved photoemission study [Phys. Rev. B **80** 075312 (2009)].

9:12AM V5.00007 Lattice relaxation as the origin of the insulating nature of the alkali/Si(111):B surface, LAURENT CHAPUT, CEDRIC TOURNIER-COLLETTA, LOUIS CARDENAS, BERTRAND KIERREN, YANNICK FAGOT-REVURAT, DANIEL MALTERRE, Institut Jean Lamour, PATRICK LEFEVRE, FRANCOIS BERTRAN, synchrotron soleil, ANTONIO TEJEDA, Institut Jean Lamour, AMINA TALEB, synchrotron soleil — *Ab initio* density-functional theory calculations, photoemission spectroscopy (PES), scanning tunneling microscopy, and spectroscopy (STM, STS) have been used to solve the $2\sqrt{3} \times 2\sqrt{3}R30$ surface reconstruction observed previously by LEED on 0.5 ML K/Si:B. It is found that the large K-induced vertical lattice relaxation obtain in the calculations and occurring only for 3/4 of Si adatoms is shown to quantitatively explain both the chemical shift of 1.14 eV and the ratio 1/3 measured on the two distinct B 1s core levels. A gap is observed between valence and conduction surface bands by ARPES and STS which is shown to have mainly a Si-B character using the *ab initio* calculations. Finally, the calculated STM images agree with our experimental results. Therefore, the insulating character of alkali/Si:B interfaces has been captured to an excellent accuracy, from the low lying 1s state of boron, to the unoccupied states above the gap, within a one-electron approach. This work solves the controversy about the origin of the insulating ground state of alkali-metal/Si(111):B semiconducting interfaces which were believed previously to be related to many-body effects

9:24AM V5.00008 First-Principles Study of One-Dimensional Metal-Molecule Hybrid Chains Self-Assembled on Ag Substrate, BON-GIL KOO, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University — We explore the formation mechanism and the structural and electronic properties of one-dimensional metal-molecule hybrid chain self-assembled on Ag(111) substrate using *ab initio* density functional theory. It is observed that such a hybrid chain is formed by spontaneous transformation from 4,4''-dibromo-*p*-terphenyl (DBTP) molecules when deposited on Ag(111) substrate at room temperature. We find that the chain is composed of *p*-terphenyl (TP) connected through an Ag atom to form (TP-Ag)_n. Our study shows that Ag(111) surface plays a catalytic role removing two Br atoms (DB) from DBTP and connecting the remaining TP through an Ag atom, which is a similar phenomenon as the Ullmann cross coupling reaction occurred on Cu surface. We find that those Br atoms detached from DBTP play important roles for spontaneous formation of well-aligned pattern. Our calculated electronic structures and simulated scanning tunneling microscopy (STM) images of (TP-Ag)_n hybrid chain exhibit remarkably different charge distributions depending on the energy values, which are related to the tip voltage in STM experiments. We also investigate the end state of the hybrid chain, which can be spatially resolved.

9:36AM V5.00009 Quantum Monte Carlo studies of surface adsorptions, CHING-MING WEI, CHENG-RONG HSING, IAMS, Academia Sinica, Taipei 10617, Taiwan — Surface adsorption is the first step to the study of surface catalytic reaction. The most common used tool is the Density Functional Theory (DFT) based on exchange-correlation approximations and the accuracy usually has not been checked carefully by highly accurate quantum many-body approaches. We have performed calculations of the surface adsorptions using the state-of-the-art diffusion quantum Monte Carlo (QMC) method to examine the accuracy of LDA and GGA (PBE) functionals in the study of surface adsorptions. The systems examined include the H₂O and OH adsorptions on various types of surfaces such as NaCl(100), MgO(100), TiO₂(110), graphene, Si(100)-(2x2) and Al(100). By comparing GGA (PBE) results with DMC, our results indicate that (i) for the H₂O adsorption, PBE predicts the correct adsorption energies; (ii) for the OH adsorption, PBE has predicted a large over-binding effect except on graphene and Si(100) surfaces. This fact indicates that one needs to be cautious when using DFT to study the surface adsorptions of OH free radical.

9:48AM V5.00010 Resistivity of thin gold films on mica induced by electron-surface scattering from a self-affine fractal surface¹, RAUL C. MUNOZ, CLAUDIO GONZALEZ-FUENTES, RICARDO HENRIQUEZ, MARCOS FLORES, Department of Physics, University of Chile — We present a rigorous comparison between resistivity data and theoretical predictions involving the theory of Palasantzas [G. Palasantzas et al., *Phys. Rev. B* **56** 7726 (1997)], and the mSXW-fractal theory [R. C. Munoz et al., *Phys. Rev. B* **66** 205401 (2002)], regarding the resistivity arising from electron scattering by a self affine fractal surface on gold films *using no adjustable parameters*. We find that both theories lead to an approximate description of the temperature dependence of the resistivity data. However, the description of charge transport based upon fractal scaling seems oversimplified, and the predicted increase in resistivity arising from electron-surface scattering seems at variance with other experimental results. If the samples are made up of grains such that the mean grain diameter $D > L(300)$, the electronic mean free path in the bulk at 300 K, then the predicted increase in resistivity at 4 K is of the order of a few percent. This contradicts published measurements of magnetomorph effects arising from size effects where *electron-surface scattering is the dominant electron scattering mechanism at 4 K*. On the contrary, if the samples are made out of grains such that $D < L(300)$, then *the dominant electron scattering mechanism controlling the resistivity is not electron-surface scattering but rather electron-grain boundary scattering, and the latter electron scattering mechanism is not included in either theory*.

¹Funded by FONDECYT 1085026.

10:00AM V5.00011 Electronic confinement imposed by a nanoporous network: Band formation from coupled quantum dots, KATHRIN MUELLER, MEIKE STOEHR, University of Groningen, The Netherlands, MANFRED MATENA, University of Basel, Switzerland, JORGE LOBO-CHECA, Centre d'Investigacio en Nanociencia i Nanotecnologia, Spain, THOMAS JUNG, Paul-Scherrer-Institut, Switzerland, LUTZ GADE, University of Heidelberg, Germany — The electronic and optical properties of crystalline solids exhibit characteristics that derive to a large extent from the periodic arrangement and interactions of their component quantum systems, such as atoms or molecules. Quantum effects due to confinement of electronic states have been extensively studied for surface states of noble metals which are characterized by a quasi 2D electron gas. The design of such periodic 2D structures on surfaces is more readily achieved using molecular self-assembly from building blocks instead of atom by atom manipulation. We chose a perylene derivative (DPDI) as organic building block which is known to form a highly ordered porous network on Cu(111) upon thermal dehydrogenation. To study the interaction between the electronic surface state and our porous network structure, scanning tunneling spectroscopy (STS) and angle-resolved photoemission (ARPES) was used. Each pore of our porous network confines the surface state of the Cu substrate what can be described as a 0D quantum dot. This work can lead to artificially created electronic structures by modification of the dimensions of the molecular network periodicities together with the appropriate choice of the substrate and the building block.

10:12AM V5.00012 ABSTRACT WITHDRAWN —

10:24AM V5.00013 First-Principles Investigations of Oxygen Vacancies on SnO₂ Nanofilms¹, DANIEL CELLUCCI, STEVEN LEWIS, University of Georgia — In recent years multiple critical advances in nanofabrication have allowed for the well-controlled formation of nanocrystals of the n-type semiconductor tin oxide (SnO_2). Because gas sensing in SnO_2 involves changes in surface resistivity as a function of gas concentration, the high surface-to-volume ratio of SnO_2 nanocrystals could be leveraged to produce a gas sensor with significantly enhanced sensitivity. A key feature of the sensing mechanism is the facile formation and destruction of oxygen vacancies at (or near) the surface. In this talk I will discuss our ongoing first-principles investigations of surface oxygen vacancies in SnO_2 nanofilms. We have focused on vacancy formation among the so-called bridging oxygen atoms on the (110) surface of rutile SnO_2 as a function of vacancy concentration and film thickness and have studied the effect on local atomic and electronic structure. From a set of first-principles Density Functional Theory calculations on ordered vacancy structures, we have parametrized and tested a lattice-gas model describing vacancy-vacancy interactions. Using this model we have conducted extensive Monte Carlo simulations to investigate the oxygen vacancy phases on SnO_2 (110) as a function of temperature and oxygen vapor pressure.

¹National Science Foundation, Grant #CMMI-0856719.

10:36AM V5.00014 Orbital tomography: Deconvoluting photoemission spectra of organic molecules¹, PETER PUSCHNIG, University of Leoben, EVA-MARIA REINISCH, THOMAS ULES, GEORG KOLLER, University of Graz, Austria, SERGEY SOUBATCH, Forschungszentrum Juelich, Germany, MARKUS OSTLER, University Erlangen-Nuernberg, Germany, LORENZ ROMANER, University of Leoben, Austria, F. STEFAN TAUTZ, Forschungszentrum Juelich, Germany, CLAUDIA AMBROSCH-DRAXL, Humboldt University Berlin, Germany, MICHAEL G. RAMSEY, University of Graz, Austria — We study the interface of an organic monolayer with a metallic surface, *i. e.*, PTCDA (3,4,9,10-perylene-tetracarboxylic-dianhydride) on Ag(110), by means of angle-resolved photoemission spectroscopy (ARPES) and *ab initio* electronic structure calculations. We present a tomographic method which uses the energy and momentum dependence of ARPES data to deconvolute spectra into individual orbital contributions beyond the limits of energy resolution. This provides an orbital-by-orbital characterization of large adsorbate systems without the need to invoke sophisticated theory of photoemission, allowing us to directly estimate the effects of bonding on individual orbitals. Moreover, this experimental data serves as a most stringent test necessary for the further development of *ab initio* electronic structure theory.

¹Austrian Science Fund (FWF), projects S97, P21330-N20 and P23190-N16

10:48AM V5.00015 Two-Dimensional Band Structure Study of Bi_{1-x}Sb_x Thin Films, SHUANG TANG, MILDRED DRESSELHAUS, Massachusetts Institute of Technology, DRESSELHAUS GROUP TEAM — Alloys of Bi_{1-x}Sb_x, are considered as one of the best thermoelectric materials for low temperature applications below 200 K. The band structure of Bi_{1-x}Sb_x varies as a function of stoichiometry. At a temperature below 77 K, it does not change with temperature. At a certain Sb composition ($x=0.04$), the conduction band and the valence band touch each other at the L point, and the band-crossing occurs. The electronic dispersion relation becomes linear at the L point, which implies that a Dirac cone is formed at each of the three L points. By making the alloys of Bi_{1-x}Sb_x into thin films, we have two more parameters to vary the band structure, namely film thickness and growth orientation. In our present work, the rich variety of band structure configurations, as well as various phases, of Bi_{1-x}Sb_x thin films has been revealed.

Thursday, March 1, 2012 8:00AM - 11:00AM —

Session V6 DMP: Focus Session: Carbon Nanotube Optics I: Spectroscopy and Excitons 206B

8:00AM V6.00001 High Throughput Optical Imaging and Spectroscopy of Individual Carbon Nanotubes, JIWOONG PARK, Cornell University — Laser-based imaging and characterization of individual carbon nanotubes provides a number of significant advantages over other imaging techniques, including its high throughput, spectral characterization capability, and relatively simple sample preparation. We recently reported a novel on-chip Rayleigh imaging technique using widefield laser illumination to measure optical scattering from individual single-walled carbon nanotubes (SWNTs) on a solid substrate with high spatial and spectral resolution. This method accurately measures the resonance energies and diameters for a large number of SWNTs in parallel. This technique can be used for fast mapping of key SWNT parameters, including the electronic-types and chiral indices for individual SWNTs, position and frequency of chirality-changing events, and intertube interactions in both bundled and distant SWNTs. Further Rayleigh characterization showed that SWNTs can form ideal optical wires. Interestingly, the spatial distribution of the radiation scattered by the nanotubes is determined by their shape, but the intensity and spectrum of the scattered radiation are determined by exciton dynamics and other intrinsic properties. Moreover, the nanotubes display a uniform peak optical conductivity, suggesting universal behavior similar to that observed in nanotube conductance. Finally, two other high-throughput optical imaging techniques, widefield Raman imaging and confocal absorption microscopy, and their applications in nanotube imaging will be discussed.

8:36AM V6.00002 Plasmon Nanooptics with Pristine and Hybrid Nanotube Systems¹, IGOR BONDAREV, North Carolina Central University, USA, MAXIM GELIN, WOLFGANG DOMCKE, Technical University of Munich, Germany — In general, plasmons cannot be excited by light in optical absorption since they are longitudinal excitations while photons are transverse. In small-diameter (~ 1 nm) semiconducting carbon nanotubes (CNs), light polarized along the CN axis excites excitons which, in turn, can couple to the nearest (same-band) interband plasmons [1,2]. Both of these collective excitations originate from the same electronic transitions and, therefore, occur at the same (low) energies ~ 1 eV, as opposed to bulk semiconductors where they are separated by tens of eVs. They do have different physical nature and properties. Their coexistence at the same energies in CNs is a unique feature of confined quasi-1D systems where the transverse electronic motion is quantized to form 1D bands and the longitudinal one is continuous. We discuss how low-energy interband plasmon excitations can efficiently mediate enhanced electromagnetic absorption in pristine semiconducting CNs and bipartite entanglement in hybrid metallic CN systems. We develop a theory for (non-linear) optical monitoring and control of the phenomena above.

[1] I.V.Bondarev, JCTN7, 1673(2010).

[2] I.V.Bondarev, L.M. Woods, and K. Tatur, PRB80, 085407(2009).

¹Support from ARO (W911NF-11-1-0189), DOE (DE-SC0007117), NASA (NNX09AV07A), NSF (ECCS-1045661 & HRD-0833184), and Munich Center for Advanced Photonics (DFG), is acknowledged.

8:48AM V6.00003 Photoluminescence from suspended individual ¹³C-enriched nanotubes¹, T. SHIMADA, A. YOKOYAMA, A. ISHII, J. SHIOMI, S. MARUYAMA, Y.K. KATO, The University of Tokyo — We investigate isotope effects on the electronic structure of single-walled carbon nanotubes by photoluminescence microscopy. In order to suspend nanotubes for luminescence measurements, trenches are formed on SiO₂/Si substrates by electron beam lithography and dry etching processes. No-flow chemical vapor deposition is used to grow carbon nanotubes with small amounts of isotopically enriched ethanol with 99% ¹³C. Optical measurements are done in air at room temperature using a laser scanning confocal microscope with a wavelength tunable Ti:sapphire laser as an excitation source. We have successfully identified suspended ¹³C-enriched nanotubes by photoluminescence imaging and assigned their chirality with excitation spectroscopy.

¹This work is supported by the Mitsubishi Foundation, Ogasawara Foundation, Ishikawa Carbon Foundation, KAKENHI, and Global COE Program of MEXT, Japan.

9:00AM V6.00004 Circular dichroism in air-suspended single-walled carbon nanotubes¹, A. YOKOYAMA, A. ISHII, M. YOSHIDA, T. SHIMADA, Y.K. KATO, The University of Tokyo — Chiral carbon nanotubes lack inversion symmetry and are expected to show circular dichroism. We have investigated the helicity dependence of absorption in air-suspended single-walled carbon nanotubes by using photoluminescence intensity for detection. Patterned chemical vapor deposition is used to grow carbon nanotubes over trenches etched on SiO₂/Si substrates. We identified suspended carbon nanotubes by taking photoluminescence images with a home-built laser-scanning confocal microscope and characterized them by excitation spectroscopy. A quarter-wave plate is inserted in the excitation laser path, and the photoluminescence intensity is measured as a function of the angle of the wave plate. We observe differences in the luminescence intensity between left- and right-circularly polarized light.

¹This work is supported by KAKENHI and the Photon Frontier Network Program of MEXT, Japan.

9:12AM V6.00005 Visible fluorescence from 5-Angstrom single-wall carbon nanotubes, YASUMITSU MIYATA, TOSHIYA NAKAMURA, MIHO FUJIHARA, HONG EN LIM, RYO KITaura, HISANORI SHINOHARA, Nagoya University — We report the observation of visible fluorescence from the ultrathin single-wall carbon nanotubes (SWCNTs) with diameters of less than 5-Angstrom. Such ultrathin nanotubes were prepared by extracting the inner shells of double-wall carbon nanotubes using ultrasonication [1]. The extracted sample shows two visible photoluminescence (PL) peaks at 700 and 720 nm under light excitation at 410 and 540 nm, respectively. These peaks can be assigned, respectively, as the PL of (4,3) and (5,3) SWCNTs by comparison with the experimental Kataura plot proposed by Weisman et al. [2]. The present findings provide an important insight for the studies of the structural stability and electric structure of ultrathin SWCNTs. [1] Y. Miyata et al. ACS Nano. 4, 5807 (2010), [2] R. Weisman et. al., Nano Lett. 3, 1235 (2003).

9:24AM V6.00006 Symmetry-breaking of carbon nanotubes vibrational modes induced by transversal deformations, NEWTON M.B. NETO, Universidade Federal de Uberlândia, HELIO CHACHAM, ADO JORIO, SABRINA S. CARARA, JAQUELINE SOARES, Universidade Federal de Minas Gerais, RONALDO J.C. BATISTA, Universidade Federal de Ouro Preto, ERNESTO JOSE-LEVICH, Weizmann Institute of Science, MILDRED DRESSSELHAUS, PAULO ARAUJO, Massachusetts Institute of Technology — In this work we combine an atomic force microscope (AFM) with a setup to perform confocal Raman spectroscopy to follow, *in situ*, the evolution of the G-band feature of a Single Wall Carbon Nanotube (SWNT) with transversal pressure applied to the nanotube via the AFM probe. We observe a previously elusive and fundamental symmetry-breaking effect of the totally symmetric tangential optical TO modes in the G-band feature which exhibits two distinct Raman active modes with an anomalous frequency behavior with increasing applied pressure, while the totally symmetric longitudinal optical LO component remains unaltered. We propose a simple analytical model based on a mass-spring ring system, which satisfactorily explains the main observed effects and shows that the pressure effects change with tube flattening.

9:36AM V6.00007 Non-Radiative Exciton Decay in Single-Walled Carbon Nanotubes, MARK HARRAH, JUDE SCHNECK, Boston University, ALEXANDER GREEN, Wyss Institute, Harvard University, MARK HERSAM, Northwestern University, LAWRENCE ZIEGLER, ANNA SWAN, Boston University — We report on the exciton dynamics for an ensemble of individual, suspended (6,5) single-walled carbon nanotubes via single color E_{22} pump-probe spectroscopy for a wide range of pump fluences. The calculated initial exciton population ranges from ~ 5 to 120 excitons per ~ 725 nm long nanotube, putting the high fluence experiment well into the nonlinear regime. The pump-probe data is not well described by multi-exponential decay or by power law behavior for all fluences. We have developed a single model that describes all data, ranging over two decades of pump fluence and three decades of delay times. The signal decay at low fluence is dominated by a stretched exponential that is consistent with the distribution of relaxation rates resulting from diffusion-limited contact quenching for a nanotube ensemble. The change in dynamics as a function of increasing pump intensity is attributed to exciton-exciton Auger de-excitation in the E_{11} subband and, to a lesser extent, in the E_{22} subband. The initial sub-picosecond decay of the observed response is attributed to E_{22} excitons rapidly acquiring non-zero momentum while remaining in the E_{22} subband.

9:48AM V6.00008 Fine structure of exciton levels in carbon nanotubes: A semianalytical approach¹, SERGUEI GOUPALOV², Jackson State University — We propose a new approach [1] toward excitons in carbon nanotubes whereby the matrix elements of the electron-hole Coulomb interaction are expanded into a series over the nanotube's one-dimensional reciprocal lattice vectors. We show that only a few terms of this expansion give a non-vanishing contribution to the Coulomb matrix elements. The proposed approach allows one to single out Fourier components of the Coulomb potential responsible for the intervalley coupling and formation of the exciton fine structure for each particular nanotube chirality.

[1] S.V. Goupalov, Phys. Rev. B 84, 125407 (2011).

¹NSF PHY05-51164, NSF HRD-0833178

²also with Ioffe Institute, Russian Academy of Sciences

10:00AM V6.00009 Dynamical crossovers, universality and long-range interactions of excitons on carbon nanotubes, JEREMY ALLAM, TARIQ SAJJAD, RICHARD SUTTON, SOPHIA SIDDIQUE, ZHONGYANG WANG, KONSTANTIN LITVINENKO, University of Surrey, QUAN-HONG YANG, Tianjin University, TOM BROWN, University of Southampton, WEI LOH, University of Southamp — Simple microscopic interactions in non-equilibrium systems give rise to complex emergent macroscopic phenomena. There has been much theoretical work to understand dynamics of different systems, and equilibrium concepts of scaling, criticality and universality have proved useful. However there is a noted lack of experimental studies. Here we show that exciton reactions on carbon nanotubes display the rich kinetics of the prototypical 1D coalescence reaction $A+A \rightarrow A$. An Auger-like exciton interaction¹ and anomalous kinetics² have already been reported. Here we demonstrate the existence of four distinct dynamical regimes: (1) early dynamics determined by spatial ordering of excitons due to Pauli repulsion at high concentrations; (2) a classical mean-field region with exciton population n decaying as t^{-1} ; (3) a self-organized critical state with anomalous reaction kinetics limited by diffusion and characterized by $n \sim t^{-1/2}$, which we show to be universal with respect to the initial population; and (4) an exponential approach towards an absorbing state corresponding to one exciton per nanotube. The abrupt crossover between regimes indicates a long-range exciton interaction, which introduces a non-scaling dimension that breaks universality at intermediate length-scales.

¹Y.-Z. Maet al, Phys Rev Lett 94, 157402 (2005).

²R. M. Russo et al. Phys Rev B 74, 041405 (2006).

10:12AM V6.00010 Exciton transport and exchange self-energy in semiconducting carbon nanotubes, JARED CROCHET, Los Alamos National Laboratory, JAY SAU, Harvard University, MARVIN COHEN, University of California at Berkeley and Lawrence Berkeley National Laboratory, JUAN DUQUE, Los Alamos National Laboratory, LAURENT COGNET, Universite de Bordeaux and CNRS, STEPHEN DOORN, Los Alamos National Laboratory — We present direct measurements of S_1 exciton transport in (6,5) carbon nanotubes. Exciton diffusion lengths associated with end quenching, photoluminescence lifetimes, and homogeneous emission linewidths provide a basis for determining an intrinsic diffusion constant of $5 \text{ cm}^2\text{s}^{-1}$ within the dispersion of light. Exciton diffusion is modeled in terms of an anomalous dispersion within a marginal Fermi liquid description of the exciton exchange self-energy and acoustic phonon scattering.

10:24AM V6.00011 Quantum Interference Between the Third and Fourth Excitonic States in Semiconducting Carbon Nanotubes, HAGEN TELG, JUAN G. DUQUE, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, HANG CHEN, ANNA K. SWAN, Department of Electrical and Computer Engineering, and Photonics Center, Boston University, Boston, MA 02215, U.S.A., XIAOMIN TU, MING ZHENG, Polymers Division, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD 20899-8540, U.S.A., ANDREW P. SHREVE, STEPHEN K. DOORN, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — We exploit an energy level cross-over effect¹ to probe quantum interference in the resonance Raman response from carbon nanotube samples highly enriched in the single semiconducting chiralities of (8,6), (9,4), and (10,5). UV Raman excitation profiles of G-band spectra reveal unambiguous signatures of interference between the third and fourth excitonic states (E33 and E44). Both constructive and destructive responses are observed and lead to anomalous intensity ratios in the LO and TO modes. Especially large anomalies for the (10,5) structure result from nearly identical energies found for the two Eii transitions. The interference patterns demonstrate that the sign of the exciton-phonon coupling matrix elements changes for the LO mode between the two electronic states, and remains the same for the TO mode. Significant non-Condon contributions to the Raman response are also found.²

¹Háro , E. H. *et al.*; *Phys. Rev. B.* **2008**, 77, 125405

²Duque, J. G. *et al.*; *ACS Nano* **2011**, 5, 5233–41

10:36AM V6.00012 New Fundamental Optical Behaviors of Single-Wall Carbon Nanotubes at Cryogenic Temperatures: Closer to their Intrinsic Behavior¹, JUAN DUQUE, CHRISTOPHER HAMILTON, JARED CROCHET, ANDREW DATTELBAUM, SCOTT CROOKER, STEPHEN DOORN, Los Alamos National lab — Development of single walled carbon nanotube (SWNT) materials for optoelectronics and nanophotonics has been especially challenging in that SWNT optical properties are highly sensitive to environmental interactions, which can be particularly severe in composite matrices. Here, we present for the first time an innovative approach to obtain highly photoluminescent (PL) solid-state SWNT-nanocomposites, which provides access to novel photophysical properties. Strongly blue-shifted spectral features, and significant increase ($\sim 3\times$) in PL intensities at cryogenic temp in comparison to room temp or previous reports. This difference can be understood as arising from a significantly slower relaxation of excitons from bright to dark states in our SWNTs, as a result of much weaker interaction with the environment. That is, the bright/dark exciton distribution is highly non-thermal, even at the lowest temperatures. In our SWNT-nanocomposites, environmental interactions are minimized, thus bright excitons *cannot* relax efficiently to the dark state, causing a highly non-equilibrium exciton distribution and a correspondingly large PL intensity, even at low temperatures.

¹Thanks to the Department of Energy through the LDRD program

10:48AM V6.00013 Coherent anti-stokes spectroscopy as a probe of chemical disorder in isolated carbon nanotubes, TATYANA SHEPS, JORDAN BROCIOS, ERIC O. POTMA, PHILIP G. COLLINS, University of California, Irvine — We use a third-order coherent anti-stokes (CAS) optical technique to study chemical disorder in individual carbon nanotubes. The CAS response is highly sensitive to this disorder, to the extent that a few chemical defects can appreciably decrease the overall signal. The experiments are performed on individual single- and multi-walled carbon nanotubes (SWNTs and MWNTs) connected in a transistor geometry and subjected to varying degrees of controlled, electrochemical oxidation. The overall CAS intensity can be used to probe the extent of chemical modification, and inhomogeneities along a nanotube resolve local coherent electron density fluctuations. We find that the CAS signal is also strongly affected by substrate interactions: aligned SWNTs grown on single crystal quartz are quenched compared to SWNTs on fused quartz. Finally, CAS spectroscopy on individual SWNTs and MWNTs using picosecond pulses resolves the third-order vibrational signal component at the G-band frequency. The ratio of electronic to vibrational CAS signal components is diameter dependent and in small diameter SWNTs the vibrational component is dominated by the electronic CAS signal. However, in MWNTs, this technique is a first step toward chemically sensitive CARS imaging on a single nanotube level.

Thursday, March 1, 2012 8:00AM - 10:48AM –
Session V7 DMP DCOMP: Focus Session: Computational Design of Materials - Engineering of Electronic Structure Materials 207

8:00AM V7.00001 Band-edge engineering of Silicon by Surface Functionalization: a Combined Ab-initio and Photoemission Study¹, YAN LI, Computational Science Center, Brookhaven National Laboratory, LESLIE OLEARY, NATHAN LEWIS, Department of Chemistry, California Institute of Technology, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis — The electrode material choice is limited in solar to fuel formation devices because of the requirement of band-edge matching to the fixed fuel formation potential. This limitation can be relieved via band-edge engineering. The changes of band-edge positions of Si electrodes induced by the adsorption of H-, Cl-, Br- and short-chain alkyl groups were investigated by combining density functional (DFT), many-body perturbation theory (MBPT), and ultraviolet photoelectron spectroscopy. The band edge shifts are related to the formation of surface dipole moments, and determine the barrier height of electrons and holes in doped silicon surfaces. We find that the trends of the sign and magnitude of the computed surface dipoles as a function of the adsorbate may be explained by simple electronegative rules. We show that quasi-particle energies obtained within MBPT are in good agreement with experiment, while DFT values may exhibit substantial errors. However computed band edge differences are in good agreement with spectroscopic and electrical measurements even at the DFT level of theory. [1] Y. Li and G. Galli, Phys. Rev. B 82, 045321 (2010). [2] Y. Li, L. O'Leary, N. Lewis and G. Galli, to be submitted.

¹YL was supported by Brookhaven Science Associates, LLC under Contract No. DE-AC02-98CH10886 with the U.S. Department of Energy. Part of the work was funded by NSF-CHE-0802907.

8:12AM V7.00002 Genetic engineering of band-edge optical absorption in Si/Ge superlattices¹, MAYEUL D'AVEZAC, JUN-WEI LUO, NREL, THOMAS CHANIER, University of Iowa, ALEX ZUNGER, University of Colorado — Integrating optoelectronic functionalities directly into the mature Silicon-Germanium technology base would prove invaluable for many applications. Unfortunately, both Si and Ge display indirect band-gaps unsuitable for optical applications. It was previously shown (Zachai *et al.* PRL 64 (1990)) that epitaxially grown $[(\text{Si})_n(\text{Ge})_m]_p$ (i. e. a single repeat unit) grown on Si can form direct-gap heterostructures with weak optical transitions as a result of zone folding and quantum confinement. The much richer space of *multiple-period* superlattices $[(\text{Si})_{n_1}(\text{Ge})_{n_2}(\text{Si})_{n_3}(\text{Ge})_{n_4} \dots \text{Ge}_{n_N}]_p$ has not been considered. If $M = \sum n_i$ is the total number of monolayers, then there are, roughly, 2^M different possible superlattices. To explore this large space, we combine a (i) genetic algorithm for effective configurational search with (ii) empirical pseudopotential designed to accurately reproduce the inter-valley and spin-orbit splittings, as well as hydrostatic and biaxial strains. We will present multiple-period SiGe superlattices with large electric dipole moments and direct gaps at Γ yielded by this search. We show this pattern is robust against known difficulties during experimental synthesis.

¹This work is supported through the Center for Inverse Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

8:24AM V7.00003 New mechanism for work-function tuning: ZnO surfaces modified by a strong organic electron acceptor, YONG XU, OLIVER T. HOFMANN, RINKE PATRICK, MATTHIAS SCHEFFLER, Fritz Haber Institute Berlin, RAPHAEL SCHLESINGER, NORBERT KOCH, Humboldt University Berlin, ANTJE VOLLMER, Helmholtz-Zentrum Berlin — A key task for optimizing optoelectronic devices comprising hybrid inorganic/organic systems is to control the energy level alignment at interfaces. The use of interlayers provides a pathway to solve this challenge. To demonstrate the concept we investigated the polar surfaces of ZnO, modified by the prototypical organic electron acceptor 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) theoretically and experimentally. DFT-PBE Δ SCF calculations of the O 1s surface core-level shifts combined with XPS measurements suggest that ZnO(000-1)/ZnO(0001) are H/OH covered. Depositing F4TCNQ on these surfaces considerably increases the work function that is shown to be insensitive to the doping level in PBE+vdW. F4TCNQ on ZnO(0001) exhibits an extraordinary high work function due to the appearance of upright adsorption. The PBE+vdW results are in line with the UPS data that shows work-function increases up to 1.4/2.8 eV on ZnO(000-1)/ZnO(0001). In contrast to F4TCNQ on metals, where pronounced bidirectional charge transfer occurs, the charge transfer from ZnO to F4TCNQ is small, pinning the LUMO close to the Fermi level. The polarization of the system, caused by strong charge rearrangement within the adsorbate, is the main mechanism for the large work-function increase.

8:36AM V7.00004 Quantum Monte Carlo Characterization of Excited States and Energy-Level Alignment at Oligomer/Quantum-Dot Interfaces, YOSUKE KANAI, The University of North Carolina, Chapel Hill / Lawrence Livermore National Laboratory, JONATHAN L. DUBOIS, DONGHWA LEE, Lawrence Livermore National Laboratory — Charge separation of excitons in materials is one of the most important physical processes that need to take place in excitonic solar cells and in photocatalytic devices. Heterogeneous interfaces with the so-called type-II character are often employed for inducing the exciton dissociation through interfacial charge transfer. As the simplest criterion for designing such an interface, the energy alignment of the quasi-particle states is often discussed in literature, together with the exciton binding energy of electron-donating materials. Therefore, accurate characterization of the interfacial energy-level alignment and the exciton binding energy using first principles calculations is important for making systematic progresses in designing better materials for solar energy conversion. However, Density Functional Theory calculations need to be employed with caution in this context. First principles calculations such as Many-Body Perturbation Theory and Quantum Monte Carlo are promising alternatives for accurate characterization, but much more work is needed in this area to assess how well these methods perform in practice. In this talk, we will discuss our preliminary results using diffusion Quantum Monte Carlo on calculating the excited states and energy-level alignment of popular Oligomer/Quantum-Dot interfaces.

8:48AM V7.00005 Shape managing the cross-section of a semiconductor nanowire as a method for fine tuning electro-optical properties¹, OSMAN BARIS MALCIOGLU, JEAN-YVES RATY, University of Liege, SORIN MELINTE, Université Catholique de Louvain — Geometry design in nanowire and nanopillar arrays is used to create photon managing structures in a number of optical applications ranging from photovoltaics to field emission devices. The diameter dependence of the intrinsic properties of the material at the nanoscale provides further tunability and significantly improved performance. Using ab-initio methods (TDDFT), we explore the additional possibility of tuning and enhancing the optical properties by fine structuring the cross-sectional geometry.

¹The authors acknowledge support from the FNRS (FRFC grant 2.4509.09) and the Belgian Federal Government.

9:00AM V7.00006 Dimensional Reduction: A design tool for new semiconductor compounds for radiation detection¹, B.W. WESSELS, J.A. PETERS, Z. LIU, Dept. of Materials Science and Engineering, Northwestern University, J. ANDROULAKIS, M.G. KANATZIDIS, Dept. of Chemistry, Northwestern University, H. JIN, A.J. FREEMAN, Dept. of Physics, Northwestern University, Evanston, IL 60208 — To address the need for new wide gap semiconductors for efficient radiation detection, we present a new design tool called *dimensional reduction* (DR). The method is based on reducing the dimensionality of highly dense but low bandgap (<1 eV) compounds to create comparably dense wide bandgap (>1.6 eV) semiconductors without compromises on their mass density. We utilize electronic band structure calculations of bandgap and effective mass to aid in the selection among the wide variety of compounds that can be formed by DR. As a proof of the concept, we report on computational design as well as optical characterization of three such dimensionally reduced materials based on β -HgS, HgSe, and CdTe compounds. These compounds, namely, Cs₂Hg₆S₇, Cs₂Hg₃Se₄, and Cs₂Cd₃Te₄, show great promise as detector materials. Band structure calculations show that they have direct bandgaps of 1.28, 1.97, and 2.35 eV, respectively, in good agreement with experimental values of 1.63, 2.2 and 2.5 eV, respectively. Measured electrical resistivity values of $\sim 10^6$, 10^7 , and 10^9 Ω -cm, respectively, are high enough for further evaluation of these materials for hard radiation detection. Computational design of other wide gap semiconductors is underway.

¹This work is supported by the Defense Threat Reduction Agency through grant no. HDTRA1 09-1-0044.

9:12AM V7.00007 First principles study of LaGaO₃/MgAl₂O₄ (001) polar interfaces¹, ALEJANDRO REBOLA, PETER ZAPOL, JEFFREY EASTMAN, Argonne National Laboratory, SERDAR OGUT, University of Illinois at Chicago — Materials with high oxygen ion conductivity have been the center of much attention due to both fundamental interest and technological applications. One of the most remarkable ionic conductors and an excellent candidate for future solid oxide fuel cells is LaGaO₃ (LGO), as it exhibits very high ionic conductivity when doped with Sr or Mg. To achieve enhanced ionic transport in this system, where oxygen vacancies (V_O) are the dominant carriers, we propose a negatively charged interface as a way of inducing a V_O enrichment layer. In this study, the interface is comprised of LGO and the spinel MgAl₂O₄, both of which exhibit nominally charged (001) planes. We consider an interface where the (GaO₂)¹⁻ layer of LGO is in contact with the (AlO₂)¹⁻ layer of the spinel. Such negatively charged interfaces require compensating defects, providing a strong driving force for enhancing the V_O concentration, and hence, the in-plane ionic conductivity in the space charge region adjacent to the boundary. We report results from first-principles calculations which provide information on the structure and relative stability of these polar interfaces, compensation mechanisms, and defect formation energies as a function of distance from the interface.

¹Supported by the Office of Basic Energy Sciences, Division of Materials Sciences, U.S. Department of Energy, under Contract No. DE-AC02-06CH11357

9:24AM V7.00008 Theory-driven design of hole-conducting transparent oxides¹, G. TRIMARCHI, H. PENG, IM J., A.J. FREEMAN, V. CLOET, A. RAW, K.R. POEPELMEIER, Northwestern University, Evanston, IL 60208, K. BISWAS, S. LANY, NREL, Golden, CO 80401, A. ZUNGER, University of Colorado, Boulder, CO 80309 — The design of *p*-type transparent conducting oxides (TCOs) aims at *simultaneously* achieving transparency and high hole concentration and hole conductivity in one compound. Such design principles (DPs) define a multi-objective optimization problem that is to be solved by *searching* a large set of compounds for optimum ones. Here, we screen a large set of ternary compounds, including Ag and Cu oxides and chalcogenides, by calculating via first-principles methods the design properties of each compound, in order to search for optimum *p*-type TCOs. We first select Ag₃VO₄ as a case study of the application of *ab-initio* methods to assess a compound as a candidate *p*-type TCO. We predict Ag₃VO₄ (i) to have a hole concentration of $\approx 10^{14}$ cm⁻³ at room temperature, (ii) to be at the verge of transparency, and (iii) to have lower hole effective mass than the prototype *p*-type TCO CuAlO₂. We then map the hole effective mass *vs.* the band gap in the selected compounds and determine those that best meet the DPs by having simultaneously minimum effective mass and a band gap large enough for transparency.

¹Funded by the DOE Energy Frontier Research Center for Inverse Design.

9:36AM V7.00009 Screw Dislocated ZnO and Si Nanostructures Studied with Objective Molecular Dynamics, EVGENIYA AKATYEVA, ILIA NIKIFOROV, DONG-BO ZHANG, TRAIAN DUMITRICA, University of Minnesota — Objective molecular dynamics [1] coupled with tight-binding density functional-based models makes it possible to investigate the stability and electronic structure of ZnO and Si nanotubes [2] and nanowires [3] containing axial screw dislocations. The dislocated structures adopt twisted configurations that stabilize the dislocation at the center despite the close vicinity of surfaces, in excellent agreement with Eshelby's elasticity model of cylinders containing an axial screw dislocation. Coupled to this elasticity model, our simulations represent a new efficient method of calculating the core energy of a dislocation and allow to rationalize the stability of chiral hollow nanowires. The uncovered mechanical and electronic behaviors have implications for a broad class of nanomaterials grown by engaging a screw dislocation. 1. T. Dumitrica and R.D. James, J. Mech. Phys. Sol. 55, 2206-2236 (2007). 2. D.-B. Zhang, E. Akatyeva, and T. Dumitrica, Phys. Rev. B 84, 115431 (2011). 3. I. Nikiforov, D.-B. Zhang, and T. Dumitrica, J. Phys. Chem. Lett. 2, 2544 (2011).

9:48AM V7.00010 Tunable band gaps in transition metal dichalcogenides, ASHWIN RAMASUBRAMANIAM, University of Massachusetts Amherst, DORON NAVEH, ELIAS TOWE, Carnegie Mellon University — We investigate band-gap tuning in transition-metal dichalcogenide bilayers by external electric fields applied perpendicular to the layers. Using density functional theory, we show that the fundamental band gap of MoS₂, MoSe₂, MoTe₂, and WS₂ bilayer structures continuously decreases with increasing applied electric fields, eventually rendering them metallic. We interpret our results in the light of the Giant Stark Effect and obtain a robust relationship, which is essentially characterized by the interlayer spacing, for the rate of change of band gap with applied external field. Our study expands the known space of layered materials with widely tunable band gaps beyond the classic example of bilayer graphene and suggests potential directions for fabrication of novel electronic and photonic devices.

10:00AM V7.00011 Growth of Monolayer Boron Sheet on Metal and Metal Boride Surface, YUANYUE LIU, QINGBO YAN, Dept. of Mech. Eng. & Mat. Sci., Rice U., HOONKYUNG LEE, Dept. of Mech. Eng. Mat. Sci., Rice U., BORIS YAKOBSON, Dept. of Mech. Eng. & Mat. Sci., Rice U., COMPUTATIONAL MATERIALS SCIENCE TEAM — Monolayer boron (B) sheet has attracted lots of interests recently due to its metallic conductivity. However, their experimental synthesis has not been achieved so far, which calls for theoretical investigation. Using first principles calculations, we study the possibility of growing monolayer B sheets on metal (Ag, Au) and metal boride (MgB₂, TiB₂) surface as catalytic substrate. It is shown that after decomposition from precursor, B atoms will aggregate to cluster, then to sheets, while three dimensional bulky B is prohibited due to high nucleation barrier. Charge transfer between substrate and B sheet shifts its stability dependence on hexagon vacancy density. B sheet with specific vacancy density can have cleavage energy as small as graphite thus should be easily peeled off. This work suggests promising approach to synthesize B sheets and would possibly pave the way towards their applications to electronic, optic, and mechanic nano-devices.

10:12AM V7.00012 Understanding the properties of hexagonal Semiconducting Nanomembranes, RODRIGO AMORIM, XIAOLIANG ZHONG, SAIKAT MUKHOPADHYAY, RAVINDRA PANDEY, Michigan Tech, SHASHI KARNA, Army Research Laboratory — Nanomembranes are an interesting material with novel applications, such as their integration into electronic devices. We can highlight the high degree of bendability of nanomembranes that can be important to device integration and the possibility of modifying electronic properties by changing the roughness. Using density functional theory (DFT) combined with non-equilibrium green's function (NEGF) theory, we investigate different hexagonal semiconducting nanomembranes (e.g. BN, AlN and GaN). We will show the stability, electronic and transport properties of these nitride membranes and look into their possible integration with graphene.

10:24AM V7.00013 Single-atom Magnetic Anisotropy on a Surface, CHIUNG-YUAN LIN, JING-NENG YAO, Department of Electronics Engineering, National Chiao Tung University — Studying single-atom magnetic anisotropy on surfaces enables the exploration of the smallest magnetic storage bit that can be built. In this work, magnetic anisotropy of a single rare-earth atom on a surface is studied for the first time, both computationally and theoretically. The substrate surface is chosen to be a copper-nitrite surface, where single transition-metal magnetic atoms on the same surface were previously studied one atom at a time by STM.¹ We propose unconventional *f* and *d* subshell symmetries so that following first-principles calculations, simple pictorial analyses of such anisotropy can be performed for the first time, independently for both rare-earth and transition-metal adatoms. The analyses explain the spin-density distribution of a single adatom, and derive the spin orientation of its largest spin-orbit coupling. The magnetic anisotropy energy of the present study is calculated to be a factor of five larger than the previous highest one.

¹C. F. Hirjibehedin, C.-Y. Lin, A. F. Otte, M. Ternes, C. P. Lutz, B. A. Jones, A. J. Heinrich, Science 317, 1199 (2007).

10:36AM V7.00014 Computer Simulated Cold Welding of Metal Nanowires, EDISON DA SILVA, ZENNER PEREIRA, Institute of Physics "Gleb Wataghin", UNICAMP, 13083-970, Campinas - SP, Brazil — Metallic contacts are of great importance in electronic devices, the ability of welding them without temperature change is quite remarkable and of interest. Recently cold welding was achieved in gold and silver nanowires (NWs) with diameters in the range of 4 to 10 nm [1]. In the present work we use computer simulations to produce cold welding in gold, silver and silver-gold NWs at room temperature. We used molecular dynamics with many body effective potentials based on the embedded-atom method EAM using the LAMMPS code to simulate first the braking of gold and silver NWs. The two produced NWs are then cold welded and similarly as occurred in the experiments the newly welded NWs showed fcc structures as the printine samples. The structural analysis is done with two independent methods [2] and strain stress curves of the breaking and welding are present. Our computer simulation compare very well with the experiments. This work is supported by CNPq CAPES and FAPESP and FAEPEX. ZSP is supported by CAPES. CENAPAD-SP and IFGW are acknowledged for computer time.

[1] Y. Lu, *et al.* Nature Nanotechnology 5, 218 - 224 (2010)

[2] E. Z. da Silva and Z.S. Pereira, Phys. Rev. B **81**, 195417 (2010).

Thursday, March 1, 2012 8:00AM - 11:00AM – Session V8 DMP GMAG: Focus Session: Frustrated Magnetism - Kagome II 208

8:00AM V8.00001 Monte Carlo simulations of the fcc Kagomé lattice¹, VAHID HEMMATI, MARTIN PLUMER, JOHN WHITEHEAD, Memorial University of Newfoundland, BYRON SOUTHERN, University of Manitoba — For many years, Ir-Mn alloys have been widely used by the magnetic storage industry in thin-film form as the antiferromagnetic pinning layer in GMR and TMR spin valves [1]. Despite the technological importance of this structure, it has not previously been noted that the magnetic Mn-ions of fcc IrMn₃ reside on Kagomé layers ABC stacked along <111> axes normal to the film plane [2,3]. Results of Monte Carlo simulations will be reported on the bulk fcc Kagomé lattice for both XY and Heisenberg models including the eight NN exchange interactions. Degeneracies persist in the 3D case and there is strong evidence for a fluctuation-driven first-order transition to well-defined long-range order characterized as the layered “*q*=0” 120-degree spin structure. Effects of varying the inter-layer coupling are also examined.

[1] M. Tsunoda *et al.*, Appl. Phys. Lett. **97**, 072501 (2010).

[2] I. Tomeno *et al.*, J. Appl. Phys. **86**, 3853 (1999).

[3] L. Szunyogh *et al.*, Phys. Rev. B **79**, 020403(R) (2009).

¹Supported by NSERC and ACEnet.

8:12AM V8.00002 Phase Control of Magnetic Order in (Y,Lu)BaCo₄O₇, JOHN MITCHELL, SEVDA AVCI, OMAR CHMAISSEM, Argonne National Laboratory, LAURENT CHAPON, Institut Laue Langevin, DMITRY KHALYAVIN, ISIS Facility, Rutherford Laboratory — The RBaCo₄O₇ (R=Ca, Y, Tb-Lu) system provides a novel topology for studying geometric frustration, in which face-sharing tetrahedra of magnetic ions link to form trigonal bipyramids on a Kagomé lattice. Here we describe the structural and magnetic behavior of the Lu member and the solid solution joining Lu to Y as a chemical means to tune between magnetically ordered and disordered ground states. Mean-field models of the generic magnetic phase diagram of RBaCo₄O₇ determined recently by our group (D. D. Khalyavin *et al.* Physical Review B **82**, 094401 (2010)) show a variety of magnetic states as a function of two exchange parameters: *J_{ab}* and *J_c*, where *J_{ab}* links Co ions in the Kagomé planes and *J_c* links Co ions from the Kagome plane to the interleaving triangular layer. Experimentally, we find that YBaCo₄O₇ has a long-range ordered antiferromagnetic ground state, while LuBaCo₄O₇ appears to be disordered above 2 K with very slow dynamics measured by neutron scattering. We use the solid solution to interpolate between these endpoints and discuss these results with respect to the mean-field phase diagram.

8:24AM V8.00003 Spin dynamics in the extended kagomé $\text{YBaCo}_4\text{O}_{7.1}$ ¹, MICHAEL HOCH, PHILIP KUHN, TIGLET BESARA, ARNEIL REYES, National High Magnetic Field Laboratory at Florida State University, Tallahassee, FL, JOHN MITCHELL, Argonne National Laboratory, Argonne, IL — The extended kagomé system YBaCo_4O_7 consists of antiferromagnetically coupled Co^{2+} and Co^{3+} ions arranged in stacks with alternating kagomé and triangular layers in ab planes in the orthorhombic lattice. The oxygen-stoichiometric material orders below 110 K. The system exhibits interesting exchange topology with both trigonal bipyramids and triangular kagomé clusters of Co ions. Model calculations and neutron scattering experiments, made by other workers, have provided considerable information on the magnetic structure. Ordered chains are found for the apical ions along the c-axis with neighbor chains having oppositely directed polarizations perpendicular to c in an antiferromagnetic configuration. Only short range order is present in the kagomé planes at temperatures as low as 2 K. The present pulsed NMR measurements, made on a single crystal, both in zero magnetic field and in low applied fields, distinguish the Co ion sites and provide information on the evolution of the spin dynamics for the plane and chain sites as a function of temperature in the range 1.7 - 50 K above which signal wipe-out occurs. A dramatic change in the spin dynamics is found below 5 K.

¹Supported under grants NSF DMR-0654118 and DE-AC02-06CH211357.

8:36AM V8.00004 Spectral Signature of Neodymium Dopants in Frustrated Gadolinium Gallium Garnet Lattice¹, CHRISTOPHER FERRI, MICHAEL TENNENBAUM, SAYANTANI GHOSH, University Of California, Merced, 95348, School Of Natural Sciences — We investigate the spectral emission of Nd^{3+} dopant ions (1% at. wt) in the frustrated magnet Gadolinium gallium Garnet (GGG) as a function of temperature and magnetic field. We concentrate on the low energy excitations centered at 1064 nm and 935 nm, which show a multiplet structure at room temperature. As temperature decreases the emission spectra demonstrate changes in relative intensities that undergo a cross-over at 122 K under zero field cooled conditions. This cross-over is magnetic field dependent and changes as we field-cool the sample. Typically, with decreasing temperature the line widths of the spectral peaks decrease, as is expected. However, when cooled below 10 K selective peaks start exhibiting broadening, even when zero-field cooled. We follow this line broadening as a function of magnetic field and dopant concentration and speculate it is a result of the dopant ions coupling to the internal magnetic fields of the host lattice.

¹We acknowledge funding from NSF CAREER DMR-1056860.

8:48AM V8.00005 Investigating the nature of magnetic correlations in the anti-ferromagnetic hyper-kagome material, $\text{Yb}_3\text{Ga}_5\text{O}_{12}$, KATE ROSS, KATHARINA FRITSCH, McMaster University, ROBERT BEWLEY, TATIANA GUIDI, ISIS, Rutherford Appleton Laboratory, YIMING QIU, CNR, NIST, CHRIS WIEBE, University of Winnipeg, HAIDONG ZHOU, Florida State University, HANNA DABKOWSKA, BRUCE GAULIN, McMaster University — The magnetic Yb^{3+} ions in $\text{Yb}_3\text{Ga}_5\text{O}_{12}$ (YbGG) reside on a hyper-kagome lattice, which has the same connectivity as the planar kagome lattice but in higher dimensions. For anti-ferromagnetically (AFM) coupled spins the hyper-kagome lattice provides a highly-frustrated geometry in three-dimensions. YbGG is isostructural with the well-studied $\text{Gd}_3\text{Ga}_5\text{O}_{12}$ (GGG), which enjoys an exotic magnetic phase diagram. In GGG, the effects of geometric frustration manifest as a disordered, partial spin-glass ground state down to 25mK in zero-field. The application of an external magnetic field first induces an intermediate spin liquid state, then a long range AFM ordered phase. Much less is known about YbGG, though all experimental evidence indicates a lack of LRO in zero-field down to 30mK. We have recently produced single crystals of YbGG and have performed neutron scattering experiments over a range of temperatures (80mK - 10K) and magnetic field strengths (0T - 8T). The results indicate low-energy, fluctuating spin correlations at 80mK, 0T, as well as a dramatic response to an applied magnetic field. At zero-field, we also observe a low-energy dispersionless spin excitation that softens as the temperature is increased above the Schottky anomaly in the specific heat.

9:00AM V8.00006 Spatially anisotropic kagome antiferromagnet with Dzyaloshinskii-Moriya interaction, VLADIMIR A. ZYUZIN, GREGORY A. FIETE, University of Texas at Austin — We theoretically study the spatially anisotropic spin-1/2 kagome antiferromagnet with Dzyaloshinskii-Moriya (DM) interaction using a renormalization group analysis in the quasi-one-dimensional limit. We identify the various temperature and energy scales for ordering in the system. For very weak DM interaction, we find a low-temperature spiral phase with the plane of the spiral selected by the DM interaction. This phase is similar to a previously identified phase in the absence of the DM interaction. However, above a critical DM interaction strength we find a transition to a phase with coexisting antiferromagnetic and dimer order, reminiscent of one-dimensional antiferromagnetic systems with a uniform DM interaction. Our results help shed light on the fate of two dimensional systems with both strong interactions and significant spin-orbit coupling.

9:12AM V8.00007 ABSTRACT WITHDRAWN —

9:24AM V8.00008 Dimensional reduction, avalanches and disorder in artificial kagome spin ice¹, REMO V. HUGLI, GERARD DUFF, HANS-BENJAMIN BRAUN, University College Dublin — In collaboration with an experimental team at the Swiss Light Source we have recently demonstrated that emergent monopoles and associated Dirac strings can directly be observed in real space via x-ray circular dichroism in a kagome lattice geometry. Here we build on the fact that the experimental results are in excellent agreement with MC simulations of a lattice of point dipoles with disorder realized in the form of random switching fields. We demonstrate that within a large range of physical parameters such as interdipolar coupling and randomness, magnetization reversal proceeds via a novel 1D avalanche behaviour whose hallmark is an exponential avalanche size distribution. After presenting simple arguments for the origin of such dimensional reduction we demonstrate that such 1D avalanche behavior also occurs in a model where the dipoles are stretched into magnetic charge dumbbells which provides a more realistic model for nanolithographic islands. Finally we demonstrate how a judicious design of the island anisotropy can be used to achieve controlled switching and avalanche propagation which paves the way for spintronic applications

¹Supported by Science Foundation Ireland (08/RFP/PHY1532, 05/IN1/I853 and 08/RFP/PHY1532 - STTF 11)

9:36AM V8.00009 Propagation of monopole defects and flux channels in an artificial square spin-ice lattice, YIMEI ZHU, V.V. VOLKOV, SHAWN POLLARD, Brookhaven National Laboratory — The recent development of artificial lattices of magnetic islands in which competing interactions give rise to macroscopic analogs of atomically frustrated spin ices has opened up a new field of research, in which the interaction, frustration and evolution of individual magnetic elements can be directly observed in real space. We investigate the magnetic reversal along the (11) symmetry axis of permalloy islands in an artificial “square” spin-ice geometry with in-situ Lorentz transmission electron microscopy. Novel differential transport-of-intensity allows for the identification of “monopole”-like defects and flux channels, similar to Dirac strings, that link them. We track the growth and propagation of these defects and flux channels throughout the reversal process. Simulations are used to compare with experiment to show how nucleation and propagation of defects affect the reversal of the lattice as a whole. We find that interactions between defects and flux channels can explain the saturation of defect populations at low net magnetizations. This work was supported by U.S. Department of Energy, Office of Basic Energy Science, Material Sciences and Engineering Division, under Contract No. DE-AC02-98CH10886.

9:48AM V8.00010 Magnetization dynamics in artificial spin ice lattices¹, OLLE HEINONEN, SEBASTIAN GLIGA, Argonne National Laboratory — Artificial spin ice lattices (ASIL) consist of regular arrays of single-domain nanomagnets displaying ice rule ordering. Frustration is introduced through shape anisotropy. ASILs have been shown to exhibit complex behavior, with rich phase diagrams and quasi-static magnetization reversal. In particular, topological defects, such as Dirac monopoles and Dirac strings, play a fundamental role in the quasi-static behavior of ASILs. In this work, we use micromagnetic simulations to investigate the resonant frequencies of square lattice ASILs consisting of stadium-shaped nanomagnets. We calculate the evolution of the fundamental modes of a single element when elements are combined in four-stadia configurations and large lattices. In a cross-shaped four-stadium configuration for example, the Dirac monopole splits the frequencies of the lowest (near)-degenerate symmetric and antisymmetric edge modes of a single stadium. This splitting increases in a 24-stadium system with two monopoles. We also calculate the evolution of the spectral characteristics as the monopoles move farther apart in the lattice, but stay connected through a Dirac string. Our work suggests that these topological defects have distinct spectral signatures that can be detected experimentally.

¹Part of this work was carried out at Argonne National Laboratory (ANL), a US DOE Science Laboratory operated under contract no. DE-AC02-06CH11357 by UChicago Argonne, LLC. We also acknowledge use of the Center for Nanoscale Materials at ANL.

10:00AM V8.00011 Study of system-size effects on the emergent magnetic monopoles and Dirac strings in artificial kagome spin ice¹, ALEJANDRO LEON, Universidad Diego Portales — In this work we study the dynamical properties of a finite array of nanomagnets in artificial kagome spin ice at room temperature. The dynamic response of the array of nanomagnets is studied by implementing a "frustrated cellular automata" (FCA), based in the charge model. In this model, each dipole is replaced by a dumbbell of two opposite charges, which are situated at the neighbouring vertices of the honeycomb lattice. The FCA simulations, allow us to study in real-time and deterministic way, the dynamic of the system, with minimal computational resource. The update function is defined according to the coordination number of vertices in the system. Our results show that for a set geometric parameters of the array of nanomagnets, the system exhibits high density of Dirac strings and high density emergent magnetic monopoles. A study of the effect of disorder in the arrangement of nanomagnets is incorporated in this work.

¹The author acknowledge the financial support of Fondecyt program grant 11100045.

10:12AM V8.00012 Magnetic reversal of an artificial square ice: dipolar correlation and charge ordering, JASON MORGAN, University of Leeds, AARON STEIN, Center for Functional Nanomaterials, SEAN LANGRIDGE, ISIS,, CHRISTOPHER MARROWS, University of Leeds — Artificial spin ices are lithographically patterned arrays of single domain nanomagnets [1-4]. The elongated elements form a 2D system of interlinked vertices at which Ising-like dipole moments meet with incompatible interactions. They are directly analogous to 3D bulk spin ice materials [5]. We report on the magnetic reversal of an athermal artificial square ice pattern subject to a sequence of magnetic fields applied slightly off the diagonal symmetry axis, investigated via magnetic force microscopy of the remanent states that result [1]. From an initial diagonally polarised state, sublattice independent reversal is observed via bulk-nucleated incrementally-pinned flipped moment chains along parallel channels of magnetic elements, as evident from analysis of vertex populations and dipolar correlation functions. Weak dipolar interactions between adjacent chains favour antialignment and give rise to weak charge ordering of "monopole" vertices during reversal.

[1] J. P. Morgan, A. Stein, S. Langridge & C.H. Marrows, New Journal of Physics (2011), 13, 105002.

[2] R. F. Wang et al., Nature (2006), 439, 303-306.

[3] E. Mengotti et al., Nature Physics (2011), 7, 68-74.

[4] J. P. Morgan et al., Nature Physics (2011), 7, 75-79.

[5] M. J. Harris et al., PRL (1997), 79, 2554-255

10:24AM V8.00013 Experimental Realization of Isotropic Ising Spins in Frustrated and Unfrustrated Artificial Spin Ice with Perpendicular Anisotropy¹, SHENG ZHANG, JIE LI, IAN GILBERT, YU PAN, PAUL LAMMERT, KRITI KOHLI, RAJIV MISRA, VINCENT CRESPI, NITIN SAMARTH, PETER SCHIFFER, Department of Physics and Materials Research Institute, Pennsylvania State University, University Park, PA 16802, USA, CRISTIANO NISOLI, Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, MIKE ERICKSON, CHRIS LEIGHTON, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455, USA — We have studied lithographically defined arrays of magnetostatically interacting single domain ferromagnetic islands with moments normal to the plane, leading to fully isotropic magnetostatic interactions. Probing both frustrated kagome and unfrustrated honeycomb array geometries, we find that the spin configurations can be reproduced with models based on only nearest-neighbor correlations. While the honeycomb geometry displays ordering of moments in well-defined domains, the kagome geometry has only short range correlations that show striking similarities to those of analogous in-plane systems and are closely comparable to expectations for a simple Ising system.

¹We acknowledge the financial support from DOE and Army Research Office.

10:36AM V8.00014 Hysteresis and Return Point Memory in Artificial Spin Ice Systems, CYNTHIA REICHHARDT, Los Alamos National Laboratory, ANDRAS LIBAL, Babes-Bolyai University, CHARLES REICHHARDT, Los Alamos National Laboratory — We investigate hysteresis loops and return point memory for artificial square and kagome spin ice systems by cycling an applied bias force and comparing microscopic effective spin configurations throughout the hysteresis cycle. Return point memory loss is caused by motion of individual defects in kagome ice or of grain boundaries in square ice. In successive cycles, return point memory is recovered rapidly in kagome ice. Memory is recovered more gradually in square ice due to the extended nature of the grain boundaries. Increasing the amount of quenched disorder increases the defect density but also enhances the return point memory since the defects become trapped more easily.

10:48AM V8.00015 Collective Magnetic Behavior of Geometrically Frustrated Arrays with Perpendicular Anisotropy, Y. PAN, K.K. KOHLI, R. FRALEIGH, A.L. BALK, D. FINKEL, S. ZHANG, J. LI, I. GILBERT, P.E. LAMMERT, R. MISRA, V.H. CRESPI, P. SCHIFFER, N. SAMARTH, Dept. of Physics, Penn State University, University Park PA 16802, M. ERICKSON, C. LEIGHTON, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455 — We use the magneto-optical Kerr effect (MOKE) to study the global and local magnetic behavior of geometrically frustrated arrays of single domain ferromagnetic islands with perpendicular anisotropy. MOKE measurements over macroscopic length scales probe the global properties of arrays with different lattice geometries and island spacings. The variation of switching field as a function of island spacing gives us insight into the influence of local frustration on the collective magnetic response of the arrays. The experimental results are compared with mean field calculations. Finally, we use spatially resolved Kerr microscopy to probe nucleation and domain propagation in the magnetization reversal process. Supported by U.S. Department of Energy Award DE-SC0005313. Lithography performed with the support of the National Nanotechnology Infrastructure Network

Thursday, March 1, 2012 8:00AM - 11:00AM –
Session V9 GMAG DMP: Focus Session: Magnetic Oxide Thin Films And Heterostructures -
Transport Properties 209

8:00AM V9.00001 Scaling of the anomalous Hall effect in SrRuO_3 , NOAM HAHAM, YISHAI SHPERBER, MOTY SCHULTZ, NETANEL NAFTALIS, EFRAT SHIMSHONI, Department of Physics, Nano-magnetism Research Center, Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Ramat-Gan 52900, Israel, JAMES REINER, Department of Applied Physics, Yale University, New Haven, CT 06520-8284, LIOR KLEIN, Department of Physics, Nano-magnetism Research Center, Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Ramat-Gan 52900, Israel — Being one of the most intriguing manifestations of a transport phenomenon that is sensitive to spin and topology, the anomalous Hall effect (AHE) is at the focus of considerable theoretical and experimental efforts. SrRuO_3 has played a pivotal role in the study of the AHE and numerous attempts have been made to elucidate its complicated behavior. By using SrRuO_3 films with a wide range of thicknesses that vary considerably in the temperature-dependence of their resistivity, we show that the AHE scales with resistivity. The scaling provides a compelling piece of evidence that resistivity, *irrespective of its sources or nature (elastic or inelastic)*, determines the AHE of SrRuO_3 in the entire ferromagnetic phase. This observation strongly suggests that changes in Berry phase due to assumed temperature-dependent exchange splitting cannot explain the complicated temperature dependence of the AHE. On the other hand side jumps mechanism combined with Karplus-Luttinger (Berry phase) mechanism that takes into account effects of finite scattering time may explain the observed behavior.

8:12AM V9.00002 Optical spectroscopy of magnetic exchange splitting above the Curie temperature in ferromagnetic SrRuO_3 thin film, D.W. JEONG, C.H. KIM, C.H. SOHN, S.H. CHANG, H.J. PARK, T.D. KANG, Seoul National University, Y.S. LEE, Soongsil University, J.J. YU, T.W. NOH, Seoul National University — SrRuO_3 is a representative itinerant ferromagnetic material with the Curie temperature about 150K. To investigate the relation between magnetism and electronic structure, we measured temperature dependent optical spectra of SrRuO_3 thin film on SrTiO_3 substrate. With decreasing temperature, spectral weight transfer between 2.5eV and 3.2eV transition was observed. Comparing to the first-principles calculation, we attributed the weight transfer as a magnetic exchange splitting due to the Stoner transition. Interestingly, the exchange splitting remained above the Curie temperature, and destroyed near the room temperature. This observation indicates the long range magnetic ordering of SrRuO_3 is destroyed at the Curie temperature due to the transverse spin fluctuation not a Stoner transition. Moreover, using the optical sum rule of optical spectra, we systematically and quantitatively studied the ferromagnetic property of SrRuO_3 thin film.

8:24AM V9.00003 Electronic and magnetic properties of $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ epitaxial thin films¹, LUDI MIAO, WENYONG ZHANG, PUNAM SILWAL, XIAOLAN ZHOU, ILAN STERN, JIN PENG, Tulane University, LEONARD SPINU, University of New Orleans, ZHIQIANG MAO, DAEHO KIM, Tulane University — Strongly correlated $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ (CSRO) has attracted much attention for its rich physical properties such as Mott metal-insulator (MI) transition, antiferromagnetism (AFM), and spin-triplet superconductivity. We have grown epitaxial CSRO thin films on LaAlO_3 (001) substrates using a pulsed laser deposition method and investigated their electronic and magnetic properties. Ca_2RuO_4 thin films show strong compressive strain leading to an itinerant ferromagnetic (FM) phase coexisting with insulating AFM phase in the ground state and a suppressed broad and gradual MI transition. This is in sharp contrast to bulk Ca_2RuO_4 , which exhibits an AFM Mott-insulating ground state and sharp MI transition. While the $x=0.1$ and 0.5 CSRO films also exhibit coherent strain, the MI transition and itinerant ferromagnetism are partially suppressed in the $x=0.1$ film and fully suppressed in the $x=0.5$ film. In contrast, Sr_2RuO_4 thin films are not susceptible to strain on any perovskite substrates including LaAlO_3 ; superconductivity in these films is suppressed due to disorders resulting from strain relaxation.

¹This research is supported by DOD ARO under Grant No. W911NF0910530 and the LA-SIGMA program

8:36AM V9.00004 Optical properties of ferrimagnetic NiFe_2O_4 thin films, DIPANJAN MAZUMDAR, Center for Materials for Information Technology, University of Alabama, QI SUN, KEN O NEAL, BRIAN HOLINSWORTH, HUNTER SIMS, Chemistry Department, University of Tennessee, JIANXING MA, ARUNAVA GUPTA, WILLIAM BUTLER, JANICE MUSFELDT, Center for Materials for Information Technology, University of Alabama, U ALABAMA TEAM, U TENNESSEE TEAM — Magnetic insulators like NiFe_2O_4 are attracting attention due to the high Curie temperature (850 K), which is rare among oxides. We recently demonstrated the growth of high-quality NiFe_2O_4 thin films practically down to room temperature, which permits investigation of the optical properties over wide growth temperatures. Our spectroscopic work reveals that NiFe_2O_4 displays both direct and indirect band gaps. A plot of $(\alpha E)^2$ vs. energy places the 300 K direct gaps for the highest quality films at 2.77 and 2.36 eV for the majority and minority channels, respectively whereas a plot of $(\alpha E)^{0.5}$ vs. energy places the indirect band gap at 1.64 eV. For the indirect case, we extract a coupling phonon energy of ~ 50 meV (400 cm^{-1}), which corresponds to an infrared active O-Fe-O bending mode. The difference between the direct and indirect gap energies reveals an opportunity to obtain spin-polarized carriers via optical excitation. These features have strong overlap with the solar spectrum.

8:48AM V9.00005 Effects of Strain in Highly Ordered $\text{Sr}_2\text{CrReO}_6$ Epitaxial Films¹, A.J. HAUSER, J.R. SOLIZ, M. DIXIT, R.E.A. WILLIAMS, M.A. SUSNER, B. PETERS, L.M. MIER, T.L. GUSTAFSON, M.D. SUMPTION, H.L. FRASER, P.M. WOODWARD, F.Y. YANG, The Ohio State University — $\text{Sr}_2\text{CrReO}_6$, a double-perovskite ferrimagnet, has attracted much attention because of its Curie temperature well above room temperature and predictions of half-metallicity. We have deposited pure-phase $\text{Sr}_2\text{CrReO}_6$ epitaxial films on several (001)-oriented substrates and buffer layers by ultrahigh vacuum off-axis magnetron sputtering, in order to study tensile and compressive strain effects due to lattice mismatches up to 1.5%. Triple-axis x-ray diffractometry was used in tandem with direct observations via HAADF STEM to confirm film epitaxy, phase purity, Cr/Re ordering, and strain via film lattice constants. Magnetic characterization shows a marked effect on the saturation magnetization due to strain, with slight changes in the Curie temperatures. Finally, electrical and optical characterization suggest that $\text{Sr}_2\text{CrReO}_6$ is a gapped material under both unstrained and strained systems, and will be discussed in detail as well.

¹This work is supported by the Center for Emergent Materials at the Ohio State University, a NSF Materials Research Science and Engineering Center (DMR-0820414).

9:00AM V9.00006 Probing of polarization reversal and charge conduction in epitaxial (Ga,Fe)₂O₃ thin films on conducting oxide SrRuO₃, R.H. SHIN, S.H. OH, J.H. LEE, W. JO¹, Department of Physics, Ewha Womans University, Korea, C. LEFEVRE, A. TOMASSON, F. ROULLAND, C. MENY, N. VIART, Institut de Physique et Chimie des Matériaux de Strasbourg, France — Ga_{2-x}Fe_xO₃ (GFO) thin films are the promising room-temperature multiferroics since their magnetic T_C has been reported up to 370 K at x=1.4. However, most polarization hysteresis loops of the GFO thin films have been showed lossy behaviors due to the large leakage current. The origin probably lies on charge movement between Fe³⁺ and Fe²⁺ sites which is generated by oxygen vacancy. We report the large reduced leakage current of the GFO thin films by chemical doping to reduce Fe²⁺. The doped GFO thin films were deposited by pulsed laser deposition at 750°C for 15 min in oxygen partial pressure of 200 mTorr on SrRuO₃/SrTiO₃ substrates with various doping concentration. Epitaxy of b-axis orientation in out-of plane was confirmed by x-ray diffraction. The leakage current was reduced up to 5~6 order of magnitude depending on doping concentration. In order to investigate their conduction mechanism, temperature dependent macroscopic I-V curves were measured. Ferroelectric polarization and switching of the films were acquired over a wide range of temperature as well. Scanning probe microscopy has been used to measure local leakage currents as well as polarization reversal as a mode of conductive atomic force microscopy and piezoelectric microscopy, respectively. Local investigation of their electrical properties alludes to ferroelectricity in GFO.

¹a corresponding author

9:12AM V9.00007 Manipulating magnetic phase competition in manganites¹, T. ZAC WARD, ZHENG GAI, XIAOSHAN XU, Oak Ridge National Laboratory, HANGWEN GUO, WENBIN WANG, University of Tennessee — We will discuss recent investigations attempting to isolate single order parameters in the spin-charge-orbital-lattice hierarchy in order to further understand how these complex interactions govern macroscopic electronic and magnetic properties. Specifically, we will present recent findings on strongly correlated thin films of [LaCa]MnO₃, [LaSr]MnO₃, and [LaPrCa]MnO₃. We have developed new experimental methods that allow for both spin engineering and strain engineering at an interface to be tested on these materials; this has allowed us a glimpse at the interplay driving emergent phenomena. We have found that it is possible to exert a measure of control over the electronic phase competition leading to colossal magnetoresistance and the metal-insulator transition in manganites. This work has also been coupled with novel confinement techniques that allow us to observe single domain transitions using basic resistivity measurements which has led to several new discoveries on the formation and dynamics of electronic domains. These studies offer new means to quantitatively investigate the balanced energetics that drive complex materials and promise an ability to tune critical temperatures and desired electronic/magnetic properties.

¹Supported by US DOE Office of Basic Energy Sciences, Materials Sciences and Engineering Division

9:24AM V9.00008 Role of Interface Transport in the Magnetoresistance of Strained Rare Earth Manganite Thin Films¹, PARUL SRIVASTAVA, TYLER GOEHRINGER, CACIE HART, GILLES DONGMO-MOMO, EKEMBU KEVIN TANYI, GRACE YONG, VERA SMOLYANINOVA, DAVID SCHAEFER, RAJESWARI KOLAGANI, Towson University — We are studying the temperature and field dependence of magnetoresistance in epitaxial thin films of rare earth manganites which are subject to lattice mismatch strain, with the goal of investigating the possible role of transport across strain-induced internal interfaces. We will present our results, comparing La_{0.67}Ca_{0.33}MnO₃ (LCMO) thin films grown on by Pulsed laser deposition on different substrates with varying degrees of compressive or tensile lattice mismatch. Strained films of thickness ~ 10 nm, show a large magnetoresistance in fields < 1 Tesla, which continues to increase with decrease in temperature, similar to magnetoresistance associated with grain boundary transport. The temperature dependence of MR in these films does not correlate with the temperature dependence of resistivity and thus seems to originate from effects other than Mn spin alignment. Lattice mismatch strain is known to suppress the insulator-metal transition and enhance charge and orbital ordering, leading to the coexistence of insulating and ferromagnetic metallic phases. Our results suggest possible contributions to the magnetoresistance from transport across the interfaces between the different phases.

¹TG,CH and GD acknowledge support from Undergraduate Research grants from Fisher College of Science and Mathematics and Towson University Undergraduate research Committee.

9:36AM V9.00009 Correlation between the transport properties, atomic structure and oxygen vacancies of perovskites thin films, JUAN RUBIO-ZUAZO, PILAR FERRER, IGOR MADARIAGA, JONANDER GALLASTEGUI, GERMAN R. CASTRO, CRG SpLine at the ESRF, CRG SPLINE-BM25 TEAM — We present a study of the role of the oxygen vacancies on the atomic structure and the transport properties of a 20 nm thick La_{0.7}Ca_{0.3}MnO₃ thin film grown by the pulsed laser deposition method on a SrTiO₃ (001) substrate. The results show that the manganite lattice can accommodate up to 13% of oxygen vacancies maintaining high crystalline order. Under such conditions the atomic structure is characterized by the movement of the La/Ca cations to the perovskite regular position, by the absence of the MnO₆ basal plane rotation, and by a cooperative tilting of the octahedra along the out-of-plane direction. The metal-to-insulator transition temperature decreases from 265K for the fully oxygenated sample to 28 K for the sample with 13% of oxygen deficiency..

9:48AM V9.00010 The metal-insulator transition in a phase-separated manganite studied by in situ STS¹, P.C. SNIJDERS, ORNL, M. GAO, IOP, CAS, Beijing, China and ORNL, H. GUO, ORNL, Univ. of Tennessee, T.Z. WARD, ORNL, H.-J. GAO, IOP, CAS, Beijing, China, J. SHEN, Univ. of Tennessee and Fudan Univ. Shanghai, China, Z. GAI, ORNL — Electronic phase separation (EPS) is a key feature at the heart of the wide variety of electronic and magnetic properties in complex oxides. One consequence of EPS is that electronic transport experiments in bulk materials or 2D films mostly probe the low resistivity electronic phases due to the percolative path of the current. We study oxygen deficient La_{5/8-x}Pr_xCa_{3/8}MnO₃ (LPCMO) thin films using both *in situ* scanning tunneling spectroscopy (STS) and *ex situ* transport experiments. The oxygen deficiency is known to decrease the metal-insulator transition (MIT) temperature or even completely suppress the MIT in conventional transport experiments. We show that *in situ* STS is able to detect the MIT even in systems where conventional transport experiments do not show an MIT at zero magnetic field.

¹Research sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy.

10:00AM V9.00011 Electroresistance and Joule heating effects in manganite thin films, BENJAMIN MARTINEZ, LUIS PENA, REGINA GALCERAN, ZORICA KONSTANTINOVIC, ALBERTO POMAR, BERNAT BOZZO, LLUIS BALCELLS, FELIP SANDIUMENGE, ICMAB-CSIC. Campus de Bellaterra, Bellaterra-08193. SPAIN, NANOSTRUCTURED MAGNETIC MATERIALS TEAM — Electroresistance (ER), i.e. electric field- and/or current-induced resistance switching, has attracted much attention recently because of the possibility of using it for the implementation of resistance random access memories (ReRAM). Although ER is a quite common phenomenon in transition metal oxides, that has been extensively studied both theoretically and experimentally, the precise mechanism involved is not clear yet. In this work we report on the ER measurements in patterned La_{2/3}Sr_{1/3}MnO₃ (LSMO) thin films prepared by sputtering. In order to analyze Joule heating effects we have evaporated a Pt layer on top of the LSMO path to have access to the actual temperature of the sample while measuring resistance of LSMO path or I(V) characteristic curves. I(V) curves have been measured at different temperatures and the corresponding resistance values are compared with that of the R(T) curve taking into account the actual temperature of the sample in order to clarify the role of Joule heating in the observed change of the resistance.

10:12AM V9.00012 Anisotropic magnetoresistance in thin films of the Mott metal CaVO_3 ¹, JIWEI LU, MAN GU, University of Virginia — Bulk CaVO_3 (CVO) is a Pauli paramagnetic metal with a single 3d electron. Some unusual drastic changes in the magneto-resistance, magnetic susceptibility and the Hall effect have been reported in single crystal CVO. We have simultaneously synthesized epitaxial CVO films grown on three differently oriented SrTiO_3 substrates. Colossal magneto-resistance (MR) as well as large crystalline anisotropic was observed at low temperatures. The maximum MR, defined as $(R(7\text{ T})-R(0\text{ T}))/R(0\text{ T})*100\%$, was over 1,000% at 2 K and 35 Tesla (parallel magnetic field) on the CVO films deposited on a (110) SrTiO_3 single crystal substrate, and didn't show any sign of saturation. When the magnetic field was perpendicular, MR was dropped to 6,000%. The MR ratio was much larger than that of single crystal CVO. We have also investigated the magneto-transport behaviors of CVO films deposited on (111) and (100) STO and will discuss the dependence of MR in CVO on the crystal orientation as well as the orientation of external magnetic field.

¹We are thankful to the support from ARO

10:24AM V9.00013 Magnetoelectric effects in Fe_3O_4 thin films, JARED WONG, ADRIAN SWARTZ, RENJING ZHENG, ROLAND KAWAKAMI, Dept. of Physics and Astronomy - University of California, Riverside — Recently, there has been great interest in voltage-induced manipulation of magnetic properties inside magnetic materials. One attractive avenue is using magnetic oxides, which could be susceptible to manipulation of magnetic properties by electric fields at the interface and/or directly altering the electronic behavior within strongly correlated systems, for example. Magnetite (Fe_3O_4) is quite interesting because it exhibits many interesting properties such as ferrimagnetism, ferroelectricity (at low temperatures) and a metal-insulator phase transition near 120 K known as the Verwey transition. Single crystal Fe_3O_4 samples are deposited through reactive molecular beam epitaxy (MBE) on MgO (001) substrates and the structural quality is confirmed through XRD, RHEED, and LEED. Magnetic properties are examined through magneto-optic Kerr effect (MOKE) measurements and 4-probe I-V / Van Der Pauw measurements were used to determine the electronic properties. Samples are incorporated into an electrically gated structure by the addition of a dielectric layer and metallic top electrode and we report our results and observations of voltage-induced manipulation of the magnetic properties inside thin films of Fe_3O_4 .

10:36AM V9.00014 Dynamics of multiple phases in manganite as revealed by dielectric spectroscopy¹, ZHIGAO SHENG, CERG, ASI-RIKEN, Japan, MASAO NAKAMURA, CERG & CMRG ASI-RIKEN, Japan, MASASHI KAWASAKI, YOSHINORI TOKURA, CERG & CMRG ASI-RIKEN, Japan; University of Tokyo, Japan — Phase separation is a very important feature in correlated electron oxides. The coexistence and competition of multiple phases give rise to gigantic response to tiny stimuli, producing dramatic changes in magnetic, transport, and other properties in these compounds [1]. It is crucial to probe the physical properties of each phase separately for a comprehensive understanding of correlated electron oxide materials and their phase separation, but it is difficult due to their nano-scale distribution. Here we report dynamic properties of multiple phases in manganite thin films by using dielectric spectroscopy with a unique $p-N$ junction configuration. The multiple dielectric relaxations have been detected and we distinguished their corresponding multiple phases. The activation energy and dielectric properties of different phases have been deduced separately. We also elucidated their phase evolution with changing of temperature or applied magnetic field from viewpoint of dielectric response. These results provide a guideline to explore the electronic phase separation phenomena in correlated electron oxides.

[1] Y. Tokura et al. Rep. Prog. Phys. 69, 797 (2006).

¹We acknowledge the support from Japan Society for the Promotion of Science (JSPS) through its “Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST Program).”

10:48AM V9.00015 Interface induced giant magnetoelectric coupling in multiferroelectric superlattices, HONGWEI WANG¹, LIXIN HE², Key Laboratory of Quantum Information, University of Science and Technology of China, XIFAN WU³, Department of Physics and Institute for Computational Molecular Science, — AMnO_3 ($A=\text{Ca}, \text{Sr}, \dots$) are good candidates as building blocks for the multiferroic superlattices, because they have several competing instabilities coupled to the magnetic ordering. The coupling between the spin, the AFD modes and the FE modes depends on the relative energetics of these instabilities. Unfortunately in bulk AMnO_3 , there is a strong AFD instability associated with a large oxygen octahedral rotation that suppresses the FE mode. As a result, the linear magnetoelectric (spin-ferroelectricity) coupling is usually found to be weak. We take the $\text{CaMnO}_3(\text{CMO})/\text{BaTiO}_3(\text{BTO})$ SLs as our model systems. We find that the MnO_6 octahedral rotation will be strongly suppressed by the neighboring BaO layers, leading to the enormous enhancement of magnetoelectric coupling and the local electric polarizations in the CMO layers are significant, comparable to that in the BTO layers. This enhancement will be strengthened with the increasing density of interfaces and reaches its maximum at the shortest SL, (i.e., $n=1$) where one observes a huge change of electric polarization between the antiferromagnetic (AFM) and ferromagnetic (FM) states.

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Thursday, March 1, 2012 8:00AM - 11:00AM —

Session V10 GQI DAMOP: Invited Session: Quantum Entanglement in Many-Body Systems

210A

8:00AM V10.00001 Entanglement, teleportation and memory in atomic spin ensembles, EUGENE POLZIK, Niels Bohr Institute, Copenhagen University — Recent experimental progress with entanglement generation and processing in macroscopic atomic spin ensembles will be reviewed. It includes atomic entanglement maintained for an unlimited time via engineered collective dissipation mediated by light and teleportation of collective atomic spin states. A proposal for quantum memory assisted detection of strongly coupled systems will be presented.

8:36AM V10.00002 Entanglement and real-space renormalization group methods for quantum field theories, FRANK VERSTRAETE, University of Vienna — We will demonstrate how the reformulation of the density matrix renormalization group as a variational method within the class of matrix product states has led to a wide class of novel applications and insights into strongly correlated quantum systems in 1 dimension. The discussion will detail the crucial role of entanglement and area laws, and then focus on the generalization of matrix product state methods to quantum field theories and the prospects of simulating experiments with cold gasses. Joint work with I. Cirac, J. Haegeman, T. Osborne.

9:12AM V10.00003 Entangled States of Trapped Ions¹, DIETRICH LEIBFRIED, National Institute of Standards and Technology — Entangled states of the internal degrees of freedom are an important resource in Quantum Information Processing (QIP) and Quantum Simulation (QS) with trapped ions. Most basic requirements for QIP and QS have been demonstrated for trapped ions, with two big challenges remaining: Improving operation fidelity and scaling up to larger numbers of qubits. In the last few years, steady progress has been achieved with laser-based entanglement schemes with demonstrated fidelities of deterministically produced Bell states of 99.3% and up to 14 ion-qubits entangled in generalized GHZ-states. Scalable architectures have been proposed; one scheme, where ion-qubits are moved through a multi-zone trap array, is studied in several laboratories. Sympathetic cooling with a second ion species, which initializes the motional states for multi-qubit operations, has been demonstrated in an experiment where arbitrary operations on two qubits were implemented. Micro-fabrication approaches to ion-trap-arrays have yielded structures that should be capable of holding and manipulating large numbers of ions. Recently, with the use of microwaves, single-qubit rotations with fidelities of 99.998% per gate operation were demonstrated and two ion-qubit gates have been implemented. Microwave control could potentially be easier to scale by directly integrating microwave-lines on micro-fabricated trap devices. It also eliminates several sources of decoherence that are present in laser-based schemes by exclusively coupling to long lived hyperfine ground states.

¹NIST work has been supported by IARPA, DARPA, NSA, ONR and the NIST Quantum Information Program.

9:48AM V10.00004 Topological order and long range quantum entanglements, XIAO-GANG WEN, Dept. of Physics, MIT — What is the origin of fractional charges and fractional statistics in FQH states? What is the origin of light? It turns out that long range entanglement is the reason why fractional charges and fractional statistics can appear FQH state. Long range entanglement is also the reason why waves that satisfy Maxwell equation can appear in some qubit (spin) systems. Long range entanglement also lead to a deeper understanding of gapped quantum phases. It allows us to obtain a classification of interacting topological insulators/superconductors, as well as the much more general symmetry protected topological phases, and intrinsic topological phases.

10:24AM V10.00005 Entangled states as resources in quantum complexity theory, SCOTT AARONSON, MIT Dept. of Electrical Engineering and Computer Science — No abstract available.

Thursday, March 1, 2012 8:00AM - 11:00AM –
Session V11 DMP: Focus Session: Graphene Structure, Stacking, Interactions: Edges and Grain Boundaries 210B

8:00AM V11.00001 Theory and hierarchical calculations of [0001] tilt grain boundaries in graphene, JOHAN CARLSSON, Accelrys Ltd, Cambridge (UK) and Fritz-Haber-Institut, D-14195, Berlin, LUCA M. GHIRINGHELLI, Fritz-Haber-Institut der MPG, D-14195, Berlin, A. FASOLINO, Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands — Several experiments have revealed the presence of grain boundaries in graphene that may change its electronic and elastic properties. Here, we present a general theory for the structure of [0001] tilt grain boundaries in graphene based on the coincidence site lattice (CSL) theory. We show that the CSL theory uniquely classifies the grain boundaries in terms of the misorientation angle θ and periodicity d . The structure and formation energy of a large set of grain boundaries generated by the CSL theory for $0^\circ < \theta < 60^\circ$ (up to 15 608 atoms) were optimized by a hierarchical methodology and validated by density functional calculations. We find that low-energy grain boundaries in graphene can be identified as dislocation arrays. In contrast to three-dimensional materials, the strain created by the grain boundary can be released via out-of-plane distortions that imply to an effective attractive interaction between dislocation cores. This leads to a (secondary) minimum structure at $\theta = 32.2^\circ$, where the grain boundary is made of a flat zigzag array of only 5- and 7-rings. We discuss the importance of these findings for the interpretation of recent experimental results.

8:12AM V11.00002 Localized states at grain boundaries in graphite¹, ADINA LUCAN-MAYER, GUOHONG LI, Department of Physics and Astronomy, Rutgers University, GABRIEL AUTES, OLEG YAZYEV, Ecole Polytechnique Federale de Lausanne (EPFL), Switzerland, EVA Y. ANDREI, Department of Physics and Astronomy, Rutgers University — Scanning Tunneling Microscopy and Spectroscopy at low temperature and in magnetic field was used to characterize the electronic states near grain boundaries on the surface of graphite. Topographic surface maps show the grain boundaries as narrow stripes within which the lattice is reconstructed into a periodic pattern whose period is determined by the relative orientation between adjacent grains. In spectroscopy the grain boundaries produce sharp peaks in the density-of-states at energies that are characteristic of the misorientation between adjacent grains. Spatial maps of the density-of-states at these peak energies show that the peaks correspond to electronic states that are localized on the grain boundaries. We will present measurements of these localized electronic states, their evolution with magnetic field and misorientation angle between grains. The experimental results will be compared with theoretical calculations.

¹Work supported by DOE under DE-FG02-99ER45742, by the Lucent-Alcatel foundation and by NSF under NSF-DMR-0906711, Swiss NSF (grant No. PBELP2-123086)

8:24AM V11.00003 Altering graphene line defect properties using chemistry¹, SMITHA VASUDEVAN, George Washington University, CARTER WHITE, DANIEL GUNLYCKE, Naval Research Laboratory — First-principles calculations are presented of a fundamental topological line defect in graphene that was observed and reported in Nature Nanotech. 5, 326 (2010). These calculations show that atoms and smaller molecules can bind covalently to the surface in the vicinity of the graphene line defect. It is also shown that the chemistry at the line defect has a strong effect on its electronic and magnetic properties, e.g. the ferromagnetically aligned moments along the line defect can be quenched by some adsorbates. The strong effect of the adsorbates on the line defect properties can be understood by examining how these adsorbates affect the boundary-localized states in the vicinity of the Fermi level. We also expect that the line defect chemistry will significantly affect the scattering properties of incident low-energy particles approaching it from graphene.

¹This work was supported by the Office of Naval Research, directly and through the Naval Research Laboratory.

8:36AM V11.00004 Imaging the Structure of Grains, Grain Boundaries, and Stacking Sequences in Single and Multi-Layer Graphene¹, DAVID MULLER, Cornell University — Graphene can be produced by chemical vapor deposition (CVD) on copper substrates on up to meter scales [1, 2], making their polycrystallinity [3,4] almost unavoidable. By combining aberration-corrected scanning transmission electron microscopy and dark-field transmission electron microscopy, we image graphene grains and grain boundaries across six orders of magnitude. Atomic-resolution images of graphene grain boundaries reveal that different grains can stitch together via pentagon-heptagon pairs. We use diffraction-filtered electron imaging to map the shape and orientation of several hundred grains and boundaries over fields of view of a hundred microns. Single, double and multilayer graphene can be differentiated, and the stacking sequence and relative abundance of sequences can be directly imaged. These images reveal an intricate patchwork of grains with structural details depending strongly on growth conditions. The imaging techniques enabled studies of the structure, properties, and control of graphene grains and grain boundaries [5].

[1] X. Li *et al.*, *Science* **324**, 1312 (2009).

[2] S. Bae *et al.*, *Nature Nanotechnol.* **5**, 574 (2010).

[3] J. M. Wofford, *et al.*, *Nano Lett.*, (2010).

[4] P. Y. Huang, *et al.*, *Nature* **469**, 389–392 (2011); *arXiv:1009.4714*, (2010)

[5] In collaboration with Pinshane Y. Huang, C. S. Ruiz-Vargas, A. M. van der Zande, A. W. Tsen, L. Brown, R. Hovden, F. Ghahari, W. S. Whitney, M.P. Levendorf, J. W. Kevek, S. Garg, J. S. Alden, C. J. Hustedt, Y. Zhu, N. Petrone, J. Hone, J. Park, P. L. McEuen

¹Supported by the Cornell Center for Materials Research, an NSF MRSEC, (NSF Grants DMR 1120296 and DMR-0520404), NSF NSEC (EEC-0117770, 064654), ARO, the AFOSR, DARPA-MTO and the MARCO FRC on Materials, Structures, and Devices.

9:12AM V11.00005 Experimentally Controlling the Edge Termination of Graphene Nanoribbons, XIAOWEI ZHANG, OLEG YAZYEV, University of California, Berkeley and Lawrence Berkeley National Laboratory, JUANJUAN FENG, University of California, Berkeley and Lanzhou University, Lanzhou, China, CHENGGANG TAO, YEN-CHIA CHEN, University of California, Berkeley and Lawrence Berkeley National Laboratory, LIMING XIE, Stanford University, Stanford, STEVEN LOUIE, ALEX ZETTL, University of California, Berkeley and Lawrence Berkeley National Laboratory, HONGJIE DAI, Stanford University, Stanford, MICHAEL CROMMIE, University of California, Berkeley and Lawrence Berkeley National Laboratory — The edges of graphene exhibit several unique features, such as the presence of localized edge states, and are anticipated to be a powerful means of controlling the electronic properties of this two-dimensional material. Understanding such properties, however, requires a precise knowledge of the atomic-scale structure and chemical composition of the edge. In this work, the edges of graphene nanoribbons (GNRs) are controlled by hydrogen plasma and are investigated through a combination of high-resolution scanning tunneling microscopy (STM) and first-principles calculations. We recover the atomic structure of the edge termination in atom-by-atom fashion and establish the chemical nature of terminating functional groups at graphene edge segments of different orientation – (i.e., zigzag, armchair and chiral). These results allow us to conclude that the edges of hydrogen-plasma-etched GNRs are generally free of structural reconstructions and are terminated by hydrogen atoms with no rehybridization of the outermost carbon edge atoms. Both zigzag and chiral edges show the presence of edge states.

9:24AM V11.00006 Tunable magnetism at graphene edges, MANUEL SCHMIDT, RWTH Aachen, Institute for Theoretical Solid State Physics — Electron-electron interactions drive clean graphene zigzag edges to a ferromagnetic state, known as edge magnetism. In this state, the spin of specific one-dimensional electronic modes, that are localized at the edge (the so-called edge state), is fully polarized. I will discuss a mechanism by which the edge magnetism can be manipulated via electric fields. One possible realization of this mechanism is based on graphene/graphane interfaces. As the field strength is varied, the graphene edge undergoes two phase transitions: (1) from fully polarized edge magnetism to a ferromagnetic Luttinger liquid (fLL) and (2) from the fLL to an ordinary Luttinger liquid. The intermediate phase (fLL) is a realization of the unusual itinerant one-dimensional ferromagnet and is therefore in seeming contradiction with the Lieb-Mattis theorem, which forbids such one-dimensional magnetism. The resolution of this seeming contradiction is shortly discussed.

9:36AM V11.00007 Dynamics of Graphene Edges Interaction under Joule-heating, XU ZHANG, Department of Electrical Engineering and Computer Science, MIT, Cambridge, MA, XIAOTING JIA, Department of Materials Science and Engineering, MIT, Cambridge, MA, EDUARDO CRUZ-SILVA, Department of Physics, Rensselaer Polytechnic Institute, Troy, NY, LEE-PING WANG, Department of Chemistry, MIT, Cambridge, MA, JESSICA CAMPOS-DELGADO, Laboratory for Nanoscience and Nanotechnology Research (LINAN), México, PAULO ANTONIO ARAUJO, Department of EECS, MIT, Cambridge, MA, VINCENT MEUNIER, Department of Physics, Rensselaer Polytechnic Institute, NY 12180, MAURICIO TERRONES, Department of Physics, Pennsylvania State University, PA, TOMAS PALACIOS, Department of Electrical Engineering and Computer Science, MIT, Cambridge, MA, MILDRED DRESSELHAUS, Department of Electrical Engineering and Computer Science, Department of Physics, MIT, Cambridge, MA — The edge physics of graphene plays an essential role in the electronic properties of nanometer scale graphene. Studying the Joule-heating of a graphene sample supported by an integrated TEM-STM instrument is an effective way to sharpen graphene edges, and therefore produce smooth graphene nanoribbons, which will be studied in this work. Through observation of the movement of graphene platelets heat-treated within a crystalline domain of graphene substrate underneath, we advance our understanding about the mechanism of edge reconstruction, edge-edge interaction, in addition to the graphene substrate interaction for single layer graphene.

9:48AM V11.00008 Structure, Stability and Electronic Properties of Graphene Edges on Co(0001), DEBORAH PREZZI, S3 CNR-Nano, IT, DAEJIN EOM, Columbia University, NY, KWANG T. RIM, Columbia University, HUI ZHOU, MICHAEL LEFENFELD, COLIN NUCKOLLS, TONY F. HEINZ, GEORGE W. FLYNN, Columbia University, NY, MARK S. HYBERTSEN, Brookhaven National Laboratory, NY — We recently demonstrated the growth of epitaxial graphene flakes on Co(0001) surfaces [1]. Here we combine low-temperature scanning tunneling microscopy (STM) measurements and DFT calculations to study graphene edge stability and electronic properties, as resulting from the coupling with the substrate. Graphene edges display straight well-ordered structure with zigzag orientation. DFT calculations provide insights into their stability by comparing several edge morphologies with both armchair and zigzag orientation. Simulated images indicate that different edge structures can be clearly distinguished in topography at low bias. The calculated electronic properties for the low energy edge structures are consistent with the measured STS tunneling spectra, which show a prominent edge-localized peak at low bias. [1] D. Eom *et al.*, *Nano Lett.* **9**, 2844 (2009).

10:00AM V11.00009 Chemical versus Thermal Folding of Graphene Edges¹, NINGHAI SU, MIAO LIU, FENG LIU, Department of Materials Science and Engineering, University of Utah — Using molecular dynamics (MD) simulations, we have investigated the kinetics of the graphene edge folding process. The lower limit of the energy barrier is found to be ~ 380 meV/Å (or about 800 meV per edge atom) and ~ 50 meV/Å (or about 120 meV per edge atom) for folding the edges of intrinsic clean single-layer graphene (SLG) and double-layer graphene (DLG), respectively. However, the edge folding barriers can be substantially reduced by imbalanced chemical adsorption, such as of H atoms, on the two sides of graphene along the edges. Our studies indicate that thermal folding is not feasible at room temperature (RT) for clean SLG and DLG edges and is feasible at high temperature only for DLG edges, whereas chemical folding (with adsorbates) of both SLG and DLG edges can be spontaneous at RT. These findings suggest that the folded edge structures of suspended graphene observed in some experiments are possibly due to the presence of adsorbates at the edges.

¹This work was supported by DOE (#DE-FG02-03ER46027, DE-SC0001061); NSF-DMR (#0909212).

10:12AM V11.00010 Edge effects in Zigzag Graphene Nanoribbons¹, WEN YING RUAN, School of Physics, Georgia Institute of Technology, YIYANG SUN, SHENG BAI ZHANG, Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute, Troy, NY 12180, USA, MEI-YIN CHOU, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332, USA, and Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan — Analytical and numerical results based on the tight binding model are presented for zigzag graphene nanoribbons with z1 and z12₁₂ edges. We show the crucial importance of the symmetry of the two edges in determining the electronic structures of the system. Examples of significant band gap narrowings due to symmetry breaking are illustrated.

¹Supported by US DOE grant No. DEFG02-97ER45632 and DE-SC0002623.

10:24AM V11.00011 Mapping edge-state wavefunctions in chiral graphene nanoribbons, YEN-CHIA CHEN, DIMAS G. DE OTEYZA, XIAOWEI ZHANG, DAVID STRUBBE, Department of Physics, University of California at Berkeley, LIYING JIAO, Department of Chemistry and Laboratory for Advanced Materials, Stanford University, ALEX ZETTL, Department of Physics, University of California at Berkeley, HONGJIE DAI, Department of Chemistry and Laboratory for Advanced Materials, Stanford University, STEVEN G. LOUIE, MICHAEL F. CROMMIE, Department of Physics, University of California at Berkeley — The electronic behavior of graphene is readily tunable through nanoscale patterning. A particularly important structural motif is the nanoribbon (GNR), a narrow strip of graphene defined by its width, length, and edge properties. GNRs, due to quantum confinement and edge effects, have been predicted to exhibit many novel behaviors, such as tunable energy gaps and the presence of magnetic edge states. Here we report measurement of the local electronic structure of GNRs with highly ordered edges obtained by unzipping carbon nanotubes. Due to variation in the precursor nanotubes, this synthesis method generally produces single- or multi-layered nanoribbons with varying widths, lengths and chiralities. We have combined scanning tunneling microscopy (STM) and spectroscopy (STS) to simultaneously characterize the structural and electronic properties of these GNRs at the atomic scale. In particular, we observe 1D edge states that exhibit an energy gap that is dependent on nanoribbon width and the chirality. We have further spatially mapped patterns in the electronic local density of states associated with different GNR spectroscopic resonances. These patterns are compared with theoretical simulations.

10:36AM V11.00012 Effects of edge-potential on armchair graphene open boundary and nanoribbon, CHI-HSUAN CHIU, CHON-SAAR CHU, ElectroPhysice department, National Chiao Tung University, Taiwan — The physics for the edge state formation and gap opening at an armchair graphene open boundary and nanoribbon due to an edge potential are investigated. At an open boundary, the edge-potential U_0 is shown to turn on pseudospin-flipped (intravalley) scattering even though U_0 does not post an apparent breaking of the AB site (basis atoms) symmetry. The interference between the pseudospin conserving (intervalley) and nonconserving (intravalley) processes in the scattering state leads to a finite out-of-plane pseudospin density. Similar two-waves feature in the evanescent regime leads to the formation of the edge state. This physical origin of the edge state is different from that for the Tamm states in semiconductors. For an armchair graphene nanoribbon with gapless energy spectrum, applying U_0 to both edges opens up an energy gap. In addition, dispersive edge state can be found inside the energy gap for the bulk-like states. The U_0 -induced out-of-plane pseudospin density vanishes for the armchair graphene nanoribbon, but we expect it to be finite, for more general cases, at an armchair graphene open boundary.

10:48AM V11.00013 Formation of unconventional standing waves at graphene edges, CHANG-WON PARK, Department of Physics and Astronomy, Seoul National University, HEEJUN YANG, Graphene Research Center, Samsung Advanced Institute of Technology, Samsung Electronics, JISOON IHM, Department of Physics and Astronomy, Seoul National University, GUNN KIM, Department of Physics and Graphene Research Institute, Sejong University — The electron scattering properties of graphene edge have been investigated by the interference images using the scanning tunneling microscopy (STM). A conventional metal with a terrace and a step can be modeled as a two-dimensional electron gas with a hard wall and this behavior was directly observed at the steps of Au(111) and Cu(111) surfaces by STM. Now, a question arises as to how two sublattices and two inequivalent valleys in graphene affect the scattering and the standing wave formation. We present how the contributions from two valleys vary in the scattering at different graphene edges. For the zigzag edge, only intravalley scattering is possible due to the different edge-direction crystal momentum of two valleys. For the armchair edge, in contrast, the wave is reflected mostly via intervalley scattering and as a result, an atomic-scale nodalike pattern and beats in the standing wave are generated near the edge. When the incident angle is small, this intervalley scattering process is quite robust in the presence of defects so that we can still observe nodal patterns even for edges of relatively high defect densities.

Thursday, March 1, 2012 8:00AM - 11:00AM –
Session V12 DMP DCMP: Graphene: Optical Properties and Responses 210C

8:00AM V12.00001 Temperature dependence of hot carrier-assisted photoresponse in graphene, QIONG MA, NATHANIEL GABOR, NITYAN NAIR, Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Namiki 1-1, Tsukuba, Ibaraki 305-0044, Japan, PABLO JARILLO-HERRERO, Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA — We report on temperature dependent photocurrent measurements of high-quality dual-gated monolayer graphene p-n junction devices. Over temperatures ranging from 5 K to 300 K, we find that the photocurrent at the p-n interface peaks at an intermediate temperature, and decreases at higher and lower temperatures. Spatial photocurrent microscopy (at wavelength 850 nanometers) shows that the photocurrent measured as a function of distance away from the p-n interface also varies with temperature. We consider various electronic cooling processes in graphene to explain the photocurrent temperature dependence. Our measurements may reveal novel energy loss processes that reduce the electronic temperature of photoexcited charge carriers in graphene, and give additional insight into hot carrier photoresponse.

8:12AM V12.00002 Hot-Carrier cooling at Graphene-Metal Contact Interface¹, JASON ROSS, Department of Materials Science & Engineering, University of Washington, Seattle, GRANT AIVAZIAN, DONG SUN, AARON JONES, Department of Physics, University of Washington, Seattle, WANG YAO, Department of Physics and Center of Theoretical and Computational Physics, The University of Hong Kong, DAVID COBDEN, XIAODONG XU, Department of Physics, University of Washington, Seattle — There has been a recent surge of interest in using graphene as broadband and ultrafast optoelectronics, however the mechanisms of photodetection are not yet fully understood. Our previous measurements at a top gated graphene pn junction and at a monolayer-bilayer interface have found the dominating mechanism to be photothermoelectric (PTE) in nature, whereas most graphene-metal contact (GM) studies attribute photocurrent to the photovoltaic effect. By performing comprehensive ultrafast optical pump-probe measurements of photocurrent as a function of temperature, Fermi level, and laser power at various GM interfaces, the current work differentiates the contributions of PTE and photovoltaic effects to the photocurrent and identifies a hot-carrier relaxation time of ~ 2 ps at room temperature and ~ 7 ps at cryogenic temperatures. This work provides valuable insight to the design of new graphene based optoelectronic devices for sensing and communication.

¹We thank the support of DARPA YFA.

8:24AM V12.00003 Time Resolved Carrier Distributions in Graphene, STEVE GILBERTSON, GEORGI DAKOVSKI, TOMASZ DURAKIEWICZ, JIAN-XIN ZHU, KESHAV DANI, ADITYA MOHITE, ANDREW DATTELBAUM, GEORGE RODRIGUEZ, Los Alamos National Laboratory — Graphene, a recently discovered two-dimensional form of carbon, is a strong candidate for many future electronic devices. A question of central importance in optoelectronics, particularly high-speed applications, is how photoexcited carriers behave on ultrashort time scales. Even though time-resolved studies have provided a wealth of information, fundamental questions concerning the quantum descriptions of the transient electron-hole plasma remain. On one hand, conflicting views on the relaxation dynamics go as far as precluding the possibility of observing some predicted phenomena, such as THz lasing or tunable lasers while the observation of phenomena such as ultrafast photoluminescence and carrier multiplication are already established. Here, by employing the technique of time-resolved photoemission, we directly obtain the evolving Fermi-Dirac distributions of the electrons and holes: on an ultrashort 500 fs time scale the electron and hole populations can be described by two separate Fermi-Dirac distributions, while on longer time scales the populations coalesce to form a single Fermi-Dirac distribution at an elevated temperature. This unusual behavior is a consequence of graphene's unique band structure and has important implications for possible applications.

8:36AM V12.00004 Gate-tunable nanoplasmonic effects in single- and bi-layer graphene, ZHE FEI, GREGORY ANDREEV, University of California, San Diego, WENZHONG BAO, University of California, Riverside, ALEKSANDR RODIN, ALEXANDER MCLEOD, University of California, San Diego, LINGFENG ZHANG, Boston University, ZENG ZHAO, University of California, Riverside, GERARDO DOMINGUEZ, MARK THIEMENS, MICHAEL FOGLER, University of California, San Diego, ANTONIO CASTRO-NETO, National University of Singapore, CHUNNING LAU, University of California, Riverside, FRITZ KEILMANN, Max Plank Institute of Quantum Optics, DIMITRI BASOV, University of California, San Diego — We employed near-field infrared (IR) nanoscopy and nanoimaging to study mid-IR nanoplasmonic effects of both single-layer graphene (SLG) and bilayer graphene (BLG) on SiO₂/Si substrate. In our previous study, we found that SLG enhanced and blueshifted the surface phonon resonance of SiO₂ due to plasmon-phonon coupling [Z. Fei et al. Nano. Lett. 2011]. Here we report that both these effects are also observed in BLG. Using back-gate we were able to systematically change the carrier density in both SLG and BLG while monitoring the evolution of the hybrid plasmon-phonon resonance. New data are in accord with our point-dipole modeling results. IR imaging with nanoscale resolution revealed fringe patterns extending along the edges of both SLG and BLG. We ascribe these patterns to the interference of plasmon waves launched by the near-field probe with those reflected from the edges. Detailed analysis allowed us to observe gate-induced changes in the plasmon dispersion of both SLG and BLG, which are consistent with the notion of massless Dirac fermions in SLG and massive carriers in BLG.

8:48AM V12.00005 Atomically Localized Plasmon Enhancement in Monolayer Graphene, JUAN CARLOS IDROBO, Oak Ridge National Laboratory, WU ZHOU, JAEKWANG LEE, Vanderbilt University, JAGJIT NANDA, Oak Ridge National Laboratory, SOKRATES T. PANTELIDES, Vanderbilt University, STEPHEN J. PENNYCOOK, Oak Ridge National Laboratory — Graphene has attracted significant attention due to its exceptional properties and very promising applications, including optoelectronics and nanoplasmonics. All localized plasmon resonances observed so far in materials have been limited to the sub-10 nanometer scale, with a reported record of $\lambda/40$, where λ is the wavelength of the related plasmon excitation. In this talk, using aberration-corrected scanning transmission electron microscopy and total energy first-principles calculations, we show that single point defects can enhance the π and $\pi + \sigma$ plasmons of monolayer graphene at the atomic level. Our study shows that point defects in monolayer graphene represent a length scale smaller than $\lambda/200$, and suggest that the physical limit for the size of plasmonic and optoelectronic devices can be down to the single atom level. This research was supported by NSF grant No. DMR-0938330 (WZ, J-CI), DOE grant DE-F002-09ER46554 (STP), by the Shared Research Equipment (SHaRE) User Facility, Oak Ridge National Laboratory, which is sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences (J-CI), and by the Office of Basic Energy Sciences, Materials Sciences and Engineering Division, U.S. Department of Energy (JL, JN, SJP).

9:00AM V12.00006 Effect of nonhomogenous dielectric background on the plasmon modes in graphene double-layer structures¹, SAMVEL BADALYAN, PREDRAG KRSTAJIC, FRANCOIS PEETERS, Department of Physics, University of Antwerp, B-2020 Antwerpen, Belgium — We have calculated the plasmon modes in graphene double layer structures, taking into account the non-homogeneity of the system dielectric background. The effective dielectric function is obtained from the solution of the Poisson equation in three-layer dielectric medium with the graphene sheets located at the interfaces, separating different materials. Due to the momentum dispersion of the effective dielectric function, the intra- and inter-layer bare Coulomb interactions in graphene double layer systems acquire additional momentum dependence—an effect of the order of inter-layer interaction itself. It has been shown that in the long wavelength limit the energies of optical and acoustical plasmons, respectively, with the square root and linear dispersions are determined by different dielectric permittivities.

¹The work has been supported by the Flemish Science Foundation (FWO-VI), the Belgian Science Policy (IAP).

9:12AM V12.00007 Measurement of plasmon dispersion in graphene: tunable graphene plasmonics¹, BEN D. DAWSON, MIKE S. LODGE, Department of Physics and Nanoscience Technology Center, University of Central Florida, Orlando FL 32816, NIMA NADER ESFAHANI, R.E. PEALE, Department of Physics, University of Central Florida, Orlando FL 32816, M. ISHIGAMI, Department of Physics and Nanoscience Technology Center, University of Central Florida, Orlando FL 32816 — Graphene is an intriguing material for plasmonics. We have measured the transmission spectrum of large area graphene, grown using chemical vapor deposition, using Fourier transform infrared spectroscopy. By varying the Fermi level of graphene, we are able to explore the energy dispersion of plasmons in graphene. Our result lays the foundation for tunable plasmonic devices based on graphene.

¹This was supported by the Intelligence Community Postdoctoral Fellowship Program and by AFOSR grant FA95501010030, Program Manager Gernot Pomrenke.

9:24AM V12.00008 Scattering theory for graphene plasmons near edges and interfaces, ALEKSANDR RODIN, MICHAEL FOGLER, UCSD — Motivated by recent infrared nano-imaging experiments, we study eigenmodes of graphene plasmons near sample boundaries, corners, and interfaces. Such modes can be understood as standing-wave patterns formed by multiple scattering of elementary waves. We derive the rules of the corresponding scattering theory by analyzing the integro-differential equation for the plasmon dynamics. Our analytical results include the solution for the edge reflection problem in uniform graphene and a quasiclassical formalism for graphene of slowly varying density. Numerical simulations are employed for more complicated boundary geometries (wedge, constriction, etc.) and for singular density distributions that exist near the edge of a gated graphene.

9:36AM V12.00009 Edge Functionalization and Optical Excitations in Graphene Nanoflakes, CATERINA COCCHI, S3 CNR-Nano, IT and University of Modena, IT, DEBORAH PREZZI, S3 CNR-Nano, IT, ALICE RUINI, S3 CNR-Nano, IT and University of Modena, IT, MARILIA J. CALDAS, University of Sao Paulo, BR, ELISA MOLINARI, S3 CNR-Nano, IT and University of Modena, IT — We investigate the effects of edge covalent functionalization on the opto-electronic properties of finite elongated graphene nano-flakes (GNFs). Following our previous work on nanojunctions[1], we compute mean-field ground state electronic properties and configuration-interaction UV-vis optical excitations at varying size and functionalization by means of semi-empirical methods. The character of the lowest energy excitations and the influence exerted on them both by length/width modulation and by the specific chemical properties of the terminating groups are analyzed in details. The role of local distortions spontaneously arising upon geometrical optimization is inspected. Nanoplasmonic-like features related to the spectrum of these elongated finite graphene nanostructures are also discussed. [1] C. Cocchi et al. J. Phys. Chem. Lett. 2, 1315 (2011)

9:48AM V12.00010 Theory of double-resonant Raman spectra in graphene: intensity and line shape of defect-induced and two-phonon bands, PEDRO VENEZUELA, Universidade Federal Fluminense - Brazil, MICHELE LAZZERI, FRANCESCO MAURI, Université Pierre et Marie Curie - France — We calculate the double resonant Raman spectrum of graphene associated to both phonon-defect processes (such as the D and D' lines), and two-phonons ones (such as the $2D$, $2D'$ and $D + D''$ lines). For an excitation energy of 2.4 eV, the agreement with measurements is very good and calculations reproduce the relative intensities among phonon-defect or among two-phonon lines and the measured small widths of the D , D' , $2D$ and $2D'$ lines. We determine how the spectra depend on the excitation energy, on the light polarization, on the electronic linewidth, on the kind of defects and on their concentration. The intensity ratio between the D and D' lines depends on the kind of model defect, suggesting that this ratio could be used to identify actual defects. The present analysis reveals that, for both D and $2D$ lines, the dominant DR processes are those in which electrons and holes are both involved in the scattering. The most important phonons belong to the $\mathbf{K} \rightarrow \Gamma$ direction (*inner* phonons) and not to the $\mathbf{K} \rightarrow \mathbf{M}$ one (*outer* phonons), as usually assumed. The small $2D$ line width at $\epsilon_L = 2.4$ eV is a consequence of the interplay between the opposite trigonal warpings of the electron and phonon dispersions.

10:00AM V12.00011 A TD-DFT study on the Optical and dielectric properties of graphene nanoflakes, CARLOS RAMOS, EDUARDO CIFUENTES, ROMEO DE COSS, CINVESTAV Unidad Merida — Optical and dielectric properties of graphene nanostructures are of current interest because the potential applications in electronic and photonics devices. Recently, it has been reported important progress in the synthesis of graphene nanoflakes and their applications as quantum dots. In this work, the size and geometric shape effects on the optical spectrum and dielectric constant of graphene nanoflakes are studied by using an ab-initio approach. The calculations were performed using the Time-Dependent Density Functional Theory (TD-DFT) as implemented in the plane wave method and the results provide insights about controlling the optical properties of graphene using the size and shape of the nanostructure. This research was supported by Conacyt-México under Grant No. 83604.

10:12AM V12.00012 Two-photon absorption measurements in graphene fragments: Role of electron-electron interactions¹, A. SANDHU, Dept of Physics and OSC, Univ of Arizona, A. ROBERTS, OSC, Univ of Arizona, K. ARYANPOUR, Dept of Physics, Univ of Arizona, A. SHUKLA, Dept of Physics, IIT Bombay, S. MAZUMDAR, Dept of Physics, Univ of Arizona — Many-body interactions in graphene are an active field of research. There is a clear evidence of strong electron correlation effects in other carbon based materials which have the same sp^2 hybridization as graphene. For example, in linear-polyenes, the electron-electron interactions are considered responsible for the occurrence of lowest two-photon state below the optical one-photon state. The electronic correlation in these linear systems is a strong function of the chain length. Thus, it is pertinent to question if the two-dimensional graphene fragments also exhibit strong correlation effects and how these effects scale with fragment size. Using a white light super-continuum source, we perform z-scan measurements to extract frequency-dependent two-photon absorption coefficients in symmetric molecular fragments of graphene, e.g. coronene and hexabenzocoronene. A comparison of one-photon and two-photon absorption coefficients is then used to uncover the extent of correlation effects. In the smallest fragment, coronene, our results indicate a strong signature of the Coulomb interactions. We will discuss how the importance of electron-electron interaction varies with system size and its implication for the correlation effects in graphene.

¹Supported by the DoD SMART Fellowship.

10:24AM V12.00013 Pump-probe study of electron dynamics in bilayer graphene, LONG JU, TSUNG-TA TANG, FENG WANG, UC Berkeley, FENG WANG'S GROUP TEAM — Bilayer graphene exhibit many unusual physical properties, including a gate tunable electronic bandgap, and there is great interest in using it for novel electronic and optical devices. Understanding ultrafast dynamics in bilayer graphene is a prerequisite for many of its potential applications. We use ultrafast pump-probe spectroscopy to investigate such ultrafast electron relaxation behavior in bilayer graphene. In this talk, I will discuss the observed dynamic relaxations taking place in femto- and pico-second time scales..

10:36AM V12.00014 Theory of Two-Photon Absorptions in Graphene Fragments¹, K. ARYANPOUR, Dept of Physics, Univ of Arizona, A. SHUKLA, Dept of Physics, IIT Bombay, S. MAZUMDAR, Dept of Physics, Univ of Arizona, A. SANDHU, Dept of Physics and OSC, Univ of Arizona, A. ROBERTS, OSC, Univ of Arizona — Electron-electron correlations in graphene is currently an active field of research [1-3]. The carbon atoms in graphene have the same sp^2 hybridization as in strongly correlated π -conjugated polymer systems. The low energy behavior in graphene however appears to be reasonably described within the one-electron Dirac massless fermions model. Historically, the occurrence of the lowest two-photon state *below* the optical one-photon state provided the strongest proof for strong electron correlations in linear polyenes [4]. We systematically study the Coulomb interaction effects on the ground state and nonlinear absorptions in graphene fragments as a function of system size, beginning from the smallest stable fragment coronene. We report high order calculations of one- vs two-photon spin singlet and triplet states, in coronene, hexabenzocoronene and other molecular fragments that clearly indicate the strong role of electron-electron interactions. We will discuss the implications of our work on molecular systems for the thermodynamic limit of graphene.

[1] Siegel David A.; et al., PNAS, v108, 28, 11365-11369 (2011)

[2] Grönqvist J. H.; et al., arXiv: 1107.5653v1

[3] Uchoa B.; et al., arXiv: 1109.1577v1

[4] Ramasesha S.; et al., J. Chem. Phys. 80, 3278 (1984)

¹US NSF grant DMR-0705163 and the Univ of Arizona WEES program.

10:48AM V12.00015 Floquet Spectrum and Transport Through an Irradiated Graphene Ribbon¹, H.A. FERTIG, ZHENGHAO GU, Indiana University, DANIEL AROVAS, University of California, San Diego, ASSA AUERBACH, Technion — Graphene subject to a spatially uniform, circularly-polarized electric field supports a Floquet spectrum with properties akin to those of a topological insulator, including non-vanishing Chern numbers associated with bulk bands and current-carrying edge states. Transport properties of this system however are complicated by the non-equilibrium occupations of the Floquet states. We address this by considering transport in a two-terminal ribbon geometry for which the leads have well-defined chemical potentials, with an irradiated central scattering region. We demonstrate the presence of edge states, which for infinite mass boundary conditions may be associated with only one of the two valleys. At low frequencies, the bulk DC conductivity near zero energy is shown to be dominated by a series of states with very narrow anticrossings, leading to super-diffusive behavior. For very long ribbons, a ballistic regime emerges in which edge state transport dominates.

¹The authors thank the NSF and the Binational Science Foundation for financial support, and the Aspen Center for Physics where this work was initiated.

Thursday, March 1, 2012 8:00AM - 11:00AM –
Session V13 DMP GMAG: Focus Session: Magnetic Nanostructures-Domain Walls 211

8:00AM V13.00001 Domain-wall dynamics in ferromagnetic nanowires¹ , OLEG TRETIKOV, Texas A&M University — Current-induced domain-wall (DW) dynamics is studied in a thin ferromagnetic nanowire. We derive effective equations of motion describing the dynamics of the DW soft modes with or without topological defects. Because the DWs are topological objects with a rigid spin structure, these equations are rather universal. The DW rigidity makes the microscopic details irrelevant, and it allows us to solve the DW dynamics for a very general class of spin Hamiltonians. We show that the DW dynamics is described by simple equations with only four parameters. Based on these equations, we study DW dynamics in a ferromagnetic wire with Dzyaloshinskii-Moriya interaction (DMI). We find spin spiral DW structure and how the critical current required to move the domain wall depends on DMI. We also investigate the DW dynamics driven by time-dependent currents. We find the most efficient (with the lowest Ohmic losses) way to move the DWs by resonant current pulses. In addition, we propose a procedure to unambiguously determine the DW dynamics parameters by all-electric measurements of the time-dependent voltage induced by moving DW. Furthermore, based on the derived DW dynamics equations for the translationally non-invariant nanowires, we show how to make potential magnetic memory nanodevices much more energy efficient.

¹This work was supported by the NSF Grant No. 0757992 and Welch Foundation (A-1678).

8:36AM V13.00002 Reduction in critical current for domain wall injection by ion irradiation of perpendicular magnetic anisotropy nanowires , TIMOTHY PHUNG, IBM Almaden Research Center/Stanford University, LUC THOMAS, SEE-HUN YANG, CHARLES RETTNER, KWANG-SU RYU, JOHN BAGLIN, BRIAN HUGHES, STUART PARKIN, IBM Almaden Research Center — One of the key problems for realization of domain wall motion devices is the reliable and energy efficient injection of domain walls (DWs) into magnetic nanowires. In this work, we explore the injection of domain walls in perpendicular magnetic anisotropy nanowires (Co/Ni multilayers) which are locally softened by ion irradiation. We observe a minimum in the domain wall injection critical current, which occurs where the anisotropy of the irradiated region transitions from out of plane to in plane anisotropy. Furthermore, we find that the irradiated site acts as a pinning site for the DWs. At the irradiation site, we are able to create localized nanosecond long pulsed magnetic fields used to inject the DWs. By performing DC resistance measurements after each injection event, we are able to probe for the existence of the domain wall, and also find the strength of the ion irradiated pinning site. Using the above technique, we have demonstrated a five fold reduction in the domain wall injection current.

8:48AM V13.00003 360 Degree DW formation during vortex to vortex switching in thin ferromagnetic nanorings in an applied circular field¹ , YINENG SUN, ABBY GOLDMAN, ABIGAIL LICHT, YIHAN LI, NIHAR PRADHAN, Mount Holyoke College, MA, TIANYU YANG, MARK TUOMINEN, University of Massachusetts Amherst, MA, KATHERINE AIDALA , Mount Holyoke College, MA — We present simulations of the switching process between clockwise and counterclockwise vortex states in ferromagnetic nanorings in an applied circular field, relevant to potential data storage devices. This circular field can be experimentally generated by passing current through the solid metal tip of an atomic force microscope, which has achieved vortex-to-vortex switching in thicker asymmetric rings [1]. We find that in sufficiently thin rings, the vortex switching process occurs through the nucleation and annihilation of pairs of 360 degree domain walls (DW), with opposite topological indices. The DW with the same circulation as the vortex annihilates first. We can control which DW annihilates first by offsetting the center of our circular field to target a specific DW. Both exchange energy and demagnetization energy must be considered in predicting the energy barrier to DW annihilation. [1] T. Yang, N.R. Pradhan, A. Goldman, A.S. Licht, Y. Li, M. Kemei, M.T. Tuominen, K.E. Aidala. APL, 98, 242505 (2011).

¹NSF grant No. DMR-0906832, DMR-097201. NSF Center for Hierarchical Manufacturing (CMMI- 0531171). Simulations were performed with the facilities at the Center for Nanoscale Systems (CNS) (NSF award ECS-0335765)

9:00AM V13.00004 Individual domain wall manipulation in a local oersted circular field¹ , XIAOLIN HU, Mount Holyoke College, HUAJIE KE, NIHAR PRADHAN, University of Massachusetts, YINENG SUN, Mount Holyoke College, MARK TUOMINEN, University of Massachusetts, KATHERINE AIDALA, Mount Holyoke College — Understanding domain wall (DW) motion in nanoscale ferromagnetic structures reveals intriguing physics, with potential applications in nanoscale devices and DW data storage. One challenge is to create and move individual DWs in arbitrary locations. We developed a technique to generate localized circular magnetic field by applying a current through the tip of the atomic force microscope (AFM) and thereby manipulating the state of ferromagnetic rings [1]. Now we extend our ability to control domain walls in various structures, such as straight wires with notches and zigzag wires. By placing the tip near a 180 DW in a vertex of a zigzag wire, we can move the 180 DW along the wire and form a stable 360 DW in nearby vertex. We can also move 360 DWs with the local magnetic field around the AFM tip. We will discuss simulations and experimental implementations.

[1] T. Yang, N. R. Pradhan, A. Goldman, A. Licht, Y. Li, M. T. Tuominen and K. E. Aidala, Applied Physics Letter, http://apl.aip.org/resource/1/applab/v98/i24/p242505_s1 98, 242505, (2011)

¹NSF grant No. DMR-0906832, DMR-097201, DMR-097201, NSF Center for Hierarchical Manufacturing (CMMI- 0531171). Simulations were performed with the facilities at the Center for Nanoscale Systems (CNS) (NSF award ECS-0335765).

9:12AM V13.00005 Probing and manipulating magnetization at the nanoscale , NITIN SAMARTH, Dept. of Physics, Penn State University, University Park PA 16802 — Combining semiconductors with magnetism in hetero- and nano-structured geometries provides a powerful means of exploring the interplay between spin-dependent transport and nanoscale magnetism. We describe two recent studies in this context. First, we use spin-dependent transport in ferromagnetic semiconductor thin films to provide a new window into nanoscale magnetism [1]: here, we exploit the large anomalous Hall effect in a ferromagnetic semiconductor as a nanoscale probe of the reversible elastic behavior of magnetic domain walls and gain insight into regimes of domain wall behavior inaccessible to more conventional optical techniques. Next, we describe novel ways to create self-assembled hybrid semiconductor/ferromagnet core-shell nanowires [2] and show how magnetoresistance measurements in single nanowires, coupled with micromagnetic simulations, can provide detailed insights into the magnetization reversal process in nanoscale ferromagnets [3]. The work described here was carried out in collaboration with Andrew Balk, Jing Liang, Nicholas Deltas, Mark Nowakowski, David Rench, Mark Wilson, Roman Engel-Herbert, Suzanne Mohny, Peter Schiffer and David Awschalom. This work is supported by ONR, NSF and the NSF-MRSEC program.

[1] A. L. Balk et al., Phys. Rev.Lett. **107**, 077205 (2011).

[2] N. J. Deltas et al., Appl. Phys. Lett. **97**, 072505 (2010).

[3] J. Liang *et al.*, in preparation.

9:48AM V13.00006 Beyond a compact magnetic domain wall, PHILIPP EIB, CARL ZINONI, ANTOINE VAN-HAVERBEKE, GIAN SALIS, RETO SCHLITTLER, ANDREAS BISCHOF, ROLF ALLENSPACH, IBM Research - Zurich, Säumerstr. 4, CH-8803 Rüschlikon, Switzerland — The generally accepted concept that limits magnetic domain wall velocity is the Walker breakdown. This is the magnetic field at which wall motion becomes oscillatory capping the performance of domain wall-based spintronic devices. To understand the limiting mechanisms, we study vortex walls in $\text{Ni}_{80}\text{Fe}_{20}$ wires with widths between 300 and 900 nm. We detect the walls by time-resolved magneto-optical Kerr effect in a pump-probe technique setup. The wires are fabricated by electron-beam lithography and by a nanostencil tool [1]. We find the dynamics of vortex walls to depart significantly from the current description of a compact entity evolving along the wire. Instead, the wall is composed of several substructures propagating in different dynamic regimes with very different velocities. Wire edges crucially affect this dynamics and can be influenced by variation of growth parameters. Extensive, parallelized micromagnetic simulations reveal the unusual wall structure and complement the experimental findings [2]. Possibilities how to overcome the limits imposed by the Walker breakdown will be discussed.

[1] L. Gross *et al.*, *Nanotechnology* **21**, 325301 (2010)

[2] C. Zinoni *et al.*, *Phys. Rev. Lett.* **107**, 207204 (2011)

10:00AM V13.00007 Domain walls in ultrathin magnetic nanowires at finite temperatures, THOMAS MICHAELS, ALESSANDRO VINDIGNI, DANILO PESCIA, Laboratory for Solid State Physics, ETH Zurich, Switzerland — The possibility of inducing domain-wall (DW) motion in magnetic nanowires by means of electric currents has recently renewed theoretical interest in this field. The problem is usually modelled on a micromagnetic approach, but ignoring thermal fluctuations. However, some relevant experimental facts - like the correct order of magnitude of the critical current needed for DW motion - still lack satisfactory explanations. We thus developed a one-dimensional stochastic model for DW dynamics, which allowed us to take into account both thermal fluctuations and external drifts (magnetic field and electric spin-polarized current) simultaneously. We also provided a general theoretical framework, which highlights the crucial role played by thermal fluctuations at the centre of DWs. The latter, for example, qualitatively accounts for the shrinking of magnetic domains observed in Fe films on Cu(001) with increasing temperature and the renormalisation of the critical current for DW motion in magnetic nanowires at finite temperatures.

10:12AM V13.00008 Antiferromagnetic Domain Wall Engineering in Chromium Films, JONATHAN LOGAN, HYEKYUNG KIM, University of Chicago, ERIC ISAACS, Argonne National Laboratory, OLEG SHPYRKO, University of California, San Diego, DANIEL ROSENMAN, Center for Nanoscale Materials, Argonne National Laboratory, ZHONGHOU CAI, Advanced Photon Source, Argonne National Laboratory, RALU DIVAN, Center for Nanoscale Materials, Argonne National Laboratory — We have engineered an antiferromagnetic domain wall by utilizing a magnetic frustration effect of a thin iron cap layer deposited on a chromium film. Through lithography and wet etching we selectively removed areas of the Fe cap layer to form a patterned ferromagnetic mask over the Cr film. Removing the Fe locally removes magnetic frustration in user-defined regions of the Cr film. We present x-ray microdiffraction results confirming the formation of an antiferromagnetic spin-density wave propagation domain wall in Cr. This domain wall nucleates at the boundary defined by our Fe mask. We have characterized the region surrounding the domain wall using x-ray microdiffraction and microfluorescence with a resolution of 1 micron.

10:24AM V13.00009 Formation and structure of 360 and 540 degree domain walls in thin magnetic stripes¹, MARK MASCARO, YOUNGMAN JANG², Massachusetts Institute of Technology, S.R. BOWDEN, J. UNGURIS, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, C.A. ROSS, Massachusetts Institute of Technology — A method is presented for forming a 360° domain wall (DW) and more complex structures such as a 540° DW in a wire attached to an injection pad by applying an alternating in-plane field perpendicular to the wire. SEMPA, MFM measurements and OOMMF micromagnetic simulations give a consistent picture of the magnetic structure and stray field distribution of the 360° DW. Equilibrium 360° DWs in wires have a well-defined structure and size, persist over a wide field range, and can be distinguished from configurations consisting of two 180° DWs pinned near each other. The formation and stability of these complex walls has implications in memory and logic devices based on field- or current-induced DW motion, where impingement of adjacent 180° DWs can produce composite DWs whose behavior and stray field distribution differ significantly from that of a 180° DW, and these structures could also be used to examine intriguing resonant behavior as predicted by modeling. [*Phys. Rev. B* **82**, 214411; *Phys. Rev. B* **82**, 134411]

¹Support of the National Science Foundation and the INDEX Center is gratefully acknowledged.

²Present address: Samsung Advanced Institute of Technology (SAIT), Gyeonggi-Do 446-712, Republic of Korea

10:36AM V13.00010 Polarization Dependent Switching of Asymmetric Nanorings with a Circular field¹, NIHAR PRADHAN, Mount Holyoke College and UMass Amherst, MARK TUOMINEN, UMass Amherst, MA 01003, KATHERINE AIDALA, Mount Holyoke College, South Hadley, MA 01075 — We present experimental switching from the onion to vortex states in asymmetric cobalt nanorings in an applied circular field. We initialize the onion state in two polarizations, along the symmetric or asymmetric axes. We apply a circular field by passing current through a solid metal AFM tip positioned at the center of the ring [1]. The asymmetry of the ring leads to different switching fields depending on the location of the domain walls (DWs) and direction of applied field. For polarization along the asymmetric axis, the field required to move the DWs to the narrow side of the ring is smaller than moving the DWs to the larger side of the ring. The direction of the DW motion is controlled by the circular field. When polarizing the ring along the symmetric axis, establishing one DW in the narrow side and one on the wide side, the field required to switch to the vortex state is an intermediate value. We will be presenting detail of the switching field of cobalt nanoring by circular field with two different direction of polarization.

(1) T. Yang, N. R. Pradhan, A. Goldman, A. Licht, Y. Li, M. T. Tuominen and K. E. Aidala, *Applied Physics Letter*, **98**, 242505, (2011)

¹This work was supported by NSF grants No. DMR- 0906832 and DMR-097201, the Research Corporation for Science Advancement grant No. 7889, and the NSF Center for Hierarchical Manufacturing at the University of Massachusetts, Amherst (CMMI-0531171)

10:48AM V13.00011 Non-volatile electric field tuning of magnetic domains in permalloy thin films coupled to ferroelastic PZT bilayers¹, ICHIRO TAKEUCHI, ANBUSATHAIAH VARATHARAJAN, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20424, SAMUEL BOWDEN, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA, SEAN FACKLER, TIEREN GAO, PARIS ALEXANDER, JOHN CUMINGS, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20424, DAN PIERCE, JOHN UNGURIS, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA, UNIVERSITY OF MARYLAND TEAM, NIST COLLABORATION — We are investigating electric field controlled magnetic domain motion in Py films on $\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$ (PZT) bilayers. Previously, we have shown that bilayered heterostructures consisting of a tetragonal $\text{PbZr}_{0.3}\text{Ti}_{0.7}\text{O}_3$ film (70 nm) above a rhombohedral $\text{PbZr}_{0.7}\text{Ti}_{0.3}\text{O}_3$ film (70 nm) display large ferroelastic domains in tetragonal PZT layer. The reversible non-volatile ferroelastic domain wall motion in this layer can serve as a basis for inducing controlled strain on magnetic thin films. This results in different ferroelastic domain configurations in the tetragonal PZT layer. This in turn leads to changes in magnetic domains of Py film. We find that a Py film on the ferroelastic PZT layer exhibits sharp magnetic domain patterns usually associated with out-of-plane magnetization by MFM. SEMPA imaging reveals that the magnetic domains are indeed in-plane magnetized as expected for Py films. OOMMF analysis indicates presence of unusual metastable in-plane anisotropy modulation in the Py film.

¹This work is supported by NSF MRSEC.

Thursday, March 1, 2012 8:00AM - 11:00AM —

Session V14 DMP GMAG: Focus Session: Spins in Carbon - Spins and Magnetism in Carbon

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8:00AM V14.00001 Inducing Magnetization by Flexing Graphene Nanoribbon, RENAT SABIRIANOV, NABIL AL-AQTASH, University of Nebraska at Omaha — Zigzag graphene nanoribbons (ZGNRs) are antiferromagnetic in the ground state with zero net magnetization due to the compensation of contributions from opposite edges. The uniform deformations (both shear and axial) do not produce magnetization due to the symmetry restrictions. However, we report the results of first-principles calculations that predict that the induction of net magnetization in the graphene nanoribbon upon non-uniform strain applied to the nanoribbon. Using density functional theory (DFT) method implemented in SIESTA code, we show that the bending or twisting of nanoribbon produces magnetization because in the presence of strain gradient the induced magnetization on opposite edges are not compensating each other. We estimate an average magnetization of $\sim 3.3\mu_B$ that produced from the bending of nanoribbon with the sinusoidal profile $\delta x = A \sin(2\pi z/L)$ with $A = 3\text{\AA}$ and $L = 87.4\text{\AA}$ ($z = 0..L/2$, i.e. the half of the period). Our study suggests that the induced magnetization can be used for the control of magnetic structure in graphene including the trap of the domain walls.

8:12AM V14.00002 Numerical studies of the magnetism in graphene nanoribbons and graphene dot, TIANXING MA, Department of Physics, Beijing Normal University, Beijing 100875, China, ZHONGBING HUANG, Faculty of Physics and Electronic Technology, Hubei University, Wuhan 430062, China, HAI-QING LIN, Beijing Computational Science Research Center, Beijing 100084, China — Within determinant quantum Monte Carlo simulation, the magnetic properties of graphene nanoribbons and graphene dot are studied. It is predicted that the armchair graphene nanoribbons show carrier mediated ferromagnetism as electron filling is lower than 0.8. The uniform magnetic susceptibility increase as the width of nanoribbons decrease, and it increases greatly as the next-nearest-neighbor hopping energy increases. It is also shown that strain may induce magnetism in doped square graphene dot having zigzag edge. The resultant ferromagnetism in graphene-based system may facilitate the development of spintronics.

8:24AM V14.00003 g-Tensor control in a bent carbon nanotube quantum dot, RUBY LAI, HUGH CHURCHILL, CHARLES MARCUS, Harvard University — We report low-temperature transport measurements of a carbon nanotube quantum dot containing a bend along its length. The bend occurred naturally in CVD growth, with a bend angle of 140 degrees and a radius of curvature of $\sim 1\mu\text{m}$. The device was contacted across the bend, with a global back gate and a top gate proximal to one arm of the bend. We measured the magnetic field angle dependence of conductance, tunneling rates, and bandgap in a 3-axis vector magnetic field. We characterize key signatures of carbon nanotube bends in the Kondo regime, comparing these dependencies in perpendicular and in-plane magnetic fields. We also demonstrate control of the electron spin g-tensor using gate voltages. Support from IBM, NSF-MWN, NSF-NRI through the INDEX Center, and Harvard University is acknowledged.

8:36AM V14.00004 Magnetic impurities and Kondo conductance anomalies in nanotubes: the importance of being “in”¹, ERIO TOSATTI, SISSA and ICTP, Trieste, PIERPAOLO BARUSELLI, SISSA Trieste, MICHELE FABRIZIO, SISSA and ICTP, Trieste — Transition metal impurities should yield zero bias anomalies in the conductance of well contacted metallic carbon nanotubes, but relevant temperatures and lineshapes cannot be anticipated without accurate ab initio calculations. Applying the density functional plus numerical renormalization group approach of Lucignano et al [1] to Co and Fe impurities in (4,4) and (8,8) nanotubes, we discover a huge difference of behaviour between outside versus inside impurity adsorption. The predicted Kondo temperatures and zero bias anomalies, tiny when the impurity is outside the nanotube [2] turn large and strongly radius dependent inside, owing to a change of symmetry of the magnetic orbital. These results foreshadow interesting field and temperature dependent nanotube electrical transport, to be addressed in future experiments.

[1] P. Lucignano, et al., Nature Materials 8, 563 (2009).

[2] P. Baruselli, et al., Physica E (2011) doi:10.1016/j.physe.2011.05.005

¹Research sponsored by PRIN/COFIN contract 20087NX9Y7.

8:48AM V14.00005 Spin-orbit coupling and electronic transport in carbon nanotubes in external fields¹, GINETOM DINIZ, S. E. ULLOA, Ohio University — We have investigated theoretically the role of spin-orbit coupling (SOC) on the conductance response of carbon nanotubes (CNT) in the presence of external electric and magnetic fields. We use an equilibrium Green's function formalism to calculate the spin resolved conductance by using a four-orbital orthogonal tight-binding representation in real space, taking into account curvature effects that induce orbital hybridization and are responsible for sizable SOC enhancements [1]. Different directions of external magnetic and electric fields (transverse and longitudinal to the CNTs), as well as length and chirality of the CNT, are shown to strongly affect the transport behavior of the systems. In particular, this results in stronger SOC effects for tubes with smaller radii. The interplay of electric and magnetic fields on the possible spin polarization of conductance will be discussed, as the sizable SOC effects result in effective control of the spin selective transport in these versatile nanoelectronic devices.

[1] J. Klinovaja et al. PRL 106, 156809 (2011).

¹Supported by CAPES-Fulbright, NSF-PIRE and NSF-MWN/CIAM

9:00AM V14.00006 Spin-orbit induced strong coupling of a single spin to a nanomechanical resonator, PHILIPP STRUCK, University of Konstanz, ANDRAS PALYI, Eotvos University, Budapest, MARK RUDNER, Harvard University, Cambridge, KARSTEN FLENSBERG, Niels Bohr Institute, University of Copenhagen, GUIDO BURKARD, University of Konstanz — We theoretically investigate the coupling of an electron spin to vibrational motion due to curvature-induced spin-orbit coupling in suspended carbon nanotube quantum dots. Our estimates indicate that, with current capabilities, a quantum dot with an odd number of electrons can serve as a realization of the Jaynes-Cummings model of quantum electrodynamics in the strong-coupling regime. A quantized flexural mode of the suspended tube plays the role of the optical mode and we identify two distinct two-level subspaces, at small and large magnetic field, which can be used as qubits in this setup. The strong intrinsic spin-mechanical coupling allows for detection, as well as manipulation of the spin qubit, and may yield enhanced performance of nanotubes in sensing applications.

9:12AM V14.00007 Distinctive Magneto Conductance and Universal Scaling in One Dimensional Polymer Nanofibers, AJEONG CHOI, KYUNG HO KIM, SUNG JU HONG, Seoul National University, MUNJU GOH, KAZUO AKAGI, Kyoto University, RICHARD B. KANER, UCLA, YUNG WOO PARK, Seoul National University — The conducting polymers are one dimensional organic hydrocarbon systems where the non-linear local excitations such as solitons, polarons and bipolarons were predicted based on the electron-phonon interactions. The local excitations have different spin-charge relations in different kinds of polymers. In this work, the magneto conductance (MC) of polymer nanofibers is investigated in high magnetic field at low temperature to understand both spin (magneto) and charge (conductance) of the charge carriers simultaneously. We discovered the distinctive zero MC in polyacetylene nanofibers while the finite MC in polyaniline and polythiophene nanofibers. On the other hand, the charge transports of polymer nanofibers as a function of temperature and bias are observed to be scaled onto the universal curve. We conclude that the universal scaling and the zero MC (the finite MC) in polyacetylene (polyaniline and polythiophene) nanofibers are from the interacting spinless charged solitons (interacting polarons which have both spin and charge).

9:24AM V14.00008 Magneto-Photoinduced Absorption in Organic Polymer Films, BHOJ GAUTAM, THO NGUYEN, Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112, EITAN EHRENFREUND, Physics Department, Technion-Israel Institute of Technology, Haifa, Israel, Z. VALY VARDENY, Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112 — In order to elucidate the underlying mechanism of magneto-conductivity (MC) in OLEDs we studied magneto-photoinduced absorption (MPA) response in polymer films. The films were based on the MEH-PPV polymer in three different forms, namely: pristine film; film exposed to prolonged UV illumination; and MEH-PPV/PCBM blend having weight ratio 1:1. In pristine film we show that the MPA at low excitation intensity is due to sublevel spin mixing of triplet excitons; whereas at high excitation intensity the MPA is dominated by the triplet-triplet annihilation process. In UV illuminated MEH-PPV films that support photogenerated polarons we show that the MPA is due to sublevel spin-mixing of polaron-pairs via the hyperfine interaction with the closest hydrogen atoms to the chain. This mechanism also explains the MC response of OLED based on MEH-PPV, since its response is similar to that of MPA. Finally we found that the MPA in MEH-PPV/PCBM blend films is dominated by spin mixing of polaron-pair on the polymer and fullerene molecules, via the Δg mechanism. Supported by the NSF DMR-1104495, the NSF MRSEC at the UoU, and the BSF program.

9:36AM V14.00009 Tunnel magnetoresistance in Self-Assembled Monolayers Based Tunnel Junctions, RICHARD MATTANA, CLÉMENT BARRAUD, SERGIO TATAY, MARTA GALBIATI, PIERRE SENEOR, KARIM BOUZEHOUE, ERIC JACQUET, CYRILE DERANLOT, ALBERT FERT, FRÉDÉRIC PETROFF, Unité Mixte de Physique CNRS/Thales — Organic/molecular spintronics is a rising research field at the frontier between spintronics and organic chemistry. Organic molecule and semiconductors were first seen as promising for spintronics devices due to their expected long spin lifetime. But an exciting challenge has also been to find opportunities arising from chemistry to develop new spintronics functionalities. It was shown that the molecular structure and the ferromagnetic metal/molecule hybridization can strongly influence interfacial spin properties going from spin polarization enhancement to its sign control in spintronics devices. In this scenario, while scarcely studied, self-assembled monolayers (SAMs) are expected to become perfect toy barriers to further test these tailoring properties in molecular magnetic tunnel junctions (MTJs). Due to its very high spin polarization and air stability LSMO has positioned itself as the electrode of choice in most of the organic spintronics devices. We will present a missing building block for molecular spintronics tailoring: the grafting and film characterization of organic monofunctionalized long alkane chains over LSMO. We have obtained 35% of magnetoresistance in LSMO/SAMs/Co MTJs. We will discuss the unusual behaviour of the bias voltage dependence of the TMR.

9:48AM V14.00010 Electrical spin injection from an organic-based ferrimagnet in a hybrid organic/inorganic heterostructure¹, EZEKIEL JOHNSTON-HALPERIN, Department of Physics, The Ohio State University — The development of organic-based magnets with room temperature magnetic ordering and semiconducting functionality promises to broaden the field of semiconductor spintronics, providing a route to all-organic spintronic devices and hybrid organic/inorganic structures capable of exploiting the multifunctionality and ease of production in organic systems as well as the well established spintronic functionality of inorganic materials. Our work demonstrates the successful extraction of spin polarized current from the organic-based room temperature ferrimagnetic semiconductor $V[TCNE]_x$ ($x \sim 2$, TCNE: tetracyanoethylene; $T_C > 400$ K, $E_G \sim 0.5$ eV, $\sigma \sim 10^{-2}$ S/cm) and its subsequent injection into a GaAs/AlGaAs light-emitting diode (LED) [1]. The spin current is detected by monitoring the polarization state of the photons emitted from the LED structure and tracks the magnetization of $V[TCNE]_{x \sim 2}$, is weakly temperature dependent, and exhibits heavy hole / light hole asymmetry. This result opens the door to a new class of active, hybrid spintronic devices with multifunctional behavior defined by the optical, electronic and chemical sensitivity of the organic layer. In addition, spin transport in these hybrid structures provides the opportunity to leverage well-characterized inorganic materials as a probe of spin physics in organic and molecular systems and to explore the impact of the hybrid interface on spin injection efficiency. Initial studies exploring the impact of surface passivation of the inorganic layer with self-assembled monolayers of various chemistries will be presented, and additional experimental probes of the interfacial exchange interaction will be discussed.

[1] "Electrical Spin Injection from an Organic-Based Ferrimagnet in a Hybrid Organic-Inorganic Heterostructure," Lei Fang, K. Deniz Bozdog, Chia-Yi Chen, P.A. Truitt, A.J. Epstein and E. Johnston-Halperin, *Phys. Rev. Lett.* **106**, 156602 (2011).

¹Funding for this research was provided by the Center for Emergent Materials at the Ohio State University, a NSF MRSEC (Award Number DMR-0820414).

10:24AM V14.00011 The effect on the properties of V(TCNE) grown on bare substrates and self assembled monolayers, MEGAN HARBERTS, HOWARD YU, MARK GUSEMAN, Department of Physics, The Ohio State University, YU LU, Department of Chemistry, The Ohio State University, EZEKIAL JOHNSTON-HALPERIN, Department of Physics, The Ohio State University, ARTHUR EPSTEIN, Departments of Chemistry and Physics, The Ohio State University — V(TCNE) is a room temperature T_C larger than 400K organic based magnetic semiconductor. It has been shown that this fully-spin polarized material can be used as a spin injector in hybrid organic inorganic spin-light emitting diode (spin-LED) as well as hybrid and all organic spin valves [1,2]. Attempts to improve the spin signal from a spin LED device are focusing on surface passivation of the III-V heterostructure surface by including a self-assembled monolayer (SAM). We present a comparison of the properties of V(TCNE) grown by chemical vapor deposition (CVD) on various SAM's and bare substrates. We find that the successful growth of uniform, thin films of CVD V(TCNE) requires careful purification of the SAM precursors. We observe bulk magnetic properties of V(TCNE) grown on SAM's to be consistent with or better than films grown on bare substrates. Therefore the presence of the SAM does not appear to adversely affect the desired properties of the V(TCNE) for use as a spin injector, dramatically expanding the range of potential hybrid device geometries.

[1] L. Fang, *Phys Rev Lett*, **106** (15), (2011).

[2] J. W. Yoo, *Nat Mater*, **9** (2010).

10:36AM V14.00012 Spin multiplicity and symmetry breaking in vanadium-benzene complexes¹, IVAN STICH, LUCIA HORVATHOVA, MATUS DUBECKY, Institute of Physics, Slovak Academy of Sciences, LUBOS MITAS, Dept. of Physics, North Carolina State University — Despite use of vanadium-benzene complexes in spintronics applications [1], reliable theoretical and experimental knowledge of energetics, dissociation energy, spin multiplicity, etc. of these systems is missing. Fixed-node DMC calculations have been done with the quest to elucidate electronic and atomic structure of vanadium-benzene half-sandwiches. At variance with DFT results which favor either low- or high-spin state, depending on the functional used [2], DMC predicts degenerate energies for spin multiplicities 2, 4, and 6, irrespective of DFT functional used to fix the nodal hypersurfaces. Ultimately, we predict high-spin ground-state, based on comparison of experimental/theory ionization energy [3]. Based again on DMC, we predict vastly different gaps for spin-up/-down electrons. The DMC results indicate that both DFT [2] as well as experimental results [4] may be biased. [1] V. V. Maslyuk *et al.*, Phys. Rev. Lett. **97**, 097201 (2006) [2] R. Pandey, B. K. Rao, P. Jena, M. A. Blanco, J. Am. Chem. Soc. **123**, 3799 (2001) [3] T. Kurikawa, *et al.*, Organometallics **18**, 1430 (1999). [4] R. L. Hettich, T. C. Jackson, E. M. Stanko, B. S. Freiser, J. Am. Chem. Soc. **108**, 5086 (1986).

¹Financial support from APVV projects APVV-0091-07, LPP-0392-09 is acknowledged. This research was supported in part also by ERDF OP R&D, Project CE meta-QUTE ITMS 26240120022, and via CE SAS QUTE.

10:48AM V14.00013 Total Scattering Study of Vanadium Tetracyanoethylene, D.M. PAJEROWSKI, NIST Center for Neutron Research, National Institute of Standards and Technology, J.L. ARTHUR, Dept. Chem., Univ. Utah, K. PAGE, LANSCE, Los Alamos National Laboratory, J.S. MILLER, Dept. Chem., Univ. Utah, J.W. LYNN, NIST Center for Neutron Research, National Institute of Standards and Technology — Vanadium tetracyanoethylene powder prepared in deuterated dichloromethane (henceforth V-TCNE) was studied using neutron and X-ray diffraction. V-TCNE is a molecule-based magnet that has been shown to display magnetic order above room temperature¹ as well as photocontrol of magnetism at cryogenic temperatures.² To date, all reported synthesis preparations of V-TCNE yield amorphous compounds that lack Bragg peaks in diffractograms. In the absence of long range structural order, diffraction experiments may still elucidate short range structural order. The experimental results, which display short range correlations, will be presented and compared to Monte Carlo simulations.

¹J.M. Manriquez, G.T. Yee, R.S. McLean, A.J. Epstein, and J.S. Miller, Science **252**, 1415-1417 (1991).

²J.-W. Yoo, R.S. Edelstein, D.M. Lincoln, N.P. Raju, and A.J. Epstein, Phys. Rev. Lett. **99** 157205 (2007).

Thursday, March 1, 2012 8:00AM - 11:00AM — Session V16 DCMP: Heavy Fermions- 1-1-5 Systems and Others 251

8:00AM V16.00001 Fermi surface of Ce₂RhIn₈ studied by angle-resolved photoemission spectroscopy¹, RUI JIANG, R.S. DHAKA, CHANG LIU, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa, 50011, USA, C. PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY, 11973, USA, ADAM KAMINSKI, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa, 50011, USA — The superconductivity in heavy fermion compounds is one of most interesting, outstanding problems in condensed matter physics. In this family of materials, Ce₂RhIn₈ and related compounds is unique because its electronic properties are believed to be quasi 2D. Here, we use angle-resolved photoemission spectroscopy to measure its electronic properties. The lack of significant *k_z* dispersion confirms the quasi two dimensionality of the electronic structure. Fermi surface is quite complicated and consists of several hole and electron sheets. There are several extended segments of the Fermi surface which are likely nested. This provides clues to understanding of their unusual transport and thermodynamical properties.

¹The Ames Laboratory is operated for the US Department of Energy, Basic Energy Sciences, by Iowa State University under contract no. DE-AC02-07CH11358.

8:12AM V16.00002 Anomalous superfluid response in the layered heavy fermion compound Ce₂PdIn₈ near a magnetic quantum critical point, KENICHIRO HASHIMOTO, YUTA MIZUKAMI, RYO KATSUMATA, MINORU YAMASHITA, HIROAKI IKEDA, TAKASADA SHIBAUCHI, YUJI MATSUDA, Department of Physics, Kyoto University, DANIEL GNIDA, DARIUSZ KACZOROWSKI, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, ANTONY CARRINGTON, H. H. Wills Physics Laboratory, University of Bristol — The recently discovered layered heavy fermion superconductor Ce₂PdIn₈ (*T_c* = 0.7 K) has attracted a great interest because of the appearance of unconventional superconductivity near a quantum critical point. Here we report high-precision measurements of magnetic penetration depth λ down to 60 mK ($\sim 0.1T_c/T_c$) by using a tunnel diode oscillator operating at ~ 13 MHz. A strong power-law temperature dependence of λ demonstrates low-energy excitations of quasiparticles, which is consistent with recent thermal conductivity measurements indicative of nodal superconductivity. The observed $T^{1.5}$ behavior at low temperatures, which is commonly seen in superconductors with line nodes near a magnetic quantum critical point such as CeCoIn₅ or organics, can be attributed to the enhancement of effective mass towards zero temperature due to quantum magnetic fluctuations even in the superconducting state.

8:24AM V16.00003 Magnetism in 2D Heavy Fermion Superconductor CePt₂In₇, NICHOLAS APROBERTS-WARREN, JOHN CROCKER, ADAM DIOGUARDI, PETER KLAIVINS, CHING LIN, KENT SHIRER, ABIGAIL SHOCKLEY, NICHOLAS CURRO, University of California at Davis — CePt₂In₇ was first synthesized in 2008, and it was discovered to be a superconductor under pressure shortly thereafter in 2009. It is closely related to the well-studied crystal class CeMIn₅ (*M* = Ir, Co, Rh), but CePt₂In₇ is considerably more anisotropic with a *c/a* ratio more than twice as large as the 115's. We present here nuclear quadrupole resonance results for the ¹¹⁵In nucleus, and follow it from the paramagnetic heavy fermion state into the anti-ferromagnetic state below *T_N* = 5.2 K. The NQR data will show a rich magnetic phase diagram, with a commensurate magnetic order parameter directly below *T_N*, and more complex magnetic states emerging as the material is further cooled. Additionally, we will present some additional results on how hydrostatic pressure affects the magnetic order in CePt₂In₇.

8:36AM V16.00004 Electric transport measurements on micro-structured CePt₂In₇ single crystals in a diamond anvil cell, J. KANTER, P. MOLL, Laboratory for Solid State Physics, ETH Zurich, Switzerland, F. RONNING, E. BAUER, P. TOBASH, J. THOMPSON, Los Alamos National Laboratory, Los Alamos, New Mexico, USA, B. BATLOGG, Laboratory for Solid State Physics, ETH Zurich, Switzerland — We report Shubnikov-de Haas and resistivity measurements of CePt₂In₇ samples under hydrostatic pressures using a diamond anvil cell. CePt₂In₇ belongs to the *C_{em}M_nIn_{3m+2n}* heavy fermion family. Compared to the CeMIn₅ members of this group, the structure of CePt₂In₇ has a more two dimensional character, but also exhibits an antiferromagnetically ordered and a superconducting phase. Upon increasing pressure the AFM order is suppressed with the Néel temperature extrapolating to a quantum critical point. The fluctuations associated with the QCP are thought to stabilize the unconventional superconducting phase. To investigate the weight of the different scattering channels the anisotropy of the resistivity above the Néel temperature was measured for various applied pressures. Shubnikov-de Haas measurements were conducted to deduce the changes in the effective electron masses in the AFM and superconducting phases under applied hydrostatic pressure. To this end we developed a method to conduct four terminal resistance measurements on micro-structured samples inside a diamond anvil cell.

8:48AM V16.00005 SmPt₄Ge₁₂ – a filled skutterudite with exotic heavy-fermion properties

ANDREAS LEITHE-JASPER, ROMAN GUMENIUK, WALTER SCHNELLE, HELGE ROSNER, MICHAEL NICKLAS, MICHAEL SCHÖNEICH, ULRICH SCHWARZ, YURI GRIN, Max-Planck-Institute for Chemical Physics of Solids — Ternary samarium-filled platinum-germanium skutterudite SmPt₄Ge₁₂ was prepared at a pressure of 5.0(0.5) GPa and a temperature of 1070(70) K. The compound crystallizes in the cubic space group $Im\bar{3}$ ($a = 8.6069(4)$ Å) and is isotopic with LaFe₄P₁₂. X-ray absorption spectroscopy measurements show that samarium in SmPt₄Ge₁₂ has a temperature-independent intermediate valence ($\nu = 2.90 \pm 0.03$). Magnetization data reveal van-Vleck paramagnetism above ~ 50 K. The low-temperature specific heat displays a broad anomaly centred at 2.9 K and a large linear coefficient $\gamma' = 450$ mJ mol⁻¹ K⁻² suggesting heavy-fermion behaviour. This state is remarkably field-independent and resembles the physics of SmOs₄Sb₁₂. [1] R. Gumeniuk et al. New J. Physics 12 (2010) 103035.

9:00AM V16.00006 Physical properties and Ce-valence of the filled skutterudite CePt₄Ge₁₂

WALTER SCHNELLE, ROMAN GUMENIUK, MICHAEL NICKLAS, HELGE ROSNER, ANDREAS LEITHE-JASPER, YURI GRIN, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, KRISTINA O. KVASHNINA, ESRF, Grenoble, France, YURI SKOURSKI, HLD, Helmholtz-Zentrum Dresden-Rossendorf, Germany — Filled skutterudite compounds MPt₄Ge₁₂ with a Pt-Ge framework structure show intriguing physical ground states (conventional ($M = \text{Sr, Ba}$) and unconventional superconductivity ($M = \text{Pr}$), heavy-fermion behavior ($M = \text{Sm}$), magnetic ordering), similar to the well-known transition-metal pnictogen skutterudites. Here, we report on the electronic, magnetic, and transport properties of CePt₄Ge₁₂ [1]. High-resolution X-ray absorption spectroscopy (XANES) measurements at the cerium L_{III} edge demonstrate that Ce in this compound has a temperature-independent valence close to three. However, magnetic susceptibility, thermopower, Hall effect, and electronic specific heat reveal broad maxima at $T_{\text{max}} = 65\text{--}80$ K, suggesting the presence of valence fluctuations. The Sommerfeld coefficient $\gamma = 105$ mJ mol⁻¹ K⁻² indicates moderately enhanced band masses for CePt₄Ge₁₂. We discuss these findings and conclude that CePt₄Ge₁₂ represents a system at the border between intermediate valence (IV) and Kondo lattice behavior.

[1] R. Gumeniuk et al. J. Phys.: Condensed Matter 23 (2011) 456601.

9:12AM V16.00007 Cu-NMR and magnetization in disordered nFL system UCu₄Ni¹, O.O. BERNAL,

A. VALDEZ, M. CHIANG, Department of Physics and Astronomy, California State University, Los Angeles, CA 90032, D.E. MACLAUGHLIN, Department of Physics and Astronomy, University of California, Riverside, CA 92125, G.R. STEWART, J.S. KIM, Department of Physics, University of Florida, Gainesville, FL 32611 — We present a study of the NMR spectra in a random powder of UCu₄Ni as a function of frequency (40–70 MHz) and temperature (5–300 K). Two types of spectral lines for each of the two isotopes of naturally abundant Cu in the material are clearly evident in the spectra. Their behavior is followed for temperature and field variations and compared/contrasted with the more studied case of UCu₄Pd, where only one type of Cu-NMR line has been observed clearly. Unlike in UCu₄Pd, the appearance of two types of signal from Cu nuclei in the Ni compound is unambiguous evidence of site disorder in UCu₄Ni. This alone is indication that the amount of site disorder in the Ni sample is larger than in the Pd system; however, the NMR line intensities reveal that the Ni ions do not seem to go completely randomly in the two available crystallographic sites of the underlying crystal structure as would be expected from ionic-size considerations alone. The NMR parameters for both types of spectral lines, together with complementary measurements of magnetic susceptibility performed on the same powder samples, will be discussed from the point of view of magnetic disorder and non-Fermi liquid behavior.

¹Work supported by NSF/DMR-0604015 and 1105380

9:24AM V16.00008 Effect of pressure on CeGe_{2-x} single crystals, S.L. BUD'KO, Ames Laboratory US DOE and

Dept. of Physics and Astronomy, ISU, Ames, IA 50011, USA and SPSMS, UMR-E CEA/UJF-Grenoble 1, INAC, 38054 Grenoble, France, D. BRAITHWAITE, B. SALCE, SPSMS, UMR-E CEA/UJF-Grenoble 1, INAC, 38054 Grenoble, France, E. COLOMBIER, Ames Laboratory US DOE and Dept. of Physics and Astronomy, ISU, Ames, IA 50011, USA, M.S. TORIKACHVILI, Dept. of Physics and Astronomy, ISU, Ames, IA 50011, USA, and Dept. of Physics, SDSU, San Diego, CA 92182, USA, H. HODOVANETS, P.C. CANFIELD, Ames Laboratory US DOE and Dept. of Physics and Astronomy, ISU, Ames, IA 50011, USA — At ambient pressure CeGe_{2-x} has an antiferromagnetic (AFM) transition at $T_N \sim 7$ K and, on further cooling, a second transition, to a weak ferromagnetic (WFM) state, at $T_C \sim 4$ K. Under pressure the T_N goes through a broad maximum, and then is completely suppressed with a critical point at ~ 85 kbar, grossly following the Kondo-necklace picture. The WFM phase evolves into apparent AFM phase under moderate pressure of ~ 10 kbar, with T_N joining T_N at ~ 60 kbar. Resulting $P - T$ phase diagram and comparison with CeRu₂Ge₂ under pressure will be presented.

9:36AM V16.00009 A THz spectroscopy investigation of the heavy fermion state in CeCu₂Ge₂¹

GRACE BOSSE, L. BILBRO, R. VALDES AUGILAR, JHU Dept. of Physics and Astronomy, Y. LI, J. ECKSTEIN, Dept. of Physics, University of Illinois, N.P. ARMITAGE, JHU Dept. of Physics and Astronomy — We present time-domain THz spectroscopy data of a thin film of the heavy fermion compound CeCu₂Ge₂. Measurements to obtain the frequency dependent complex conductivity were taken as a function of temperature down to temperatures well below the onset of magnetic order. At low temperatures a narrow Drude-like peak forms, which is likely associated with the heavy fermion or spin density wave state. Using this data in conjunction with DC resistivity measurements, we obtain the frequency dependence of the scattering rate and the mass renormalization through an extended Drude model analysis.

¹This has been supported at JHU by the Gordon and Betty Moore Foundation. At UIUC, this work has been supported by the Center for Emergent Superconductivity, funded by the DOE award DE-AC0298CH1088.

9:48AM V16.00010 Influence of charge carrier doping on the T^* -scale in YbRh₂Si₂¹, PHILIPP

GEGENWART, H.S. JEEVAN, Y. TOKIWA, M. SCHUBERT, M. MCHALWAT, E. BLUMENROETHER, I. Physik. Institut, Goerg-August University Goettingen — YbRh₂Si₂ is a prototype heavy-fermion metal which displays a magnetic field-induced antiferromagnetic (AF) quantum critical point (QCP). It has attracted much attention due to an additional low-energy scale $T^*(B)$ merging at the QCP, whose origin is controversially discussed. Here, we report measurements of the electrical resistivity $\rho(T, B)$ on different single crystalline samples of charge-carrier doped Yb(Rh_{1-x}T_x)₂Si₂ (T=Fe, Ni) at temperatures down to 15 mK and in magnetic fields up to 7 T. The partial substitution of Rh by either Fe or Ni introduces holes or electrons, respectively. The evolution of the single-ion Kondo scale is similar as for isoelectronic Co substitution and in accordance with the chemical pressure effect. However, while chemical pressure has little influence on $T^*(B)$, we observe a drastic reduction or increase of $B^*(T = 0)$ by Fe- or Ni-doping, respectively. Most interestingly, $B^*(T = 0)$ is always pinned at the field-induced AF QCP, in contrast to chemical pressure results. As AF order is completely suppressed by Fe-doping, a heavy Fermi liquid ground (without $T^*(B)$ anomaly) is observed.

¹Work supported by the DFG through the research unit 960 (Quantum phase transitions).

10:00AM V16.00011 Quantum Criticality in the strongly correlated 3d electron system $\text{YFe}_2\text{Al}_{10}$, L.S. WU, Stony Brook University, K. PARK, Y. JANSSEN, M.S. KIM, C. MARQUES, Brookhaven National Lab, M.C. ARONSON, Stony Brook University, Brookhaven National Lab — $\text{YFe}_2\text{Al}_{10}$ has recently been identified as a strongly correlated 3d -electron system that is located very close to a quantum critical point (QCP). At low temperatures, divergences were found in the ac magnetic susceptibility ($\chi' \propto T^{-1.3}$) and magnetic specific heat ($C_M/T \propto T^{-0.47}$) based on the measurements carried out on single crystals. The magnetic Grüneisen ratio determined from these measurements ($\Gamma/H = -\frac{1}{T} \frac{\partial S/\partial B}{\partial S/\partial T} = -\frac{\partial M/\partial T}{C}$) also shows a strong divergence as $T \rightarrow 0$, which is suppressed in fields indicating a quantum critical point at $B=0$. When applying magnetic field, Fermi liquid like behavior with an enhanced magnetic susceptibility χ_0 and Sommerfeld coefficient C/T emerges at $T < T_{FL}$, and this enabled us to establish a field temperature (B - T) phase diagram with a crossover temperature $T_{FL}(B)$ coming out from the QCP at $B=0$. This is very similar to the quantum critical behavior observed in many f-electron based heavy fermion (HF) systems, and it makes $\text{YFe}_2\text{Al}_{10}$ an interesting 3d- electron candidate for studying quantum criticality.

10:12AM V16.00012 Small-angle neutron scattering study of the vortex lattice in $\text{PrOs}_4\text{Sb}_{12}$, ALEXANDRE DESILETS-BENOIT, ANDREA BIANCHI, University of Montreal, SIMON GERBER, NIKOLA EIGETENMEYER, JORGE GAVILANO, MICHEL KENZELMANN, Paul Scherrer Institut, CHRISTIAN PFLEIDERER, Technische Universität München, SEBASTIAN MUEHLBAUER, ETH Zürich, RYAN BAUMBACH, BRIAN MAPLE, University of California at San Diego — We carried out a small angle neutron scattering study of the vortex lattice in the Pr based heavy Fermion superconductor $\text{PrSb}_4\text{Os}_{12}$ with H applied along the c-axis. With a critical temperature T_c of 1.85 K and a H_{c2} of 2.5T, $\text{PrOs}_4\text{Sb}_{12}$ is the first Pr based heavy fermion superconductor (SC). Although $\text{PrOs}_4\text{Sb}_{12}$ crystallizes in a filled Skutterudite structure with a cubic lattice, this structure has a tetrahedral point group symmetry. In consequence, with the application of a magnetic field along the c-direction, the a and b-axis are no longer equivalent. Measurements of the angular dependence of the thermal conductivity in $\text{PrOs}_4\text{Sb}_{12}$ suggest a change of the superconducting order parameter deep inside the SC phase diagram from a two fold symmetry to a fourfold symmetry. Three ways of applying field were tested and wiggle field cooling was found to produce the highest intensity. We observed a twinned distorted hexagonal VL up to 1T of applied field which is consistent with s-wave superconductivity. We did not observe a field dependent phase transition associated with a change in symmetry of the VL. We found a rapidly decreasing form factor $-F^{-2}$ of the vortex lattice (VL) in $\text{PrOs}_4\text{Sb}_{12}$ with increasing field.

10:24AM V16.00013 In plane vortex lattice of the heavy Fermion superconductor CeCoIn_5 , A.D. BIANCHI, Université de Montréal, P. DAS, University of Notre Dame, J.S. WHITE, Paul Scherrer Institut, A.T. HOLMES, E.M. FORGAN, University of Birmingham, M. KENZELMANN, M. ZOLLIKER, S. GERBER, J.L. GAVILANO, Paul Scherrer Institut, E.D. BAUER, J.L. SARRAO, Los Alamos National Laboratory, C. PETROVIC, Brookhaven National Laboratory, M.R. ESKILDSEN, University of Notre Dame — We present a small angle neutron scattering study of the vortex lattice (VL) in the unconventional superconductor CeCoIn_5 for magnetic fields H applied in the crystallographic ab -plane. CeCoIn_5 is a $d_{x^2-y^2}$ superconductor with the lines nodes of the superconducting gap oriented along the $[110]$ direction. At low fields H applied parallel to $[100]$, and $[110]$, we observed a distorted hexagonal VL with an opening angle of about 80° . However, for $[110]$ we find a reorientation transition for fields above 9 T where the vortex lattice is rotated by 90° . The H -dependence of the form factor of the vortex lattice is similar to what we observed previously along the c-axis: The scattering intensity increases with increasing H due to Pauli paramagnetism. For fields where the transition into the SC state becomes first order, we observe a broadening of the VL.

10:36AM V16.00014 Low-energy magnetic excitations in single-crystalline CeCu_2Ge_2 in fields up to 10 T, MICHAEL LOEWENHAUPT, IFP/TU Dresden, ASTRID SCHNEIDEWIND, ENRICO FAULHABER, HZB/PANDA, OLIVER STOCKERT, MPI-CPFS — CeCu_2Ge_2 is a magnetically ordered ($T_N = 4.1$ K) Kondo lattice with a moderate enhanced Sommerfeld coefficient of 140 mJ/molK^2 . Calculations of the Fermi surface showed that the observed incommensurate antiferromagnetic order can only be explained by involving an itinerant component of the Ce 4f-moments in addition to their local character. We performed low-energy inelastic neutron scattering experiments on a 2 g single crystal of CeCu_2Ge_2 using the cold triple-axis spectrometer PANDA at FRM II. Data were taken at 1.5 K and in magnetic fields up to 10 T applied perpendicular to the (110/001) scattering plane. At zero field the magnetic excitations show an energy gap of 0.5 meV at all investigated Γ points in the (110/001) plane with similar intensities. Away from the Γ points the magnetic excitations become dispersive merging into a band of excitations around 1 meV. For increasing magnetic fields the gap energy decreases indicating opposite action of external and internal fields. The results will be discussed in the framework of local, crystal field related, and non-local, spin-wave-like, magnetic excitations.

10:48AM V16.00015 Universal Kondo effect in $\text{Ti}_{0.94}\text{M}_{0.06}\text{O}_2$ ($M = \text{Nb, Ta}$) Thin Films, KALON GOPINADHAN, NUSNNI-NanoCore, National University of Singapore, Singapore 117576, A. ROY BARMAN, A. ANNADI, T.P. SARKAR, Department of Physics, National University of Singapore, Singapore 117542, W.M. LU, NUSNNI-NanoCore, National University of Singapore, Singapore 117576, Z.Q. LIU, AMAR SRIVASTAVA, - ARIANDO, Department of Physics, National University of Singapore, Singapore 117542, SANKAR DHAR, T. VENKATESAN, NUSNNI-NanoCore, National University of Singapore, Singapore 117576 — We show that $\text{Ti}_{0.94}\text{M}_{0.06}\text{O}_2$ ($M = \text{Nb, Ta}$) thin films are Kondo systems by angle dependent magneto-resistance measurement. Surprisingly, the data fitted by both Goldhaber-Gordon and Hamann formula yield comparable carrier dependent Kondo temperatures (10 - 60 K). The Kondo temperature dependence on carrier density was different for Ta and Nb incorporated in TiO_2 but this result could be understood on the basis of the formation of compensating defects (Ti vacancies) which also act as localized magnetic scattering centers. Using the unitarity-limit resistivity and Kondo temperature estimated from these fits the normalized resistivity versus temperature for all these films collapse into a universal curve consistent with data observed in metallic systems. However, the size of the Kondo scattering is at least an order of magnitude larger than in metallic systems. Further, from the extrapolation of the Kondo temperature we are able to predict that Ta is a better candidate for observation of ferromagnetism versus Nb.

Thursday, March 1, 2012 8:00AM - 10:48AM –

Session V17 DMP: Focus Session: Electron, Ion, and Exciton Transport in Nanostructures - Junctions 252A

8:00AM V17.00001 Effects of electron-phonon coupling in the Kondo regime of a two-orbital single-molecule junction¹, EDSON VERNEK, GISELE IORIO, Universidade Federal de Uberlândia, LILI DENG, KEVIN INGERSENT, University of Florida - USA, ENRIQUE ANDA, Pontificia Universidade Católica do Rio de Janeiro - Brazil — Single-molecule junctions (SMJs) are electronic devices formed by a molecule bridging the gap between two metallic contacts. Despite their apparent simplicity, such systems have attracted much attention for the rich variety of experimentally accessible physics that they display. The spatial confinement of electrons in molecules can lead to collective phenomena such as Coulomb blockade and the Kondo effect, as well as to strong coupling of electrons to molecular vibrations. We explore the interesting interplay of electron-electron and electron-phonon interactions in a model of an SMJ in which the central molecule has two active orbitals. The nonperturbative numerical renormalization group method is used to treat the many-body Kondo physics and electron-phonon coupling on equal footing. Electron-phonon coupling renormalizes the energies and Coulomb interactions of the molecular orbitals. The effects are most pronounced in cases where both molecular orbitals lie close to the Fermi energy of the contacts. Here, a sufficiently strong phonon-assisted inter-orbital tunneling can suppress the Kondo effect and cause a crossover to a phonon-dominated regime having very different electrical transport properties.

¹We would like to thank FAPEMIG and CNPq for financial support.

8:12AM V17.00002 Rectification in Symmetric Conjugated Molecules with Asymmetric Linkers, ARUNABH BATRA, Dept. of Applied Physics and Applied Mathematics, Columbia University, JEFFREY S. MEISNER, Dept. of Chemistry, Columbia University, JONATHAN R. WIDAWSKY, EEK HUISMAN, Dept. of Applied Physics and Applied Mathematics, Columbia University, COLIN NUCKOLLS, Dept. of Chemistry, Columbia University, LATHA VENKATARAMAN, Dept. of Applied Physics and Applied Mathematics, Columbia University — Demonstrating single-molecule rectification is an important step towards the realization of molecule-based electronic devices. Most molecules put forward as potential rectifiers employ asymmetric molecular backbones. In contrast, we show that we can create rectifying junctions by designing asymmetry only into the linker groups used to bond the molecule to metal electrodes. Our molecules consist of a conjugated backbone terminated with methylsulfide on one end and methyl-trimethyltin on the other. These molecules couple to Au electrodes through an Au-SMe donor acceptor bond, which serves as the electronically weak link, and a Au-C covalent bond, which is created in-situ after the SnMe_3 cleaves off [1]. We create thousands of molecular junctions using a modified STM setup in a solution of molecules, measure their current-voltage (IV) characteristics and create averaged IV curves. We find that asymmetrically terminated molecules show non-linear IV curves with significant rectification, while molecules terminated symmetrically with either SMe or SnMe_3 do not show substantial rectification. We also find that the rectification direction is dependent on molecular orientation in the junction. [1] Chen, W., et al., J. Am. Chem. Soc., 2011. 133(43): p. 17160-17163

8:24AM V17.00003 Simultaneous Determination of Conductance and Thermopower of Single Molecule Junctions¹, JONATHAN WIDAWSKY, Department of Applied Physics and Applied Mathematics, Columbia University, PIERRE DARANCET, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, LATHA VENKATARAMAN, Department of Applied Physics and Applied Mathematics, Columbia University — We present a study of concurrent determination of conductance (G) and thermopower (S) of single-molecule junctions via direct measurement of electrical and thermoelectric currents. The junctions are created using the STM-based break-junction technique where a cold Au tip is repeatedly brought in and out of contact with a hot Au-on-mica substrate in an environment of the target molecule. We explore several amine-Au and pyridine-Au linked molecules that are predicted to conduct through either the highest occupied molecular orbital (HOMO) or the lowest unoccupied molecular orbital (LUMO), respectively. We find that the Seebeck coefficient is negative for pyridine-Au linked LUMO-conducting junctions and positive for amine-Au linked HOMO-conducting junctions. From histograms of thousands of junctions, we use the most probable Seebeck coefficient to determine a power factor, GS^2 , for each junction studied, and find that GS^2 generally increases with G .

¹Funded Primarily by the Energy Frontier Research Center of DOE under Award Number DE-SC0001085

8:36AM V17.00004 Theory of Solvent-Mediated Environmental Effects on Molecular-Scale Transport, MICHELE KOTIUGA, Department of Physics, UC Berkeley & Molecular Foundry, LBNL, PIERRE DARANCET, Molecular Foundry, LBNL, VALLA FATEMI, Department of Physics, MIT, BIRGER HENNINGS, MICHAEL FREI, LATHA VENKATARAMAN, Department of Applied Physics and Applied Mathematics, Columbia, JEFFREY NEATON, Molecular Foundry, LBNL — Single-molecule junctions, formed with well-defined and robust metal-molecule contacts, can provide an ideal model system to study mechanisms of charge transport at the molecular scale. However, the presence of solvent is often unavoidable, and recent experiments have shown that the junction conductance can be altered by a factor of two depending on the solvent present [1]. It has been proposed that the binding of the solvent to the gold electrodes changes their local work function, which in turn alters the conductance of the junction in a predictable manner. Here, we use a first-principles scattering-state approach, based on self-energy corrected density functional theory, to explore the transmission and conductance of bipyridine- and diaminestilbene-Au molecular junctions in the presence of solvent molecules, using an analytical model to compare with experimental results. We acknowledge DOE for support, and NERSC for computational resources.

8:48AM V17.00005 Tailoring IV Characteristics and Rectification in Single-Molecule Junctions¹, PIERRE DARANCET, Lawrence Berkeley National Laboratory, JONATHAN WIDAWSKY, Columbia University, HYOUNG JOON CHOI, Yonsei University, LATHA VENKATARAMAN, Columbia University, JEFFREY NEATON, Lawrence Berkeley National Laboratory — Asymmetry in the current-voltage characteristics, or current rectification, of nanoscale junctions is a critical property for many optoelectronic and energy conversion applications using nanostructured materials. Here, we compute the conductance, IV characteristics, and bias-dependent rectification of a class of molecular junctions, consisting of donor-acceptor molecules in contact with Au electrodes, using quantitative first-principles calculations [1]. We relate the rectification to the identities of the donor and acceptor moieties through the junction energy level alignment and dipole moments and find, surprisingly, that a large asymmetry in the contact coupling leads to weak rectification. We explain our results with an analytic coherent tunneling model, and suggest concrete strategies for obtaining high rectification in experimentally-achievable systems. [1] Darancet et al., submitted (2011).

¹We acknowledge DOE-BES for support and NERSC for computational resources.

9:00AM V17.00006 Electronic transport properties of functional single molecule junctions, E.S. TAM, H.D. ABRUNA, D.C. RALPH, Cornell University — We report experimental studies of single molecule conductance using two techniques: statistical measurements with repeatedly-formed breakjunctions in ambient conditions and low-temperature measurements with electromigrated breakjunctions. In each case, we chose molecules with specific functions. With statistical measurements, we measured the nonconducting open and conducting closed forms of dithienylethene, a photochromic (optically switchable) molecule. These molecules were synthesized with pyridine endgroups to achieve relatively well-defined and stable contacts to Au electrodes. For the closed isomer, we find a conductance of $(3.3 \pm 0.5) G_0$, while that of the open isomer is below the noise floor of our measurement. We can therefore set a lower limit of 30 for the on/off ratio of this molecule. We are currently investigating the use of electromigrated graphene nano-constrictions and breakjunctions for spin-polarized single molecule conductance measurements and plan to present initial results for this technique.

9:12AM V17.00007 Bias-Dependent Noise Measurements in Individual Electromigrated Nanoscale Junctions, PATRICK WHEELER, RUOYU CHEN, DOUGLAS NATELSON, Department of Physics Rice University — Shot noise provides insight into the correlated motion of electrons in nanostructures. Previous measurements have examined shot noise in mechanically controlled break junctions (MCBJs), looking at a large ensemble of junction configurations at room temperature. Electromigrated, lithographically created Au structures at liquid nitrogen and helium temperatures allow for noise measurements of individual junction configurations. High frequency excess noise is amplified by a RF amplifier chain and measured in combination with lock-in techniques simultaneously with the dc conductance. Noise measurements across bias and temperature are compared to previous experiments performed with MCBJs at room temperature, with an emphasis on the dependence of the noise on bias conditions. We find that measured noise in individual junctions can exhibit nonlinearities with bias as well as asymmetries as a function of the polarity of bias current. Individual junctions can also switch stochastically between different atomic configurations with nearly identical conductances but strikingly different noise properties. We discuss these observations in the context of “traditional” shot noise, bias-dependent noise processes, and $1/f$ contributions to the measured noise.

9:24AM V17.00008 Shot noise measurements as a function of bias in STM-style gold junctions¹

, RUOYU CHEN, PATRICK WHEELER, DOUGLAS NATELSON, Physics & Astronomy, Rice University — Shot noise measurements provide more detailed information regarding conductance channels than transport alone. Because of nearly fully transmitted modes, shot noise in nanoscale junctions is suppressed strongly near certain conductance values. In this experiment, we use a gold tip in a STM-style geometry to make nanoscale junctions, which function as the noise source when under bias. Peaks of conductance histograms and related mean square, radio frequency shot noise are successfully measured simultaneously at room temperature, at a series of voltage biases. Those peaks and related shot noise suppressions appear near integer multiples of the conductance quantum G_0 , especially the first three. We are able to measure shot noise at biases as low as tens of millivolts, and make use of even lower biases to estimate the systematical background existing in our measurements. Combined with a radio frequency reflection measurement, we convert the measured signal to current noise across the junction. The relevant noise processes and their evolution with bias across the junctions will be discussed.

¹This work is supported by NSF award DMR-0855607.

9:36AM V17.00009 Testing the charge transport mechanism in molecule-nanoparticle networks by molecular exchange

, VENKATA KAMALAKAR, IPCMS CNRS-University of Strasbourg, EDWIN DEVID, Leiden University, JEAN-FRANCOIS DAYEN, BERNARD DOUDIN, IPCMS CNRS-University of Strasbourg, SENSE JAN VAN DER MOLEN, Leiden University — Nanoparticles molecular networks have recently emerged as useful toolbox for molecular electronics studies. Nanoparticles bridging the size gap between molecules and macroscopic electrical interconnects make possible the realization of large self-assemblies of particles interlinked by molecules, with unique advantage of high reproducibility and robustness. This results from averaging over ensembles of molecules and make possible applications ranging from electrical, optical, mechanical, to spintronics devices. Electronic properties of well-organized two-dimensional networks, where Coulomb blockade regime is expected to be predominant, make these materials of high interest as model systems. We present temperature-dependent transport properties of networks bridging high aspect ratio trenches, making possible measurements over a wide temperature range. We study how the charge transport is modified when reversible molecular exchange is performed, tailoring the intrinsic conductance of the molecule. Quantitative agreement with experiments is obtained using a model clarifying the role played by the intrinsic conduction properties of the molecules and the geometry of the network.

9:48AM V17.00010 Quantum phase transitions arising from competing electron-electron and electron-phonon interactions in a two-orbital single-molecule junction¹

, LILI DENG, KEVIN INGERSANT, U. Florida, GISELLE LUIZ, EDSON VERNEK, U. Fed. Uberlandia, Brazil, ENRIQUE ANDA, PUC-Rio, Brazil — Electron-electron and electron-phonon interactions both play important roles in determining the transport properties of nanostructures such as single-molecule junctions. We use the numerical renormalization group to study a molecule with two active electronic orbitals connecting a pair of metallic leads. We focus on quantum phase transitions (QPTs) that can be accessed by varying couplings to a local vibrational mode, particularly the strength of phonon-assisted tunneling between the two molecular orbitals. One type of QPT arises in situations where, in the absence of electron-phonon interactions, one of the molecular orbitals manifests the many-body Kondo effect with its characteristic zero-bias anomaly in the electrical conductance through the junction. At a critical coupling, the system undergoes a first-order QPT to a low-conductance phase in which the electron-phonon interaction overwhelms the strong bare electron-electron repulsion and Kondo physics is completely destroyed. A second type of first-order QPT is found in cases where there is also a Holstein coupling of local phonons to the molecular charge. We will explain the conditions that give rise to QPTs, as opposed to crossovers, between different ground states of this system.

¹Supported by the NSF and CNPq through the Inter-American Materials Collaboration.

10:00AM V17.00011 Motion and Photon Emission of Single Molecules in Space-Time¹

, JOONHEE LEE, SHAWN PERDUE, ALEJANDRO RODRIGUEZ PEREZ, V. ARA APKARIAN, University of California, Irvine, DEPARTMENT OF CHEMISTRY TEAM — We have visualized tunneling electron induced motion of single Zn-Etioporphyrin molecules adsorbed on the thin oxide film grown on NiAl(110) surface using scanning tunneling microscopy (STM). When tunneling electrons are injected resonantly to an unoccupied molecular orbital, nearly bistable switching in tunneling current occurs and the molecule starts exhibiting vibronic progression in its photon emission spectra. The switching behavior was spatially mapped by recording time traces on individual pixels of an STM image. We reconstruct the motion using the spatial distribution of amplitude, frequency, and on-time of the switching, and interpret it as the planar hindered rotation shuttling between two different adsorption configurations. The angle of rotation is close to 45 degrees, and the on-time reveals the nature of local potential barrier. Due to the two fold symmetry of the molecules under interrogation, the conductance switching shows different polarities. The electronic excitation of the molecule leads to vibronic transition in which the molecule emits photons and vibrates inside the local potential wells. Considering significant corrugation of oxide surfaces, rotation mediated by quantum tunneling of ethyl groups of the molecule will be discussed.

¹This research was made possible through NSF Center for Chemistry at the Space-Time Limit (Grant no. CHE-082913)

10:12AM V17.00012 Atomic-scale motor driven by the current-induced forces

, YU-CHANG CHEN, BAILEY C. HSU, ALLEN TSENG, Department of Electrophysics, National Chiao Tung University, 1001 University Road, Hsinchu 30010, Taiwan — From first-principles approaches, we investigate the current-induced forces in an asymmetric molecular junction using Hellmann-Feynman type theorem in the framework of density functional theory in scattering approaches. We observe that it is possible to construct atomic-scale systems where the current-induced forces can be used to rotate the atoms. As an example, we consider a junction formed by the benzene molecule which directly connected to the Pt electrodes, where the benzene molecule is highly tilted. The highly tilted benzene molecule causes the streamline flow of the current to curve considerably to one side of the benzene ring. This could cause a net torque due to the unbalanced current-induced forces, which tend to rotate the benzene molecule in a manner similar to a stream of water rotates a waterwheel. Thus, the highly asymmetric single molecule junctions offer the atomic-scale systems to explore the possibility of nano-motors driven by non-equilibrium electron transport. The authors thank National Science Council (Taiwan) for support under Grant NSC 100-2112-M-012-MY3

10:24AM V17.00013 Capacitance variations of a Nanocapacitor in the Field Emission Regime¹

, CARLOS UNTIEDT, Dep. Fisica Aplicada. Universidad de Alicante. Spain, GIOVANNI SAENZ-ARCE, Dep. Fisica Aplicada. Univ. Alicante. Spain, JOSE IGNACIO PASCUAL, Institut für Experimentalphysik. Freie Universität Berlin, Germany — The electronic transport properties and mechanical forces between two metallic electrodes separated by a nanometer-sized vacuum gap have been studied using a Scanning Tunneling Microscope combined with a Tuning Fork Force sensor. When applying a voltage difference to the electrodes above their work function energy, the Field Emission regime can be accessed at which Field Emission Resonances take place. Under these circumstances a decrease of the capacitance has been found to occur showing a new mechanism of capacitor leaking in the quantum regime.

¹Spanish Government Support through grants FIS2010-21883-C02-01 and CONSOLIDER CSD2007- 0010; and University of Alicante through ACIE11-09

10:36AM V17.00014 Probing Water Structures in Nanopores via Tunneling¹, PAUL BOYNTON, MASSIMILIANO DI VENTRA, University of California, San Diego — We study the effects of volumetric constraints on the structure and electronic transport properties of distilled water in a synthetic nanopore. Combining classical molecular dynamics simulations with the Landauer approach to scattering theory as originally done in the context of DNA sequencing [1], we develop a relationship between the electronic current and the structure the water assumes in the confining pore-electrode system. Prior research in the field shows a tendency for the tunneling current through water to fluctuate due to local cavities in the water's structure. We show a shift in the tunneling current's dependence on pore diameter at the transition from exclusion of water to a monolayer. Furthermore, we argue that the current with respect to pore diameter does not follow a simple exponential curve at this transition as one would expect from tunneling. This research develops our understanding of water as a complex medium and describes fundamental physics of aqueous solutions.

[1] J. Lagerqvist, M. Zwolak, and M. Di Ventra, *Fast DNA sequencing via transverse electronic transport*, Nano Lett. **6**, 779 (2006).

¹Work supported in part by NIH

Thursday, March 1, 2012 8:00AM - 11:00AM –
Session V18 DMP: Focus Session: Interfaces in Complex Oxides - Interface and Surface Conductivity in SrTiO₃ 252B

8:00AM V18.00001 Surface charges & adsorbates tune the electron gas at the LaAlO₃/SrTiO₃ interface, YANWU XIE, CHRISTOPHER BELL, YASUYUKI HIKITA, HAROLD Y. HWANG, Department of Applied Physics and Stanford Institute for Materials and Energy Science, Stanford University, Stanford, California 94305, USA — The physical properties of the LaAlO₃/SrTiO₃ heterointerface are substantially determined by the density and mobility of the electron gas at the buried interface. Here, we present two ways to tune the electron gas from the LaAlO₃ surface. First, the electron gas can be locally tuned by using biased atomic force microscope probe [1]. Our studies show that this is caused by the accumulation of charge on the LaAlO₃ surface [2], and can change the density by up to $3 \times 10^{13} \text{ cm}^{-2}$ [3], comparable to the maximum modulation achieved in normal field effect devices. Second, we found that the electron gas can be dramatically tuned by the surface adsorption of common polar solvents such as acetone, ethanol and water [4]. This strong surface-interface coupling provides a new technique for manipulating the interface-confined electrons. Most significantly, adsorbates induce an insulator to metal transition when the thickness of the LaAlO₃ is 3 unit cells, suggesting sensor applications with extremely large sensitivity.

[1] C. Cen *et al.*, *Nature Mater.* **7**, 298 (2008).

[2] Y. Xie *et al.*, *Nano Lett.* **10**, 2588 (2010).

[3] Y. Xie *et al.*, *Adv. Mater.* **23**, 1744 (2011).

[4] Y. Xie *et al.*, *Nature Commun.* **2**, 494 (2011).

8:12AM V18.00002 Unexpected Two Dimensional Electron Gas at the LaAlO₃/SrTiO₃ (110) Interface¹, A. ANNADI, X. WANG, K. GOPINADHAN, W.M. LV, Z.Q. LIU, A. ROY BARMAN, A. SRIVASTAVA, S. SAHA, S. DHAR, NUSNNI-Nanocore, National University of Singapore, Singapore, H. HILGENKAMP, University of Twente, The Netherlands, T. VENKATESAN, - ARIANDO, NUSNNI-Nanocore, National University of Singapore, Singapore — The observation of two dimensional electron gas (2DEG), superconductivity and magnetism at the interfaces of LaAlO₃/SrTiO₃ has further amplified the potential of complex oxides for novel electronics. These multifunctional properties are strongly believed to originate from the polarization discontinuity at the interface between the two oxides along (001) direction. In this scenario, the crystal orientation plays an important role and no conductivity would be expected for e.g., the interface between LaAlO₃ and (110)-oriented SrTiO₃, which should not have a polarization discontinuity. In this talk, we will show the observation of conductivity at the LaAlO₃/SrTiO₃ interface prepared on (110)-oriented SrTiO₃. The strong evidence for 2DEG at the interface of LaAlO₃/SrTiO₃ (110) is the observed thickness dependence of insulator-metal transition at 3-4 u.c. of LaAlO₃. Directional dependent electrical transport is observed in resistance versus temperature measurements. We propose some models for explaining the observed phenomena.

¹We thank National Research Foundation (NRF) Singapore under the Competitive Research Program (CRP) "Tailoring Oxide Electronics by Atomic Control" NRF2008NRF-CRP002-024 and Ministry of Education (MOE) FRC-ARF Grant No. R-144-000-278-112.

8:24AM V18.00003 Temperature Dependent Strain Relaxation in LaAlO₃ Thin Films on SrTiO₃ Substrates, GUOZHEN LIU, KE CHEN, QINGYU LEI, Department of Physics, Temple University, QUN LI, LONGQING CHEN, Department of Materials Science and Engineering, Penn State University, XIAOXING XI, Department of Physics, Temple University — LaAlO₃/SrTiO₃ interface has attracted great interest due to discoveries of rich interfacial properties. Strain and strain relaxation in LaAlO₃ films on SrTiO₃ substrates directly impact the lattice distortions and defects at the interface and therefore will influence the interfacial properties. Combining grazing incident x-ray diffraction and reciprocal space mapping, we directly measured the in-plane lattice constants of LaAlO₃ films on SrTiO₃ with thickness ranging from 4 u.c. to 250 u.c. We found a strong relationship between the strain relaxation behavior and the growth temperature of the LaAlO₃ films. Cracks were observed when the strain relaxed rapidly, consistent with the fracture theory. The processing temperature-dependent strain relaxation significantly affects the LaAlO₃/SrTiO₃ interface properties.

8:36AM V18.00004 The origin of the 2DEG at oxide polar-non polar interfaces: electron reconstruction versus defect doping¹, CLAUDIA CANTONI, Oak Ridge National Laboratory, FABIO MILETTO GRANOZIO, CARMELA ARUTA, Università di Napoli Federico II & CNR-SPIN, JAUME GAZQUEZ, MARK OXLEY, ANDREW LUPINI, MARIA VARELA, STEPHEN PENNYCOOK, Oak Ridge National Laboratory, UMBERTO SCOTTI DI UCCIO, PAOLO PERNA, Università di Napoli Federico II & CNR-SPIN, DANIELE MARRÈ, Università di Genova & CNR-SPIN — In spite of intense research efforts, the microscopic mechanism underlying the formation of a 2DEG at the LaAlO₃(LAO)/SrTiO₃(STO) interface is still controversial. In particular, there is no consensus on whether the interface charge stems from an electronic reconstruction or from mobile electrons introduced by oxygen vacancies and/or cation doping. We present direct, atomic-column-resolved scanning transmission electron microscopy and electron energy loss measurements in LAO/STO and LaGaO₃(LGO)/STO interfaces. We find that both the measured injected charge, the low concentration of point defects, and the lattice polarization are consistent with a model of electronic reconstruction in LAO/STO. On the other hand, LGO/STO interfaces grown in the same conditions show negligible polar lattice distortions and an injected charge incompatible with electronic reconstruction. Conductivity here is explained by the observed cation intermixing and the presence of oxygen vacancies.

¹ORNL research sponsored by US DOE Office of Science, Materials Science and Engineering Division.

8:48AM V18.00005 Computational study of oxygen vacancy defects in perovskite oxides, SrTiO₃ and LaAlO₃, CHANDRIMA MITRA, CHUNGWEI LIN, University of Texas at Austin, JOHN ROBERTSON, Cambridge University, ALEXANDER DEMKOV, University of Texas at Austin — Insulating perovskite oxides, SrTiO₃ (STO) and LaAlO₃ (LAO) have attracted a lot of attention due to the observed two dimensional electron gas at the interface of these two insulating oxides. Oxygen vacancies, which are easily incorporated in these oxide systems during various processes such as growth, annealing and redox reactions, form an n-type defect in these systems. Hence they are responsible for modifications of various physical properties such as conductivity and optical properties to name a few. As such, there is still a lack of comprehensive theoretical understanding of these important defects in these materials. In this work we present first principles calculations of neutral (V^0) and charged (V^+ , V^{++}) oxygen vacancies in STO and LAO. Density functional theory within the local density approximation proves insufficient in reliably predicting the defect levels due to their well known band gap problem. We therefore employ the Heyd, Scuseria, and Ernzerhof (HSE) hybrid functional to study these defects. Band gaps of 3.01 eV and 5.0 eV are obtained for bulk STO and LAO which are in excellent agreement to experimental values. In STO we find a localized V^0 defect state at 0.7 eV below the conduction band edge (CBE) while in LAO it is a deep lying level at 2.13 eV below the CBE. A band alignment of the defect levels in these two materials shows that upon stabilizing the singly ionized state, charge transfer could take place from the V^+ LAO state to the V^+ STO state which lies at 1.19 eV below the former.

9:00AM V18.00006 Oxygen vacancy shuttle across the LaAlO₃/SrTiO₃ interface, EVGENY Y. TSYMBAL, TULA R. PAUDEL, YONG WANG, J.D. BURTON, University of Nebraska, Lincoln — There have been several recent indications of a switchable piezo-response in oxide materials not associated with ferroelectric polarization. We explore a LaAlO₃/SrTiO₃ (LAO/STO) heterostructure as a model system to understand this behavior by considering oxygen vacancies as the origin. Using first-principles calculations based on a supercell approach and an adequate electrostatic model, we show that the oxygen vacancy formation energy has two local minima: one at the surface of LAO and another in STO few unit cell below the interface. Due to inbuilt electric field in the system, electrons forming the oxygen vacancies in LAO transfer to the interface leaving behind two holes at the vacancy site irrespective of their spatial position, whereas those in the STO exhibit such a behavior only when lying within a finite distance ~ 1 nm associated with the screening length of the electric field in STO. The two local minima may accommodate oxygen vacancies reversibly when the applied electric field changes its polarity producing a switchable piezo-response behavior in the LAO/STO system.

9:12AM V18.00007 Electronic phase separation at the LaAlO₃/SrTiO₃ interface¹, - ARIANDO, NUSNNI-Nanocore & Department of Physics, National University of Singapore, Singapore — In the last few years we have seen a number of new properties to emerge at the interface between two insulating oxides. However the origin of these properties remains unclear and needs further investigation. In this talk I will discuss our recent studies on oxide interfaces in which we vary various parameters such as oxygen content and crystal orientation, and use different polar layers and heterostructures. Surprisingly, at the LaAlO₃/SrTiO₃ interface a remarkable combination of strong diamagnetism (superconductor like), paramagnetism and ferromagnetism can coexist with the quasi two dimensional electron gas (Q2DEG) when prepared under a more oxidizing condition. The ferromagnetic phase is stable even above room temperature and the diamagnetism below a relatively high temperature of 60 K. Our measurements show that the free surface of SrTiO₃ may be responsible for all these fascinating phenomena. The phenomena are explained due to the selective occupancy of interface/surface sub-bands of the nearly degenerate Ti orbital in the SrTiO₃. On changing the interface orientation, we unexpectedly can also obtain conductivity at the LaAlO₃/SrTiO₃ interface prepared on (110)-oriented SrTiO₃. The conductivity is found to be highly anisotropic, which is a novel feature for these oxide Q2DEGs and of potential interest for applications. I will discuss various possible models that can explain this intriguing observation and also review various interfaces prepared using different polar layers coupled to other functional materials which result in new phenomena.

¹We thank National Research Foundation (NRF) Singapore under the Competitive Research Program (CRP) “Tailoring Oxide Electronics by Atomic Control” NRF2008NRF-CRP002-024 and Ministry of Education (MOE) FRC-ARF Grant No. R-144-000-278-112.

9:48AM V18.00008 Effect of cation-nonstoichiometry in the SrTiO₃ layer on the interfacial conductance of LaAlO₃/SrTiO₃ heterostructures, SUSANNE HOFFMANN-EIFERT, FELIX GUNKEL, SEBASTIAN WICKLEIN, FZ Juelich, PGI-7 and JARA-FIT, Juelich, Germany, PETER BRINKS, MARK HUIJBEN, JOSEE E. KLEIBEUKER, GERTJAN KOSTER, GUUS RIJNDERS, Mesa+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands, REGINA DITTMANN, RAINER WASER, FZ Juelich, PGI-7 and JARA-FIT, Juelich, Germany — A study of the interface conductivity in LaAlO₃/SrTiO₃ (LAO/STO) heterostructures will be presented with focus on the defect chemical state of the SrTiO₃ close to the interface. SrTiO₃ layers with a controlled deviation from cation stoichiometry ($Sr/Ti=1$) were grown to investigate the effect of cation-nonstoichiometry in the SrTiO₃ layer on the resulting interface conductance of the corresponding LAO/STO heterostructures. The study comprises structural information and electrical properties derived from Hall measurements and high-temperature conductance measurements performed under equilibrium oxygen atmospheres. According to the model of defect chemistry the results give further evidence for the importance of charge compensation through defects on cation lattice sites.

10:00AM V18.00009 Nature of localized states induced by an oxygen vacancy in SrTiO₃¹, CHUNGWEI LIN, CHANDRIMA MITRA, ALEXANDER DEMKOV, Department of Physics, University of Texas at Austin — Combining the density function theory and model analysis, we study the nature of localized states induced by an oxygen vacancy (OV) in SrTiO₃. The key effect caused by an OV is that it introduces a local mixing between $3z^2 - r^2$ and $4s$, $4p$ orbitals of Ti next to the vacancy. According to our analysis, the OV-induced localized state is highly one-dimensional and is mainly composed of Ti $3z^2 - r^2$ orbitals along the Ti-OV-Ti axis (defined as the z -axis) and Ti $4s$, $4p$ at the OV site. Ti t_{2g} based localized states are ruled out. We suggest the $4s$, $4p$ components of the OV induced localized state should be reflected in the x-ray adsorption spectroscopy when Ti $4s$, $4p$ are served as final states. Our analysis and conclusion apply to general transition metal perovskites.

¹This work is supported by the U.S. Department of Energy (DOE) under Grant No. DESC0001878 and all DFT computations have been done at the Texas Advanced Computing Center.

10:12AM V18.00010 Oxygen deficiency on the p(1x1) structure of SrTiO₃ (001) surface¹, LINA CHEN, ZHAOLIANG LIAO, VON BRAUN NASCIMENTO, YI LI, A.C. ANTONY, E.W. PLUMMER, JIANDI ZHANG, Department of Physics and Astronomy, Louisiana State University, LA, 70810 USA — SrTiO₃(STO) is one of the most common substrates used for epitaxial film growth of oxide materials. However, the structure and stoichiometry of STO are still unclear even though they may dictate the interface properties. We have studied the STO(001) surface structure by Low Energy Electron Diffraction (LEED) and angle-resolved X-ray Photoelectron Spectroscopy (AR-XPS). The unreconstructed $p(1 \times 1)$ STO(001) surface terminated with TiO₂ layer is obtained by simple chemical etching which is always accompanied by oxygen deficiency. Both LEED and AR-XPS results suggest that the surface has a considerable oxygen deficiency, but LEED I(V) analysis indicates the existence of more oxygen vacancies than that from AP-XPS results. The structural analysis indicates a surface polarization due to a surface buckling combined with oxygen deficiency, which is consistent with recent surface x-ray scattering results [1] with important implications on surface ferroelectric phenomena in STO. The annealing effect of the as-etched surface in oxygen atmosphere on surface oxygen deficiency as well as reconstruction will also be discussed.

[1] R. Herger et al., Phys. Rev. Lett. 98, 076102(2007).

¹Supported by U.S. DOE under Grant No. DOE DE-SC0002136.

10:24AM V18.00011 Strain effects on the electron effective mass in SrTiO_3 ¹, ANDERSON JANOTTI, DANIEL STEIAUF, CHRIS G. VAN DE WALLE, Materials Department, University of California Santa Barbara — Strain can greatly affect the electronic properties of thin layers in epitaxial heterostructures, leading to improved transport properties. In SrTiO_3 -based heterostructures, strain can lift the degeneracy and modify the order of the states near the conduction-band minimum. Using density functional theory with the screened hybrid functional of Heyd, Scuseria, and Ernzerhof (HSE) we study the effects of strain on the energetic ordering and effective mass of the lowest-energy conduction-band states in SrTiO_3 . We predict that biaxial stress in the (001) or (110) planes results in the lowest-energy conduction-band state having significantly smaller electron mass in the in-plane directions compared to unstrained SrTiO_3 , thus suggesting that pseudomorphic growth is a promising route to increasing the electron mobility in epitaxial films. We propose possible substrates that may lead to SrTiO_3 films with enhanced electron mobilities, and report deformation potentials that allow accurate prediction of conduction-band splittings for arbitrary strain configurations.

¹Work supported by ARO and NSF.

10:36AM V18.00012 Electrical Transport in SrTiO_3 Under Biaxial Strain¹, ADAM KAJDOS, UC Santa Barbara - Materials, BHARAT JALAN, University of Minnesota - Chemical Engineering and Materials Science, JAMES ALLEN, UC Santa Barbara - Physics, SUSANNE STEMMER, UC Santa Barbara - Materials — Mobility engineering with strain is widely used for conventional semiconductors, but has only recently been proposed for complex oxides such as SrTiO_3 . The conduction band structure of SrTiO_3 is complicated with multiple degenerate bands derived from the Ti 3d orbitals. Strain is thus expected to have a significant effect by lifting this degeneracy and altering the occupancy and curvature of the bands. Indeed, a 300% increase in the electron mobility with values exceeding $128,000 \text{ cm}^2/\text{Vs}$ at 1.8 K was demonstrated in MBE-grown SrTiO_3 films subjected to *uniaxial* compressive strain [1]. For heterostructure engineering, the effect of *biaxial* strain is relevant. Here, the electron mobilities in SrTiO_3 subjected to biaxial strain are investigated through growth of coherent films on lattice-mismatched substrates. Lightly-doped (high-mobility) strained SrTiO_3 films below the critical thickness are insulating because of significant surface depletion, which increases with decreasing temperature due to the high dielectric constant of SrTiO_3 . We show that highly-doped, low-mobility capping layers address this problem, but require a multilayer model to analyze the Hall data in terms of the mobility in the lightly doped layer. [1] B. Jalan et al., Appl. Phys. Lett. **98**, 132102 (2011)

¹This work is supported by NSF Award No. DMR-1006640 and the UCSB MRL through NSF Award No. DMR-1121053.

10:48AM V18.00013 The Influence of Oxygen in Transition Metal Oxides, P.L. BACH, V. LEBORAN, F. RIVADULLA, University of Santiago de Compostela — The existence of a 2D metallic state at the interface between LaAlO_3 and SrTiO_3 (LAO/STO) has generated much excitement. Its origin has been attributed to charge redistribution to avoid a dielectric catastrophe; however, oxygen vacancies in TiO_2 -terminated STO can play a significant role in the electronic properties of the interface. In order to determine the nature and origin of the metallic phase, we have induced vacancies in TiO_2 -terminated STO single crystal substrates by annealing under controlled vacuum conditions. We report resistivity, Hall effect, and thermopower measurements on these materials and discuss their implications for the nature of the 2D electron gas at the STO surface. We have explored the possibility of gate-tuning these systems in order to fabricate single-oxide based devices. This work was supported by the Ministerio de Ciencia e Innovación (Spain), grant MAT2010-16157, and the European Research Council, grant ERC-2010-StG 259082 2D THERMS.

Thursday, March 1, 2012 8:00AM - 11:00AM –

Session V19 DCMP: Invited Session: Holography and Strongly Correlated Electron Matter
253AB

8:00AM V19.00001 Why black holes may be useful for condensed matter physics, SEAN HARTNOLL, Stanford University — I will give an overview of recent applications of black hole physics to strongly correlated electron systems, via the holographic correspondence. I will briefly review the thermodynamic nature of black hole horizons and explain how black holes exhibit quantum critical dissipation. I proceed to argue that black holes are associated with fractionalized phases of matter and provide a simple setting in which transport and other properties of such phases can be nonperturbatively studied. Black holes furthermore have natural instabilities to superconducting phases. The onset of superconductivity is described in a qualitatively different way than in BCS-derived theories of pairing. The superconductivity emerges from a non-Fermi liquid state of matter, without well-defined quasiparticles, and may suggest emphasis on different classes of observables.

8:36AM V19.00002 Holography and Mottness: A Discrete Marriage¹, PHILIP PHILLIPS, Dept. of Physics, University of Illinois, Urbana, IL 61801 — Gauge-gravity duality has allowed us to solve the physics of certain strongly coupled quantum mechanical systems using gravity. I will show how a space-time consisting of a charged black hole and a bulk Pauli coupling corresponds to a boundary theory with a dynamically generated gap (with no obvious symmetry breaking) and a massive rearrangement of the spectral weight as in classic Mott systems such as VO_2 . In this holographic set-up, the gap opens only when discrete scale invariance is present. This raises the possibility that the elusive symmetry that might be broken in Mott insulators, in general, might pertain to scale invariance. The relevance of this claim to recent theories of Mott systems that possess massless charged bosons is explored.

¹NSF DMR-0940992 and the Center for Emergent Superconductivity, a DOE Energy Frontier Research Center, Award Number DE-AC0298CH1088.

9:12AM V19.00003 Charge fractionalization and gauge-gravityduality¹, LIZA HUIJSE, Harvard University — We discuss zero temperature phases of compressible quantum matter, i.e. phases in which the expectation value of a globally conserved $U(1)$ density, Q , varies smoothly as a function of parameters. Provided the global $U(1)$ and translational symmetries are unbroken, such phases are expected to have Fermi surfaces, and the Luttinger theorem relates the volumes enclosed by these Fermi surfaces to $\langle Q \rangle$. We distinguish three compressible states: Landau's Fermi Liquid (FL), the fractionalized Fermi Liquid (FL*) and the non-Fermi Liquid (NFL). The motivation for this classification stems from the fact that compressible phases seem to be the rule rather than the exception in theories studied in the context of gauge-gravity duality. We argue that the three compressible phases we identify are indeed present in two paradigmatic supersymmetric gauge-theories underlying the duality. We then describe a gravity theory with an asymptotic electric flux dual to a zero temperature gauge theory at finite chemical potential. The flux can be sourced either by explicit charged matter in the bulk, by an extremal black hole horizon, or both. We argue that these three cases show important similarities with the three compressible states of matter. By tuning a relevant parameter we can study zero temperature phase transitions between the three phases in the dual description. The work I present was done in collaboration with S. Sachdev and S. Hartnoll.

¹The Netherlands Organization for Scientific Research (NWO)

9:48AM V19.00004 Emergent dimensions and quantum critical points¹, SUNG-SIK LEE, McMaster University / Perimeter Institute — When quantum many-body systems are strongly correlated, the underlying particles may dynamically organize themselves to show novel collective behaviors. Under certain conditions, collective fluctuations behave as if they are living in a space which has one more dimension than the space where the original particles are defined. In this talk, I will discuss about an example where an 'external' space emerges at a quantum critical point of a non-abelian gauge theory. A close analogy will be drawn between this phenomenon and fractionalization which can be viewed as an example of emergent 'internal' spaces. I will also discuss about non-trivial quantum orders associated with emergent dimensions.

¹This research was supported by NSERC, the Ontario Ministry of Research and Innovation and the Government of Canada.

10:24AM V19.00005 Embedding Fermi liquids in string theory, STEVEN GUBSER, Princeton University — Evidence of Fermi surfaces in strongly coupled gauge theories comes from calculations in the gauge-string duality based on the propagation of fermion fields in charged black hole backgrounds. Most of these calculations have been done without reference to explicitly known string theory constructions. When calculations based on the most universal sector of string theory constructions were at last done, no Fermi surface was found. In addition to reviewing the work just described, I will present new work showing that Fermi surfaces do exist in the next-to-simplest string theory constructions.

Thursday, March 1, 2012 8:00AM - 10:24AM —
Session V20 FIAP: Invited Session: High k Dielectrics for High Carrier Mobility Channel Applications 253C

8:00AM V20.00001 Materials and Device Aspects of III-V 3D Transistors, PEIDE YE, Purdue University — Recently, III-V MOSFETs with high drain currents ($I_{ds} > 1\text{mA}/\mu\text{m}$) and high transconductances ($g_m > 1\text{mS}/\mu\text{m}$) have been achieved at sub-micron channel lengths (L_{ch}), thanks to the better understanding and significant improvement in high-k/III-V interfaces. However, to realize a III-V FET at beyond 14nm technology node, one major challenge is how to effectively control the short channel effects (SCE). Due to the higher permittivity and lower bandgap of the channel materials, III-V MOSFETs are more susceptible to SCE than its Si counterpart. The scaling of planar devices stops at around 150nm L_{ch} . The dramatic increase in DIBL beyond 150nm indicates severe impact from 2D electrostatics. Therefore, the introduction of 3-dimensional (3D) structures to the fabrication of sub-100nm III-V FETs is necessary. In this talk, we will review the materials and device aspects of III-V 3D transistors developed very recently [1-3].

[1] Y. Q. Wu *et al.* IEDM Tech. Dig. 331 (2009).

[2] M. Radosavljevic *et al.*, IEDM Tech. Dig. 126 (2010).

[3] J. J. Gu *et al.* IEDM Tech Dig. 2011 (in press).

8:36AM V20.00002 Pushing the material limit and physics novelty in high κ 's/high carrier mobility semiconductors for post Si CMOS, MINGHWEI HONG, Department of Physics and Graduate Institute of Applied Physics, National Taiwan University, Taipei, Taiwan 10617 — The semiconductor industry is now facing unprecedented materials/physics challenges due to the scaling-limitation of Si CMOS transistor arising from non-scaling of matters, namely gate dielectrics and channel mobility. The new technology using high- κ plus metal gate on high carrier mobility semiconductors of InGaAs and Ge will lead to faster speed at lower power. The tasks for realizing the new devices equivalent oxide thickness (EOT) $< 1\text{ nm}$, interfacial density of state (D_{it}) $\leq 10^{11}\text{ eV}^{-1}\text{cm}^{-2}$, self-aligned process, low parasitic, and integration with Si, have been solved or are being feverishly studied. The key of achieving the above goals is to understand/tailor interfaces of the high κ 's/InGaAs (Ge). Tremendous progress has been made using molecular beam epitaxy (MBE) and atomic layer deposition (ALD) high κ 's of Ga_2O_3 (Gd_2O_3), Al_2O_3 , and HfO_2 , and the novel ALD/MBE dual dielectrics in attaining an EOT of 0.5 nm, D_{it} of low $10^{11}\text{ eV}^{-1}\text{cm}^{-2}$ (with a flat D_{it} distribution versus energy), and thermal stability at high temperatures higher than 800°C of the MOS structures. Electronic/electrical characteristics of the hetero-structures have been studied using in-situ synchrotron radiation photo-emission, cross-sectional scanning tunneling spectroscopy, capacitance (conductance)-voltage under various temperatures, and charge pumping methods. Device performance in world-record drain currents, transconductances, sub-threshold swings, etc. in self-aligned inversion-channel high κ 's/InGaAs and /Ge MOSFET's will also be presented. This work has been supported by Nano National Program (NSC 100-2120-M-007-010) of the NSC of Taiwan, and the AOARD of the US Air Force.

In collaboration with J. Kwo, W. C. Lee, M. L. Huang, T. D. Lin, Y. C. Chang, Y. H. Chang, C. A. Lin, Y. M. Chang (NTHU and NTU in Taiwan), T. W. Pi, C. H. Hsu (NSRRC in Taiwan), Y. P. Chiu (NSYSU in Taiwan), C. Merckling (IMEC in Belgium), J. I. Chyi (NCU, Taiwan), and G. J. Brown (AFRL, USA).

9:12AM V20.00003 Bonding principles of the Passivation Mechanism at III-V – oxide Interfaces, JOHN ROBERTSON, Cambridge University — It has always been much more difficult to make FETs from GaAs than Si, because of 'Fermi level pinning' and the difficulty of passivating its surfaces and interfaces. These issues have been discussed from the early days of PCSI by Spicer *et al* [1] with their "unified defect model." Hasegawa [2] introduced the idea of "Disorder Induced Gap states" (DIGS). Since 1997 it has been possible to make inverted MOSFETs on GaAs using the epitaxial Gadolinium gallium oxide [3], but the main impetuous has been since 2003 to use atomic layer dpeosition to make scalable FETs, as recently acheived by Intel [4]. The obvious question is why GaAs is so much more difficult to passivate than Si. The early answer was that the native oxide was poor. But since the advent of good deposited ALD oxides on Si such as HfO_2 or Al_2O_3 , this answer is no good, as they should also work on GaAs. They do to an extent, but the interfacial density of states is still too large and the CV p lots are distorted. The cause of the defects is cannot be due to stress. The reason must be some underlying chemical reason. I show that the reason is the polar nature of bonding in GaAa and other III-Vs, and the driving force to keep the Fermi level in a gap. The electron counting rule of Pashley [5] that describes surface reconstruction is shown to be a variant of auto-compensation, and it is proposed to work more generally, at each layer deposition or growth on GaAs [6]. This leads to a continuous generation of defects if it is not satisfied. So the answer is to deposit oxide layers that meet this rule, and also break up any surface reconstructions that would lead to As-As dimers [6].

[1] W E Spicer, Phys Rev Lett **44** 420 (1980)

[2] H Hasegawa, J Vac Sci Technol B **5** 1097 (1987)

[3] M Hong *et al*, Science **283** 1897 (1997)

[4] M Radosavljevic, *et al*, IEDM (2009) p13.1

[5] M D Pashley, Phys Rev B **40** 10481 (1989)

[6] J Robertson, L Lin, App Phys Letts (submitted), App Phys Lett **98** 082903 (2011)

9:48AM V20.00004 Exploring Ge and III-V devices to scale CMOS beyond the Si roadmap

, MARC HEYNS, imec — There is lots of interest in the use of germanium and III-V compounds as channel material in future CMOS generations. Direct growth of Ge and III-V in Si trenches allows to co-integrate these materials on bulk Si substrates. The formation of antiphase domain boundaries during epitaxy of III-V materials can be avoided by creating double atomic steps at the bottom of the trench through controlled Ge surface profiling. Much effort was dedicated to the electrical passivation of the interface between the high-k dielectric and these materials. Despite its relatively poor stability GeO₂-like passivation of Ge has been demonstrated for both pMOS and nMOS devices. Si capping layers of only a few monolayers were used to fabricate short channel Ge pMOS devices with high drive currents. Other successful Ge passivation methods are based on surface treatments such as in situ H₂S or wet (NH₄)₂S. Devices in III-V materials often suffer from Fermi level pinning associated with a high density of defect states near the high-k/III-V interface. These defects can be suppressed by optimized (in-situ) surface treatments and precise control of the oxidation states at the high-k/III-V interface. The Al₂O₃/InGaAs interface has been extensively investigated, often concentrating on the possibility to remove Ga and As oxides by exposure to trimethylaluminum (TMA) during atomic layer deposition (ALD), but good passivation has also been demonstrated with various other high-k materials. Since most III-V materials have a low conduction band density of states, the surface potential travels far into the conduction band before the necessary amount of mobile charge is accumulated at the interface. Therefore, the defect density at these energy levels must also be reduced, including border traps in the high-k layer that cause frequency dispersion in the capacitance-voltage behaviour. Finally, it is noteworthy to mention that the introduction of these advanced materials also allows the development of new device concepts, such as Implant-Free Quantum Well devices, heterojunction TunnelFETs and nanowire devices, that can fully exploit the properties of these new materials.

Thursday, March 1, 2012 8:00AM - 11:00AM –

Session V21 DCMP: Superconductivity: Mostly Cuprates 254A

8:00AM V21.00001 Evidence of strong correlations at the Van Hove singularity in the scanning-tunneling spectra of superconducting Bi₂Sr₂CaCu₂O_{8+δ} single crystals¹

, ARUN BANSIL, Northeastern University, JOUKO NIEMINEN, ILPO SUOMINEN, Tampere University of Technology, Finland, TANMOY DAS, ROBERT MARKIEWICZ, Northeastern University — We present realistic multiband calculations of scanning tunneling spectra in Bi₂Sr₂CaCu₂O_{8+δ} over a wide doping range. Our modeling incorporates effects of a competing pseudogap and pairing gap as well as effects of strong electronic correlations, which are included by introducing self-energy corrections in the one-particle propagators. The calculations provide a good description of the two-gap features seen in experiments at low energies. In particular, the Van Hove singularity (VHS) in the underlying electronic states is found to split into a prominent incoherent feature at high energies and a weaker coherent part near the Fermi level which is strongly involved in gap formation. The progressive hybridization of the localized VHS into the Fermi surface with increasing doping is suggestive of Kondo physics which has been proposed previously for cuprates and heavy fermion compounds.

¹Supported in part by the US DOE.

8:12AM V21.00002 Local correlations and deviations of energy scales from SI-STM in Bi-2212

, KYLE MCELROY, JACOB ALLDREDGE, University of Colorado Boulder, KAZUHIRO FUJITA, Cornell University, GENDA GU, Brookhaven National Laboratory, HIROSHI EISAKI, Institute of Advanced Industrial Science and Technology, S. UCHIDA, Department of Physics, University of Tokyo — One of the key difficulties in understanding the cuprate superconductors is reconciling the many probes that have been used to investigate them. In particular, in one of the most studied materials BSCCO-2212, this comparison is complicated by the striking atomic scale inhomogeneity that is seen in the electronic structure. We will present spectroscopic imaging scanning tunneling microscopy studies which show that the dominate energy scales are tied together not only as a function of doping but locally. This implies a single parameter that allows much of the low energy structure to be predicted. In addition, local structures which cause deviations in the ability of this single parameter to fit the data correspond to other phenomena previously described.

8:24AM V21.00003 Doping dependent study of non-equilibrium quasiparticle dynamics in the superconducting and normal state of La_{2-x}Sr_xCuO₄ thin films

, FAHAD MAHMOOD, DARIUS TORCHINSKY, Department of Physics, Massachusetts Institute of Technology, Cambridge MA 02139, A. BOLLINGER, I. BOZOVIC, Brookhaven National Laboratory, NUH GEDIK, Department of Physics, Massachusetts Institute of Technology, Cambridge MA 02139 — We report on measurements of non-equilibrium quasiparticle dynamics in La_{2-x}Sr_xCuO₄ thin films via ultrafast optical pump probe spectroscopy. Quasiparticles are excited into the thin films using ultrashort laser pulses. The transient change in the quasiparticle density causes a corresponding change in the reflectivity of the sample, allowing time resolved measurements of quasiparticle recombination. We describe the doping dependence of these measurements both above and below T_c and discuss their implications on the nature of the electron-boson coupling in the cuprates.

8:36AM V21.00004 Doping-dependence of Scattering Interference in Cuprates

, KAZUHIRO FUJITA, MOHAMMAD HAMIDIAN, INES FIRMO, SOURIN MUKHOPADHYAY, Cornell University, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology, SHIN-ICHI UCHIDA, University of Tokyo, J.C. DAVIS, Cornell University — Evolution of the k-space electronic structure from the strongly underdoped to overdoped regime upon doping is studied. At the doping level coincident with the disappearance of the pseudogap phenomenology a crossover in the scattering processes is identified [1]. We discuss the significance of such transition in conjunction with other experimental facts.

[1] K. Fujita, M. Hamidian, I. A. Firmo, S. Mukhopadhyay, H. Eisaki, S. Uchida, and J. C. Davis *Submitted* (2011).

8:48AM V21.00005 Time resolved reflectivity study of electron and hole doped cuprate superconductors

, JAMES HINTON, UC Berkeley, LBNL, JAKE KORALEK, LBNL, GUICHUAN YU, MUN CHAN, University of Minnesota, NEVEN BARISIC, University of Minnesota, University of Stuttgart, XUDONG ZHAO, Jilin University, MARTIN GREVEN, University of Minnesota, JOSEPH ORENSTEIN, UC Berkeley, LBNL — We study both the hole-doped cuprate HgBa₂CuO_{4+δ} (Hg1201) and the electron-doped cuprate Nd_{2-x}Ce_xCuO_{4+δ} (NCCO) using time-resolved optical reflectivity. In this technique, the sample is excited using an ultrashort 800 nm laser pulse, and the induced change in reflectivity is measured as a function of time after excitation. We focus on the temperature range above the superconducting transition; the fluctuating antiferromagnetic phase in NCCO and the pseudogap phase in Hg1201. In both cases we compare our results directly to neutron experiments, highlighting the relationship of the ultrafast optical response to magnetically ordered phases.

9:00AM V21.00006 Magnetic, Structural and Resistivity Characterization of New $R_3\text{Gd}_3\text{Ba}_2\text{Ca}_2\text{Cu}_7\text{O}_{10}:\text{Li}$ Compounds ($R=\text{rare earth}$), C. AGUILAR, Instituto de Investigaciones en Materiales, UNAM, Mexico, DF 04510, E.E. MARINERO, Hitachi San Jose Research Center, 3403 Yerba Buena Road, San Jose, CA 95135, E. CHAVIRA, Instituto de Investigaciones en Materiales, UNAM, Mexico, DF 04510, L. BUCIO, Instituto de Fisica, UNAM, Mexico, DF 04510, H. PFEIFFER, Instituto de Investigaciones en Materiales, UNAM, Mexico, DF 04510 — We report on the synthesis of $R_3\text{Gd}_3\text{Ba}_2\text{Ca}_2\text{Cu}_7\text{O}_{10}:\text{Li}$ compounds with different rare earth elements ($R=\text{Dy, Ho}$) by solid state reaction. Reaction products during the synthesis were identified by XRD and their thermal stability measured by Thermo-Gravimetric Analysis (TGA). Rietveld refinement of the XRD spectra enabled us to identify two coupled phases: a tetragonal one and an orthorhombic component. Magnetic measurements were conducted in the range of 5 to 300K to determine their Curie point and evidence for superconducting transitions. We find that in spite of the fact that both the Dy and Ho containing samples have the same crystalline structure, they exhibit different magnetic behavior over the temperature range studied. Evidence for a critical temperature at 15K for the Dy containing sample is observed exhibiting the characteristic M_s vs. T dependence ascribed to superconducting behavior. Detailed structural characterization results and measurements of R vs. T will be presented to confirm that the behavior observed at 15K is evidence for superconducting behavior.

9:12AM V21.00007 External vs. “internal” pressure effect on the anti-ferromagnetic super-exchange energy, J , in $\text{LnBa}_2\text{Cu}_3\text{O}_6$ ($\text{Ln}=\text{La, Nd, ..., Lu}$), BEN MALLETT, The MacDiarmid Institute, Victoria University of Wellington, JEFFERY TALLON, The MacDiarmid Institute, Industrial Research Limited, GRANT WILLIAMS, The MacDiarmid Institute, Victoria University of Wellington, THOMAS WOLF, Karlsruhe Institute of Technology, Institute of Solid State Physics — What causes the difference between the effect of “internal” pressure, as caused by ionic substitution, and external pressure on T_c^{max} in the cuprates [1]? Is it the density of states, the pairing boson energy scale (ω_B), condensation energy (which governs fluctuations), or ...? Many models of high temperature superconductivity put the energy scale of ω_B as the anti-ferromagnetic super-exchange energy, J , between adjacent Cu(2) ions in the CuO_2 plane. We therefore investigated Raman B_{1g} two-magnon scattering in high quality $\text{LnBa}_2\text{Cu}_3\text{O}_6$ ($\text{Ln}=\text{La, Nd, Sm, Eu, Gd, Dy, Yb, Lu}$), at ambient pressure to determine the effect of internal pressure on J . Comparing with measurements of J under external pressure reveals that internal and external pressure have *quantitatively* the same effect on J . However, and most surprisingly, we find an anticorrelation between J and T_c^{max} when ion size or internal pressure is the implicit variable. Given the opposite effects of internal and external pressure on T_c^{max} , this result suggests that some energy scale other than short range anti-ferromagnetic interactions has a more dominant effect on T_c^{max} .

[1] e.g. M. Marezio, Physica C, 341-348, 375 (2000)

9:24AM V21.00008 Anomalous High-Energy Spin Excitations in the High- T_c Superconductor Parent Antiferromagnet La_2CuO_4 , STEPHEN HAYDEN, NEIL HEADINGS, University of Bristol, RADU COLDEA, University of Oxford, TOBY PERRING, Rutherford Appleton Laboratory — Inelastic neutron scattering is used to investigate the collective magnetic excitations of the high-temperature superconductor parent antiferromagnet La_2CuO_4 . We find that while the lower energy excitations are well described by spin-wave theory, including one- and two-magnon scattering processes, the high-energy spin waves are strongly damped near the $(1/2, 0)$ position in reciprocal space and merge into a momentum dependent continuum. This anomalous damping indicates the decay of spin waves into other excitations, possibly unbound spinon pairs. The spinon dispersion that can explain the observed spin-wave damping in our experiments has the same form as the pseudogap dispersion observed in superconducting cuprates, with a minimum at $(1/4, 1/4)$.

9:36AM V21.00009 Charge transfer at the interface between ferromagnetic $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ and superconducting $\text{EuBa}_2\text{Cu}_3\text{O}_7$ probed by STM/STS, YINGHAO LIU, JIE XIONG, JASON HARALDSEN(2), LI YAN, ALEXANDER BALATSKY(2), QUANXI JIA, ANTOINETTE TAYLOR, DMITRY YAROTSKI, MPA-CINT and Theoretical Division(2), Los Alamos National Laboratory, NM 87545 — $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (LSMO) is a ferromagnetic half-metallic compound with nearly 100% spin polarization at room temperature, making it an ideal candidate for applications in spintronic devices. However, this useful functionality disappears when the thickness of LSMO film grown on SrTiO_3 substrate is reduced to below 4 nm, limiting its application in nanoscale devices. Here, we show that metallic and ferromagnetic properties of ultrathin ($< 4\text{nm}$) LSMO film can be restored by interfacing it with a superconductor $\text{EuBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (EBCO). We use scanning tunneling microscopy and spectroscopy to probe the evolution of the electronic structure of LSMO film grown on EBCO as functions of LSMO layer thickness and aging of bilayer LSMO/EBCO. Our results reveal that the charge (hole) transfer at LSMO/EBCO interface is responsible for driving LSMO film (of only five-unit-cell thickness) to metallic state. The conductive behavior of aged LSMO/EBCO bilayers varies systematically with the thickness of LSMO layer, allowing us to estimate the charge-transfer depth to be 4~5 nm on the LSMO side.

9:48AM V21.00010 Muon spin rotation investigation of the pressure effect on the magnetic penetration depth in $\text{YBa}_2\text{Cu}_3\text{O}_x$ ¹, ALEXANDER MAISURADZE, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland, ALEXANDER SHENGELAYA, Tbilisi State University, GE-0128 Tbilisi, Georgia, ALEX AMATO, EKATERINA POMJAKUSHINA, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland, HUGO KELLER, Physics Institute of University of Zurich, CH-8057 Zurich, Switzerland, UNIVERSITY OF ZURICH TEAM, PAUL SCHERRER INSTITUTE TEAM, TBILISI STATE UNIVERSITY TEAM — The pressure dependence of the magnetic penetration depth λ in polycrystalline samples of $\text{YBa}_2\text{Cu}_3\text{O}_x$ with different oxygen concentrations $x = 6.45, 6.6, 6.8$, and 6.98 was studied by muon spin rotation (μSR). The pressure dependence of the superfluid density $\rho_s \propto 1/\lambda^2$ as a function of the superconducting transition temperature T_c is found to deviate from the usual Uemura line. The ratio $(\partial T_c / \partial P) / (\partial \rho_s / \partial P)$ is factor of $\simeq 2$ smaller than that of the Uemura relation. In underdoped samples, the zero temperature superconducting gap Δ_0 and the BCS ratio $\Delta_0 / k_B T_c$ both increase with increasing external hydrostatic pressure, implying an increase of the coupling strength with pressure. The relation between the pressure effect and the oxygen isotope effect on λ is also discussed. In order to analyze reliably the μSR spectra of samples with strong magnetic moments in a pressure cell, a special model was developed and applied.

¹This work was partially supported by MaNEP

10:00AM V21.00011 Ultrafast spectroscopy of the stripe phase of underdoped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ thin films, DARIUS TORCHINSKY, FAHAD MAHMOOD, MIT, A. BOLLINGER, I. BOZOVIC, Brookhaven National Laboratory, NUH GEDIK, MIT — We have performed ultrafast measurements on high- T_c thin films of underdoped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. In these experiments, femtosecond pulses create photoexcitations derived from both the superconducting and striped phase fraction whose evolution and decay are probed as a function of time. We discuss the separate dynamics of these two electronic components as a function of temperature and excitation density.

10:12AM V21.00012 Nonlinear Response of the High-Temperature Superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ to the Transmission of Intense Terahertz Pulses¹, IWA O KAWAYAMA, Osaka Univ. and PRESTO-JST, ANDREAS GLOSSNER, Osaka Univ. and Universität Erlangen-Nürnberg, CAIHONG ZHANG, SHINYA KIKUTA, HIRONARU MURAKAMI, Osaka Univ., PAUL MÜLLER, Universität Erlangen-Nürnberg, MASAYOSHI TONOUCHI, Osaka Univ. — High-Power Terahertz Time-Domain Spectroscopy (THz-TDS) was used to examine $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ thin films when transmitted by intense single-cycle THz pulses. This allowed for an investigation of the nonlinear, time-resolved behavior of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ in the presence of strong THz electric fields for the first time. High field strengths of tens of kV cm^{-1} were achieved by improving the efficiency of optical rectification in LiNbO_3 through the tilted-pulse-front method and by ensuring a tight focusing of the THz beam. In the case of low field strengths, the behavior of the thin films agrees with previous examinations of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ by means of conventional, low-power THz-TDS. However, for strong THz electric fields, it was found by analysis with the two-fluid model that the superfluid population decreases dramatically, possibly due to Cooper pair breakup. This was accompanied by a drop in the imaginary part of the conductivity in the investigated frequency range of 0.2 to 0.8 THz. The results further suggest a decrease of the effective mass of the carriers for strong THz fields.

¹This work is partially supported by Grant-in-Aid A22246043, JSPS, and Industry-Academia Collaborative R&D, JST.

10:24AM V21.00013 Carrier mobility of insulating cuprates from time-resolved terahertz photoconductivity measurements, J. STEVEN DODGE, Dept. of Physics, Simon Fraser University, JESSE C. PETERSEN, Dept. of Physics, Oxford University, AMIR D. FARAHANI, Dept. of Physics, Simon Fraser University, RUIXING LIANG, Dept. of Physics and Astronomy, University of British Columbia, IVAN BOZOVIC, Brookhaven National Laboratory — We study the ultrafast transient photoconductivity of three insulating cuprates, $\text{Sr}_2\text{CuO}_2\text{Cl}_2$, $\text{YBa}_2\text{Cu}_3\text{O}_6$, and La_2CuO_4 . Terahertz spectroscopy reveals mobile dilute carriers, with a conductivity that appears promptly and decays non-exponentially in picoseconds. The peak photoconductivity is orders of magnitude larger than the static photoconductivity but smaller than that of chemically doped samples, with fast dynamics that depends weakly on material, concentration, and temperature. Decay dynamics indicate hopping transport with a low activation energy, suggesting weak to intermediate polaronic binding.

10:36AM V21.00014 Study of the radiation line width and shape from the Bi212 mesa structure¹, TAKANARI KASHIWAGI, TAKASHI YAMAMOTO, KAZUYA ISHIDA, MANABU TSUJIMOTO, KAVEH DELFANAZARI, RYO NAKAYAMA, TAKEO KITAMURA, MASASHI SAWAMURA, HIDEHIRO ASAI, HIDETOSHI MINAMI, KAZUO KADOWAKI, University of Tsukuba — Continuous electromagnetic waves in terahertz (THz) range have been observed from mesa structures of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (Bi212) single crystals¹. It has been established that the radiation frequency is determined by both the ac Josephson frequency and the resonance condition of the geometrical cavity². In order to understand the mechanism of the radiation from the intrinsic Josephson junctions (IJJs) in Bi212 , we studied the radiation line width and shape. These might depend upon the physical parameters of the Bi212 single crystal such as the number of IJJs the fluctuations of the quasiparticles and pairs, the non-linearity and non-equilibrium conditions, and the stability of the electrical circuit including the IJJs. However, technical difficulties have been delayed the line width measurements in the THz range. Recently, we succeeded in measuring the radiation line width using a frequency mixer. These results will be compared to those from a single junction 1) L. Ozyuzer *et al.*, Science **318** (2007) 1291., 2) K. Kadowaki *et al.*, J. Phys. Soc. Jpn. **79** (2010) 023703

¹This work was supported by CREST-JST and WPI-MANA project(NIMS). This work is in part performed in collaboration with Dr. Wai Kwok and his group in Argonne National Lab.

10:48AM V21.00015 High resolution copper M-Edge resonant inelastic X-ray scattering at MERLIN, LEWIS WRAY, YI-DE CHUANG, Lawrence Berkeley National Laboratory — The Advanced Light Source MERLIN RIXS spectrometer (beamline 4.0.3) is a new user endstation for resonant inelastic X-ray scattering at the Advanced Light Source. I will discuss new scientific explorations that are expected to be possible with the system, including preliminary data obtained during the commissioning period on cuprate samples. Because very few previous studies have been performed at the M-Edge, the presentation will review how M-Edge scattering data at MERLIN resemble and differ from the more broadly studied transition metal K- and L-edges, including critical parameters of the excitation process such as fitted intermediate state lifetimes, X-ray penetration depth, spin-orbit coupling and scattering intensity for different types of excitation mode.

Thursday, March 1, 2012 8:00AM - 11:00AM –
Session V22 DMP DCOMP: Focus Session: Fe-based Superconductors - Magnetism and Anisotropy 254B

8:00AM V22.00001 In Plane Resistivity Anisotropy in iron Chalcogenides¹, JIUN-HAW CHU, CHRIS KUCHARCZYK, IAN FISHER, Stanford University — FeTe suffers a bicollinear antiferromagnetic ordering, with a $(\frac{1}{2} \ 0)$ ordering wave-vector, in contrast to the $(\frac{1}{2} \ \frac{1}{2})$ ordering wave-vector found in underdoped “122” and “1111” iron pnictides. At the optimal doping the static $(\frac{1}{2} \ 0)$ order disappears and a spin resonance at the $(\frac{1}{2} \ \frac{1}{2})$ wave-vector emerges. Here we report measurements of the in-plane resistivity anisotropy of single crystals of $\text{Fe}_{1+\delta}\text{Te}_{1-x}\text{Se}_x$ for underdoped and optimally doped compositions. The underdoped compounds were partially detwinned by applying uni-axial strain along the $(\frac{1}{2} \ 0)$, revealing a larger resistivity along the antiferromagnetic ordering direction. However, for optimal doping uni-axial strain induces the largest resistivity anisotropy along the $(\frac{1}{2} \ \frac{1}{2})$ direction, similar to the “122” family of compounds. This behaviour suggests that in addition to the presence of spin resonance, a divergent nematic susceptibility might be a key feature associated with optimal doping in iron based superconductors.

¹This work is supported by the Department of Energy, Office of Basic Energy Sciences under contract DE-AC02-76SF00515.

8:12AM V22.00002 The temperature dependence of the conductance anisotropy of the pnictides studied via Monte Carlo simulation of the Spin-Fermion model, SHUHUA LIANG, CENGIZ SEN, ADRIANA MOREO, ELBIO DAGOTTO, Department of Physics, University of Tennessee and Materials Science and Technology Division, ORNL, GONZALO ALVAREZ, Computer Science and Mathematics Division and Center for Nanophase Materials Sciences, ORNL — The undoped three-orbital (xz , yz , xy) spin-fermion model for the pnictides is studied via Monte Carlo (MC) simulations [1], using both the standard exact diagonalization of the fermionic sector (supplemented by cooling down procedures) developed in the manganite context [2], as well as the truncated polynomial expansion techniques [3]. The magnetic order is found to be the expected $(\pi, 0)$ wavevector and the angle-resolved photoemission signal is in good agreement with experiments. The low-temperature conductance reveals the experimentally observed anisotropy between the ferromagnetic and the antiferromagnetic (AFM) directions, with the largest conductance for the AFM case, similarly as observed in recent investigations using the Hartree-Fock approximation to the Hubbard model [4]. The finite temperature MC analysis also produces results in good agreement with transport experiments. [1] S. Liang, G. Alvarez, C. Sen, A. Moreo, and E. Dagotto, submitted for publication. [2] C. Sen, S. Liang, and E. Dagotto, arXiv: 1109.1797 ; and references therein. [3] C. Sen, G. Alvarez, Y. Motome, N. Furukawa, I. A. Sergienko, T. Schulthess, A. Moreo, and E. Dagotto. Phys. Rev. B 73, 224430 (2006). [4] X. Zhang and E. Dagotto, Phys. Rev. B 84 132505 (2011).

8:24AM V22.00003 Anisotropy in BaFe₂Se₃ single crystals with double chains of FeSe tetrahedra, HECHANG LEI, HYEJIN RYU, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, ANATOLY FRENKEL, Physics Department, Yeshiva University, CEDOMIR PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory — Since two-dimensional (2D) FePn or FeCh (Pn = pnictogens, Ch = chalcogens) tetrahedron layers are the common structural ingredient in all iron based superconductors, they are probably related to high temperature superconductivity. In order to fully understand the nature of iron-based superconductivity, study of materials containing similar FePn or FeCh tetrahedron as building blocks is of significant interest. BaFe₂Se₃ contains one-dimensional (1D) double chains of edge shared Fe-Se tetrahedra along the b-axis, in contrast to iron chalcogenide superconductors which feature two-dimensional (2D) Fe-Se planes. We report the anisotropic physical properties and local crystal structure of Ba_{1.00(4)}Fe_{1.9(1)}Se_{3.1(1)} single crystals. It shows that BaFe₂Se₃ is a semiconductor with a short-range AFM correlation at the room temperature and a long-range AFM order below 255 K. Composition analysis indicates that all crystallographic sites are fully occupied. X-ray absorption near edge structure (XANES) result shows that the valence of Fe is about 1.87+.

8:36AM V22.00004 Towards an understanding of magnetic interactions and anisotropies in iron superconductors, ELENA BASCONES, Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC) — The itinerant or strong coupling origin of magnetism in iron pnictides is still unsettled. The localized description generally assumes AF exchange constants satisfying $2J_2 > J_1$, with J_1 and J_2 referring to first and second nearest neighbors respectively. The itinerant picture relies on the nesting of the Fermi surface. Both descriptions reproduce the columnar ordering found experimentally. The role played by the Hund's coupling J_H and the orbital degree of freedom are also highly debated. Orbital ordering has been invoked to explain the anisotropic resistivity and optical conductivity. We make connection between these two pictures by studying the same five-orbital model within Heisenberg and mean field descriptions [1]. We have found that J_2/J_1 strongly depends on the charge and orbital filling what results in an unexpected sensitivity of the AF ordering to crystal field parameters. J_1 and J_2 can become ferromagnetic at large J_H . Consistent results are obtained in the mean field description. We also analyze the resistivity and optical conductivity anisotropies and show that they are a consequence of magnetism and not of orbital ordering [2].

[1] M.J. Calderón et al, arXiv:1107.2279. E. Bascones et al, PRL 104, 227201 (2010).

[2] B. Valenzuela et al, PRL 105, 207202 (2010).

9:12AM V22.00005 Nematic order and its implications to the iron pnictides: pseudogap behavior, orbital order, and magneto-structural phase diagram, R.M. FERNANDES, Columbia University and Los Alamos National Lab, A.V. CHUBUKOV, University of Wisconsin-Madison, J. KNOLLE, Max-Planck-Institut für Physik komplexer Systeme, Dresden, I. EREMIN, Institut für Theoretische Physik III, Ruhr-Universität Bochum, J. SCHMALIAN, Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie — We present an electronic model for the emergence of nematic order in the iron pnictides. In particular, we show that the degeneracy of the magnetic ground state, allied to spin fluctuations, gives rise to a state that spontaneously breaks the tetragonal symmetry of the system, but preserves its spin-rotational symmetry. The nematic state displays several anisotropic properties, inducing a weak orbital polarization as well as a small orthorhombic distortion of the lattice. Nematic order also enhances the magnetic fluctuations and facilitates the magnetic phase transition, leading to a joint magnetic and meta-nematic transition, as well as to a pseudogap behavior due to magnetic precursors. Finally, we discuss the characters of the magnetic and structural phase transitions, showing that electron doping tends to split both transitions, whereas pressure and lattice softness tend to make them simultaneous. Our model provides a simple framework to understand the interplay between the different degrees of freedom present in the iron pnictides, shedding light on the primary role played by magnetism in these materials.

9:24AM V22.00006 Impurity-Induced Electronic Nematic State in Iron-Pnictide Superconductors¹, YUICHI YAMAKAWA, YOSHIO INOUE, HIROSHI KONTANI, Nagoya University — We propose that impurity-induced electronic nematic state is realized above the orthorhombic structure transition temperature T_S in iron-pnictide superconductors [1]. In the presence of strong orbital fluctuations near T_S , it is theoretically revealed that a single impurity induces non-local orbital order with C_2 -symmetry, consistently with recent STM/STS measurements. Each impurity-induced C_2 orbital order aligns along a-axis by applying tiny uniaxial pressure along b-axis. In this impurity-induced nematic phase, the resistivity shows sizable in-plane anisotropy ($\rho_b/\rho_a \sim 2$) even above T_S , actually observed in various “detwinned” samples. The present study indicates the existence of strong orbital fluctuations in iron-pnictide superconductors. [1] Y. Inoue, Y. Yamakawa and H. Kontani, arXiv:1110.2401.

¹This study has been supported by Grants-in-Aid for Scientific Research from MEXT of Japan, and by JST, TRIP.

9:36AM V22.00007 Effect of uniaxial strain on the structural and magnetic phase transitions in BaFe₂As₂, CHETAN DHITAL, Boston College, Z. YAMANI, Canadian Neutron Beam center, Canada, WEI TIAN, Oak ridge National Laboratory, Oakridge, TN, J. ZERETSKY, Ames Laboratory, A.S. SEFAT, Oak ridge National Laboratory, Oakridge, TN, ZIQIANG WANG, Boston College, R.J. BIRGENEAU, University of California, Berkeley, STEPHEN WILSON, Boston College — We report neutron scattering experiments probing the influence of uniaxial strain on both the magnetic and structural order parameters in the parent bilayer iron pnictide compound BaFe₂As₂. Under the application of modest strain fields along the in-plane orthorhombic b-axis, we observe an upward shift in the onset of both the structural and magnetic phase transition temperatures. Our data show that modest strain fields can affect significant changes in phase behavior simultaneous to the removal of structural twinning effects. As a result, we demonstrate in BaFe₂As₂ samples detwinned via uniaxial strain that the in-plane C_4 symmetry is broken by both the structural lattice distortion and long-range spin ordering at temperatures far above the nominal, strain-free, phase transition temperatures. The relevance of our measurements to earlier transport measurements in detwinned crystals of BaFe₂As₂ is discussed.

9:48AM V22.00008 Anisotropic transport properties of the paramagnetic state of iron-based superconductors, JOERG SCHMALIAN, Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, ELIHU ABRAHAMS, University of California Los Angeles, RAFAEL FERNANDES, Columbia University and Los Alamos National Lab — Recent experiments in detwinned iron-pnictide samples have revealed strong anisotropies in the in-plane transport properties of the paramagnetic state. Since these anisotropies cannot be attributed solely to the small orthorhombic distortion of the lattice, it has been proposed that an underlying anisotropic electronic order is at play. One of the candidates is the Ising-nematic order that emerges due to the degeneracy of the magnetic ground state. Here we present a microscopic model for the transport properties of this nematic phase, considering both the elastic scattering by impurities as well as the inelastic scattering by anisotropic spin fluctuations. We show that the interference between these two scattering channels give rise to anisotropic non-Fermi liquid transport properties. In particular, we explain the observed sign of the resistivity anisotropy in electron-doped samples and predict a sign-change for sufficiently hole-doped samples. We also address the suppression of the resistivity anisotropy with sample annealing, as well as its dependence on alkaline-earth substitution. Finally, we discuss the predictions of our model to the thermopower anisotropy.

10:00AM V22.00009 Anisotropic magnetoelastic coupling in iron arsenide superconductors: an x-ray diffraction study in high magnetic field, J.P.C. RUFF, R.K. DAS, Z. ISLAM, Advanced Photon Source, Argonne National Laboratory, J.-H. CHU, H.-H. KUO, I.R. FISHER, Stanford University, H. NOJIRI, Tohoku University — We report high-resolution single crystal x-ray diffraction measurements of underdoped $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ in pulsed magnetic fields as high as 28 Tesla. Our direct measurements confirm earlier reports of strong and highly anisotropic magnetoelastic coupling in iron arsenides. We observe magnetic field induced de-twinning of orthorhombic samples, and characterize the magnitude of the effect as a function of temperature and field. We identify a range of field and temperature where samples can be 100% de-twinned by magnetic fields less than 30 Tesla. The effect shows a notable insensitivity to SDW ordering, but varies rapidly in the vicinity of the superconducting transition.

10:12AM V22.00010 In-plane structural and electronic anisotropy in de-twinned $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$, ERICK BLOMBERG, M.A. TANATAR, W.E. STRASZHEIM, The Ames Laboratory, Ames, IA, USA., B. SHEN, H.H. WEN, Nanjin University, Nanjin, China., R. PROZOROV, The Ames Laboratory, Ames, IA, USA. — The iron-pnictides undergo a tetragonal to orthorhombic structural transition below a doping - dependent temperature T_s . In the absence of external stress or strain, the orthorhombic phase is divided into four degenerate, equally populated, “twin” structural domains, obscuring direct measurement of in-plane anisotropy. This degeneracy may be broken through mild mechanical stress or strain leaving the sample de-twinned. The properties of detwinned $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$ with $x=0.1, 0.18$ (hole under-doped) were discussed previously [1]. Here we report polarized-light microscopy and AC transport measurements of strain-detwinned $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$ with a doping range from $x=0.15$ to $x=0.35$. Our results provide new insight into a region of coexisting magnetic and superconducting order parameters.

[1] J. J. Ying, et al. Phys. Rev. Lett. **107** 067001 (2011).

10:24AM V22.00011 Nematic phase persisting above the superconducting dome of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$, S. KASAHARA, H.J. SHI, K. HASHIMOTO, T. SHIBAUCHI, T. TERASHIMA, Y. MATSUDA, Kyoto University, T. FUKUDA, JAEA Spring-8, K. SUGIMOTO, JASRI Spring-8, A.H. NEVIDOMSKYY, Rice University — Strongly interacting electrons can exhibit novel collective phases, among which the electronic nematic phases are perhaps the most surprising as they spontaneously break rotational symmetry of the underlying crystal lattice. Here, we provide the first thermodynamic evidence in pure crystals of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ that the nematicity develops well above the structural transition and persists to the nonmagnetic superconducting regime, resulting in a new phase diagram strikingly similar to the pseudogap phase diagram in the cuprates. Our highly sensitive magnetic anisotropy measurements using microcantilever torque-magnetometry under in-plane field rotation reveal pronounced two-fold oscillations, which break the tetragonal symmetry. Combined with complementary high-resolution synchrotron X-ray and resistivity measurements, our results consistently identify two distinct temperatures—one at T^* , signifying a true nematic transition, and the other at $T_s (< T^*)$, which we show to be not a true phase transition, but rather what we refer to as a “meta-nematic transition”, in analogy to the well-known metamagnetic transition in the theory of magnetism.

10:36AM V22.00012 Unusual giant negative thermal expansion in La-doped CaFe_2As_2 superconducting single crystal¹, ALWYN REBELLO, JOHN J. NEUMEIER, Montana State University, ZHAOSHUN GAO, YANPENG QI, YANWEI MA, Chinese Academy of Sciences — Large negative thermal expansion (NTE), wherein a material substantially shrinks on heating, is a phenomenon that occurs only in very rare materials.^{2,3} Here we present results on anisotropic and unusually large NTE in single crystalline $\text{Ca}_{0.8}\text{La}_{0.2}\text{Fe}_2\text{As}_2$ (CLFA), a recently discovered high temperature superconducting material. The volume thermal expansion coefficient in CLFA remains negative over the entire measured temperature range and reaches a maximum of $\Omega = -90 \times 10^{-6} \text{ K}^{-1}$ near 65 K, which is remarkably large compared to the thermal expansion (TE) of most other materials. Furthermore, we do not observe signatures of any structural transition in the linear TE in the a , b and c axes. Our results on TE and heat capacity behavior in the vicinity of superconducting transition temperature ($T_C = 42.7 \text{ K}$) indicate non-bulk superconductivity in the sample. The observed large NTE in our sample is attributed to anomalous transverse modes which may vibrate in a quartic potential as in ScF_3 .⁴

¹Supported by NSF Grant DMR-0907036

²T. A. Mary et al. Science, **272**, 90 (1996)

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10:48AM V22.00013 Lower critical field, anisotropy, and two-gap features of LiFeAs , KALYAN SASMAL, Department of Physics and TCSUH, University of Houston, Houston, Texas 77204-5002, USA, B. LV, Z. TANG, Department of Chemistry and TCSUH, University of Houston, Houston, Texas 77204-5003, USA, F. WEI, Y. XUE, Department of Physics and TCSUH, University of Houston, Houston, Texas 77204-5002, USA, A. GULOY, Department of Chemistry and TCSUH, University of Houston, Houston, Texas 77204-5003, USA, CHING-WU CHU, Department of Physics and TCSUH, University of Houston, Houston, Texas 77204-5002; Lawrence Berkeley National Laboratory, 1 Cyclotron Road, USA — The magnetic properties of LiFeAs , as single crystalline and polycrystalline samples, were investigated. The lower critical field deduced from the vortex penetration of two single crystals appears to be almost isotropic with a temperature dependence closer to that of two-gap superconductors. The parameters extracted from the reversible magnetizations of sintered polycrystalline samples are in good agreement with those from the single-crystal data.

**Thursday, March 1, 2012 8:00AM - 11:00AM –
Session V23 DCMP: Superconductivity: Mostly Transport 255**

8:00AM V23.00001 Thermal Conductivity Data Near T_c as a Probe of Unconventional Superconductivity, BRIAN SALES, Oak Ridge National Laboratory — In classical phonon-mediated superconductors, the thermal conductivity, κ , just below T_c decreases since electrons in the superfluid state carry no heat. A decrease in κ occurs just below T_c even for BCS superconductors with relatively high transition temperatures such as Nb_3Sn and MgB_2 . By contrast, in all of the unconventional superconductors, of which the author is aware, the thermal conductivity always increases just below T_c . It is hypothesized in these unconventional superconductors that magnetic or some other type of fluctuation that scatters phonons above T_c are frozen out below T_c , resulting in a larger κ . This suggests that a relatively simple thermal conductivity measurement may be a way of identifying superconductors with an unusual pairing mechanism. Although this phenomenology does not help identify new superconductors, it may help determine which materials have the potential for a much higher T_c . Several related examples of the effects of magnetic fluctuations or excitations on thermal transport also will be presented. This research was supported by the Materials Sciences and Engineering Division, Office of Science, U. S. Department of Energy.

8:12AM V23.00002 Critical currents in thin-film superconductors via two-coil mutual inductance measurements, JOHN DRASKOVIC, JIE YONG, MICHAEL HINTON, ADAM AHMED, Department of Physics, The Ohio State University, SONG WANG, Department of Physics, Stanford University, STANLEY STEERS, THOMAS LEMBERGER, Department of Physics, The Ohio State University — Following Claassen et al. (RSI 1991), we determine the critical current density, $J_c(T)$, in a superconducting thin film by measuring the inductive coupling between two coils located on opposite sides of the film as a function of temperature. For several values of the AC drive magnetic field, we record the temperature at which inductive coupling between the coils jumps dramatically. The peak current density in the film at such temperature is computed by numerical simulation. For thin niobium films, we obtain $J_c(0)$ values greater than 10 percent of the Ginzburg-Landau (GL) prediction with the correct temperature dependence. This suggests the possibility of practical measurement of the GL coherence length in thin films without need for the strong magnetic fields used to measure B_{c2} . Application of this technique to cuprates and pnictides will be discussed.

8:24AM V23.00003 Anomalous dependence of interface superconductivity on carrier density in metal-insulator bilayer, JIE WU, Brookhaven National Laboratory & National High Magnetic Field Laboratory, OSHRI PELLEG, GENNADY LOGVENOV, ANTHONY BOLLINGER, Brookhaven National Laboratory, GREG BOEBINGER, National High Magnetic Field Laboratory, IVAN BOZOVIC, Brookhaven National Laboratory — The interface superconductivity is of particular interest for its higher superconducting temperature (T_c) and close connection to the HTS study. However, despite of the experimental and theoretical progress, the answer to the following key question still remains ambiguous: can the underlying mechanism of the interface superconductivity be interpreted solely in terms of charge transfer and Sr interdiffusion? One experimental approach to answer this question is to study the dependence of T_c on the carrier density of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4/\text{La}_2\text{CuO}_4$ (LSCO/LCO) bilayer by changing the doping level in the metallic LSCO layer. The charge transfer and cation interdiffusion at the interface is proportional to the carrier density in LSCO layer; therefore, T_c of the interface is expected to show a significant and non-monotonic dependence on the carrier density. To exam this prediction, we synthesized a series of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4/\text{La}_2\text{CuO}_4$ bilayers with x ranging in 0.27 to 0.47 by atomic layer-by-layer molecular beam epitaxy (ALL-MBE). The uniqueness of these samples is a 4% Sr doping gradient of the central doping level across the 10mm width of the substrate. These combinatorial samples realize an extremely fine tuning of doping and enable us to construct a phase diagram that is 30 times denser than a normal method can achieve.

8:36AM V23.00004 Magnetotransport of $\text{La}_{(2-x)}\text{Sr}_x\text{CuO}_4$ with Nearly Continuous Doping, ZACHARY STEGEN, JIE WU, JONATHON KEMPER, GREG BOEBINGER, Florida State University, SCOTT RIGGS, Stanford University, FEDOR BALAKIREV, ALBERT MIGLIORI, Los Alamos National Laboratory, IVAN BOZOVIC, Brookhaven National Laboratory — Hall resistivity and longitudinal magnetoresistance were measured in fields up to 35 T. The samples were grown using Combinatorial Molecular Beam Epitaxy (COMBE) where the strontium doping changes continuously across the sample. Thirty simultaneous transport measurements were taken on a sample from a single growth, which allows for unprecedented resolution in doping ($\Delta p \approx 0.0002$). A series of these measurements were performed with the goal of examining the phase diagram of the hole-doped cuprates, particularly an increase in the Hall number around optimum doping.

8:48AM V23.00005 Decoupling of superconducting planes of $\text{La}_{1.905}\text{Ba}_{0.095}\text{CuO}_4$ in a transverse magnetic field¹, JOHN TRANQUADA, Brookhaven National Lab, Z. STEGEN, G.S. BOEBINGER, National High Magnetic Field Lab, SU JUNG HAN, JIE WU, ZHIJUN XU, GENDA GU, QIANG LI, Brookhaven National Lab — We have measured the resistivity parallel and perpendicular to the CuO_2 planes in single crystals of $\text{La}_{1.905}\text{Ba}_{0.095}\text{CuO}_4$ for magnetic fields up to 35 T applied along the c -axis. Below the zero-field superconducting transition temperature of 32 K, we observe that, above a threshold field, the c -axis resistivity grows with field, eventually reaching a maximum and then decreasing. At the resistivity maximum, interlayer pair tunneling becomes insignificant. Under the same field and temperature conditions, the in-plane resistivity remains quite low, reflecting robust superconductivity. We identify a regime in which the superconducting planes are effectively decoupled. At 20 K, a field much greater than 35 T would be required to destroy the in-plane pairing, despite the fact that the field also induces both charge and spin stripe order (J.S. Wen *et al.*, arXiv:1009.0031).

¹Work at BNL supported by Office of Basic Energy Sciences, US DOE, under Contract No. DE-AC02-98CH10886. NHMFL is supported by NSF under Cooperative Agreement No. DMR-084173.

9:00AM V23.00006 Spatial Inhomogeneity in Oxygen Modulated Potassium Tungsten Oxide Thin Films: implications for superconductivity and metal-insulator transitions¹, KO MUNAKATA, KATHERINE LUNA, Geballe Laboratory for Advanced Materials, Stanford University, AKIO TSUKADA, Department of Applied Physics, Tokyo University of Science, SUBHASH RISBUD, THEODORE GEBALLE, MALCOLM BEASLEY, Geballe Laboratory for Advanced Materials, Stanford University — High quality potassium tungsten oxide ($\text{K}_{0.33}\text{WO}_y$) films were synthesized by pulsed laser deposition followed by annealing in vacuum. Oxygen concentration modulated anomalous correlation of metal-insulator and superconductivity transitions were studied; a similar scenario was recently suggested in the literature [1] for polycrystalline rubidium tungsten oxide samples. Detailed studies of the transport properties below and above the superconducting transition temperature exhibit a diversity of unexpected behavior. Some of our results can be interpreted as a signature of reduced dimensionality in the ab -plane in oxygen-rich insulating samples, implying a formation of spatially inhomogeneous electronic structure. We compare such phenomenology to the behavior of other materials with strong electron-phonon interactions, and discuss its implication for the possible high temperature superconducting anomaly in sodium tungsten oxides reported in the literature [2]. [1] D. C. Ling et. al., J. Phys. Conf. Ser. 150, 052141 (2009). [2] S. Reich, and Y. Tsabba, Eur. Phys. J. B 9, 1 (1999).

¹This work is supported by the AFOSR and was supported initially by US DOE.

9:12AM V23.00007 Thermal Hall effect in YBCO: Probing Fermi-surface reconstruction inside the superconducting state, OLIVIER CYR-CHOINIÈRE, FRANCIS LALIBERTÉ, SOPHIE DUFOUR-BEAUSÉJOUR, GAËL GRIS-SONNANCHE, RYAN T. GORDON, NICOLAS DOIRON-LEYRAUD, LOUIS TAILLEFER, Université de Sherbrooke, Canada, BRAD J. RAMSHAW, RUIXING LIANG, DOUG A. BONN, WALTER N. HARDY, University of British Columbia, Canada, CYRIL PROUST, LNCMI, France — The thermal Hall (Righi-Leduc) effect was measured in the cuprate superconductor YBCO at a doping $p = 0.11$, as a function of magnetic field H up to 29 T. At temperatures well below the zero-field superconducting T_c , the thermal Hall conductivity κ_{xy} is positive at low field and then turns over to become negative at fields above 15 T. The negative κ_{xy} is consistent with the negative Hall and Seebeck coefficients observed in the normal state above 25 T [1,2]. This further supports our interpretation: the Fermi surface of YBCO contains a small electron-like pocket [3] in that region of the phase diagram, the result of a Fermi-surface reconstruction attributed to stripe order [4]. In the $T = 0$ limit at $H = 29$ T, we find reasonable agreement with the Wiedemann-Franz law, $\kappa_{xy}/T = L_0\sigma_{xy}$. The fact that κ_{xy} changes sign at $H \approx 15$ T is consistent with a scenario of phase competition whereby stripe order emerges only at finite field, in agreement with recent NMR studies that detect the onset of charge-stripe order above 15 T [5].

[1] LeBoeuf *et al.*, *PRB* **83**, 054056 (2011); [2] Laliberté *et al.*, *Nat. Commun.* **2**, 432 (2011); [3] LeBoeuf *et al.*, *Nature* **450**, 533 (2007); [4] Chang *et al.*, *PRL* **104**, 057005 (2010); [5] Wu *et al.*, *Nature* **477**, 191 (2011).

9:24AM V23.00008 On the magnetic tricritical point in $\text{BaFe}_{2(1-x)}\text{Co}_{2x}\text{As}_2$, COSTEL ROTUNDU, Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, ROBERT BIRGENEAU, Department of Physics, Department of Materials Science and Engineering, University of California, Berkeley, CA 94720, USA — We present here high resolution magnetization measurements on high-quality $\text{BaFe}_{2(1-x)}\text{Co}_{2x}\text{As}_2$, $0 \leq x \leq 0.046$ as-grown single crystals. The results confirm the existence of a magnetic tricritical point in the (x, T) plane at $x_{tr}^m \approx 0.022$ [1,2]. We show that the extrapolated T_c onset doping could be close to the magnetic tricritical point x_{tr}^m . It has been speculated that the magnetic critical point is relevant to the superconductivity in this series [3]. Finally, we comment on the universality of the tricritical point in the superconducting 122s.

[1] M. G. Kim *et al.*, *Phys. Rev. B* **83**, 134522 (2011).
 [2] C. R. Rotundu and R. J. Birgeneau, *Phys. Rev. B* **84**, 092501 (2011).
 [3] G. Giovannetti *et al.*, *Nature Communications* **2**, article number 398 (2011).

¹This work was supported by the Director, Office of Science, Office of Basic Energy Sciences, US Department of Energy.

9:36AM V23.00009 $\text{Rb}_x\text{Fe}_2\text{Se}_2$: A study of superconductivity under high pressure, MELISSA GOOCH, BING LV, LIANGZI DENG, Dept. of Physics at the University of Houston and TcSUH, TAKAKI MURAMATSU, Geophysical Laboratory, Carnegie Institution of Washington, JIM MEEN, Dept. of Chemistry at the University of Houston and TcSUH, YUYI XUE, BERND LORENZ, Dept. of Physics at the University of Houston and TcSUH, CHING-WU CHU, Dept. of Physics at the University of Houston and TcSUH; Lawrence Berkeley National Laboratory — Superconductivity was reported in $\text{Rb}_x\text{Fe}_2\text{Se}_2$ in early 2011, after the discovery of similar Fe-based chalcogenides, $\text{K}_x\text{Fe}_2\text{Se}_2$ and $\text{Cs}_x\text{Fe}_2\text{Se}_2$ in December 2010. These Fe-based chalcogenides have similar structures to the iron pnictides, with a superconducting transition of approximately 30 K. Here we report the results of the physical characterization and the subsequent high-pressure study on two samples with slightly different compositions of $\text{Rb}_x\text{Fe}_2\text{Se}_2$. From resistivity measurements, $\text{Rb}_{0.93(2)}\text{Fe}_{1.70(2)}\text{Se}_2$ (sample A) was found to be superconducting and $\text{Rb}_{0.90(1)}\text{Fe}_{1.78(1)}\text{Se}_2$ (sample B) was found to be semiconducting. Further sample characterization was conducted through magnetic and thermoelectric power measurements, which support the initial resistivity findings. High pressure resistivity measurements were conducted with a BeCu clamp cell up to approximately 1.8 GPa. Initially, the T_c of sample A increases slightly until p reaches ~ 1 GPa. However, at further increasing pressure, T_c starts to decrease and superconductivity is completely suppressed at about 6 GPa. Sample B was not found to be superconducting up to 1.8 GPa.

9:48AM V23.00010 Unusual superconducting state in Pr-doped CaFe_2As_2 , LIANGZI DENG, BING LV, MELISSA GOOCH, FENGYAN WEI, YANYI SUN, Dept. of Physics at the University of Houston and TcSUH, JAMES MEEN, Dept. of Chemistry at the University of Houston and TcSUH, YUYI XUE, BERND LORENZ, Dept. of Physics at the University of Houston and TcSUH, CHING-WU CHU, Dept. of Physics at the University of Houston and TcSUH, Lawrence Berkeley National Laboratory — We report the detection of unusual superconductivity up to 49 K in Pr-doped single crystalline CaFe_2As_2 as evidenced from the resistive, magnetic and thermoelectric measurements. This superconducting transition observed suggests the possible existence of two phases: a field as low as 500 Oe can totally suppress the observed diamagnetic susceptibility above 21K. The 49 K part has a low critical field < 4 Oe, and the other at 21K, with a high upper critical field > 5 T. Our observations are in strong contrast to previous reports of doping or pressurizing layered compounds AeFe_2As_2 (Ae122), where Ae = Ca, Sr, or Ba. In Ae 122, hole-doping has been previously observed to generate superconductivity with a transition temperature (T_c) only up to 38 K and pressurization has been reported to produce superconductivity with a T_c up to 30 K. The experiment results of resistivity and inductance measurements of Pr-doped Ca122 under pressure up to 2.0 GPa will also be discussed.

10:00AM V23.00011 Fermi-liquid behavior of quasiparticle scattering in the normal state of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$, YING JIA, LEI FANG, ULRICH WELP, ALEXEI KOSHELEV, GEORGE CRABTREE, WAI-KWONG KWOK, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA — We present studies of the galvanomagnetic effects of compensated $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ ($x=0.32\sim 0.6$) superconductors. The magnetoresistance follows the relaxed Kohler's scaling for all doping levels. Using a two-band model, we quantitatively extracted the scattering parameter m^*/τ and the carrier density of the electron and hole bands. The temperature dependence of the carrier concentration reveals the semimetal properties of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$. The Fermi-liquid behavior, $m^*/\tau \sim T^2$, is observed from optimally doped $x=0.32$ to over-doped $x=0.6$ crystals, suggesting that the proximity of the SDW state does not play an important role in transport. Our analysis suggests that the normal state transport properties of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ can be well understood in the framework of a compensated two-band Fermi-liquid semimetal.

¹Crystal synthesis was supported by the Energy Frontier Research Center funded by the US DOE-BES (YJ, LF, WKK, GWC), materials characterization and theoretical support were provided by the DOE-BES (UW, AEK), under Contract No. DE-AC02-06CH11357.

10:12AM V23.00012 Pressure effect on the electronic transport properties of $\text{Fe}_{1+y}\text{Te}_{1-x}\text{Se}_x$, STEVAN ARSENIJEVIĆ, RICHARD GAÁL, HENRIK RØNNOW, Institute of Condensed Matter Physics, Swiss Federal Institute of Technology, EPFL, CH-1015 Lausanne, Switzerland, ROMAIN VIENNOIS, ENRICO GIANNINI, DIRK VAN DER MAREL, DPMC, University of Geneva, 24 Quai E.-Ansermet, 1211 Geneva, Switzerland, LÁSZLÓ FORRÓ, Institute of Condensed Matter Physics, Swiss Federal Institute of Technology, EPFL, CH-1015 Lausanne, Switzerland — We present a systematic study of electronic transport as function of pressure up to 25 kbar of $\text{Fe}_{1+y}\text{Te}_{1-x}\text{Se}_x$ single crystalline samples (with $y = 0.02, 0.05$, and $x = 0, 0.2$, and 0.3). Pressure is demonstrated to be a clean control parameter to drive the system with high Fe-excess through the metal-insulator (MIT) transition, in analogy with increasing the Se-doping or reducing the Fe-excess. The scaling of resistivity $\rho(T, p)$ below 50 K identified a critical pressure of $p_c = 8$ kbar which separates non-metallic and metallic temperature dependences. At the p_c the low-temperature sheet resistance is in the 6.5 k Ω /square range. The Seebeck coefficient (S) at p_c changes sign from negative to positive indicating a change in the electronic structure and in the balance between the electron and hole carriers. The S at the highest pressure exhibits low positive values similar to the metallic, superconducting cuprates. The critical MIT behavior, related to a quantum phase transition, indicates a universality of the Fe- and Cu-based high- T_c superconductors.

10:24AM V23.00013 DC transport properties of Fe(Se,Te) crystals: Effects of Se substitution into Te site, SEIKI KOMIYA, MASAFUMI HANAWA, ICHIRO TSUKADA, Central Research Institute of Electric Power Industry, JST-TRIP, ATSUTAKA MAEDA, University of Tokyo, JST-TRIP — FeTe is an antiferromagnetic semimetal and superconductivity shows up when Te is substituted with Se, but effects of Se substitution are still unclear. To elucidate this issue, we study the behavior of Hall resistance in detail using single crystalline $\text{FeSe}_x\text{Te}_{1-x}$ with $x = 0$ to 0.4. Single crystals are grown by Bridgman method, and Hall resistance is analyzed within the standard 2-carrier model. We find that the electron density n_e is larger than the hole density n_h for $x \leq 0.3$ samples, but n_h becomes greater than n_e for $x = 0.4$ crystal. We also find that electron mobility enhances especially at low temperatures with Se substitution.

10:36AM V23.00014 Ferroelectricity and magnetoelectric coupling in underdoped $\text{La}_2\text{CuO}_{4+x}$, Z. VISKADOURAKIS, I. RADULOV, IESL-FORTH, A.P. PETROVIC, Division of Physics and Applied Physics, Nanyang Technological University, Singapore, S. MUKHERJEE, B. ANDERSEN, Niels Bohr Institute, University of Copenhagen, Denmark, G. JELBERT, Cavendish Laboratory, University of Cambridge, U.K., N.S. HEADINGS, S.M. HAYDEN, H. H. Wills Physics Laboratory, University of Bristol, U.K., K. KIEFER, S. LANDSGESELL, Helmholtz-Zentrum-Berlin für Materialien und Energie, Germany, D.N. ARGYRIOU, European Spallation Source ESS AB, Sweden, C. PANAGOPOULOS, IESL-FORTH and Department of Physics, University of Crete, Greece — La_2CuO_4 is an archetypal antiferromagnetic Mott insulator. Upon oxygen doping, a wide range groundstates may be accessed, including glassy magnetic phases and high- T_c superconductivity. However, determining the nature of the charge correlations coexistent with magnetic order has remained elusive, particularly in the highly underdoped limit. In this study, we show that the first holes added to La_2CuO_4 drive the formation of a ferroelectric phase below 4.5K, with slow charge fluctuations developing below 40K. We invoke the formation of polar nanoregions – which are a natural consequence of non-stoichiometric oxygen doping – to explain the emergent ferroelectricity. An anisotropic magnetoelectric coupling is observed and attributed to the Dzyaloshinskii-Moriya interaction. Although this interaction is not responsible for the electronic ordering (unlike in other multiferroic perovskites), the presence of weak magnetoelectricity allows us to confirm charge carrier doping as the cause of ferroelectricity in $\text{La}_2\text{CuO}_{4+x}$.

10:48AM V23.00015 Surface pinning effects in Ag doped superconducting polycrystalline $\text{Y}_1\text{Ba}_2\text{Cu}_3\text{O}_{7-x}$, ATILGAN ALTINKOK, MURAT OLUTAS, KIVILCIM KILIC, ATILLA KILIC, Abant Izzet Baysal University — The current-voltage measurements (I - V curves) with different current sweep rates (dI/dt) were carried out to investigate the effects of silver on the flux dynamics in Ag doped superconducting polycrystalline $\text{Y}_1\text{Ba}_2\text{Cu}_3\text{O}_{7-x}$ sample (YBCO/Ag). Standard and reverse procedures were used in the measurements of I - V curves. In the standard procedure, the dc driving current is cycled up and down; whereas, in the reverse procedure, the current is first cycled down and, then, cycled up. The reverse procedure enables us to investigate the flux motion evolving from the outer surface of the sample to its interior. Upon cycling transport current, the I - V curves of the YBCO/Ag sample exhibit hysteresis effects for both procedures and are sensitive to the variation of dI/dt . The experimental data reveal that the irreversibilities in the I - V curves of undoped YBCO are more prominent than those of YBCO/Ag. One of the main observations in the I - V curves of YBCO/Ag is the peculiar voltage jumps and drops. It was found that these instabilities depend strongly on the magnitude of external parameters dI/dt and H . The instabilities and short and long lived plateau regions observed in I - V curves were explained in terms of plastic flow of flux lines along easy motion channels which are considered mainly as metallic silver paths in the YBCO/Ag sample. In order to understand better the flux dynamics evolving in YBCO/Ag, the results of present measurements were compared to our previous studies on polycrystalline samples of undoped YBCO and MgB_2 .

Thursday, March 1, 2012 8:00AM - 11:00AM – Session V24 FIAP: Low-Dimensional Semiconductors 256

8:00AM V24.00001 $1/f$ Noise in Delta Doped GaAs/AlGaAs Heterostructures¹, YUN SUK EO, STEVEN WOLGAST, CAGLIYAN KURDAK, University of Michigan Department of Physics, L. N. PFEIFFER, K. W. WEST, Princeton University Department of Electrical Engineering — We studied $1/f$ noise of a two-dimensional electron gases (2DEG) in δ -doped $\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ heterostructures. Three samples that we measured were identical except for the δ -doping concentration: $9.1 \times 10^{18}(\text{cm}^{-2})$ (high), $1.3 \times 10^{18}(\text{cm}^{-2})$ (medium), $0.3 \times 10^{18}(\text{cm}^{-2})$ (low). These δ -doping layers are located in the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ region, 800Å above the GaAs and $\text{Al}_x\text{Ga}_{1-x}\text{As}$ interface. We fabricated Corbino and Hall bar structures with different sizes. Carrier density was varied by the persistent photoconductivity effect at low temperature (4.2K). Initially, the samples did not exhibit measurable $1/f$ noise. The high δ -doping concentration samples exhibited parallel conduction. As we increased the carrier concentration in the high and medium-doped samples, $1/f$ noised increased initially, but disappeared as the photo current was saturated. The low-doped samples did not exhibit $1/f$ noise as the carrier concentration was increased. We conclude that $1/f$ noise is caused by the remote ionized impurities in the δ -doped region. Also, changing the DX-center configuration changes the density of the ionized impurities, which then changes the magnitude of $1/f$ noise.

¹University of Michigan was funded by the NSF (DMR-1006500). Princeton University was funded by the Gordon and Betty Moore Foundation and the NSF MRSEC Program (DMR-0819860)

8:12AM V24.00002 Conductance noise in a strongly disordered 2D electron system in Si MOSFETs¹, PING V. LIN, XIAOYAN SHI, JAN JAROSZYŃSKI, DRAGANA POPOVIĆ, National High Magnetic Field Lab., Florida State Univ. — Studies have shown that the metal-insulator transition (MIT) in a 2DES in Si MOSFETs is closely related to the glassy freezing of electrons as temperature $T \rightarrow 0$. However, no glassy relaxations were seen after a T quench. Here we first study the effect of cooling in detail: the carrier density n_s is changed at a high $T \approx 20$ K, the system is then cooled to a desired T with a fixed n_s , and fluctuations of conductance G with time are measured. The analysis of the noise power spectra $S_G \propto 1/f^\alpha$ gives evidence for the onset of slow, glassy dynamics near the MIT as $T \rightarrow 0$, supporting conclusions obtained with a different protocol. While these noise measurements were done in the Ohmic regime, we have also explored the effect of high excitation voltages, deep into the nonlinear regime, on the noise statistics. The results will be discussed in detail. Finally, we show that sweeping n_s at low enough T results in a reproducible fluctuation pattern of $G(n_s)$. Such a pattern, which reflects a particular realization of disorder, does not change even after warming up to 30 K. This demonstrates that the disorder does not change at low T , and that the observed non-Gaussianity of the noise reflects the intrinsic glassiness of the 2DES.

¹Supported by NSF DMR-0905843, NHMFL via NSF DMR-0654118

8:24AM V24.00003 Extended States and Critical Behavior in 2D and 3D Amorphous Conductors, DONALD PRIOUR, Kansas City, Kansas Community College (KCKCC) — With a tight binding treatment for one, two and three dimensional systems, we calculate and analyze electronic states in a conductor with topological disorder, or no correlations among the positions of the hopping sites. The Inverse Participation Ratio (IPR) is used to characterize carrier wave functions with respect to localization. We consider an exponentially decaying hopping integral with range (or “Bohr radius”) l . Using two complementary finite size scaling techniques to extrapolate to the bulk limit (both methods exploit critical behavior in different ways to locate the energy marking the boundary between extended and localized wave functions) which nevertheless yield identical results, we obtain phase diagrams showing regions where states are extended and domains of localized states. We find exclusively localized wave functions for 1D geometries, irrespective of l . In the 2D case, states are localized below a threshold length scale $l_c \approx 1.0$, with a finite fraction of states extended for $l > l_c$. For 3D systems, the extended phase is flanked by regions of localized states and bounded by two mobility edges. The swath of extended states, broad for $l \sim 1$, becomes narrower with decreasing l , scaling asymptotically as $e^{-A/l}$ for $l \ll 1$.

8:36AM V24.00004 The disappearance of weak localization in a strongly correlated 2D hole system¹, RICHARD L.J. QIU, XUAN P.A. GAO², Dept of Physics, Case Western Reserve University, LOREN N. PFEIFFER, KEN W. WEST, Dept of Electrical Engineering, Princeton University — The origin of Metal-Insulator Transition (MIT) in strongly correlated two-dimensional (2D) electrons or holes in semiconductors has long been of great interest. We will present the low temperature (down to 0.05K) transport properties of 10nm GaAs quantum wells with metallic hole densities near the critical point of the 2D MIT (critical density $p_c \approx 0.8 \times 10^{10} \text{cm}^{-2}$). We found that 2D holes exhibit a negative magneto-resistance in small perpendicular magnetic fields, which has been attributed to weak localization in the literature. On the other hand, the magnitude of this negative magneto-resistance is much smaller than conventional 2D weak localization. What is more surprising is that the weak localization induced negative magneto-resistance peak around $B=0$ becomes weaker at lower temperature, suggesting there is a mechanism causing quasiparticles to lose coherence as temperature decreases.

¹This work is supported by NSF (DMR-0906415). The work at Princeton was partially funded by the Gordon and Betty Moore Foundation as well as the NSF MRSEC Program through the Princeton Center for Complex Materials (DMR-0819860).

²Corresponding author

8:48AM V24.00005 Strong negative magnetoresistance in high-mobility 2D electron systems, MICHAEL ZUDOV, ANTHONY HATKE, School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455, USA, JOHN RENO, Sandia National Laboratories, Albuquerque, NM 87185, USA, LOREN PFEIFFER, KEN WEST, Princeton University, Department of Electrical Engineering, Princeton, NJ 08544, USA — This talk reports on a remarkably strong negative magnetoresistance effect in high mobility GaAs/AlGaAs heterostructures and quantum wells. The effect is the strongest at about 1 kG where a deep and strongly temperature dependent minimum is observed. At low temperature, the resistivity at this minimum is a small fraction of the zero field resistivity. The talk will discuss the effects of temperature and in-plane magnetic field on this negative magnetoresistance and compare experimental findings with existing theories. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by NSF Cooperative Agreement No. DMR-0654118, by the State of Florida, and by the DOE and at the Center for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences user facility. The work at Minnesota was supported by the NSF Grant No. DMR-0548014 and by the DOE Grant No. DE-SC002567. The work at Princeton was partially funded by the Gordon and Betty Moore Foundation and the NSF MRSEC Program through the Princeton Center for Complex Materials (DMR-0819860) and the work at Sandia was supported by the Sandia Corporation under Contract No. DE-AC04-94AL85000. Sandia National Laboratories is a multi-program laboratory managed.

9:00AM V24.00006 Nonlinear response of magnetoplasmon resonance, ANTHONY HATKE, MICHAEL ZUDOV, School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455, USA, MICHAEL MANFRA, Department of Physics, West Lafayette, IN 47907 — Magnetoplasmon resonances have been observed in microwave photoresistance of Hall bar-shaped two-dimensional electron systems more than two decades ago. This talk will report on such a resonance in a very high mobility two-dimensional electron gas where it appears as a distinct photoresistivity peak superimposed on a microwave-induced zero-resistance state. In particular, we will discuss the response of this peak to dc electric field. A portion of this work was performed at the National High Magnetic Field Laboratory which is supported by NSF Cooperative Agreement No. DMR-0654118, by the State of Florida, and the DOE. The work at Minnesota was supported by DOE Grant No. DE-SC002567 and NSF Grant No. DMR-0548014. The work at Purdue was supported by DOE grant de-sc0006671.

9:12AM V24.00007 Interference effect in magneto-oscillations in two-dimensional system under bichromatic irradiation, QIANHUI SHI, University of Minnesota, MAXIM KHODAS, University of Iowa, MICHAEL ZUDOV, University of Minnesota — We report on the studies of magneto-oscillations caused by bichromatic irradiation in perpendicular magnetic field. Using quantum kinetic method, we have studied the case of ω , 2ω , and the case of ω , 3ω frequencies. In the latter case the interference part is shown to produce a phase-sensitive contribution. Also, the final answer depends on the polarizations of the two waves.

9:24AM V24.00008 Quantum lifetime of 2D electron in magnetic field¹, SCOTT DIETRICH, SERGEY VITKALOV, City College of New York, DMITRY DMITRIEV, ALEXEY BYKOV, Institute of Semiconductor Physics, 630090 Novosibirsk, Russia — The lifetime of two dimensional electrons in GaAs quantum wells, placed in weak quantizing magnetic fields, is measured using a simple transport method in broad range of temperatures from 0.3 K to 20 K. The temperature variations of the electron lifetime are found to be in good agreement with conventional theory of electron-electron scattering in 2D systems.

¹Supported by NSF (DMR 1104503) and RFBR, project no. 11-02-00925

9:36AM V24.00009 Hall viscosity in lattice models, RUDRO BISWAS, TAYLOR HUGHES, University of Illinois at Urbana-Champaign — We present results from our investigations of the Hall viscosity in lattice models. We use the insight gained from these calculations to comment on using the Hall viscosity to characterize gapped quantum fluids.

9:48AM V24.00010 Rank Saturation in finite size Entanglement Spectrum for Quantum Hall states, BENOIT ESTIENNE, BOGDAN A. BERNEVIG, Princeton University, RAOUL SANTACHIARA, LPTMS Orsay — We investigate analytically in finite size the entanglement spectrum arising from real-space cuts for fractional quantum Hall states. We provide a proof that the rank of the reduced density matrix is saturated for the Laughlin state even on finite sizes.

10:00AM V24.00011 Magnetic field spectra and many-body correlations of spin 3/2 holes confined to GaAs quantum well, GEORGE SIMION, YULI LYANDA-GELLER, Purdue University — We consider two dimensional spin 3/2 hole liquid in the presence of a perpendicular magnetic field. Single particle states of Luttinger Hamiltonian are calculated. For the semiclassical limit, the Hamiltonian is separated into the time-symmetric part treated exactly and time-antisymmetric part treated perturbatively. The angular momentum (spin) 3/2 states are characterized by the Landau level index and parity with respect to reflection about the growth direction. The single-particle spectrum exhibits level-crossings as magnetic field is varied, with or without Rashba and Dresselhaus interactions. The numerical calculations were performed for infinite barrier well, finite size barrier, well doped on one side, symmetrically doped well and parabolic well. Cyclotron mass was calculated and its dependence of the type of structure, magnetic field and symmetry of states is discussed and compared with experimental values. Landé effective factor is defined and evaluated. Shubnikov-de Haas oscillations are calculated. Electron-electron interactions are accounted using (time-dependent) mean field theories. An interesting effect is a single-well non-homogeneous spin-texture state. Possible implications of shape of hole spectra for fractional quantum Hall states are explored.

10:12AM V24.00012 Tunneling spectroscopy of 5/2 fractional quantum Hall excitations in etch defined quantum point contacts, MADHU THALAKULAM, WEI PAN, Sandia National Labs, K.W. BALDWIN, K.W. WEST, L. PFEIFFER, Princeton University — Ever since its discovery the fractional quantum Hall (FQH) state at the even denominator filling fraction $\nu=5/2$ has generated immense interests among researchers. 5/2 FQH excitations are believed to obey non-Abelian statistics and possess topological properties making them an ideal candidate for the proposed fault tolerant topological quantum computation. Theoretical proposals to characterize the topological properties of the 5/2 state are usually based on confined geometries. In this work we report the characterization of the 5/2 state using quasiparticle tunneling experiments in quantum point contacts (QPC). We have successfully fabricated QPCs on high mobility GaAs/AlGaAs heterostructures using conventional photolithography followed by etching and evaporation of Cr/Au depletion gates. Our samples show very stable FQH plateaus at $\nu = 7/3, 5/2$ and $8/3$ filling fractions. Tunneling experiments are performed in the QPCs at various temperatures and also at various pinch-off voltages to characterize the effective charge and Coulomb interaction parameters of the quasiparticles. (Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000).

10:24AM V24.00013 Quasiparticles and excitons for the Pfaffian quantum Hall state, ANTOINE STERDYNIAK, Ecole Normale Supérieure Paris, IVAN RODRIGUEZ, National University of Ireland, Maynooth, Ireland, MARIA HERMANN, Princeton University, JOOST SLINGERLAND, National University of Ireland, Maynooth, Ireland, NICOLAS REGNAULT, Ecole Normale Supérieure Paris, CNRS — We propose trial wave functions for quasiparticle and exciton excitations of the Moore-Read Pfaffian fractional quantum Hall states, both for bosons and for fermions, and study these numerically. Our construction of trial wave functions employs a picture of the bosonic Moore-Read state as a symmetrized double layer composite fermion state. We obtain the number of independent angular momentum multiplets of quasiparticle and exciton trial states for systems of up to 20 electrons. We find that the counting for quasielectrons at large angular momentum on the sphere matches that expected from the CFT which describes the Moore-Read state's boundary theory. In particular, the counting for quasielectrons is the same as for quasiholes, in accordance with the idea that the CFT describing both sides of the FQH plateau should be the same. We also show that our trial wave functions have good overlaps with exact wave functions obtained using various interactions, including second Landau level Coulomb interactions and the 3-body delta interaction for which the Pfaffian states and their quasiholes are exact ground states.

10:36AM V24.00014 Exact results for a fermion chain with fractionalized excitations, MASAAKI NAKAMURA, ZHENG-YUAN WANG, Tokyo Institute of Technology, EMIL BERGHOLTZ, Freie Universität Berlin — We present a number of exact results for a fermion chain with center of mass conservation at $1/3$ filling. The ground state of our model, which is three-fold degenerate even in the case of site dependent interactions, show striking similarities with the superconducting BCS wave functions, the AKLT spin chain, and in particular, with the Laughlin state describing the fractional quantum Hall effect. This state supports exact zero modes with fractional charge slightly below $1/3$ filling, and it has a matrix product representation which enables us to analytically calculate correlation functions, excitation gaps, and the entanglement spectrum. Reference: M. Nakamura, Z.-Y. Wang and E. J. Bergholtz, arXiv:1110.5033

10:48AM V24.00015 Polaronic effects in a single modulation doped GaAs quantum well, GERARD MARTINEZ, CLEMENT FAUGERAS, MILAN ORLITA, Laboratoire National des Champs Magnétiques Intenses, Grenoble, A. RIEDEL, R. REY, KLAUS FRIEDLAND, Paul Drude Institute, Berlin — Absolute magneto-optical transmission measurements have been performed in the far-infrared range under magnetic fields up to 32 T and at a temperature of 1.8 K on a single modulation doped GaAs quantum well (QW) with a width $d_w = 13$ nm. This QW is sandwiched between two GaAs/AlAs superlattices, the whole epilayer being lift-off from the GaAs substrate and deposited on a wedged Si substrate. The carrier concentration $N_s = 3.8 \cdot 10^{11} \text{ cm}^{-2}$ and has a mobility exceeding $10^6 \text{ cm}^2/\text{V}/\text{sec}$ at low temperatures. Due to the absence of the GaAs substrate, the magneto-transmission of the sample, mainly governed by the cyclotron (CR) absorption line, can be followed continuously over the whole range of energies. It reveals a strong polaronic interaction with the LO GaAs-phonon: the results can be interpreted quantitatively using the FHIP model [1] and the related conductivity response [2].

[1] R.P. Feynman, R.W. Hellwarth, C.K. Iddings and P.M. Platzman, Phys. Rev., 127, 1004 (1962).

[2] F.M. Peeters and J.T. Devreese, Phys. Rev. B, 28, 6051 (1983).

Thursday, March 1, 2012 8:00AM - 11:00AM — Session V25 DCOMP DCMF: High Pressure: Experiment 257A

8:00AM V25.00001 Kinetics studies across the phase transition of metals using *dynamic*-DAC, JING-YIN CHEN, WILLIAM EVANS, LLNL — We utilize the time-resolved synchrotron x-ray diffraction and in-situ optical spectroscopy to study the dynamic properties of several metals across the phase transition under different compression rates. The dynamic properties of metals across the pressure-induced phase transition, for example the mechanism of solidification or solid-solid transitions, are lacking. Obtaining the time-resolved structural evolutions of metals under rapid compression is critical to understanding material stability or metastability, and transition mechanism. In addition, the dynamical pressure changes can dramatically influence the microstructure and even phase boundaries, further affecting the properties of metals, such as toughness and strength.

8:12AM V25.00002 Phase Transition Kinetics of GST at High Pressures, ADAM CADIEN, QING YANG HU, HOWARD SHENG, George Mason University — The phase change material Ge₂Sb₂Te₅ (GST) undergoes an amorphous to ordered phase transition in nanoseconds. This ultra-fast phase transition kinetics in conjunction with drastic electrical property changes makes GST an ideal candidate for next generation optical and digital storage media. The origins of this fast transition have thus far been traced back to the atomic configurations of both the amorphous and ordered phases. However the precise configurations of both the ordered and amorphous phases are still unknown with advances from simulations constantly altering our understanding of these structures. To discover the structural dependence of the phase transition kinetics of GST, we have performed in-situ synchrotron X-ray diffraction experiments on GST using a new Hydrothermal Diamond Anvil Cell under a range of pressures and observed new patterns of phase transition of GST at elevated temperatures. Ab initio simulations have been performed to interpret the structural evolutions of GST phases at different pressures, with an emphasis on the role of vacancies in the phase transition. Our results provide new insight into the mechanism of the fast phase transition kinetics of GST.

8:24AM V25.00003 ABSTRACT WITHDRAWN —

8:36AM V25.00004 Pressure-induced phase transitions in GeS under high pressures¹ , RANGA DIAS, Institute for Shock Physics, Department of Physics, Washington State University, Pullman, Washington 99164, CHOONG-SHIK YOO, Institute for Shock Physics, Department of Chemistry, Washington State University, Pullman, Washington 99164 — We have studied the pressure-induced structural and electronic phase transitions of layered GeS (*Pnma*) to 30 GPa, using micro-Raman spectroscopy and electrical resistivity measurements in diamond anvil cells. The result shows a steady decrease in resistivity to that of metal at around 18 GPa. The visual appearance of GeS supports the insulator-metal transition: initially black GeS becomes opaque and eventually reflective with increasing pressure. The Raman result indicates that the metallization is preceded by a structural phase transition, presumably to the previously predicted *Cmcm* structure.

¹The work has been supported by the NSF (DMR-0854618)

8:48AM V25.00005 High pressure behavior of Cr₂O₃ to 62 GPa¹ , KRYSTLE CATALLI, HYUNCHAE CYNN, WILLIAM J. EVANS, Lawrence Livermore National Lab — Corundum-structured oxides are of interest for a broad range of reasons, including their mineralogical occurrences and technological uses. The high pressure behavior of Cr₂O₃ is of particular interest due to the widespread use of ruby, (Al,Cr)₂O₃, as a pressure standard in diamond anvil cells experiments. Although there have been a number of high pressure studies on Cr₂O₃, discrepancies still exist among the different data sets. Here we present synchrotron X-ray diffraction data on the structure and compressional behavior of Cr₂O₃ to 62 GPa. Although no change in crystal structure is detected within the resolution of the measurements, a change in compressional behavior occurs near 30 GPa where Cr₂O₃ changes color from red to orange.

¹Prepared by LLNL under Contract DE-AC52-07NA27344. Work performed at HPCAT, Advanced Photon Source (APS), Argonne National Lab. HPCAT is supported through funding from DOE-NNSA, DOE-BES and NSF. APS is supported by DOE-BES.

9:00AM V25.00006 Amorphous diamond – A high-pressure superhard carbon allotrope , YU LIN, Geological and Environmental Sciences, Stanford University, LI ZHANG, HO-KWANG MAO, Geophysical Laboratory, Carnegie Institution of Washington, PAUL CHOW, YUMING XIAO, High Pressure Collaborative Access Team, Geophysical Laboratory, MARIA BALDINI, High Pressure Synergetic Consortium, Geophysical Laboratory, JINFU SHU, Geophysical Laboratory, Carnegie Institution of Washington, WENDY MAO, Geological and Environmental Sciences, Stanford University — Compressing glassy carbon above 40 GPa, we have observed a new carbon allotrope with a fully *sp*³-bonded amorphous structure and diamond-like strength. Synchrotron x-ray Raman spectroscopy revealed a continuous pressure-induced *sp*²-to-*sp*³ bonding change, while x-ray diffraction confirmed the perseverance of non-crystallinity. The transition was reversible upon releasing pressure. Used as an indenter, the glassy carbon ball demonstrated exceptional strength by reaching 130 GPa with a confining pressure of 60 GPa. Such an extremely large stress difference of >70 GPa has never been observed in any material besides diamond, indicating the high hardness of this high-pressure carbon allotrope. The nanoscale transmission x-ray microscopy is being utilized for accurate pressure-volume determination of glassy carbon and its high-pressure phase.

9:12AM V25.00007 Comparison of the existing internally consistent pressure scales at high pressures and high temperatures¹ , HYUNCHAE CYNN, B.J. BAER, LLNL, Livermore, CA, S.G. MACLEOD, AWE, Aldermaston, UK, W.J. EVANS, M.J. LIPP, J.P. KLEPEIS, ZS. JENEI, J.Y. CHEN, K. CATALLI, LLNL, Livermore, CA, D. POPOV, C.Y. PARK, HP-CAT, APS — There have been several efforts to determine internally consistent pressure scales for static diamond anvil high pressure study. We decide to extend the choice of pressure scales to include W and Cu. A recent study of Cu claims that electronic theory can constrain cold curve and possibly room temperature isotherm (Greeff et al., 2006, JPCS). We will present our comparison of 6 different pressure scales in regards with the suggested Cu EOS. We have measured angle-dispersive x-ray diffraction of Au, Pt, W, Cu, Ne, and NaCl to directly compare with the current existing EOS. We will also discuss discrepancies in the precise determination of pressure of phase transformations.

¹This work performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344. HPCAT use is supported by DOE-BES, DOE-NNSA, NSF, and the W.M. Keck Foundation. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.

9:24AM V25.00008 Simultaneous measurement of pressure evolution of crystal structure and superconductivity in Fese_{0.8} using designer diamonds , WALTER UHOYA, University of Alabama at Birmingham (UAB) Birmingham, AL 35294, USA, NATHANIEL WOLANYK, Illinois Wesleyan University (IWU), Bloomington, IL 61702-2900, USA, GEORGIY TSOI, University of Alabama at Birmingham (UAB) Birmingham, AL 35294, USA, YOGESH VOHRA, Department of Physics, University of Alabama at Birmingham (UAB) Birmingham, AL 35294, USA, SISTLA M RAO, MAU-KUEN WU, Institute of Physics, Academia Sinica, Nankang, Taipei 115, Taiwan, SAMUEL WEIR, Mail Stop L-041, Lawrence Livermore National Laboratory (LLNL) Livermore, CA 94550, USA — Simultaneous high pressure x-ray diffraction and electrical resistance measurements have been carried out on (P4/nmm) PbO type α -FeSe_{0.89} compound to a pressure of 44 GPa and at low temperatures down to 4 K using a synchrotron source and designer diamond anvils technique. At ambient temperature, a structural phase transition from the tetragonal (I4/nmm) phase to orthorhombic (Pbnm) is observed at 11 GPa and persist up to 75 GPa. The superconducting transition temperature increases rapidly with pressure in a parabolic manner reaching a maximum of ~40 K at ~11GPa. It then decreases at higher pressures. We also performed a complimentary pressure dependence x-ray diffraction simultaneously with resistance measurement at low temperatures and observe superconductivity only in the low pressure orthorhombic phase (Cmma) of α -FeSe_{0.89}. Upon increasing pressure at 10 K, structural phase change from a mixed phase of orthorhombic (Cmma) and hexagonal (P63/mmc) to a high pressure orthorhombic phase (Pbnm) is observed at around 12 GPa where T_c is maximum.

9:36AM V25.00009 Melting Studies of Metals in a Paris Edinbrough Cell via Radiography , MAGNUS LIPP, ZSOLT JENEI, DAVE RUDDLE, CHANTEL ARACNE-RUDDLE, HYUNCHAE CYNN, WILLIAM EVANS, Lawrence Livermore National Laboratory, YOSHIO KONO, CURTIS KENNEY-BENSON, CHANGYONG PARK, HPCAT, Advanced Photon Source, Argonne National Laboratory — Equation-of-state measurements of amorphous solids and liquids suffer from the lack of distinct X-ray diffraction patterns that can be indexed and used for a precise and accurate volume determination. For relatively high Z materials, however, a possible remedy might be found in the application of X-ray radiography. The presentation will describe current efforts with regard to cerium and alloys of noble metals in the liquid state. This work was performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344. The X-ray studies were performed at HPCAT (Sector 16), APS/ANL. HPCAT is supported by CIW, CDAC, UNLV and LLNL through funding from DOE-NNSA, DOE-BES and NSF. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.

9:48AM V25.00010 Homoepitaxial Boron Doped Diamond Anvil as Heating Element in a Diamond Anvil Cell, JEFFREY MONTGOMERY, GOPI SAMUDRALA, YOGESH VOHRA, University of Alabama at Birmingham — Recent advances in designer-diamond technology have allowed for the use of electrically and thermally conducting homoepitaxially-grown layers of boron-doped diamond (grown at 1200 °C with a 2% mixture of CH₄ in H₂, resulting in extremely high doping levels $\sim 10^{20}/\text{cm}^3$) to be used as heating elements in a diamond anvil cell (DAC). These diamonds allow for precise control of the temperature inside of the diamond anvil itself, particularly when coupled with a cryostat. Furthermore, the unmatched thermally conducting nature of diamond ensures that no significant spatial gradient in temperature occurs across the culet area. Since a thermocouple can easily be attached anywhere on the diamond surface, we can also measure diamond temperatures directly. With two such heaters, one can raise sample temperatures uniformly, or with any desired gradient along the pressure axis while preserving optical access. In our initial experiments with these diamond anvils we report on the measurement of the thermal conductivity of copper-beryllium using a single diamond heater and two thermocouples. We augment these measurements with measurements of sample pressure via ruby fluorescence and electrical resistance of the sample and diamond heater.

10:00AM V25.00011 ABSTRACT WITHDRAWN —

10:12AM V25.00012 ABSTRACT WITHDRAWN —

10:24AM V25.00013 High pressure study of mixed valence compound CsAuI₃, SHIBING WANG, SHIGETO HIRAI, ALEXANDER KEMPER, Stanford University, MARIA BALDINI, Geophysical Laboratory, HONGWEI MA, Indiana University, SCOTT RIGGS, MAXWELL SHAPIRO, TOM DEVEREAUX, IAN FISHER, WENDY MAO, TED GEBALLE, Stanford University — CsAuI₃, chemically described as Cs₂Au^IAu^{III}I₆, is a mixed valence compound in the family of CsAuX₃ (X = Cl, Br, I), resembling the high T_c superconductor parent compound BaBiO₃. At ambient conditions it adopts a distorted perovskite structure with compressed Au^IX₆ octahedra and elongated Au^{III}X₆ octahedra along the crystallographic c-axis. The compound undergoes a pressure-induced transition into a new tetragonal phase comprising nearly equivalent AuX₆ octahedra around 5.3 GPa, which agrees with the valence transition previously reported using Mössbauer spectroscopy between 8-12 GPa. We present a thorough high pressure studies of CsAuI₃ through X-ray diffraction and Raman spectroscopy, confirming a pressure-induced band Jahn-Teller effect associated with the 5d⁹ Au^{III} ion. We will also report the reversible amorphization above 15 GPa.

10:36AM V25.00014 Pressure tuning of the thermal conductance of weak interfaces, WEN-PIN HSIEH, Stanford Institute for Materials and Energy Science, Stanford University and SLAC, AUSTIN LYONS, ERIC POP, Department of Electrical and Computer Engineering, University of Illinois, Urbana, PAWEL KEBLINSKI, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY, DAVID CAHILL, Department of Materials Science and Engineering, University of Illinois, Urbana — We use high pressure to reveal the dependence of interfacial heat transport on the stiffness of interfacial bonds. The combination of time-domain thermoreflectance and SiC anvil techniques is used to measure the pressure-dependent thermal conductance $G(P)$ of clean and modified Al/SiC interfaces at pressures as high as $P=12$ GPa. We create low-stiffness, van der Waals bonded interfaces by transferring a monolayer of graphene onto the SiC surface before depositing the Al film. For such weak interfaces, $G(P)$ initially increases approximately linearly with P , consistent with results of molecular dynamics simulations. At high pressures, $P > 8$ GPa, the thermal conductance of weak interfaces approaches the high values characteristic of strongly-bonded, clean interfaces. The results provide new insight demonstrating that interface stiffness dominates thermal transport at weak interfaces, but plays a minor role for strong interfaces with stiffness similar to that in the bulk of the materials.

10:48AM V25.00015 Target tracking in a dusty plasma: phase transitions and equations of state¹, NEIL OXTOPY, JASON RALPH, CÉLINE DURNIAK, DMITRY SAMSONOV, University of Liverpool, United Kingdom — A dusty plasma is a low-density ionized gas containing micron-sized charged dust particles. Laboratory dusty plasmas can be used as kinematic simulators of condensed matter systems, displaying phenomena such as phase transitions. The motion of individual particles is resolvable using a high-speed video camera. We use recursive state estimation (target tracking) techniques to track the dust kinematics, from which we calculate an equation of state for the toy condensed matter system.

¹Financial support from UK EPSRC grant number EP/G007918/1

Thursday, March 1, 2012 8:00AM - 11:00AM —

Session V26 DCOMP: Focus Session: Computational Frontiers in Quantum Spin Systems III

257B

8:00AM V26.00001 A dynamical Marshall sign convention, KEVIN BEACH, University of Alberta — Monte Carlo sampling of quantum spin models is only practical when it is possible to gauge away simultaneously all negative signs in the coefficients of the ground state wavefunction. The existence of such a transformation is related to the possibility of establishing a bipartite pattern of magnetic order on the lattice and to the choice of a so-called Marshall sign convention. In practice, identifying the correct Marshall sign convention is the responsibility of the QMC practitioner, and the convention itself is generally hard coded. It turns out, however, that a locally optimal sign convention can be determined dynamically within the simulation—meaning that for nonfrustrated systems the simulation quickly establishes a Marshall sign convention that leads to sign-problem-free sampling and that for frustrated systems the Marshall sign convention continually evolves in Monte Carlo time so as to minimize the severity of the sign problem. For concreteness, we focus on a worm algorithm formulated in the basis of singlet product states.

8:12AM V26.00002 Monte Carlo Simulations of Quantum Spin Systems in the Valence Bond Basis, FABIAN ZSCHOCKE, University of Alberta — We propose a quantum Monte Carlo method for frustrated spin systems that partially alleviates the sign problem — thereby extending the range of frustrated couplings over which the system can be reliably sampled. The scheme is projective and takes advantage of the overcompleteness and nonorthogonality of the valence bond basis. It provides a framework for further semi-controlled approximations that are fully sign-problem-free in which the transition weights between bond configurations take on effective, renormalized values. We present results for the frustrated (J₁-J₂), spin-half Heisenberg model on the square lattice in the vicinity of its phase transition at $J_2/J_1 \approx 0.4$.

8:24AM V26.00003 Observing spinon excitations in quantum spin models¹, YING TANG, ANDERS SANDVIK, Boston University — We develop a technique to directly study spinons (emergent spin $S = 1/2$ particles) in quantum spin models in any number of dimensions [1]. Two characteristic lengths—the size of a spinon wave packet and the size of a bound pair (a triplon)—are defined in terms of wave-function overlaps that can be evaluated by quantum Monte Carlo simulations. We find that these two lengths are well distinguishable in one-dimensional models with valence-bond-solid (VBS) ground states and explicitly dimerized models, yet hardly separable in 2-leg ladder systems. We provide some physics insights for these phenomena. We also study spinons in two-dimensional resonating-valence-bond states and models with Néel-VBS transitions.

[1] Y. Tang and A. W. Sandvik, Phys. Rev. Lett. 107, 157201 (2011).

¹NSF Grant No. DMR-1104708.

8:36AM V26.00004 Lightcone renormalization and quantum quenches in one-dimensional Hubbard models, JESKO SIRKER, TU Kaiserslautern, TILMAN ENSS, TU Muenchen — The Lieb-Robinson bound implies that the unitary time evolution of an operator can be restricted to an effective light cone for any Hamiltonian with short-range interactions. Here we present a very efficient new renormalization group algorithm based on this light cone structure to study the time evolution of prepared initial states in the thermodynamic limit in one-dimensional quantum systems. The algorithm does not require translational invariance and allows for an easy implementation of local conservation laws. We use the algorithm to investigate the relaxation dynamics of a doublon lattice in fermionic Hubbard models as well as a possible thermalization. Furthermore, we present results for a doublon impurity in a Néel background. We find that the excess charge and spin spread at different velocities, providing an example of spin-charge separation in a highly excited state.

8:48AM V26.00005 Time Evolution within a Comoving Window¹, MARTIN GANAHL, VALENTIN ZAUNER, TU Graz, TOMOTOSHI NISHINO, Kobe University, HANS GERD EVERTZ, TU Graz — We present a modification of Matrix Product State time evolution to simulate the propagation of a signal front on an infinite system. The time evolution is calculated within a finite window that moves along with the signal front, in such a way that boundary effects do not occur. Signal fronts can then be studied unperturbed for much longer times than on truly finite systems, where boundary perturbations and reflections would interfere. The entanglement within in the comoving window remains small. Our approach avoids the large entanglement which develops around the location of the signal source and therefore requires significantly lower computational effort. We verify our approach against exact results and show examples of propagating signals for the XXZ model and the transverse Ising model.

¹We acknowledge support by the Austrian Science Fund FWF (SFB F41 ViCoM) and by the NSF (KITP, PHY05-51164)

9:00AM V26.00006 Emergence of prominent bound states in the spin-1/2 Heisenberg XXZ chain after a local quantum quench¹, HANS GERD EVERTZ, MARTIN GANAHL, ELIAS RABEL, Tu Graz, FABIAN ESSLER, University of Oxford — We calculate the non-equilibrium evolution in the spin-1/2 XXZ Heisenberg chain for fixed magnetization after a *local quantum quench*. Initially an infinite magnetic field is applied to n consecutive sites in the center of a large chain, and the ground state is determined. Then the field is switched off and the time evolution of observables such as the z-component of spin is computed using the Time Evolving Block Decimation (TEBD) algorithm. We find that the observables exhibit strong signatures of propagating spinon as well as bound state excitations. These persist even when integrability-breaking perturbations are included. Since bound states (“strings”) are notoriously difficult to observe using conventional probes such as inelastic neutron scattering we conclude that local quantum quenches are an ideal setting for studying their properties. We comment on implications of our results for cold atom experiments.

¹We acknowledge support by the Austrian Science Fund FWF (SFB F41 ViCoM), by EPSRC (grant EP/I032487/1) and by the NSF (KITP, PHY05-51164)

9:12AM V26.00007 Non-local order parameters in 1D symmetry protected topological phases, FRANK POLLMANN, Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany, ARI TURNER, University of Amsterdam, 1090 GL Amsterdam, The Netherlands, EREZ BERG, Department of Physics, Harvard University, Cambridge, MA 02138, USA — A topological phase is a phase of matter which cannot be characterized by a local order parameter. It has been shown that gapped phases in 1D systems can be completely characterized using tools related to projective representations of the symmetry groups. An example of a symmetry protected topological phase is the Haldane phase of $S = 1$ chains. Here the phase is protected by any of the following symmetries: dihedral group of π -rotations about two orthogonal axes, time-reversal symmetry, or bond centered inversion symmetry. We introduce non-local order parameters for each case which can be simply calculated using numerical methods such as Density-Matrix Renormalization Group (DMRG). These non-local order parameters provide a practical tool for numerically detecting these non-trivial phases.

9:24AM V26.00008 Projected Density of Transitions for Heisenberg Models¹, ROGER HAYDOCK, C.M.M. NEX, University of Oregon — The projected density of transitions (PDoT) is the interacting analogue of the projected or local density of states. The PDoT is proportional to the probability, averaged over all states of the system, that some disturbance (the projection) induces a transition with a specific energy. It is calculated in the same way as the density of states, but using Heisenberg’s equation instead of Schrödinger’s equation. As an example we have applied it to the Heisenberg model for spin interactions of electrons on linear, square, and cubic lattices. One surprise in these calculations is what seems to be a consequence of the spin’s rotational symmetry.

¹work supported by the Richmond F. Snyder Fund

9:36AM V26.00009 Criticality in one-dimensional supersymmetric lattice fermions, MATTHIAS TROYER, Theoretische Physik, ETH Zurich, Switzerland, BELA BAUER, Station Q, Microsoft Research, Santa Barbara and Theoretische Physik, ETH Zurich, Switzerland, LIZA HUIJSE, EREZ BERG, Department of Physics, Harvard University, Cambridge, KARELJAN SCHOUTENS, Institute for Theoretical Physics, University of Amsterdam — A supersymmetric model for lattice fermions has been seen to host a plethora of interesting phenomena. On one-dimensional and quasi-one-dimensional lattices, the model naturally becomes critical and it has been conjectured that it is described by superconformal field theory. While this relation has been confirmed for the chain, establishing this link and exploring the phases adjacent to the critical point for the case of the square ladder has turned out to be a challenging problem for numerical simulations. In our work, we collect evidence in support of the conjecture and obtain insights into the adjacent phases using a variety of numerical techniques, including the density-matrix renormalization group and the multi-scale entanglement renormalization ansatz.

9:48AM V26.00010 Study of Kitaev-Heisenberg model with second-neighbor Heisenberg coupling by DMRG simulations and slave-particle theories, YI-FAN JIANG, Tsinghua University, HONG-CHEN JIANG, KITP, UCSB and Tsinghua University, HONG YAO, Stanford University and Tsinghua University — We study the effect of second-neighbor Heisenberg coupling J_2 to the first neighbor Kitaev-Heisenberg model on the honeycomb lattice by doing DMRG simulations and slave-particle theories. In the Kitaev limit, we find that the gapless spin liquid phase at $J_2 = 0$ survives up to a finite critical value J_{2c} . In an intermediate range, namely $J_{2c} < J_2 < J'_{2c}$, our results show that a new exotic (possibly a gapped chiral spin liquid) phase emerges. When J_2 is further increased beyond J'_{2c} , the ground state orders magnetically by spontaneously breaking spin-rotational and lattice translational symmetries. Possible implications of our results to the real materials Na_2IrO_3 and Li_2IrO_3 will also be discussed

10:00AM V26.00011 Thermodynamics and phase transitions of the pinwheel-distorted Kagome lattice Heisenberg model¹, EHSAN KHATAMI, Georgetown University, RAJIV R.P. SINGH, University of California, Davis, MARCOS RIGOL, Georgetown University — We study the Heisenberg model on the pinwheel-distorted Kagome lattice as observed in the material $Rb_2Cu_3SnF_{12}$. Experimentally relevant thermodynamic properties at finite temperatures are computed utilizing numerical linked-cluster expansions [1]. We introduce a Lanczos-based zero-temperature numerical linked-cluster expansion and study the approach of the pinwheel distorted lattice to the uniform Kagome lattice Heisenberg model. We find strong evidence for a phase transition before the uniform limit is reached, implying that the ground state of the Kagome lattice Heisenberg model is likely not pinwheel dimerized and is stable to finite pinwheel dimerizing perturbations [2].

[1] M. Rigol and R. R. P. Singh, Phys. Rev. Lett. 98, 207204 (2007); Phys. Rev. B 76, 184403 (2007).

[2] E. Khatami, R. R. P. Singh, M. Rigol, preprint: arXiv:1105.4147

¹This work was supported by NSF under Grants No. OCI-0904597 (EK and MR) and DMR-1004231 (RRPS).

10:12AM V26.00012 Numerical Schwinger boson approach to the Bethe lattice antiferromagnet at percolation¹, SHIVAM GHOSH, HITESH J. CHANGLANI, CHRISTOPHER L. HENLEY, Cornell University — What are the lowest energy excitations of a spin-1/2 Heisenberg antiferromagnet on a critical percolation cluster? On the square lattice, Wang et al.,² discovered anomalously low $S=1$ excitations, with energy scaling as $\Delta \sim 1/N^2$. Normally the “Anderson tower” would be the lowest, having energy $S(S+1)/2\chi N \sim 1/N$ (χ = transverse susceptibility). These anomalous excitations were attributed to “dangling spins” appearing in parts of the cluster where there was an imbalance of even and odd sites. Here, we look at the diluted $z=3$ Bethe lattice at the percolation threshold. Previous work confirmed the existence of emergent spin-1/2 degrees of freedom with an effective Heisenberg Hamiltonian but did not explain their origin. New results from DMRG (Density Matrix Renormalization Group) show strong dimerization tendency in the (singlet) ground state, yet there is long-range Neel order on the percolation cluster.³ To harmonize these results, we set up a numerical Schwinger Boson mean field calculation (with site dependent parameters); we find lowering of mean field energy and spin correlations which agree well with ED and DMRG.

¹DMR-1005466

²Phys. Rev. B 81, 054417 (2010)

³A. Sandvik, Phys. Rev. B 66,024418 (2002)

10:24AM V26.00013 Spin Mott Glass Phase in the Disordered Spin Systems, DAO-XIN YAO, NV-SEN MA, State Key Laboratory of Optoelectronic Materials and Technologies, School of Physics and Engineering, Sun Yat-sen University, ANDERS SANDVIK, Department of Physics, Boston University, MA — We use quantum Monte Carlo simulations to study a glassy ground state of $S=1/2$ quantum spins by using a dimerized J1-J2-J3 Heisenberg model on the square lattice. J1 corresponds to weak bonds, and J2 and J3 are stronger bonds which are randomly distributed on columnar rungs forming coupled 2-leg ladders. By tuning the average value of J2 and J3, the system undergoes Neel-glass-paramagnetic quantum phase transition. The size of the glass region is affected by the value of the disorder strength. In the glass phase, we find that the uniform susceptibility decreases with T according to $\exp(-b/T^a)$ with $a < 1$; thus the state is incompressible at $T=0$ and classified as a Mott glass (MG). At the Neel-MG transition, the susceptibility behaves as $T^{2/z-1}$. The dynamical exponent z is found to be larger than 1.

10:36AM V26.00014 Tuning the disorder in a bosonic superglass¹, DEREK LARSON, YING-JER KAO, National Taiwan University — We study the phase transitions associated with tuning the disorder in a Bose-Hubbard model exhibiting a superglass phase. By shifting the distribution of a nearest neighbor $\pm J$ interaction between hard-core bosons on a three-dimensional lattice, we can produce anti-ferromagnetic, glassy, and ferromagnetic (diagonal) types of ordering, each of which interacts uniquely with the superfluid (off-diagonal) ordering. Quantum Monte Carlo simulation results using the worm algorithm show that the existence of superfluidity guards against the formation of large ferromagnetic clusters, presumably due to a lowering of the cost of interfaces. This leads to a strongly-temperature-dependent phase boundary between the glassy and ferromagnetic regions.

¹Funded by Taiwan NSC under grant 100-2112-M-002-013-MY3

10:48AM V26.00015 Impact of spin-orbit coupling on the Holstein polaron, ZHOU LI, Department of Physics, University of Alberta, LUCIAN COVACI, Universiteit Antwerpen, MONA BERCIU, University of British Columbia, DEVIN BAILLIE, FRANK MARSIGLIO, University of Alberta — We utilize an exact variational numerical procedure to calculate the ground state properties of a polaron in the presence of a Rashba-like spin orbit interaction. Our results corroborate with previous work performed with the Momentum Average approximation and with weak coupling perturbation theory. We find that spin orbit coupling increases the effective mass in the regime with weak electron phonon coupling, and decreases the effective mass in the intermediate and strong electron phonon coupling regime. Analytical strong coupling perturbation theory results confirm our numerical results in the small polaron regime. A large amount of spin orbit coupling can lead to a significant lowering of the polaron effective mass

Thursday, March 1, 2012 8:00AM - 11:00AM –
Session V27 DCMP FIAP: Invited Session: Flexible and Rolled Up Semiconductor Nanomembranes 258AB

8:00AM V27.00001 Making Novel Materials Using Strain in Nanomembranes¹, MAX G. LAGALLY, University of Wisconsin-Madison, Madison WI 53706 — The controlled introduction of strain in materials offers an important degree of freedom for fundamental studies of materials as well as advanced device engineering. Strain in a crystalline solid modifies the lattice constants and reduces the crystal symmetry. Because strain energy is proportional to thickness, a free-standing crystalline thin sheet, which we call a nanomembrane (NM), can be strained to a greater degree than a bulk material with the same surface area. I show the use of nanomembrane strain engineering to make defect-free single crystals that cannot be grown any other way, and materials with strain symmetries that they do not have naturally, in both cases alloys of Si and Ge. Strain in NMs causes significant shifts in energy band edges, splitting of degenerate states, and changes in effective masses. These effects can be used to produce a desired band offset between different materials, to increase carrier mobility, and to change relative energy positions of valleys. In the latter respect, through the use of NMs it has recently become possible, using tensile strain, to make Ge direct-bandgap and light emitting at room temperature. Periodic local stress can produce strain superlattices and thus single-element heterojunctions. Work performed with the Roberto Paiella, Mark Eriksson, Feng Liu, and Irena Knezevic research groups.

¹Support provided partially by DOE, AFOSR, and NSF

8:36AM V27.00002 Strain Superlattice: A Combination of Strain Induced Self-Assembly and Strain Engineered Band Structure¹, FENG LIU, University of Utah — Semiconductor nanomembrane affords a novel 2D platform for nanoscience and nanotechnology, especially for strain engineering of nanoelectronics. Strain is well known for band engineering to improve the performance of Si devices. The evidence that the band gap of Si changes significantly with strain suggests that by alternating regions of strained and unstrained Si one creates a single-element hetero-strain-junction electronic superlattice (SL), with the carrier confinement defined by strain rather than by the chemical differences in conventional SLs. Using first-principles calculations, we map out the electronic phase diagram of a 1D pure-silicon strain SL. It exhibits a high level of phase tunability, e.g., tuning from type I to type II. Our theory rationalizes a recent observation of a strain SL in a Si nanowire and provides general guidance for the fabrication of single-element strain SLs. The low-dimensional nanoscale strain SLs extend the concept of SL to a single element that exists in different structural states. It can be made in 1D nanowires or 2D nanomembranes by nanoscale self-assembly or by nanopatterning. It expands the application of strain engineering to new territories, by combining strain induced self-assembly with strain engineered band structure.

¹This work was supported by DOE-BES

9:12AM V27.00003 Rolled-up multifunctional materials, OLIVER SCHMIDT, Institute for Integrative Nanosciences — No abstract available.

9:48AM V27.00004 Rolled-up Tube Based Nanophotonics, XIULING LI, University of Illinois — No abstract available.

10:24AM V27.00005 Nanomembrane photonics for Si photonic integration and flexible optoelectronics¹, WEIDONG ZHOU², University of Texas at Arlington — Crystalline semiconductor nanomembranes (NMs) offer unprecedented opportunities for unique electronic and photonic devices for vertically stacked high density photonic/electronic integration, high performance flexible electronics, and adaptive flexible/conformal photonics. Research progresses have been made in the areas of optical filters/modulators, spectral selective IR photodetectors, flexible LEDs, solar cells, and novel light sources, based on quantum dots, Fano resonance photonic crystal cavities, and heterogeneous integration of III-V/Si material systems. The potentials and prospects of nanomembrane photonics will also be discussed, for a wide range of applications, in the areas of hyper-spectral imaging and gas sensing (lab-on-a-chip), high capacity data network and optical computing (WDM-on-a-chip), high performance flexible inorganic displays, solid state lighting, and photovoltaic solar cells, etc.

¹The authors acknowledge the support from US AFOSR MURI program (FA9550-08-1-0337) and US ARO (W911NF-09-1-0505).

²2nd author: Zhenqiang Ma, Department of Electrical and Computer Engineering, University of Wisconsin-Madison, WI 53706, USA

Thursday, March 1, 2012 8:00AM - 9:48AM — Session V28 DMP: Semiconductor Defects and Doping 258C

8:00AM V28.00001 Transition Metal Defects in Cubic and Hexagonal Polytypes of SiC: Site Selection and Electronic Structure from ab-initio Calculations¹, ADAM GALI, VIKTOR IVÁDY, Hungarian Academy of Sciences, ANDREAS GÄLLSTRÖM, NGUYEN SON, ERIK JANZÉN, Linköping University — Relatively little is known about point defects in different polytypes of a crystal. Silicon carbide is a prototype material for polytypism. There are unidentified photoluminescence centers in SiC that are presumably originated from transition metal defects, however, the number of detected centers does not follow the number of inequivalent substitutional sites in different polytypes. In this study we applied highly convergent and sophisticated density functional theory (DFT) based methods to investigate important transition metal impurities including titanium (Ti), vanadium (V), niobium (Nb), chromium (Cr), molybdenum (Mo) and tungsten (W) in cubic 3C and hexagonal 4H and 6H polytypes of SiC. We applied DFT with PBE functional in order to calculate the ground state of the defects. We calculated the electronic structure by a screened hybrid density functional (HSE06) which was very successful in the quantitative description of native defects in SiC. We found a special asymmetric split-vacancy configuration for a class of transition metal defects. The asymmetric split-vacancy configuration exclusively prefers the hexagonal-hexagonal sites in hexagonal polytypes, thus the probability of finding these defects in 3C polytype is much smaller than in hexagonal polytypes.

¹Swedish Foundation for Strategic Research, Swedish Research Council, Swedish Energy Agency, Swedish National Infrastructure for Computing Grants No. SNIC 011/04-8 and No. SNIC001- 10-223, Knut and Alice Wallenberg Foundation

8:12AM V28.00002 Quantum Effects of Strain Influence on the Dopant Behavior in Semiconductors, DEYAN SUN, ZHENTANG WANG, East China Normal University, China, SHIYOU CHEN, East China Normal University, XIANGMEI DUAN, Ningbo University, China, SU-HUAI WEI, National Renewable Energy Laboratory, USA, XINGAO GONG, Fudan University, China — In most fields of physics, applying external strain (pressure) provides an important technique to investigate and tune the properties of materials. Quite often the theoretical treatment is based on the continuum elastic model, in which its validity is still under debate. In this talk, by using quantum mechanical theoretical analysis, we show that if the occupation change of different orbitals caused by the strain is negligible, the continuum elastic model is valid, otherwise it will fail. Our theory is confirmed by first-principles calculation of Mn-doped GaAs system. Moreover, we show that under compressive strain the hole density, thus the Curie temperature can increase in Mn-doped spintronic materials.

8:24AM V28.00003 First-principle Calculations of Donor and Acceptor Levels in PbI₂ for Ultra-fast Scintillation, GAIGONG ZHANG, Program in Applied Science, UC Davis, ANDREW CANNING¹, Computational Research Division, LBNL, NIELS GRONBECH-JENSEN², Program in Applied Science, UC Davis, LIN-WANG WANG, Materials Sciences Division, LBNL, STEPHEN DERENZO, Life Sciences Division, LBNL — In the past PbI₂ was studied as a candidate for semi-conductor gamma ray detectors as well as more recently as an ultra-fast scintillator for time-of-flight applications. The ultra-fast scintillation properties of this materials are believed to be related to donor-acceptor recombination in both the pure and doped system. This work presents first-principles electronic structure calculations of donor and acceptor levels for intrinsic defects and doped impurities in PbI₂. We performed density functional theory calculations within the generalized gradient approximation with U correction for the donor and acceptor modeling. For a more accurate description of band gaps and structures, we used more advanced methods, such as GW. Our study shows that intrinsic defects significantly affect the luminescence properties of bulk PbI₂. Moreover, the relative position of intrinsic defect levels to doped impurity levels can influence the luminosity. We will compare our theoretical work to known experimental work for this material.

¹Program in Applied Science, UC Davis

²Computational Research Division, LBNL

8:36AM V28.00004 Nonradiative lifetimes in intermediate band materials – absence of lifetime recovery¹, JACOB J. KRICH, Harvard University, Department of Chemistry and Chemical Biology, BERTRAND I. HALPERIN, Harvard University, Department of Physics, ALÁN ASPURU-GUZIĆ, Harvard University, Department of Chemistry and Chemical Biology — Intermediate band photovoltaics hold the promise of being highly efficient and cost effective photovoltaic cells. Intermediate states in the band gap, however, are known to facilitate nonradiative recombination. Much effort has been dedicated to producing metallic intermediate bands in hopes of producing *lifetime recovery* – an increase in carrier lifetime as doping levels increase. We show that lifetime recovery induced by the insulator-to-metal transition will not occur, because the metallic extended states will be localized by phonons during the recombination process. Only trivial forms of lifetime recovery, e.g., from an overall shift in intermediate levels, are possible. Future work in intermediate band photovoltaics must focus on optimizing subgap optical absorption and minimizing recombination, but not via lifetime recovery.

¹We acknowledge support from NSF Grant Nos. DMR-0934480 and DMR-0906475 and the Harvard University Center for the Environment.

8:48AM V28.00005 Imaging Defects in Semiconductors with a Snapshot Micro-Imaging Technique¹, KIRSTIN ALBERI, BRIAN FLUEGEL, DAN BEATON, ANGELO MASCARENHAS, National Renewable Energy Laboratory — Polycrystalline or metamorphically grown single crystalline thin films are ubiquitous in energy-related technologies, such as solar cells and light emitting diodes. A detailed understanding of the defects contained within these materials (i.e. dislocations, grain boundaries, inclusions) and the ability to control them play critical roles in their development. We will present the use of a novel “snapshot” micro-imaging technique to evaluate the presence and behavior of defects in a variety of materials and devices. Photoluminescence from a wide area of a sample is imaged onto a Si CCD in a single exposure, enabling real-time mapping with sub-micron resolution. A tunable liquid-crystal filter selects the exact wavelength that is imaged. Combined with a tunable excitation source, this technique is ideal for selectively investigating defects in thin films as well as individual layers in a device.

¹We acknowledge the financial support of the Department of Energy, Office of Science, Basic Energy Sciences

9:00AM V28.00006 Fluorescent nanodiamonds for biomedical thermal imaging, JUAN ENRIQUE RAMIREZ HERNANDEZ, JOSE GARCIA SOLE, MARTIN RAFAEL PEDROZA MONTERO, MARCELINO BARBOZA FLORES, DANIEL JAQUE, LAURA MARTINEZ MAESTRO, KARLA JOSEFINA SANTACRUZ GOMEZ, FRANCISCO SANZ RODRIGUEZ, NINGNING DONG, TOMAS CALDERON, None — The use of nanoparticles designed for a particular purpose in biological research has increased exponentially in the last ten years. Nanoscale particles have dimensions similar to those of most biological systems and present exceptional physical, chemical and optical properties. The optical absorption and emission of nanoparticles may be tuned by varying their shape, size and composition and recent advances in their synthesis and design suggest their potential use as probes in the detection and treatment of diseases such as cancer. One of these promising materials is nanodiamond which possesses excellent surface modification capacity and high biocompatibility. In addition to being compatible with the human body, nanodiamonds can be used as radiation sensors. In this report, the ability of nanodiamonds to be used as nanothermometers was studied by the obtention of a nanothermic scale (temperature dependence of nanodiamond's emission spectrum) to accurately measure temperature in small volumes.

9:12AM V28.00007 Laser induced local modification of material properties in a semiconductor alloy¹, YONG ZHANG, NAILI YUE, UNC-Charlotte — High energy (usually short pulse) lasers are routinely used for micromachining and surface modification of solid state materials. We demonstrate that a small power CW laser can be used to induce local modification of the electronic and optical properties of a semiconductor alloy at any desirable spatial location. The degree of modification can be precisely controlled by laser density and exposure time. The spatial resolution is determined currently by the beam size of a confocal optical system, but it can also be defined by the feature size of a lithographic method. The induced local changes in properties are measured by optical spectroscopy, and the results indicate the possibility of local structural modification.

¹Work partially supported by CRI

9:24AM V28.00008 Spatial Variation in Mobility-Lifetime Product in Bulk TlBr and CZT¹, DAVID PHILLIPS, NANCY HAEGEL, Naval Postgraduate School, KEVIN BLAINE, US Military Academy, HADONG KIM, GUIDO CIAMPI, LEN CIRIGNANO, Radiation Monitoring Devices (RMD) — The energy resolution of a semiconductor radiation detector depends on the charge transport properties of the semiconductor, and the mobility-lifetime ($\mu\tau$) product is a key figure of merit for charge transport. In this work, we investigate the effects of two impurities, Na and Cu, on the $\mu\tau$ product in bulk thallium bromide (TlBr) using cathodoluminescence (CL) and transport imaging. Transport imaging uses a scanning electron microscope to generate a line of charge carriers on the surface of a bulk sample, and the intensity and spatial distribution of the recombination luminescence are recorded. A Green's function approach is used to model the generation, diffusion, and recombination of charge carriers under steady-state conditions. The luminescence distribution is fit to the model to extract the ambipolar diffusion length and the $\mu\tau$ product, providing a high-resolution correlation between the luminescence variations due to dopants/defects and the quantitative transport behavior. The $\mu\tau$ product has been mapped across a 40 μm segment of TlBr at a resolution of 2 μm . Additionally, this approach has been used to locally map variations in ambipolar diffusion length and $\mu\tau$ product due to extended defects in cadmium zinc telluride (CZT).

¹Supported by DND Academic Research Initiative Grant NSF/ARI 083007

9:36AM V28.00009 Quantum Stress: Density Functional Theory Formulation and Physical Manifestation¹, HAO HU, FENG LIU, Department of Materials Science and Engineering, University of Utah — The concept of “quantum stress (QS)” is introduced and formulated within density functional theory (DFT), to underlie extrinsic electronic effects on the stress state of solids and thin films in the absence of lattice strain. An explicit expression of QS (σ^Q) is derived in relation to the deformation potential of electronic states (Ξ) and the variation of electron density (Δn), $\sigma^Q = \Xi(\Delta n)$, as a quantum analog of classical Hook’s law. Two distinct QS manifestations are demonstrated quantitatively by DFT calculations: (1) in the form of bulk stress induced by charge carriers; and (2) in the form of surface stress induced by quantum confinement. QS has broad implications in physical phenomena and technological applications that are based on coupling of electronic structure with lattice strain.

¹The work was supported by DOE-BES (Grant # DE-FG02-04ER46148).

Thursday, March 1, 2012 8:00AM - 10:48AM –
Session V29 GQI: Focus Session: Superconducting Qubits: Epitaxial Junctions and Two-Level Systems 259A

8:00AM V29.00001 Coherence in a transmon qubit with epitaxial tunnel junctions, MARTIN WEIDES, JEFFREY KLINE, MICHAEL VISSERS, MARTIN SANDBERG, National Institute of Standards and Technology, DAVID WISBEY, Saint Louis University, DAVID PAPPAS, National Institute of Standards and Technology, BLAKE JOHNSON, TOM OHKI, Raytheon BBN Technologies — We developed transmon qubits based on epitaxial tunnel junctions and interdigitated capacitors. This multileveled qubit, patterned by use of all-optical lithography, is a step towards scalable qubits with a high integration density. The relaxation time T_1 is $.72 - .86 \mu\text{sec}$ and the ensemble dephasing time T_2^* is slightly larger than T_1 . The dephasing time T_2 ($1.36 \mu\text{sec}$) is nearly energy-relaxation-limited. Qubit spectroscopy yields weaker level splitting than observed in qubits with amorphous barriers in equivalent-size junctions. The qubit’s inferred microwave loss closely matches the weighted losses of the individual elements (junction, wiring dielectric, and interdigitated capacitor), determined by independent resonator measurements.

8:12AM V29.00002 Superconducting qubits consisting of epitaxially-grown NbN/AlN/NbN Josephson junctions¹, YASUNOBU NAKAMURA, RIKEN/NEC, HIROTAKA TERA, NICT, KUNIHIRO INOMATA, RIKEN, TSUYOSHI YAMAMOTO, RIKEN/NEC, WEI QIU, ZHEN WANG, NICT — We demonstrate superconducting qubits using epitaxially-grown Josephson junctions. A fully epitaxial NbN/AlN/NbN trilayer on MgO (100) substrate is processed by photolithography and dry-etching into transmon qubits with a large Josephson energy. The tunnel barrier made of cubic-phase AlN, rather than the ordinary hexagonal phase, is the key to avoid piezoelectric coupling to the phonon bath. The energy-relaxation time and the spin-echo decay time of ~ 500 ns are observed in the qubits that are coupled to a monolithically-made coplanar waveguide resonator.

¹This work is partly supported by FIRST, MEXT-KAKENHI, and NICT.

8:24AM V29.00003 Josephson phase qubits incorporating high-Q crystalline dielectrics, U. PATEL, Y. GAO, L. MAURER, S. SENDELBACH, D. HOVER, Department of Physics, University of Wisconsin, Madison, Wisconsin 53706, K.H. CHO, C.B. EOM, Department of Materials Science and Engineering, University of Wisconsin, Madison, Wisconsin 53706, R. MCDERMOTT, Department of Physics, University of Wisconsin, Madison, Wisconsin 53706 — The energy relaxation times of Josephson phase qubits are currently limited by spurious coupling of the qubit to unsaturated two level system (TLS) defects of the amorphous dielectrics. It is expected that incorporation of defect-free crystalline dielectrics into qubit circuits will dramatically improve coherence. Here, we describe the growth and characterization of novel crystalline dielectrics for superconducting qubit applications, including grown Al₂O₃ on epitaxial Re underlayers. We discuss the incorporation of epitaxial dielectrics into phase qubit circuits, and present data on qubit coherence.

8:36AM V29.00004 Growth of epitaxial Al/AlO_x/Re using a sputtering PLD hybrid system with *in-situ* RHEED, KWANG-HWAN CHO, JACOB PODKAMINER, Department of Materials Science and Engineering, University of Wisconsin-Madison, UMESHKUMAR PATEL, ROBERT MCDERMOTT, Department of Physics, University of Wisconsin-Madison, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison — Our objective is the growth of epitaxial dielectrics on crystalline superconducting underlayers to improve the performance of superconducting Qubits. We have grown epitaxial Re thin films on a c-plane sapphire substrate using RF magnetron sputtering, and then transferred *ex-situ* to a pulsed laser deposition (PLD) system where dielectrics thin film layer is deposited. One drawback of this fabrication approach is the necessity to expose the sample to air when the sample is transferred to different deposition chambers. In order to avoid these drawbacks, we have employed a hybrid PLD-sputtering deposition that will allow us to grow the oxide dielectric/Re heterostructures in an *in-situ* environment without breaking vacuum. The system is also equipped with reflection high energy electron diffraction (RHEED) which will allow us to perform *in-situ* characterization of the structure and growth dynamics. We will discuss our strategy of epitaxial growth of various single crystal dielectrics on superconducting thin films in this system and their structural and electrical properties of the heterostructures.

8:48AM V29.00005 Transport Characteristics of Self-Aligned Josephson Junctions Grown using co-Deposited Molecular Beam Epitaxy¹, GUSTAF OLSON, ALLISON DOVE, ZACHARY YOSCOVITS, CHRIS NUGROHO, VLADIMIR ORLYANCHIK, DALE VAN HARLINGEN, JAMES ECKSTEIN, University of Illinois Urbana Champaign — Low noise Josephson junctions are extremely desirable in SQUIDs and qubit circuits. Sources of flux noise and critical current noise can be reduced by using both clean, single crystal junctions to lower the density of fluctuators and by decreasing the size of the junctions to lower the absolute number of fluctuators. We report transport characteristics of small, single crystal Josephson junctions grown using a co-deposited aluminum-oxide barrier molecular beam epitaxy process. We also report a novel self-aligned fabrication process that allows us to produce sub-micron junctions from these single crystal films. We show that our co-deposited junctions have more ideal transport characteristics than those junctions grown with only a diffused barrier. -

¹Work supported by IARPA grant Army UCB-00006692

9:00AM V29.00006 Internal loss of superconducting resonators induced by interacting two level systems¹ , LARA FAORO, LPTHE, CNRS, LEV IOFFE, Rutgers University — In a number of recent experiments with microwave superconducting resonators the anomalously slow dependence of the quality factor on the power was observed. This observation implies that the monochromatic radiation does not saturate two level systems in the surrounding oxides as predicted by the standard model of two-level systems (TLS). We argue that these observations suggest the importance of interactions between TLS in these materials. We show that interactions between TLS lead to a drift of their energies that result in much slower, logarithmic dependence of their absorption on the radiation power in a reasonable agreement with the data.

¹Research was supported by ARO W911NF-09-1-0395

9:12AM V29.00007 Two-level system dynamics in amorphous dielectrics probed with a dc electric field , MOE KHALIL, SERGIY GLADCHENKO, M.J.A. STOUTIMORE, University of Maryland and Laboratory for Physical Sciences, F.C. WELLSTOOD, University of Maryland, K.D. OSBORN, Laboratory for Physical Sciences — We report loss in a thin-film dc electric-field tunable LC resonator built with superconducting aluminum and silicon nitride dielectric. To measure the loss we continually apply microwave power on resonance and monitor the transmitted power. At milli-Kelvin temperatures, loss is limited by two-level systems in the dielectric which are saturated with high microwave excitation power. Measurements show that a sudden change of applied dc field causes the dielectric loss to increase to the intrinsic low power loss tangent of the dielectric. We study the subsequent relaxation of the loss tangent caused by two-level system saturation and interactions. We discuss how this arises from the dynamics of a distribution of two-level system defects and compare it with new theoretical work on interacting two-level systems.

9:24AM V29.00008 Studying two-level systems in Josephson junctions with a Josephson junction defect spectrometer , M.J.A. STOUTIMORE, M.S. KHALIL, SERGIY GLADCHENKO, Laboratory for Physical Sciences, University of Maryland, R.W. SIMMONDS, National Institute of Standards and Technology, C.J. LOBB, University of Maryland, K.D. OSBORN, Laboratory for Physical Sciences — We have fabricated and measured Josephson junction defect spectrometers (JJDSs), which are frequency-tunable, nearly-harmonic oscillators that probe two-level systems (TLSs) in the barrier of a Josephson junction (JJ). A JJDS consists of the JJ under study fabricated with a parallel capacitor and inductor such that it can accommodate a wide range of junction inductances, L_{J0} , while maintaining an operating frequency, f_{01} , in the range of 4-8 GHz. In this device, the parallel inductance helps the JJ maintain linearity over a wide range of frequencies. This architecture allows for the testing of JJs with a wide range of areas and barrier materials, and in the first devices we have tested Al/AIO_x/Al JJs. By applying a magnetic flux bias to tune f_{01} , we detect TLSs in the JJ barrier as splittings in the device spectrum. We will present our results toward identifying and quantifying these TLSs, which are known to cause decoherence in quantum devices that rely on JJs.

9:36AM V29.00009 Relaxation of a Cooper-Pair Box Coupled to Discrete Charge Fluctuators , B.S. PALMER, Laboratory for Physical Sciences, Z. KIM, F.C. WELLSTOOD, JQI, CNAM, Department of Physics, University of Maryland — Recently, Kim *et al.* have reported that the interaction of a Cooper-pair box (CPB) with discrete charge fluctuators can decrease the relaxation time (T_1) of the first excited state of a CPB when operating the CPB near the transition frequency of a charged two-level system (TLS).¹ Using a density matrix approach and a 4-level Hilbert space, we have simulated the T_1 of a CPB coupled to a TLS and a dissipative bath. We model the TLS with asymmetry and tunneling parameters which we obtain along with the CPB parameters from fits to microwave spectroscopic measurements.^{2,3} To model the bath, the CPB is coupled to a source of charge noise which causes relaxation and dephasing while the TLS is coupled to its own dissipative source of energy. Results of the simulation are presented and compared to the experimental measurements.

¹Z. Kim *et al.*, Physical Review B, **78** 144506 (2008).

²Ibid.

³F. C. Wellstood, Z. Kim, and B. S. Palmer, arXiv:0805.4429.

9:48AM V29.00010 Microwave Frequency Loss in Aluminum Nanobridge Josephson Junctions¹ , ELI LEVENSON-FALK, R. VIJAY, STEVEN WEBER, KATER MURCH, I. SIDDIQI, UC Berkeley, QNL — Dielectric loss is a major source of decoherence in many superconducting qubits. Weak link Josephson junctions have the potential advantage of eliminating any loss associated with the insulating barrier in conventional tunneling type devices. We present quality factor measurements of 6 GHz superconducting resonators realized from three dimensional aluminum nanobridges shunted by single crystal silicon overlap capacitors. We compare the measured Q values with those obtained from similar resonators with aluminum tunnel junctions, with critical currents also in the microamp range. We discuss potential relaxation mechanisms specific to weak link junctions, and describe nanobridge qubit designs.

¹ This research was supported by the DARPA YFA program.

10:00AM V29.00011 T_1 -echo sequence - Preserving the state of a qubit in the presence of coherent interaction , CLEMENS MÜLLER, Departement de Physique, Université de Sherbrooke, Quebec, Canada J1K 2R1, ALEXANDER SHNIRMAN, Institut fuer Kondensierten Materie, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany, MARTIN WEIDES, National Institute of Standards and Technology, Boulder, CO 80309-044, USA — We propose a sequence of pulses intended to preserve the state of a qubit in the presence of strong, coherent coupling to another quantum system. The sequence can be understood as a generalized SWAP and works in formal analogy to the well-known spin echo. Since the resulting decoherence rate of the qubits state is strongly influenced by the additional system, this sequence might serve to protect its quantum state. A possible area of application would be in superconducting circuits, where often spurious two-level system interact strongly with the qubits and might thus provide the necessary resource.

10:12AM V29.00012 Circuit quantum electrodynamics with a scanning qubit , WILL SHANKS, DEVIN UNDERWOOD, JAMES RAFTERY, SRIKANTH SRINIVASAN, ANTHONY HOFFMAN, ANDREW HOUCK, Princeton University — We report measurements of the coupling between a superconducting microwave resonator and a transmon qubit fabricated on a separate chip and mounted to a three-dimensional cryogenic translation stage. The qubit-resonator system reached the strong coupling regime with a coupling strength in excess of 80 MHz. We use the translation stage to explore the position dependence of the coupling strength. With a scanning qubit stage, it is possible to measure many qubits in succession and study the statistics of the fabrication process. The system can also be used as a local probe of a large array of microwave cavities and superconducting qubits.

10:24AM V29.00013 Noise and microresonance of critical current in Josephson junction induced by Kondo trap states¹, MOHAMMAD ANSARI, University of Waterloo, FRANK WILHELM, Saarland University — We analyze the impact of trap states in the oxide layer of a superconducting tunnel junctions, on the fluctuation of the Josephson critical current, thus on coherence in superconducting qubits. We use second order perturbation theory which allows to obtain analytical formulae for the interacting bound states and spectral weights, limited to small and intermediate repulsions. Remarkably, it still reproduces the main features of the model as identified from the Numerical Renormalization Group. We present analytical formulations for the subgap bound state energies, the singlet-doublet phase boundary, and the spectral weights. We show that interactions can reverse the supercurrent across the trap. We finally work out the spectrum of junction resonators for qubits in the presence of on-site repulsive electrons and analyze its dependence on microscopic parameters that may be controlled by fabrication.

¹This research was partly funded by IARPA and ODNI

10:36AM V29.00014 Probing coupling mechanism between microscopic two-level system and superconducting qubits¹, YANG YU, ZHENTAO ZHANG, Nanjing University — We propose a scheme to clarify the microscopic nature of Josephson qubits interacting with the two-level systems, coming from microscopic defects located inside insulation layer. We found that the sensitivity of the generally used spectral method in phase qubit is not sufficient to evaluate the exact form of the coupling. On the contrary, our numerical calculation shows that the coupling strength changes remarkably with flux bias for a flux qubit, providing a useful tool to investigate the coupling mechanism between the two-level systems and qubits.

¹This work was supported in part by MOST (2011CB922104, 2011CBA00200), NSFC (91021003, 10725415), and the Natural Science Foundation of Jiangsu Province (BK2010012).

Thursday, March 1, 2012 8:00AM - 11:00AM — Session V30 GQI: Focus Session: Semiconductor Qubits - Measurement 259B

8:00AM V30.00001 Single-donor spin qubits in silicon¹, ANDREA MORELLO, University of New South Wales — The idea of using the spin of a single donor atom in silicon to encode quantum information goes back to the Kane proposal [1] in 1998. We have now resolved the technical challenges involved in the readout and control of the electron and nuclear spin of a single atom. The key breakthrough was the development of a device structure where the donor is tunnel-coupled to the island of an electrostatically-induced single-electron transistor [2]. This device allowed the single-shot readout of the electron spin with visibility $> 90\%$ and $3 \mu\text{s}$ readout time [3]. More recently we have integrated the single-shot readout device with a broadband microwave transmission line to coherently control the electron and nuclear spins. The resonance frequency of the electron is found by monitoring the excess spin-up counts while sweeping the microwave frequency. At any time, one of two possible frequencies is found to be in resonance with the electron spin, depending on the state of the nuclear spin. Alternately probing the two frequencies yields the (quantum nondemolition) single-shot readout of the nucleus, with fidelity $> 99.99\%$. Then we demonstrate the coherent control (Rabi oscillations) of both the electron and the nucleus, both detected in single-shot mode. The π -pulse fidelity is $\sim 70\%$ for the electron and $\sim 99\%$ for the nucleus. Hahn echo and multi-pulse dynamical decoupling sequences allow us to explore the true coherence of the qubits, yielding $T_{2e} \sim 200 \mu\text{s}$ for the electron, and $T_{2n} \sim 60 \text{ ms}$ for the nucleus. These results are fully consistent with the bulk values for donors in a natural Si sample. Further improvements in qubit coherence can be expected by moving to isotopically pure ^{28}Si substrates.

[1] B. E. Kane, Nature **393**, 133 (1998).

[2] A. Morello *et al.*, Phys. Rev. B **80**, 081307(R) (2009).

[3] A. Morello *et al.*, Nature **467**, 687 (2010).

¹Funded by the the Australian Research Council Centre of Excellence for Quantum Computation and Communication Technology (project number CE11E0096) and the US National Security Agency and the US Army Research Office under contract number W911NF-08-1-0527

8:36AM V30.00002 Quantum read-out and fast initialization of nuclear spin qubits with electric currents¹, ROGERIO DE SOUSA, NOAH STEMEROFF, University of Victoria, BC — Nuclear spin qubits have the longest coherence times in the solid state, but their quantum read-out and initialization is a great challenge. We present a theory for the interaction of an electric current with the nuclear spins of donor impurities in semiconductors [1]. The theory yields a sensitivity criterion for quantum detection of nuclear spin states using electrically detected magnetic resonance, as well as an all electrical method for fast nuclear spin qubit initialization.

[1] N. Stemeroff and R. de Sousa, Phys. Rev. Lett. **107**, 197602 (2011).

¹We acknowledge financial support from the NSERC Discovery program.

8:48AM V30.00003 Real-time readout and lifetime measurements of single-triplet states in a Si/SiGe double quantum dot, JONATHAN PRANCE, ZHAN SHI, University of Wisconsin-Madison, CHRISTIE SIMMONS, Massachusetts Institute of Technology, DON SAVAGE, MAX LAGALLY, University of Wisconsin-Madison, LARS SCHREIBER, LIEVEN VANDERSYPEN, Kavli Institute of Nanoscience, TU Delft, MARK FRIESEN, ROBERT JOYNT, SUE COPPERSMITH, MARK ERIKSSON, University of Wisconsin-Madison — The singlet and triplet states of a two-electron double quantum dot can be used as the basis for a logical qubit that combines fast gating and robust readout via Pauli spin blockade. We present measurements of the lifetimes of these states in a Si/SiGe double dot at magnetic fields between 1T and 0T [1]. The lifetimes are found by analyzing the statistics of repeated single-shot measurements of the spin state of the system. This technique allows multiple relaxation processes to be observed simultaneously. At zero magnetic field we find that all four spin states have lifetimes of approximately 10ms. With increasing magnetic field the lifetimes of the S and T0 states show no noticeable change, while the lifetime of the T- state rises, reaching 3 seconds at 1T. [1] J. R. Prance, et al., e-print: arxiv.org/abs/1110.6431

9:00AM V30.00004 Calibrated State Tomography in Singlet-Triplet Qubits¹, OLIVER DIAL, MICHAEL SHULMAN, SHANNON HARVEY, HENDRIK BLUHM², Harvard University, VLADIMIR UMANSKY, Weizmann Institute of Science, AMIR YACOBY, Harvard University — Quantitative and accurate state tomography is becoming increasingly necessary in spin qubits to establish gate fidelities, entanglement measures, and optimize the increasingly complex gate sequences needed to perform experiments. In spin-qubits, to perform state tomography single-qubit rotations are used to map different axes of the Bloch sphere to the singlet-triplet axis, followed by projective measurement onto the singlet-triplet axis. Two orthogonal rotations are provided by two physically distinct mechanisms: magnetic field gradients and exchange rotations. The complex interplay between these mechanisms, noise sources, and pulse distortions make it difficult to accurately predict the angle and axis of rotations from first principles, leading to a circular problem: how can one calibrate tomographic rotations without any calibrated tomographic rotations? We describe and demonstrate a method which, using minimal assumptions, makes it possible to detect and correct for both axis errors in tomography and losses during the rotations associated with state tomography. This allows state tomography with unprecedented precision in these systems.

¹This work is supported through the NSA, “Precision Quantum Control and Error-Suppressing Quantum Firmware for Robust Quantum Computing” and IARPA “Multi-Qubit Coherent Operations (MQCO) Program.”

²Now RWTH Aachen University

9:12AM V30.00005 Readout and Control Technology for Spin Qubits, JAMES COLLESS, DAVID REILLY, The University of Sydney — Scale-up of spin qubits will require the development of new technological approaches that enable readout and control in multi-qubit device architectures. We report results demonstrating a fast readout method based on quantum capacitance that is well suited to detecting spin-states in qubit geometries beyond two quantum dots. Control protocols and device architectures for the selective rotation of single spins using on-chip transmission lines and ac-magnetic field gradients will be presented.

9:24AM V30.00006 Si/SiGe Quantum Dot Charge Sensing with Radio Frequency Single-Electron Transistor¹, MINGYUN YUAN, ZHEN YANG, A.J. RIMBERG, Dartmouth College, M.A. ERIKSSON, D.E. SAVAGE, University of Wisconsin — We report the operation of a radio frequency superconducting single-electron transistor (rf-SSET) as a charge sensor for single and double Si/SiGe quantum dots (QDs). The charge sensitivity is on the order of 10^{-5} to $10^{-6} e/\sqrt{Hz}$. In the reflectometry set-up, real-time electron tunneling events in a single QD are measured, which demonstrates a fast charge detection time of a few tens of microseconds. The stability diagram of a double QD is mapped out with the averaged reflected power of the rf-SSET. In addition, electron temperature is measured in a dilution refrigerator to be around 150 mK, allowing us to study spin blockade and Kondo effect.

¹This research is supported by the NSA, LPS and ARO.

9:36AM V30.00007 Study of the QPC Back-action to Electron Spin Based Qubits¹, MING XIAO, HAIYOU LI, GANG CAO, GUOPING GUO, GUANGCAN GUO, University of Science and Technology of China, HONGWEN JIANG, University of California at Los Angeles — The electron spin states in quantum dots (QD) are potential for implementing qubits. Quantum point contacts (QPC) are widely used to read-out these spin states. However, any read-out procedure inevitably causes back-action to the measured qubits. In this work we studied the back-action of a QPC to the electron spin states in a single GaAs QD. We found that the non-equilibrium effect in the QPC real-time charge counting statistics is a benchmark of the QPC back-action strength. The back-action driven excitations to higher energy levels contribute extra features which enabled us to study the QD's internal structures. The excitations between the two Zeeman states for odd number of electrons and between the spin singlet-triplet states for even number of electrons are respectively studied. This provides a way to quantitatively evaluate the influence of back-action on Zeeman or singlet-triplet based spin qubits. The dependence of the relaxation time of various spin excited states on the back-action strength was also studied.

¹This work was supported by the NFRP 2011CBA00200 and 2011CB921200, NNSF 10934006, 11074243, 10874163, 10804104, 60921091.

9:48AM V30.00008 ABSTRACT WITHDRAWN —

10:00AM V30.00009 Fast charge sensing in InAs nanowire double quantum dot devices¹, MINKYUNG JUNG, MICHAEL SCHROER, KARL PETERSSON, JIRI STEHLIK, JASON PETTA, Princeton University, PRINCETON UNIVERSITY TEAM — Fast and sensitive charge and spin state readout is one of the most important requirements for quantum computing. Radio frequency (rf) reflectometry [1] provides a simple and fast charge detection scheme for charge and spin state readout in double quantum dot (DQD) devices without a separate charge detector [2]. Here, we demonstrate charge sensing measurements in InAs nanowire DQD devices using rf-reflectometry. The source electrode of the nanowire DQD is directly coupled to the tank circuit. We correlate standard dc transport measurements with the tank circuit response. We drive the resonator at its resonant frequency and detect the reflected signal via a cryogenic and room temperature amplifier. Using rf-reflectometry, we can observe charging transitions even when the device is tuned to a regime where current through the device is below the noise floor of the setup. The sensor enables the occupancy of the quantum dot to be probed down to a few electron regime. We present preliminary results of spin state readout using rf-reflectometry.

[1] R. J. Schoelkopf *et al.*, Science **280**, 1238 (1998)

[2] K. D. Petersson *et al.*, Nano Lett. **10**, 2789 (2010)

¹Research at Princeton is supported by the Sloan and Packard Foundations, NSF, Army Research Office, and DARPA QuEST.

10:12AM V30.00010 Single charge sensing and transport in double quantum dots fabricated from commercially grown Si/SiGe heterostructures¹, K. WANG, C. PAYETTE, Y. DOVZHENKO, P. KOPPINEN, J.R. PETTA, Princeton University — We perform quantum Hall measurements on three types of commercially available modulation doped Si/SiGe heterostructures [1] to determine their suitability for depletion gate defined quantum dot devices. By adjusting the growth parameters, we are able to achieve two dimensional electron gases with low charge densities and high mobilities. We extract an electron temperature of 100 mK in the single quantum dot regime. Double quantum dots fabricated on these heterostructures show clear evidence of single charge transitions [2] as measured in dc transport and charge sensing.

[1] C. B. Simmons *et al.*, Phys. Rev. Lett. **106**, 156804 (2011).

[2] R. Hanson *et al.*, Rev. Mod. Phys. **79**, 1217 (2007).

¹Research at Princeton is supported by the Sloan and Packard Foundations, NSF, and DARPA through HRL Laboratories.

10:24AM V30.00011 Charge sensing in a silicon MOS double quantum dot¹, M. LILLY, K. NGUYEN, R. YOUNG, E. NIELSEN, N. BISHOP, J. WENDT, R. GRUBBS, T. PLUYM, J. STEVENS, J. DOMINGUEZ, R. MULLER, M. CARROLL, Sandia National Laboratories — We report charge sensing measurements on a double quantum dot fabricated in a silicon / silicon dioxide double top gated structure. Depletion gates are used to laterally define a double quantum dot, and each dot has an adjacent quantum point contact (QPC) electrometer for remote detection of the dot occupation. For charge sensing, two techniques have been employed. In one, the direct conductance of the QPC measured with a low frequency ac voltage bias, and in the other the differential change in QPC conductance is measured as an ac voltage is applied to a dot plunger gate. Simultaneous direct and differential charge sense measurements are performed using an amplitude modulation technique. We characterize the double dot using honeycomb stability diagrams and non-linear transport. Results are compared to detailed modeling of our device structure.

¹Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE

10:36AM V30.00012 Dispersive readout of spin blockade in a carbon nanotube double quantum dot, HUGH CHURCHILL, RUBY LAI, CHARLES MARCUS, Harvard University — We probe the charge states of a carbon nanotube double quantum dot by coupling superconducting resonators to the leads and a gate of a device designed for operation as a spin-valley qubit. Multiplexed dispersive readout allows rapid reflectometry measurements of the device without the need for dedicated proximal charge sensors. In this way as-grown nanotubes may be used in a bottom-gated geometry to create low-disorder devices that are freely suspended and then insulated using atomic layer deposition. These techniques are demonstrated with measurements in the spin blockade regime. We acknowledge support from IBM, NSF-MWN, NSF-NRI through the INDEX Center, and Harvard University.

10:48AM V30.00013 Relaxation hotspots and fast reset of a single electron spin in a double quantum dot¹, KATJA NOWACK², MOHAMMAD SHAFIEI, Delft University of Technology, CHRISTIAN REICHL, WERNER WEGSCHEIDER, ETH Zurich, LIEVEN VANDERSYPEN, Delft University of Technology — We measure the relaxation time of a single electron spin in a double quantum dot as a function of the energy detuning between the two dots for Zeeman splitting larger than the tunnel coupling. Close to the charge degeneracy point at which the electron delocalizes over both dots we observe two "hot spots" at which relaxation times are enhanced by almost four orders of magnitude. We identify these hot spots to occur at degeneracies of orbital and spin excitations. The spin-orbit and hyperfine interaction in the GaAs host lattice efficiently mix degenerate spin states and in combination with fast orbital relaxation this can lead to a fast pumping of the electron spin to its ground state. The enhanced spin relaxation can be exploited to achieve a fast reset of the electron spin, which might prove useful in the context of spin based quantum information processing.

¹We acknowledge funding from IARPA, FOM, ERC and the European Commission (SOLID).

²Present affiliation: Stanford University

Thursday, March 1, 2012 8:00AM - 11:00AM —
Session V31 DMP: Focus Session: Topological Insulators: Synthesis & Characterization - ARPES 260

8:00AM V31.00001 Topological Surface States in Ternary Spin-Orbit Insulators: An ARPES Viewpoint¹, MADHAB NEUPANE, S.-Y. XU, Department of Physics, Princeton University, L.A. WRAY, ALS, Lawrence Berkeley National Laboratory & Princeton University, A. PETERSEN, R. SHANKAR, Department of Physics, Princeton University, A. FEDOROV, ALS, Lawrence Berkeley National Laboratory, C. LIU, Department of Physics, Princeton University, Y.S. HOR, Department of Chemistry, Princeton University, J. XIONG, D.-X. QU, Department of Physics, Princeton University, H. LIN, Northeastern University, N.P. ONG, Department of Physics, Princeton University, A. BANSIL, Northeastern University, R.J. CAVA, Department of Chemistry, Princeton University, M.Z. HASAN, Department of Physics, Princeton University — Utilization of topological surface states is expected to lead to new vistas in electronics and fundamental physics. However, most of the known topological insulators either do not feature necessary band structure conditions (location of Dirac point with respect to the bulk band) or lack topological invariants essential for certain class of applications. Using angle-resolved photoemission spectroscopy (ARPES), we discuss the electronic band structure topology of a family of ternary spin-orbit insulators some of which feature functional electronic structure with in-gap Dirac point while others feature novel topological invariants (weak Z2 invariants) in crystalline form. We also present some of our recent results on ternary topological insulators.

¹This work is supported by DOE/BES.

8:12AM V31.00002 Rashba Spin-Splitting Control at the Surface of the Topological Insulator Bi₂Se₃, ZHIHUI ZHU, G. LEVY, B. LUDBROOK, C.N. VEENSTRA, J.A. ROSEN, R. COMIN, D. WONG, P. DOSANJH, Department of Physics and Astronomy, University of British Columbia, Vancouver, BC V6T 1Z1, Canada, A. UBALDINI, Department of Physics, University of Geneva, Switzerland, P. SYERS, N.P. BUTCH, J. PAGLIONE, CNAM, Department of Physics, University of Maryland, College Park, Maryland 20742, USA, I.S. ELFIMOV, A. DAMASCELLI, Department of Physics and Astronomy, Quantum Matter Institute, University of British Columbia, Vancouver, BC V6T 1Z1, Canada — The electronic structure of Bi₂Se₃ is studied by angle-resolved photoemission and density functional theory. We show that the instability of the surface electronic properties, observed even in ultra-high-vacuum conditions, can be overcome via *in situ* potassium deposition. In addition to accurately setting the carrier concentration, new Rashba-like spin-polarized states are induced, with a tunable, reversible, and highly stable spin splitting. *Ab initio* slab calculations reveal that these Rashba states are derived from the 5-quintuple-layer quantum-well states. While the K-induced potential gradient enhances the spin splitting, this may be present on pristine surfaces due to the symmetry breaking of the vacuum-solid interface. Phys.Rev.Lett. 107 186405 (2011)

8:24AM V31.00003 Recent Results on Topological Phase Transition and Texture Inversion in Tunable Topological Insulators¹, SU-YANG XU, YUQI XIA, Princeton University, LEWIS ANDREW WRAY, Lawrence Berkeley National Laboratory, SHUANG JIA, Princeton University, FABIAN MEIER, JAN HUGO DIL, Paul Scherrer Institute, JURG OSTERWALDER, University of Zurich, BARTOSZ SLOMSKI, Paul Scherrer Institute, ARON BANSIL, HSIN LIN, Northeastern University, ROBERT CAVA, M. ZAHID HASAN, Princeton University — The recently discovered three-dimensional or bulk topological insulators are expected to exhibit exotic quantum phenomena. It is believed that a trivial insulator can be twisted into a topological state by modulating the spin-orbit interaction or the crystal lattice, driving the system through a topological quantum phase transition. By directly measuring the topological quantum numbers, we report the observation of a phase transition in a tunable spin-orbit system, BiTi(S_{1-δ}Se_δ)₂, in which the topological state formation is visualized (S.-Y. Xu *et al.*, *Science* (2011)). In the topological state, vortex-like polarization states are observed to exhibit three-dimensional vectorial textures, which collectively feature a chirality transition as the spin momentum-locked electrons on the surface go through the zero carrier density point. Such phase transition and texture inversion can be the physical basis for observing fractional charge ($\pm e/2$) and other fractional topological phenomena. We also present some of our recent results that reveal further novel spin and electronic properties of the system close to the critical point of the topological phase transition.

¹We acknowledge support from DOE/BES.

8:36AM V31.00004 Surface Termination of Cleaved Bi_2Se_3 Investigated by Low Energy Ion Scattering, XIAOXIAO HE, ZHIYONG WANG, JING SHI, JORY YARMOFF, Department of Physics and Astronomy, University of California, Riverside — The 3D Topological Insulator, Bismuth Selenide (Bi_2Se_3), is investigated with low energy ion scattering (LEIS). Se vacancies are believed to be responsible for the metallic behavior in transport, and LEIS is uniquely sensitive to the outermost atomic layer composition. Bi_2Se_3 is comprised of Se-Bi-Se-Bi-Se quintuple layers (QLs). Since the van der Waals bonds between QLs is weaker than the covalent bonds within each QL, it has been assumed that it is Se-terminated when cleaved. This assumption has been used in previous surface studies, such as STM or ARPES, which do not provide the composition of the surface atoms. 3 keV Na^+ ions were scattered from single crystal Bi_2Se_3 cleaved in ultra-high vacuum. At room temperature, the spectra indicate a surface terminated with Bi, rather than Se, although some Se is still present. The samples display a sharp 1×1 LEED pattern, indicative of an ordered material. We conclude that Bi_2Se_3 cleaves between the QLs, but that the surface Se quickly desorbs, likely as Se_2 or Se_4 . To test this, the Se:Bi ratio was monitored by LEIS after a sample was cleaved at liquid nitrogen temperature. It was found that the ratio starts out high, but decreases over the course of hours until it reaches the same value as that of a room temperature cleave.

8:48AM V31.00005 Electronic Structure of Clean and Adsorbate-Covered Bi_2Se_3 , RICHARD HATCH, MARCO BIANCHI, TILO PLANKE, Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, JIANLI MI, BO BRUMMER-STEDT IVERSEN, Center for Materials Crystallography, Department of Chemistry, Interdisciplinary Nanoscience Center, Aarhus University, PHILIP HOFMANN, Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University — The electronic structure of the topological insulator Bi_2Se_3 was probed using angle-resolved photoemission spectroscopy (ARPES). The electronic properties of clean and adsorbate-covered samples were studied for a combination of different bulk dopings and adsorbates. Due to contamination on the surface, the Dirac point of the topological surface states moves to higher binding energies, indicating an increasingly strong downward bending of the bands near the surface. This time-dependent band bending can be accelerated by intentionally exposing the surface to carbon monoxide, alkali atoms and other species. For a sufficiently strong band bending, new spectral features in the energy region of both the valence band and the conduction band are found. These changes are explained by a confinement of the states and the formation of quantum well states. This interpretation is supported by simple calculations of the band bending effects and by photon energy-dependent ARPES measurement that show how the band dispersion in the direction perpendicular to the surface is lost and non-dispersing, sharp states appear within the energy regions of the projected bulk bands. For a strong band bending, the conduction band quantum well states are strongly Rashba split.

9:00AM V31.00006 Sharp Dirac cone at a buried superconductor/topological insulator interface, JUSTIN WAUGH, YUE CAO, QIANG WANG, University of Colorado at Boulder, ALEXEI FEDOROV, Lawrence Berkeley National Laboratory, Z.J. XU, GENDA GU, Brookhaven National Laboratory, DANIEL DESSAU, University of Colorado at Boulder — We have studied the fully buried interface of a topological insulator, Bi_2Se_3 , with the conventional superconductor Nb. We characterized the chemical reactivity at the interface using core level photoemission spectroscopy. Using ARPES we are able to observe the sharp Dirac cone at the buried interface and characterize its details; including energy positions, band dispersion, and electronic scattering rates. All these measurements are carried out over a wide range of coverages, and set the stage for more advanced studies of this interface.

9:12AM V31.00007 Mapping the Orbital Texture of the Topological Insulator Bi_2Se_3 , YUE CAO, JUSTIN WAUGH, SEUNG RYONG PARK, QIANG WANG, THEODORE REBER, University of Colorado at Boulder, SUNG-KWAN MO, Advanced Light Source, Lawrence Berkeley National Laboratory, MATTHEW BRAHLEK, NAMRATA BANSAL, SEONGSHIK OH, Rutgers, the State University of New Jersey, GENDA GU, Brookhaven National Laboratory, DANIEL DESSAU, University of Colorado at Boulder — The orbital texture of the topological insulator Bi_2Se_3 was observed with ARPES using linearly polarized light. The topological state features a superposition of all three p orbitals. We compare the measured orbitals to the existing density functional theory calculations in the literature. This illustrates some of the unusual properties of this topological state and helps clarify the origin of the currently conflicting results from the spin resolved ARPES measurements.

9:24AM V31.00008 Spin resolved photoemission on surface doped topological insulator Bi_2Se_3 ¹, ZHIHUI PAN, ELIO VESCOVO, Brookhaven National Laboratory, ALEXEI FEDOROV, Lawrence Berkeley National Laboratory, D. GARDNER, S. CHU, YOUNG S. LEE, Massachusetts Institute of Technology, GENDA GU, TONICA VALLA, Brookhaven National Laboratory — Topological insulators (TI) have attracted much attention because of their exotic properties. Bi_2Se_3 is a model TI with a relative large bulk gap and a simple surface state structure. By depositing various impurities on the surface, we were able to fill the topological surface state and higher lying Rashba splitting surface states. The spin texture of the surface electronic structure was determined in spin resolved photoemission measurement.

¹This work was supported by DOE.

9:36AM V31.00009 Controlling the Bulk-surface Spectroscopic Separation in 3D Topological “Metals” Exploiting Hybridization, YI-TING HSU, MARK FISCHER, Cornell University, TAYLOR HUGHES, University of Illinois at Urbana-Champaign, EUN-AH KIM, Cornell University — How to separately probe the surface state in 3D topological insulators (TI) with chemical potential crossing conduction bands, i.e. topological metals, is a key challenge in exploiting the topological nature of surface states. The advent of MBE grown thin films of TI's with varying thickness only adds to the importance of the issue. We study the effects of hybridization in the spirit of Fano model for the low-energy effective four-band model of Bi_2Se_3 on a slab. We find that the apparent bulk-surface spectroscopic separation in the ARPES data on 3D TI can be viewed as a *consequence of hybridization* rather than the evidence for the absence of hybridization. We describe how the separation depends on the film thickness and propose ways to control the separation using strain.

9:48AM V31.00010 Topological insulators in the quaternary chalcogenide compounds and ternary famatinite compounds, Y.J. WANG, H. LIN, Northeastern U. (NU), TANMOY DAS, LANL and NU, M.Z. HASAN, Princeton U., A. BANSIL, NU — We present first-principles calculations to predict several three-dimensional (3D) topological insulators in quaternary chalcogenide compounds of compositions $\text{I}_2\text{-II-IV-VI}_4$ and ternary famatinite compounds of compositions $\text{I}_3\text{-V-VI}_4$. Among the large number of members of these two families, we give examples of naturally occurring compounds that are mainly Cu-based chalcogenides. We show that these materials are candidates for 3D topological insulators or can be tuned to obtain topologically interesting phases by manipulating the atomic number of the various cations and anions. A band inversion can occur at a single point Γ with large inversion strength, in addition to the opening of a bulk bandgap throughout the Brillouin zone. We discuss how the two investigated families of compounds are related to each other by cross-substitution of cations in the underlying tetragonal structure. Work supported by the US DOE.

10:00AM V31.00011 Quasiparticle band structures of $\beta\text{-HgS}$, HgSe , and HgTe , NIELS E. CHRISTENSEN, AXEL SVANE, Aarhus University, Denmark, MANUEL CARDONA, Max Planck Institute FKF, Stuttgart, ATHANASIOS CHANTIS, American Physical Society, MARK VAN SCHILFGAARDE, Arizona State University, Tempe, TAKAO KOTANI, Tottori University, Japan — The electronic structures of mercury chalcogenides in the zinc-blende structure have been calculated by the LDA, GW (one-shot, G_0W_0) and quasi-particle self-consistent GW ($QSGW$) approximations including spin-orbit coupling (SO). The slight tendency to overestimation of the band gaps by $QSGW$ is avoided by using a *hybrid* scheme (20% LDA and 80 % $QSGW$). The results of G_0W_0 depend strongly starting wave functions and are thus quite different from those from $QSGW$. Within $QSGW$ HgS is found to be a semiconductor, with a Γ_6 s-like conduction-band minimum state above the valence-band top Γ_7 and Γ_8 (“negative” SO splitting). HgSe and HgTe have “negative” gaps (inverted band structure). In HgTe the Γ_7 state is below Γ_6 due to the large Te SO splitting, in contrast HgSe where Γ_6 is below Γ_7 .

10:12AM V31.00012 Exceptionally Weak Electron-Phonon Coupling on the Surface of the Topological Insulator Bi₂Se₃ - A Promise for Room Temperature Applications¹, TONICA VALLA, Z.-H. PAN, Brookhaven National Laboratory, A.V. FEDOROV, Lawrence Berkeley National Laboratory, D. GARDNER, Y.S. LEE, S. CHU, Massachusetts Institute of Technology — Gapless surface states on topological insulators are protected from elastic scattering on non-magnetic impurities which makes them promising candidates for low-power electronic applications. However, for wide-spread applications, these states should have to remain coherent at ambient temperatures. Here, we studied temperature dependence of the electronic structure and the scattering rates on the surface of a model topological insulator, Bi₂Se₃, by high resolution angle-resolved photoemission spectroscopy. We found an extremely weak broadening of the topological surface state with temperature and no anomalies in the state's dispersion, indicating exceptionally weak electron-phonon coupling. Our results demonstrate that the topological surface state is protected not only from elastic scattering on impurities, but also from scattering on low-energy phonons, suggesting that topological insulators could serve as a basis for room temperature electronic devices.

¹supported by the US Department of Energy (DOE)

10:24AM V31.00013 Persistence of Topological Order and Formation of Quantum Well States in Topological Insulators B₂(Se,Te)₃ under Ambient Conditions¹, CHAOYU CHEN, XINGJIANG ZHOU², Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — We report high resolution angle-resolved photoemission measurements on the surface state of the prototypical topological insulators, Bi₂Se₃, Bi₂Te₃ and Bi₂Se_{0.4}Te_{2.6}, upon exposing to ambient conditions. We find that the topological order persists even when the surface is exposed to air at room temperature. However, the surface state is strongly modified after such an exposure. Particularly, we have observed the formation of two-dimensional quantum well states near the surface of the topological insulators after the exposure which depends sensitively on the original composition, x, in Bi₂Se_{3-x}Te_x. These rich information are crucial in utilizing the surface state and in probing its physical properties under ambient conditions.

¹This work is supported by the NSFC (91021006) and the MOST of China (973 program No: 2011CB921703).

²Corresponding author

10:36AM V31.00014 Strong Warping Effects and Angular Momentum Structures of Topological Insulator, WONSIG JUNG, Institute of Physics and Applied Physics, Yonsei University, Seoul, Korea, Y.K. KIM, Institute of Physics and Applied Physics, Yonsei University, Seoul, Korea, B.Y. KIM, Y.Y. KOH, Institute of Physics and Applied Physics, Yonsei University, Seoul, Korea, M. MATSUNAMI, S. KIMURA, UVSOR Facility, Institute for Molecular Science and The Graduate University for Advanced Studies, Okazaki 444-8585, Japan, M. ARITA, K. SHIMADA, Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Hiroshima 739-0046, Japan, J.H. HAN, Department of Physics, Sungkyunkwan University, Suwon, Korea, B.K. CHO, School of Physics and Department of materials science and engineering, GIST, Gwangju 500-712, Korea, C. KIM, Institute of Physics and Applied Physics, Yonsei University, Seoul, Korea — We performed angle resolved photoemission (ARPES) studies on Bi₂Te₃ with circularly polarized light. The alignment of OAM is found to have a strong binding energy dependence. OAM close to Dirac point has an ideal chiral structure ($\sin\theta$) without out-of-plane component. As the binding energy decreases, warping effect comes in and circular dichroism along the constant energy contour cannot be explained by a simple $\sin\theta$ function but requires a $\sin 3\theta$ term. When the warping effect becomes even stronger near the Fermi energy, circular dichroism has $\sin 6\theta$ symmetry. Such behavior is found to be compatible with the theoretically predicted spin structure.

10:48AM V31.00015 Three-Dimensional Massive Dirac Fermion in the Bulk Band Structure of Cubic Inverse Perovskite Ca₃PbO, TOSHIKAZE KARIYADO, MASAO OGATA, the University of Tokyo — The band structure of a cubic inverse perovskite Ca₃PbO, which has been proposed as a candidate for a topological insulator, is analyzed by means of the first-principles calculation. It turns out that Ca₃PbO is actually not a topological insulator, but a close observation of the calculated band structure near the Fermi energy reveals that there exist Dirac fermions in the bulk, instead of the surface, band structure. The Dirac fermion in this material is found on the Γ -X line in the momentum space and remarkably exactly at the Fermi energy in the energy space. It should also be noted that the discovered Dirac fermion is three-dimensional and massive with a very small mass of about 10^{-2} of the bare electron mass. The origin of the Dirac fermion in Ca₃PbO and the band structure of the materials related to Ca₃PbO will also be discussed.

Thursday, March 1, 2012 8:00AM - 10:48AM –

Session V32 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides - Interfaces, Layered Materials, and Growth 261

8:00AM V32.00001 Electric-field control of magnetization in Co₄₀Fe₄₀B₂₀/Pb(Mg_{1/3}Nb_{2/3})_{0.7}Ti_{0.3}O₃ structure at room temperature¹, SEN ZHANG, Y.G. ZHAO, Department of Physics, Tsinghua University, Beijing 100084, China, S. RIZWAN, X.F. HAN, Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, Beijing 100190, China, J.X. ZHANG, R. RAMESH, Department of Materials Science and Engineering, University of California, Berkeley, California 94720, USA — Electric-field control of magnetization is important for new generation information storage technology with high integration density and low power consumption. A lot of work has been carried out on electric-field control of magnetization in artificial ferromagnetic-ferroelectric (FM-FE) two-phase systems via the piezo-strain effect. Beside strain, electric/elastic domains and phase structure also play important roles in the electric-field control of magnetization, especially in the case of amorphous FM film without magnetocrystalline anisotropy. We report a large magnetoelectric effect in a Co₄₀Fe₄₀B₂₀/Pb(Mg_{1/3}Nb_{2/3})_{0.7}Ti_{0.3}O₃ structure at room temperature. Investigations on the ferroelectric domains, phase structures, magnetic domains and strain with *in situ* electric fields reveal a new mechanism for electric-field control of magnetization. This work provides a new way to realize large magnetoelectric coupling and is significant for applications, especially in the field of CoFeB-based spin valves to achieve electric-controlled magnetic random access memories.

¹This work was supported by the 973 project of the Ministry of Science and Technology of China (Grant Nos. 2009CB929202 and 2009CB929203)

8:12AM V32.00002 Coherently Coupled ZnO and VO₂ Interface studied by Photoluminescence and electrical transport across a phase transition, AMAR SRIVASTAVA, S. SAHA, A. ANNADI, Y.L. ZHAO, K. GOPINADHAN, X. WANG, N. NAOMI, Z.Q. LIU, S. DHAR, NUSNNI-NanoCore, National University of Singapore, Singapore, T.S. HERNG, BAO NINA, Department of Mat. Sci. and Eng, National University of Singapore, Singapore, - ARIANDO, NUSNNI-NanoCore, National University of Singapore, Singapore, JUN DING, Department of Mat. Sci. and Eng, National University of Singapore, Singapore, T. VENKATESAN, NUSNNI-NanoCore, National University of Singapore, Singapore — In this work we report a study of a coherently coupled interface consisting of a ZnO layer grown on top of an oriented VO₂ layer on sapphire by photoluminescence and electrical transport measurements across the VO₂ metal insulator phase transition (MIT). The photoluminescence of the ZnO layer showed a broad hysteresis induced by the phase transition of VO₂ while the width of the electrical hysteresis was narrow and unaffected by the over layer. The enhanced width of the PL hysteresis was due to the formation of defects during the MIT as evidenced by a broad hysteresis in the opposite direction to that of the band edge PL in the defect luminescence. Unlike VO₂ the defects in ZnO did not fully recover across the phase transition. From the defect luminescence data, oxygen interstitials were found to be the predominant defects in ZnO mediated by the strain from the VO₂ phase transition. Such coherently coupled interfaces could be of use in characterizing the stability of a variety of interfaces and also for novel device application.

8:24AM V32.00003 Ferroelectricity and compositional inversion symmetry breaking in PbTiO₃/SrRuO₃ superlattices, S.J. CALLORI, J. GABEL, Department of Physics and Astronomy, Stony Brook University, D. SU, Center for Functional Nanomaterials, Brookhaven National Laboratory, J. SINSHEIMER, M.V. FERNANDEZ-SERRA, M. DAWBER, Department of Physics and Astronomy, Stony Brook University — Most work to date on artificially layered ferroelectric superlattices has utilized the insulating titanium perovskite oxides (e.g. PbTiO₃, BaTiO₃, CaTiO₃ and SrTiO₃) as “building blocks,” from which a layered structure is assembled by sequential deposition. However, the need for new functionalities, particularly related to magnetism, demands that we expand this set. The much-studied compound SrRuO₃ provides the proof of concept that metallic magnetic oxides can transform into thin-film dielectric components in certain heterostructures, in this case PbTiO₃/SrRuO₃ superlattices. Our high quality epitaxial PbTiO₃/SrRuO₃ superlattices, grown by RF magnetron sputtering on SrTiO₃ substrates (with SrRuO₃ bottom electrodes) show both ferroelectricity, and, as they have both A and B site variation, compositional breaking of inversion symmetry. We will present experimental measurements made on this system using x-ray diffraction, transmission electron microscopy, and electrical characterization, which together with first principles density functional theory simulations, demonstrate how, as the constituent layer thicknesses are varied, the metallicity of the superlattice changes and polarization evolves.

8:36AM V32.00004 Interface control of emergent ferroic order in Ruddlesden-Popper Sr_{n+1}Ti_nO_{3n+1}, TURAN BIROL, NICOLE A. BENEDEK, CRAIG J. FENNIE, School of Applied & Engineering Physics, Cornell University — We have discovered from first-principles an unusual polar state in the low n Sr_{n+1}Ti_nO_{3n+1} Ruddlesden-Popper (RP) layered perovskites in which ferroelectricity is nearly degenerate with antiferroelectricity, a relatively rare form of ferroic order. We show that epitaxial strain plays a key role in tuning the “perpendicular coherence length” of the ferroelectric mode, and does not induce ferroelectricity in these low dimensional RP materials as is well known to occur in SrTiO₃. These systems present an opportunity to manipulate the coherence length of a ferroic distortion in a controlled way, without disorder or a free surface. [T. Birol, N. A. Benedek, C. J. Fennie, Physical Review Letters, in press]

8:48AM V32.00005 Use of dimensionality to enhance tunable microwave dielectrics, D.G. SCHLOM, Cornell U., CHE-HUI LEE, R. HAISLMAIER, E. VLAHOS, V. GOPALAN, Pennsylvania State U., T. BIROL, Y. ZHU, L.F. KOURKOUTIS, N. BENEDEK, Y. KIM, J.D. BROCK, D.A. MULLER, C.J. FENNIE, Cornell U., N.D. ORLOFF, J.C. BOOTH, NIST, V. GOIAN, S. KAMBA, ASCR, M.D. BIEGALSKI, ORNL, M. BERNHAGEN, R. UECKER, Leibniz Institute for Crystal Growth, X.X. XI, Temple University, I. TAKEUCHI, U. Maryland — The miniaturization and integration of frequency-agile microwave circuits—*tunable* filters, resonators, phase shifters and more—with microelectronics offers tantalizing device possibilities, yet requires thin films whose dielectric constant at GHz frequencies can be tuned by applying a quasi-static electric field. Appropriate systems, e.g., Ba_xSr_{1-x}TiO₃, have a paraelectric-to-ferroelectric transition just below ambient temperature, providing high tunability. Unfortunately such films suffer significant losses arising from defects. Recognizing that progress is stymied by dielectric loss, we start with a system with exceptionally low loss—Sr_{n+1}Ti_nO_{3n+1} phases—where in-plane crystallographic shear (SrO)₂ faults provide an alternative to point defects for accommodating non-stoichiometry. In this talk we will establish both experimentally and theoretically the emergence of a ferroelectric and highly tunable ground state in biaxially strained Sr_{n+1}Ti_nO_{3n+1} phases with $n \geq 3$ at frequencies up to 40 GHz. With increasing n the (SrO)₂ faults are separated further than the ferroelectric coherence length perpendicular to the in-plane polarization, enabling tunability with a figure of merit at room temperature that rivals all known tunable microwave dielectrics.

9:00AM V32.00006 Ferroelectric-Antiferroelectric Phase Control: Interplay Between Octahedral Tilt, Polarization, and Chemistry at BFO-LSMO Interfaces¹, YOUNG-MIN KIM, Oak Ridge National Laboratory, PU YU, University of California Berkeley, YING-HAO CHU, National Chiao Tung University, STEPHEN PENNYCOOK, SERGEI KALININ, ALBINA BORISEVICH, Oak Ridge National Laboratory — Atomically-defined interfaces between complex oxides offer a paradigm of novel electronic and coupled functionalities. Here, we report the stabilization of the ferroelectric and antiferroelectric phases at the BFO-LSMO interface through termination control and reveal associated atomic-scale mechanisms with the help of aberration-corrected scanning transmission electron microscopy combined with Electron Energy Loss Spectroscopy. The BFO thin film grown on MnO₂-terminated surface of LSMO exhibits stabilized ferroelectric phase at the interface. The interfacial and bulk polarization are antiparallel, giving rise to head to head ferroelectric domain wall mostly parallel to the interface. In comparison, the film grown on (Sr,Li)O-terminated surface of LSMO exhibits antiferroelectric phase in the vicinity of the interface, with associated ferroelectric-antiferroelectric domain wall in the bulk. Details of tilt and polarization behavior, as well as electronic properties at the interfaces including charged domain walls and FE-AFE walls, will be presented. These results imply that the structural parameters such as octahedral tilt and ferroelectricity in BFO can be directly controlled by modifying the interface structure.

¹This research is sponsored by the MSE Division (YMK, SJP, SVK, AYB), Office of BES of the U.S. DOE.

9:12AM V32.00007 Interplay of couplings between antiferrodistortive, ferroelectric, and strain degrees of freedom in monodomain PbTiO₃/SrTiO₃ superlattices¹, PABLO AGUADO-PUENTE, PABLO GARCIA-FERNANDEZ, JAVIER JUNQUERA, DCITIMAC, Universidad de Cantabria, Avda. de los Castros s/n, 39005 Santander, Spain — We report first-principles calculations, within the density functional theory, on the coupling between epitaxial strain, polarization, and oxygen octahedra rotations in monodomain (PbTiO₃)_n/(SrTiO₃)_n superlattices. We show how the interplay between (i) the epitaxial strain and (ii) the electrostatic conditions at the interfaces can be used to control the orientation of the main axis of the system – defined by the direction of the polarization or the rotation axis of the oxygen octahedra. The electrostatic constraints at the interface facilitate the rotation of the polarization and, as a consequence, we predict large piezoelectric responses at epitaxial strains smaller than those that would be required considering only strain effects. In addition, ferroelectric (FE) and antiferrodistortive (AFD) modes are strongly coupled, with different rotation angles in the TiO₆ octahedra as a function of the polarization direction. The magnitude of the rotations cannot be explained by the usual steric arguments alone, and a covalent model is proposed to account for the large polarization-tilting coupling. The energy gain due to the FE-AFD coupling decreases with the periodicity of the superlattice, becoming negligible for $n \geq 3$.

¹Work accepted for publication in Phys. Rev. Lett. Financial support from grants FIS2009-12721-C04-02, and CP-FP 228989-2 OxIDES. Computational resources provided by the Red Española de Supercomputación.

9:24AM V32.00008 Engineered polarization rotation in $\text{PbTiO}_3/\text{CaTiO}_3$ superlattices, JOHN SINSHEIMER, SARA J. CALLORI, YUCEF BENKARA, BENJAMIN BEIN, JON DALEY, Dept of Physics and Astronomy, Stony Brook University, DONG SU, Center for Functional Nanomaterials, Brookhaven National Laboratory, MATTHEW DAWBER, Dept of Physics and Astronomy, Stony Brook University — Large piezoelectric responses, such as those seen in $\text{PbZr}_x\text{Ti}_{1-x}\text{O}_3$ in the vicinity of the compositional morphotropic phase boundary, can occur when the direction of the polarization in a ferroelectric material can rotate. Here we show experimentally that a similar enhancement of the piezoelectric response can be achieved in artificially layered epitaxial superlattices composed of alternating layers of PbTiO_3 and CaTiO_3 deposited on SrTiO_3 substrates by RF magnetron sputtering. The exceptional quality of our samples is demonstrated by x-ray diffraction and transmission electron microscopy. The structural and functional properties of the materials have been measured as a function of relative layer thickness. Electrically measured ferroelectric polarization and dielectric constants corroborate the enhancement of d_{33} we have measured experimentally using piezoforce microscopy. The structural changes, which allow polarization rotation, have been directly measured using grazing incidence in-plane x-ray diffraction (at NSLS X21 and X22C). Finally, the as-grown domain structure has been imaged with piezoforce microscopy, further confirming polarization rotation and explaining the unusual switching dynamics observed in our electrical characterization.

9:36AM V32.00009 In situ studies on ferroelectric BaTiO_3 interface¹, JUNSOO SHIN, VON BRAUN NASCIMENTO, WARD PLUMMER, JIANDI ZHANG, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, ALBINA BORISEVICH, VINCENT MEUNIER, SERGEI KALININ, ARTHUR BADDORF, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — Ferroelectric phase stability in ferroelectric films is critically dependent on the surface and interface phenomena, especially governed by electrostatic depolarization energy. Predictions for the minimum critical film thickness for ferroelectricity have continuously decreased down to few unit cells. We have examined surface/interface atomic structures of ultrathin BaTiO_3 (BTO) films grown on conductive SrRuO_3 (SRO) and Nb-doped SrTiO_3 . The surface structure of BTO/SRO was refined using in-situ Low Energy Electron Diffraction (LEED) I-V, resulting to observation of polar distortion in ultrathin (≥ 4 ML) BTO films. The in-situ Scanning Tunneling Microscopy (STM) has been performed prior and after BTO deposition on SRO. However, the unusual 2×2 reconstruction is observed for 1-2 ML BTO films and bare SRO by STM. The surface reconstruction of SRO bottom electrode is shown to affect the interface of films deposited subsequently which could be reflected in ultrathin film properties. The in-situ LEED I-V structural studies on 1-2 ML BTO interface have been performed without SRO layer, which kept ultrathin BTO films from the preclusion of reconstructed SRO films.

¹This work was supported at LSU by the DOE Grant DE-SC0002136. Research at ORNL's CNMS was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. DOE.

9:48AM V32.00010 Ellipsometric study of SrTiO_3 thin film grown Si(100), YAO TIAN, University of Toronto, CAROLINA ADAMO, Cornell Center of Materials Research, KENNETH BURCH, University of Toronto — Recently, a new method to grow SrTiO_3 thin ferroelectric film directly on Si(100) has been demonstrated by *M. P. Warusawithana, et al.* We use ellipsometry to study the film and a model based on inhomogenous gap to oxide deficiency was made to interpret the data.

10:00AM V32.00011 Valence Fluctuation in Ultrathin $\text{Ti}_{1+x}\text{O}_2$ on Rutile TiO_2 , Q.Y. CHEN¹, P.V. WADEKAR, H.J. HUNAG, S.W. YEH, N.J. HO, National Sun-Yat Sen University, Kaohsiung, Taiwan, H.W. SEO, University of Arkansas, Little Rock, AR, USA, W.K. CHU, Texas Center for Superconductivity, University of Houston, TX, USA — The physical properties of metal oxides (TMO) can change drastically depending on the non-stoichiometry of oxygen, for which rutile TiO_2 single crystals were self-implanted with Ti to acquire a layers of ~ 6 nm populated with extra Ti found in +2, +3, and +4 charge states as revealed by X-ray photoelectron spectroscopy (XPS). The formations of the TiO and Ti_2O_3 crystalline phases were verified by high-resolution transmission electron microscopy (HRTEM). Variable-temperature electrical resistivity measurement suggests the occurrence of charge ordering at low temperatures, where weak localization of the charges take hold, commonly observed in heavily doped semiconductors. The magneto-transport behaviors follow mixed scenario of band conduction and fixed range hopping, albeit with different energy scales and weighting factors demarcated by a transition temperature of MR sign change, a signature of valence fluctuation in which the ordered low-temperature phase would melt into the high-temperature disordered phase, or by condensation in reverse. This work was supported by the National Science Council, the Ministry of Education, Taiwan, the National Science Foundation, and the State of Texas through Texas Center for Superconductivity.

¹Corresponding author, also with Texas Center for Superconductivity, University of Houston, TX, USA

10:12AM V32.00012 Atomic Layer-by-Layer Growth of Homoepitaxial SrTiO_3 Films by Laser MBE, QINGYU LEI, GUOZHEN LIU, KE CHEN, Department of Physics, Temple University, SUILIN SHI, FUQIANG HUANG, CAS Key Laboratory of Materials for Energy Conversion, Shanghai Institute of Ceramics, Chinese Academy of Sciences, XIAOXING XI, Department of Physics, Temple University — Two most effective techniques for oxides film growth are reactive MBE and laser MBE. With alternating monolayer growth, reactive MBE has shown the capacity of stoichiometry control and crystalline perfection in SrTiO_3 films on SrTiO_3 , while most works of laser MBE, using compound targets, often shows non-stoichiometry and lattice defects. In order to control layer-by-layer growth to atomic level, we carried out laser MBE from separate oxide targets, for example, growing SrTiO_3 from SrO and TiO_2 targets, such that the SrO and TiO_2 layers were deposited alternatively one atomic layer at a time. X-ray diffraction spectra showed that the stoichiometric SrTiO_3 film peak overlapped with and was indistinguishable from the SrTiO_3 substrate peak, while the off stoichiometric SrTiO_3 films, either Sr rich or poor, showed lattice expansion. We conclude that laser MBE from separate oxide targets can achieve the same stoichiometry control as reactive MBE.

10:24AM V32.00013 Preparation of Atomically Flat SrTiO_3 Surfaces Using Non-acid Etching and Thermal Annealing Process, JOHN CONNELL, AMBROSE SEO, The University of Kentucky — The growth of epitaxial thin films and heterostructures requires atomically flat surfaces of substrates. So far chemical etching processes by acidic etchant have been widely used for the surface preparation of oxide substrates. Here we show that atomically flat surfaces of single crystalline SrTiO_3 substrates of both the (100) and (111) orientations can be prepared using non-acidic etching and thermal annealing techniques. Atomic force microscopy confirms the evolution of the surface of the substrates from rough to a step-terrace structure. Scanning tunneling microscopy shows that SrO segregation on the surface is removed by our etching process. This new technique replaces the use of acidic oxide etchant as the primary method for etching SrTiO_3 substrates.

10:36AM V32.00014 Effect of Mg^{2+} on the structure of amorphous CaCO_3 – A molecular dynamics simulation, HIDEKAZU TOMONO, HIROKI NADA, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, JAPAN — Molecular dynamics (MD) simulations of amorphous calcium carbonate (ACC) were carried out to investigate the effect of Mg^{2+} ions on the structure of CaCO_3 crystal nucleus formed from ACC. Our systems contained 432 CaCO_3 with several concentrations of MgCO_3 . In this study, our original ion model of Mg^{2+} was developed and combined with Raiteri model of Ca^{2+} and rigid CO_3^{2-} [1]. The simulations indicated that the fraction of vaterite-like ion arrangement was much larger than those of calcite-like and aragonite-like ion arrangements in pure ACC. However, as the Mg^{2+} concentration increased, the fraction of vaterite-like ion arrangements decreased, which suggests that Mg^{2+} ions play as inhibitors of vaterite nucleation. The result explains why calcite or aragonite is preferentially nucleated in the presence of Mg^{2+} , whereas vaterite is nucleated in the absence of them.[1] P. Raiteri, J. D. Gale, D. Quigley, and P. M. Rodger, J. Phys. Chem. C 114, 5997 (2010).

Thursday, March 1, 2012 8:00AM - 10:00AM —

Session V34 DCP: Focus Session: Impact of Ultrafast Lasers V: Applications II 107A

8:00AM V34.00001 Thermalization of photoexcited electrons in bismuth investigated by time-resolved THz spectroscopy and *ab initio* calculations¹, IURII TIMROV, Ecole Polytechnique, LSI, TOBIAS KAMPFRATH, Fachbereich Physik, Freie Universität, JEROME FAURE, NATHALIE VAST, Ecole Polytechnique, LSI, CHRISTIAN AST, Max-Planck-Institut für Festkörperforschung, CHRISTIAN FRISCHKORN, Fritz-Haber-Institut der Max-Planck-Gesellschaft, MARTIN WOLF, Fachbereich Physik, Freie Universität, PAOLA GAVA, LUCA PERFETTI, Ecole Polytechnique, LSI — The charge carrier dynamics of photoexcited bismuth generates a Drude response that evolves in time. In contrast to graphite, the plasma frequency of bismuth displays an initial increase and a subsequent decay. We have performed *ab initio* calculations of bulk bismuth within the density functional theory, and show that the non-monotonic behaviour of the plasma frequency is due to the presence of local minima in the conduction band: most of the photoexcited electrons first accumulate in these local minima, and reach the L point only 0.6 ps after photoexcitation.

¹Support from the ANR (project PNANO ACCATTONE) and from DGA are gratefully acknowledged. Computer time was granted by GENCI (project 2210).

8:12AM V34.00002 Spatio-temporal dynamics of plasmons on a metal cone, ALEJANDRO RODRIGUEZ PEREZ, JOONHEE LEE, SHAWN M. PERDUE, V. ARA APKARIAN, Department of Chemistry, University of California, Irvine — Localized surface plasmons (LSP) and propagating plasmon modes (PPM) field emit at the singularity of the metallic tip apex upon ultrafast optical excitation. Interferometric measurements, using frequency modulation-demodulation techniques, allow the characterization of the time profile of the optical field emission and the space-time profile of the propagating modes. A pump pulse launches a plasmon that oscillates on the cone and coherently interferes with a time-delayed probe pulse which is cross-polarized with respect to the pump. We present a simple model that accurately describes the experimental results. However, the observations of trapped propagating modes, their lifetime, and their polarization are not predicted by current theories, which describe tip-plasmons as strictly transverse magnetic modes.

8:24AM V34.00003 Time-Resolved ARPES Study of Ultrafast Dynamics in Cuprate Superconductor Bi2212¹, JIANQIAO MENG, Condensed Matter and Magnet Science, Materials Physics and Applications Division, Los Alamos National Laboratory, Los Alamos NM, 87545, USA, GEORGI L. DAKOVSKI, SLAC National Accelerator Laboratory, Menlo Park, CA 94025-7015, USA, JIAN-XIN ZHU, Physics of Condensed Matter and Complex Systems, Theoretical Division, Los Alamos National Laboratory, Los Alamos NM, 87545, USA, PETER S. RISEBOROUGH, Department of Physics, Temple University - Philadelphia, PA 19122, USA, GENDA GU, Condensed Matter Physics & Materials Science, Brookhaven National Laboratory, Upton, NY 11973, USA, STEVE M. GILBERTSON, GEORGE RODRIGUEZ, Center for Integrated Nanotechnologies, Materials Physics and Applications Division, Los Alamos National Laboratory, Los Alamos NM, 87545, USA, TOMASZ DURAKIEWICZ, Condensed Matter and Magnet Science, Materials Physics and Applications Division, Los Alamos National Laboratory, Los Alamos NM, 87545, USA — The momentum-dependent ultrafast dynamics in cuprate superconductor Bi2Sr2CaCu2O8 is investigated using ultra high resolution time-resolved angle-resolved photoemission spectroscopy (tr-ARPES). In this talk, we will present our observation and analysis of dynamics of the quasiparticle states in Bi2Sr2CaCu2O8 in nodal and antinodal direction as a function of doping. Work was performed with temporal resolution of 35fs. The consequences of our findings in terms of nodal-antinodal dichotomy will be discussed.

¹Support for this work was provided by LDRD program at LANL

8:36AM V34.00004 SFG and SPR Study of Sodium Dodecyl Sulfate Film Assembly on Positively Charged Surfaces¹, SANGHUN SONG, TOBIAS WEIDNER, NESAC/BIO, Univ. of Washington, MATTHEW WAGNER, The Procter and Gamble Company, DAVID CASTNER, NESAC/BIO, Univ. of Washington, NESAC/BIO TEAM, PROCTER AND GAMBLE COLLABORATION — This study uses sum frequency generation (SFG) vibrational spectroscopy and surface plasmon resonance (SPR) sensing to investigate the structure of sodium dodecyl sulfate (SDS) films formed on positively charged and hydrophilic surfaces. The SPR signals show a good surface coverage suggesting that full monolayer coverage is reached at 1 mM. SFG spectra of SDS adsorbed exhibits well resolved CH₃ peaks and OH peaks. At both 0.2 mM and 1 mM SDS concentration the intensity of both the CH₃ and OH peaks decreased close to background levels. We found that the loss of SFG signal at 0.2 mM occurs at this concentration independent of surface charge density. It is more likely that the loss of signal is related to structural inhomogeneity induced by a striped phase - stand-up phase transition. This is supported by a distinct change of the relative SFG phase between CH₃/OH near 0.2 mM. The second intensity minimum might be related to charge compensation effects. We observed a substrate dependence for the high concentration transition. We also observed distinct SFG signal phase changes for water molecules associated with SDS layers at different SDS solution concentrations indicating that the orientation of bound water changed with SDS surface structure.

¹Procter and Gamble, Univ. of Washington, NTUF, and NNIN-UW

8:48AM V34.00005 Nanoscale sensing with surface-enhanced CARS spectroscopy, DMITRI VORONINE, ALEXANDER SINYUKOV, XIA HUA, GUOWAN ZHANG, WENLONG YANG, KAI WANG, PANKAJ JHA, GEORGE WELCH, ALEXEI SOKOLOV, MARLAN SCULLY, Texas A&M University, College Station, TX 77840 — Time-resolved coherent anti-Stokes Raman scattering (CARS) is extended to the nanoscale regime where nano-molar amounts of molecules may be investigated. We show that spectral resolution of CARS generated by ultrashort laser pulses may be improved by collecting a sequence of time-resolved spectra. This procedure provides additional linewidth information and allows detecting two species of pyridine molecules in a vicinity of aggregated gold nanoparticles. Surface-enhanced CARS (SE-CARS) signals of the adsorbed pyridine monolayer are detected in the presence of a bulk pyridine background CARS signal. Time-resolved SE-CARS signals are stronger than the conventional CARS, and more sensitive to the surface environment which makes them suitable for nano-surface characterization with high molecular specificity. This technique allows measuring the vibrational dephasing time of molecules on nano-surfaces and characterizing the effects of the surface local environment on the ultrafast molecular dynamics. This technique may be applied to a variety of artificial and biological systems and complex molecular mixtures and has a potential for nanophotonic sensing applications.

9:00AM V34.00006 ABSTRACT WITHDRAWN —

9:12AM V34.00007 Time-resolved photocurrent generation in graphene $p-n$ junctions; probing $e-h$ relaxation dynamics near the Fermi level, MATT GRAHAM, SU-FEI SHI, DANIEL RALPH, JIWOONG PARK, PAUL MCEUEN, Kavli Institute at Cornell for Nanoscale Science — In this contribution we probe the relevant timescales associated with photocurrent generation by optically exciting graphene at a $p-n$ junction defined by electrostatic gates. Time-resolution of the optical and electrical response are obtained by simultaneous collection of transient photocurrent and transient absorption using a two-pulse correlation approach with 160 fs resolution. The transient absorption signal decays biexponentially in the $p-n$ junction at 0.26 and 2.2 ps; timescales similar to those recently established for hot electron and hot optical phonon cooling in graphene sheets. By contrast, we find transient photocurrent decay signal is surprisingly slow, with tails extending for 100s of ps. At 10 K, the rate coefficient for transient photocurrent decay is $2.7 \pm 0.6 \text{ ps}^{-1} \text{ nA}^{-1}$, and it increases monotonically tenfold upon warming to room temperature. We attribute the stark difference in the transient photocurrent and absorption kinetics to a photocurrent response that is sensitive to recombination processes that are occurring well below optical excitation energies, near the Fermi level. Combining the measurements, transient photocurrent alongside the well-studied transient absorption allows us to construct a rough timeline of events associated with photocurrent production at a graphene $p-n$ junction.

9:24AM V34.00008 Standoff detection of trace compounds enabled by continuum pulse shaping and coherent Raman scattering, MARSHALL T. BREMER, ORIN YUE, VADIM V. LOZOVY, MARCOS DANTUS, Michigan State University — Raman spectroscopy has long been pursued as means to detect hazards from a safe distance. This approach promises high chemical specificity, but is limited in sensitivity because of the very small Raman cross-section. We recently demonstrated detection of trace quantities using a non-linear counterpart, coherent anti-Stokes Raman scattering (CARS), which offers large signal enhancement over spontaneous Raman due to coherent signal addition. Utilizing a pulse shaper and the bandwidth inherent in a 5fs laser pulse, CARS spectra were acquired from an explosive simulant dissolved within thin polymer films. Further, the pulse shaper offers total control of the non-linear process, including selective excitation of particular vibrational modes, enabling single channel detection and associated opportunities for rapid chemical imaging. We will present standoff chemical images and associated CARS spectra acquired in a standoff configuration, demonstrating the applicability of the new spectroscopy in a realistic environment.

9:36AM V34.00009 Transient Absorption Spectroscopy for the Detection of Multiexciton States in Semiconductor Quantum Dots¹, AMANDA NEUKIRCH, OLEG PREZHDO, University of Rochester — It has been shown that excitations of quantum dots at photon energies well above the band gap can produce a superposition of single exciton (SE) and multiple exciton (ME) states. The resulting electron hole dynamics can then be monitored using transient absorption (TA) spectroscopy. We have modeled the TA signal that can be expected when $\text{Pb}_{68}\text{Se}_{68}$ and $\text{Si}_{29}\text{H}_{24}$ are excited, and subsequently probed with attosecond laser pulses. In the proposed experiment a pump pulse serves to excite the sample. The energy of the probe pulse is chosen such that any detected absorption is attributable to the presence of a ME state. Oscillations in the absorption spectrum indicate the existence of a coherent superposition. The period of the oscillation depends on the energy difference between the superimposed states. We explore how dephasing of this signal is affected by the temperature of the system, as well as the number of states involved. We predict what can and cannot be measured experimentally and propose specific attosecond experimental scenarios.

¹This work was supported by NSF grant number CHE-1050405.

9:48AM V34.00010 How much information do ultrafast spectra contain? The case for ultrafast quantum process tomography¹, ALAN ASPURU-GUZI, Department of Chemistry and Chemical Biology, Harvard University — In this talk, I will describe the concept of quantum process tomography (QPT). The QPT protocol is a novel way of thinking about ultrafast spectra that allows to design families of experiments for extracting the quantum dynamical map of any system addressable by ultrafast spectroscopy. I will explain how QPT works, and also will describe our progress towards an experimental realization in collaboration with the group of Keith Nelson (MIT).

¹This work was supported by the Department of Energy Center for Excitonics at MIT/Harvard/BNL as well as the DARPA Quantum Effects in Biological Environments (QUBE) program

Thursday, March 1, 2012 8:00AM - 11:00AM –

Session V35 DCP: Focus Session: DFT VII: Time-Dependent Processes I: Driven Systems 107B

8:00AM V35.00001 Towards the ab-initio description of photo-induced processes, E.K.U. GROSS, Max Planck Institute of Microstructure Physics — Excitons are prominent features in the optical spectra of periodic solids and molecular aggregates. Time-dependent density functional theory should, in principle, be able to describe excitonic effects. However, with standard functionals for the exchange-correlation (xc) kernel f_{xc} , such as adiabatic LDA and adiabatic GGA, excitonic features are completely absent. The construction of improved functionals for f_{xc} yielding excitons has a long history. Here we propose a new parameter-free approximation for the xc kernel through an algorithm in which the exact Dyson equation for the response is solved self-consistently with an approximate expression for the kernel in terms of the dielectric function [PRL **107**, 186401 (2011)]. We apply this to the calculation of optical spectra for various small bandgap (Ge, Si, GaAs, AlN, TiO₂, SiC), large bandgap (C, LiF, Ar, Ne) and magnetic (NiO) insulators. The calculated spectra are in very good agreement with experiment for this diverse set of materials, highlighting the universal applicability of the new kernel. These optical spectra are calculated with clamped nuclei. However, in a variety of optical phenomena, the coupling between electronic and nuclear motion plays an important role. Prominent examples are the process of vision and photo-synthesis. Standard approximations such as Ehrenfest dynamics, surface hopping, or nuclear wave-packet dynamics only partially capture the occurring non-adiabatic effects. As a first step towards a full ab-initio treatment of the coupled electron-nuclear system, we deduce an exact factorization of the complete wavefunction into a purely nuclear part and a many-electron wavefunction which parametrically depends on the nuclear configuration. We derive formally exact equations of motion for the nuclear and electronic wavefunction [PRL **105**, 123002 (2010)]. These exact equations lead to a rigorous definition of time-dependent potential energy surfaces as well as time-dependent geometric phases.

8:36AM V35.00002 Exact factorization of the time-dependent electron-nuclear wavefunction: Time-dependent potential energy surface, ALI ABEDI, FEDERICA AGOSTINI, Max-Planck-Institut für Mikrostrukturphysik Weinberg 2, D-06120 Halle, Germany, NEEPA T. MAITRA, Department of Physics and Astronomy, Hunter College and the City University of New York, 695 Park Avenue, New York, New York 10065, USA, E.K.U. GROSS, Max-Planck-Institut für Mikrostrukturphysik Weinberg 2, D-06120 Halle, Germany — We have recently proved an exact decomposition of the electronic and nuclear degrees of freedom (Phys. Rev. Lett. **105** 123002 (2010)) and introduced a set of coupled equations of motion for the electrons and nuclei that describe the evolution of the complete electron-nuclear system. The nuclear equation is particularly appealing being a Schrödinger equation with a time-dependent potential energy surface (TD PES) and a time-dependent vector potential as rigorous concepts, mediating the coupling between the nuclear and the electronic degrees of freedom in a formally exact way. By studying physically different cases, we demonstrate that the TD PES is a powerful tool to investigate molecular processes.

8:48AM V35.00003 Exact factorization of the full electron-nuclear wavefunction: A quantum-classical study, FEDERICA AGOSTINI, ALI ABEDI, EBERHARD GROSS, Max-Planck-Institut für Mikrostrukturphysik — It was recently shown in [1] that the solution of the time-dependent Schrödinger equation for a molecular system can be exactly factorized to an electronic and a nuclear contribution. In [1], the authors derived exact equations of motion for the coupled evolution of the electronic and nuclear wavefunctions, which are a good starting point to develop approximations, systematically. Based on this exact decomposition of the electron and nuclear motion, we present a quantum-classical scheme for the coupled electron-nuclear dynamics. Nuclear degrees of freedom evolve along a classical trajectory, affecting electronic motion and inducing quantum transitions, which in turn alter nuclear dynamics. Applications of the proposed method to model systems will be presented.

[1] A. Abedi, N.T. Maitra and E.K.U. Gross, *Phys. Rev. Lett.* **105** 123002 (2010).

9:00AM V35.00004 Time-dependent density functional theory for open quantum systems, DAVID TEMPEL, ALAN ASPURU-GUZI, Harvard University — We present the extension of time-dependent density functional theory (TDDFT) to the realm of open quantum systems (OQS). OQS-TDDFT allows a first principles description of electronic systems undergoing non-unitary dynamics due to coupling with a bath, such as that arising from molecular vibrations, solvent degrees of freedom or photon modes of the electromagnetic field. We first prove extensions of the Runge-Gross and van Leeuwen theorems to OQS-TDDFT, which rigorously establish it as a formally exact theory. We then discuss development of approximate OQS-TDDFT functionals, exact conditions on these functionals, as well as future challenges. Finally, we will discuss the application of OQS-TDDFT in obtaining broadened absorption spectra.

9:12AM V35.00005 Time-Dependent Electron Localization Functions, TDELFS, for Molecular Ionization and Harmonic Generation in Intense Laser Pulses¹, ANDRE D. BANDRAUK, EMMANUEL FOWE PENKA, Université de Sherbrooke — The nonlinear nonperturbative response of N₂, CO₂, OCS, CS₂ are studied numerically by solutions of Kohn-Sham (KS) orbital equations in the presence of few cycle intense $I > 10^{14}$ W/cm², 800nm laser pulses. It is found generally that ionization rates depend on different functionals and ionization also occurs from inner-shell KS orbitals. This is sensitive to laser-molecule orientation as predicted earlier [1]. Ionization rate maxima correspond to the alignment of maximum KS orbital densities with the laser polarization instead of orbital ionization potentials, I_p . These results are corroborated through time analysis of TDELFS where ionization occurs from lone pair or bond regions of the corresponding molecule at various times during the pulses. Time frequency analysis of Harmonic Generation spectra allow for identification of recollision times of ionized electrons with the parent ion.

[1] EF Penka, AD Bandrauk, *Phys Rev A* **81**, 023411(2010); **84**, 035412(2011).

¹Canada Research Chair

9:24AM V35.00006 TDDFT for nonlinear phenomena of light-matter interactions, ANGEL RUBIO, NanoBio Spectroscopy Group and ETSF Scientific Development Centre, Faculty of Chemistry University of the Basque Country — Despite the success of linear-response schemes to describe excitations of many electron systems, many physical processes stemming from the interaction of light with matter are nonlinear in nature. In this talk we will address the problems and open questions related to the description of this phenomena with the goal of providing a sound description of laser-induced-population processes within TDDFT. Through the exact solution of a few electron system interacting with a monochromatic laser we highlight some common deficiencies of all adiabatic density functionals within time-dependent density-functional theory to handle photoinduced processes leading to population changes of many-body states. One prototype case is Rabi oscillations between the ground and an excited state when a monochromatic laser with a frequency close to the resonance is applied. All adiabatic functionals are not able to discern between resonant and nonresonant (detuned) Rabi oscillations. Only the inclusion of an appropriate memory dependence can correct the fictitious time-dependence of the resonant frequency. We extend this description to dynamical induced charge transfer processes and many body tunneling. Adiabatic functionals will fail similarly in the description of all processes involving a change in the population of states. We will show our recent advances in deriving a new memory-dependent functional. The description of photo-induced processes in chemistry, physics, and biology and the new field of attosecond electron dynamics and high-intense lasers all demand fundamental functional developments going beyond the adiabatic approximation.

10:00AM V35.00007 Performance of the exact adiabatic density functional to describe Rabi physics, JOHANNA ILDEMAR FUKS, Nano-Bio Spectroscopy group and ETSF Center, Dpto. Física de Materiales, Universidad del País Vasco, Av. Tolosa 72, E-20018 San Sebastian, Spain, NICOLE HELBIG, Forschungszentrum Jülich D-52425 Jülich Germany, HEIKO APPEL, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany, ILYA TOKATLY¹, ANGEL RUBIO², Nano-Bio Spectroscopy group and ETSF Center, Dpto. Física de Materiales, Universidad del País Vasco, Av. Tolosa 72, E-20018 San Sebastian, Spain — Through the exact solution of few-electron systems interacting with a monochromatic laser we study the performance of adiabatic density functionals within time-dependent density-functional theory (TDDFT) to reproduce Rabi oscillations. The non-linear dynamics of the Kohn-Sham (KS) system shows the characteristic features of detuned Rabi oscillations even if the exact resonant frequency is used. We illustrate this effect by comparing the exact time-dependent many-body solution of a He-atom in one dimension and a few-site Hubbard model with the solution of TDDFT-KS equations for different adiabatic exchange-correlation functionals. Preventing the detuning introduces a new strong condition to be satisfied by approximate new xc-functionals.

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10:12AM V35.00008 Curing pathologies of TDDFT with semiclassical electron correlation, PETER ELLIOTT, NEEPA MAITRA, Hunter College, City University of New York — Time-dependent density functional theory (TDDFT) has been identified as a prime candidate for describing the dynamics of atoms and molecules in strong laser fields. It would be especially useful in predicting the highly non-intuitive fields needed in the optimal control problem for photonic reagents. However TDDFT encounters a number of problems when simulating these systems, both in the functional approximation of the exchange and correlation potentials, but also for observables of interest, such as momentum distributions or ionization probabilities. Recently a method to overcome some of these problems was proposed[1], whereby an auxiliary semiclassical dynamics calculation produces a correlation potential, which is then used to drive a density-matrix propagation. This method incorporates memory, initial-state dependence, changing occupation numbers, all of which are known issues for TDDFT. In this talk we build on previous work[2] and examine this scheme for a number of model 1D systems including calculations for strong field dynamics, optimal control, non-sequential ionization, and double excitations [1] A.K. Rajam, I. Raczkowska, and N.T. Maitra, *Phys. Rev. Lett.* **105**, 113002 (2010). [2] P. Elliott and N.T. Maitra, *J. Chem. Phys.* **135**, 104110 (2011).

10:24AM V35.00009 Quantum dynamics integrators in a plane-wave implementation of time-dependent density functional theory, ANDRÉ SCHLEIFE, ALFREDO CORREA, Lawrence Livermore National Laboratory, YOSUKE KANAI, The University of North Carolina at Chapel Hill — In order to develop our understanding of various dynamical phenomena in materials at the electronic-structure level, computational methods based on first-principles theory are indispensable. Such approaches can make significant contributions to improving materials for a wide range of applications reaching from photovoltaic cells to nuclear reactors. Time-dependent density functional theory is an efficient approach for describing the real-time quantum dynamics of electronic systems. However, the numerical integration of the time-dependent Kohn-Sham equations, i.e., including a density-dependent effective Hamiltonian, is highly non-trivial. We studied various integrators for propagating the single-particle wave functions explicitly in time, in order to achieve a highly-scalable implementation based on plane-waves and pseudo-potentials. We show that the fourth-order Runge-Kutta scheme is conditionally stable and accurate within this framework. Moreover, the application of our scheme to a system consisting of several hundreds of electrons unveils its excellent scalability and, hence, its applicability for large-scale simulations.

10:36AM V35.00010 The effect of cusps in time-dependent quantum mechanics¹, ZENGHUI YANG, University of Missouri - Columbia, NEEPA MAITRA, Hunter College of the City University of New York, KIERON BURKE, University of California, Irvine — Spatial cusps in initial wavefunctions can lead to non-analytic behavior in time. We suggest a method for calculating the short-time behavior in such situations. For these cases, the density does not match its Taylor-expansion in time, but the Runge-Gross proof of time-dependent density functional theory still holds, as it requires only the potential to be time-analytic.

¹ZY and KB acknowledge U.S. D.O.E funding (DE-FG02-08ER46496) and NTM acknowledges both NSF and the Research Corporation.

10:48AM V35.00011 Demonstration of the Gunnarsson-Lundqvist theorem and Lack of Hohenberg-Kohn Theorem for Excited States, XIAO-YIN PAN, YU-QI LI, BIAO LI, Ningbo University, VIRAH SAHNI, Brooklyn College CUNY — By considering two noninteracting fermions in a 1-D infinite square well we demonstrate the following: (a) The GL theorem is satisfied for the lowest excited triplet state. There exists only one potential for this density so that the HK theorem is satisfied for this lowest excited state configuration. (b) For the second excited triplet state, there exists no other potential with the original orbital configuration that reproduces the density. However, (c) for the second excited triplet state, there exist other potentials with orbital configurations different from the original that reproduce the density. Thus, there is no HK theorem for this and other excited states. The orbitals of the other set of potentials are related to the original orbitals by a rotation. The exact new eigenvalues, and solutions for the potentials and orbitals including near and at the boundaries are provided.

Thursday, March 1, 2012 8:00AM - 11:00AM – Session V36 DCP: General Chemical Physics 107C

8:00AM V36.00001 Measurement of kinetic and potential energy deposition in highly charged ion collisions with surfaces, R.E. LAKE, NIST and Clemson University, J.M. POMEROY, NIST, C.E. SOSOLIK, Clemson University — We measure craters in thin dielectric films formed by highly charged Xe^{Q+} ($26 \leq Q \leq 44$) projectiles [1]. Tunnel junction devices with ion-irradiated barriers were used to amplify the effect of charge-dependent cratering through the exponential dependence of tunneling conductance on barrier thickness. Electrical conductance of a crater $\sigma_c(Q)$ increased by 4 orders of magnitude ($7.9 \times 10^{-4} \mu\text{S}$ to $6.1 \mu\text{S}$) as Q increased, corresponding to crater depths ranging from 2 to 11 Å. By employing a heated spike model, we determine that the energy required to produce the craters spans from 8 to 25 keV over the investigated charge states where kinetic energies were $(8 \times Q)$ keV. We partition crater formation energy into potential and kinetic contributions to find that at least $(27 \pm 2)\%$ of the available ion potential energy is required. Decreasing projectile kinetic energy at constant Q , provides a new test for charge-dependent kinetic energy loss theory.

[1] R.E. Lake, J.M. Pomeroy, H. Grube, C.E. Sosolik, *Phys. Rev. Lett.* **107**, 063202 (2011)

8:12AM V36.00002 Charge transport in single photochromic molecular junctions, YOUNGSANG KIM, T. PIETSCH, ELKE SCHEER, Department of Physics, University of Konstanz, Germany, T. HELLMUTH, F. PAULY, Institute for Theoretical Solid State Physics, Karlsruhe Institute of Technology, Germany, D. SYSOIEV, T. HUHN, T. EXNER, U. GROTH, U. STEINER, Department of Chemistry, University of Konstanz, Germany, A. ERBE, Helmholtz-Zentrum Dresden Rossendorf, Germany — Recently, photoswitchable molecules, i.e. diarylethene, gained significant interest due to their applicability in data storage media, as optical switches, and in novel logic circuits [1]. Diarylethene-derivative molecules are the most promising candidates to design electronic functional elements, because of their excellent thermal stability, high fatigue resistance, and negligible change upon switching [1]. Here, we present the preferential conductance of specifically designed sulfur-free diarylethene molecules [2] bridging the mechanically controlled break-junctions at low temperatures [3]. The molecular energy levels and electrode couplings are obtained by evaluating the current-voltage characteristics using the single-level model [4]. The charge transport mechanism of different types of diarylethene molecules is investigated, and the results are discussed within the framework of novel theoretical predictions.

[1] M. Del Valle et al., *Nat Nanotechnol* **2**, 176 (2007) S. J. van der Molen et al., *Nano. Lett.* **9**, 76 (2009).

[2] D. Sysoiev et al., *Chem. Eur. J.* **17**, 6663 (2011).

[3] Y. Kim et al., *Phys. Rev. Lett.* **106**, 196804 (2011).

[4] Y. Kim et al., *Nano Lett.* **11**, 3734 (2011). L. Zotti et al., *Small* **6**, 1529 (2010).

8:24AM V36.00003 Length and temperature dependent crossover of charge transport across molecular junctions, YA-LIN LO, Department of Physics, National Taiwan University, SHIH-JYE SUN, Department of Applied Physics, National University of Kaohsiung, YING-JER KAO, Department of Physics, National Taiwan University — We study the electronic transport in a molecular junction, in which each unit is coupled to a local phonon bath, using the non-equilibrium Green's function method. We observe the conductance oscillates with the molecular chain length and the oscillation period in odd-numbered chains depends strongly on the applied bias. This oscillatory behavior is smeared out at the bias voltage near the phonon energy. For the phonon-free case, we find a crossover from tunneling to thermally activated transport as the length of the molecule increases. In the presence of electron-phonon interaction, the transport is thermally driven and a crossover from the thermally suppressed to assisted conduction is observed.

8:36AM V36.00004 Electrical properties of a layered manganese vanadate¹, VICTORIA SOGHOMONIAN, QIFAN YUAN, Virginia Tech, Physics, ELINOR SPENCER, NANCY ROSS, Virginia Tech, Geosciences — We present the electrical characteristics of a layered manganese vanadate. Octahedral Mn and tetrahedral V units form layers that in turn are connected to each other via weakly bonded strontium ions. The Mn sites are also connected to each other through bridging oxygen atoms that are partially protonated, allowing for possible proton conduction in the material. The conductivity is dependent on crystal direction. Variable temperature conductivity measurements, from 160 to 830 K, show semiconducting behavior with average activation energy of 0.35 eV. Around 670 K a dip in the conductivity is observed, correlated with loss of water from the structure inferred from thermogravimetric analysis. Above 760K, an increase in conductivity is observed. Single crystal x-ray analysis is performed on samples heated above 670 K, to probe temperature induced structural changes. Preliminary results show a contraction of one of the unit cell axes corresponding to the loss of the bridging oxygen and the ensuing movement of the two Mn sites closer to each other. Single crystal x-ray investigations of the material under hydrostatic pressure in a DAC are also performed, to probe the influence of structural changes on electronic transport properties.

¹We acknowledge support from NSF DMR-0943971

8:48AM V36.00005 Capturing Ion-Solid Interactions with MOS structures, R. SHYAM, Department of Physics and Astronomy, Clemson University, W.R. HARRELL, J.E. HARRISS, Holcombe Dept. of Electrical and Computer Engineering, Clemson University, C.E. SOSOLIK, Department of Physics and Astronomy, Clemson University — We have fabricated metal-oxide-semiconductor (MOS) devices for a study of implantation rates and damage resulting from low energy ion-solid impacts. Specifically, we seek to capture ion irradiation effects on oxides by exposing as-grown SiO₂ layers (50 nm to 200 nm) to incident beams of alkali ions with energies in the range of 100 eV to 10 keV. The oxide is analyzed post exposure by encapsulating the irradiated region under a top metallic contact or within a finished MOS device. Characterization of the resulting ion-modified MOS device involves the standard techniques of room temperature and bias-dependent capacitance-voltage (C-V) measurements. The C-V results reveal alkali ion-induced changes in the flatband voltage of irradiated devices which can be used to extract both the range and implantation probabilities of the ions. Biased C-V measurements are utilized to confirm the concentration or dosage of ions in the oxide. A triangular voltage sweep (TVS) measurement at elevated temperatures also reveals the total ionic space charge in the oxide and can be used to extract a mobility for the ions as they pass through the damaged oxide. Comparisons of these measurements to standard device models as well as to ion range calculations in the oxide are presented.

9:00AM V36.00006 Self-consistent full counting statistics of inelastic transport, TAE-HO PARK, MICHAEL GALPERIN, University of California at San Diego — The full counting statistics (FCS) of inelastic transport in molecular junctions is considered for the case of weak electron-vibration coupling. We introduce a self-consistent procedure for FCS within the non-equilibrium Green function (NEGF) method, and discuss its importance in two aspects. First, we show that in the case of FCS the self-consistent treatment provides a conserving approximation. Second, we discuss the importance of molecular vibration renormalization for the counting statistics of electron transport. We consider two-level bridge with diagonal and off-diagonal electron-vibration couplings. The latter model is shown to be especially sensitive to renormalization of the vibration. We show that heating the molecular vibration may lead to either an increase or a decrease in current through the junction depending on the strength of electron-vibration coupling in the bridge compared to molecule-contact coupling. We report an appearance of super-Poissonian noise induced by the non-equilibrium vibration at resonance, which is similar to the effect of the avalanche transport previously reported in the literature for a system with a strong electron-vibration interaction.

9:12AM V36.00007 Measurement of the Spectral Distribution of Low Energy Electrons Emitted as a Result of M₃VV Auger Transitions in Cu(100)¹, SUMAN SATYAL, PRASAD JOGLEKAR, KARTHIK SASHTRY, ALEXANDER WEISS, University of Texas at Arlington, STEVEN HULBERT, Brookhaven National Lab, STEVEN HULBERT, BROOKHAVEN NATIONAL LAB COLLABORATION — Auger Photoelectron Coincidence Spectroscopy (APECS) was used to investigate the physics of the Low Energy Tail (LET) region of the Auger spectrum of a Cu(100) sample. A beam of 200eV photons was used to probe the sample. Two Cylindrical Mirror Analyzers (CMAs) were used to select the energy of electrons emitted from the sample. An APECS technique was used to obtain an Auger spectrum with one of the CMAs fixed at the core photoemission peak. The spectrum contains the extrinsic contributions from electrons excited by the M₃VV Auger transition plus a background due to true coincidence between photo-emitted valence band electrons that undergo inelastic scattering and other valence electrons. To remove the extrinsic contribution to the LET of the Auger Spectrum, Coincidence measurements were made with the fixed analyzer set at various energies (150eV, 165eV, 180eV, 190eV and 197eV) between the core and the valence band and obtain an estimate of the background due to the inelastic scattering of the valence band electrons. The extrinsic contribution to the LET was then subtracted to get the final spectrum consisting of the secondary electrons that are intrinsic to the M₃VV Auger transition only.

¹Welch Foundation Y-1100, NSF DMR 9812682

9:24AM V36.00008 Interaction of Water Layers on Calcite Surfaces¹, RASHID HAMDAN, HAI-PING CHENG, University of Florida — Calcite is a mineral of great interest because its abundance in both geological and biological systems. While the {10 $\bar{1}$ 4} surface largely dominates the calcite morphology, other surfaces consisting of {10 $\bar{1}$ 4} terraces and steps are important for the crystal dissolution or growth in aqueous environment. We use ab-initio calculations to study the interaction of single water molecule and one and two water layers with the flat {10 $\bar{1}$ 4} calcite surface and two step surfaces: {10 $\bar{1}$ 3} and {10 $\bar{1}$ 5} made of {10 $\bar{1}$ 4} terraces offset by one atomic layer along the {10 $\bar{1}$ 1} and the {0001} surface respectively. Preliminary results show that the first layer of water bond strongly to the calcite surface. However, dissociation of the water molecules is not favored on the surface.

¹NSF/DMR grant No. 0804407

9:36AM V36.00009 Tracking Amino Acids in Chiral Quantum Corrals¹, ESMERALDA YITAMBEN, REES RANKIN, ERIN ISKI, JEFFREY GREELEY, Center for Nanoscale Materials, Argonne National Laboratory, RICHARD ROSENBERG, Advanced Photon Source, Argonne National Laboratory, NATHAN GUISSINGER, Center for Nanoscale Materials, Argonne National Laboratory — Engineering molecular superstructures on metals opens great possibilities for the control and exploration of complex nanosystems for technological applications. Of particular interest is the use of chiral molecules, such as alanine, to build self-assembled nanoscale structures for the trapping of the two-dimensional free electron gas of a metal. In the present work, molecules of D- or L-alanine were deposited on Cu(111). Scanning tunneling microscopy, spectroscopy, and density functional theory (DFT) revealed the formation of a uniform network of hexagonal chiral pores of average diameter ~ 1.2 nm. Each pore acts as a quantum corral by confining the two-dimensional electron gas of the Cu(111) surface state. Furthermore, each hexagonal pore acts as nanoscale tracks when excess alanine molecules were trapped at the inner perimeter of the pore, and were observed as rotating spatial states periodically moving between the six vertices of the hexagon. This study demonstrates the engineering of one of the smallest quantum confined structure, and the dynamics of molecular motion within these chiral potentials wells.

¹This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357

9:48AM V36.00010 Influence of ligand and environment substitution on photo-triggered linkage isomerization of photochromic ruthenium sulfoxide complexes¹, KRISTIN SPRINGFELD, VOLKER DIECKMANN, SEBASTIAN EICKE, MIRCO IMLAU, Department of Physics, University of Osnabrueck, Osnabrueck, Germany — The group of ruthenium polypyridine sulfoxides features a pronounced photochromism in the UV/VIS spectral range based on an ultrafast photo-triggered linkage isomerization located at the SO-ligand. This isomerization exhibits a tremendous photosensitivity and a high thermal stability of the two metastable structural isomers. Here, we discuss the characteristic photochromic properties of the compounds in the frame of ligand substitution and the replacement of the dielectric environment. The complex [Ru(bpy)₂(ROSO)]·PF₆ [1] (with OSO: 2-methylsulfinylbenzoate) has been modified with the groups R = H, Bn, BnCl and BnMe [2] and studied in different solvents as well as in polydimethylsiloxane. The analysis is performed by cw-pump-probe technique as a function of temperature and exposure. Our results reveal a selective adjustability of the thermal stability in the compounds, while the photosensitivity and the characteristic absorption spectra remain unchanged. We discuss the impact of sulfoxide compounds with the desired features in view of application in molecular photonic devices.

[1] V. Dieckmann et al., Opt. Express 17, 15052 (2009)

[2] V. Dieckmann et al., Opt. Express 18, 23495 (2010)

¹Financial support by the DFG (INST 190/137-1) is gratefully acknowledged.

10:00AM V36.00011 Classical models for electron capture by highly charged ions in the thin film regime, JOSH POMEROY, National Institute of Standards and Technology, RUSSELL LAKE, Clemson University — We present an extension of the classical over the barrier (COB) model[1] for highly charged ions (HCIs) that describes thin dielectric films on metal surfaces, bridging the bulk metal and bulk insulator regimes. Motivated by recent experiments [2,3], we detail the onset of charge transfer between a HCI and metal covered with a dielectric thin film. In this talk, capture distances as a function of C₆₀ film thickness on Au(111) will be presented. For ultrathin films, electron capture begins from filled levels in the metal and the C₆₀ film decreases the potential barrier for charge transfer and increases the critical distance compared to clean Au(111), increasing the time available for above-surface relaxation. This is consistent with the new observation of increasing HCI-induced electron emission yield as a function of film thickness [3]. As film thickness grows and reaches a critical value, the first captured electrons originate from the film at the distance expected for an insulator target.

[1] J. Burgdörfer et al. Phys. Rev. A 44, 5674–5685 (1991)

[2] R.E. Lake et al. Phys. Rev. Lett. 107, 063202 (2011)

[3] E. Bodewits et al. Phys. Rev. A 84, 042901 (2011)

10:12AM V36.00012 Coupling of Cobalt-Tetraphenylporphyrin Molecules in Copper Nitride Molecular Network, VINICIUS CLAUDIO ZOLDAN, Laboratório de Filmes Finos e Superfícies, Universidade Federal de Santa Catarina, CHUNLEI GAO, Max Planck Institute of Microstructure Physics, Halle, Germany, RICARDO FACCIO, Cryssmat-Lab and Centro NanoMat, Facultad de Química, Universidad de la República, Montevideo, Uruguay, ANDRÉ AVELINO PASA, Laboratório de Filmes Finos e Superfícies, Universidade Federal de Santa Catarina — We have used low temperature scanning tunneling microscopy to study the interaction between individual cobalt-tetraphenylporphyrin molecules and a molecular copper nitride network. We demonstrated that the molecular Cu₃N-Cu(110) network promotes the decoupling of the porphyrin, allowing to visualize the molecular orbitals and vibronic states of the molecule, while keeping a strong coupling of the Co atom in the center of macrocycle with the substrate. The reverse behavior was observed when the molecule was sitting on the Cu(110) metallic surface. First principle calculations confirm the assembled position of the molecule on top of N atoms and the decoupling from the surface.

10:24AM V36.00013 A New Series of Donor-Acceptor Substituted Small Organic Molecules With Large Third Order Molecular Polarizability, MARTEN BEELS, Lehigh University, IVAN BIAGGIO TEAM¹, FRANCOIS DIEDERICH COLLABORATION², MELANIE CHIU COLLABORATION³ — We report on the third-order nonlinear optical properties of a series of new small organic molecules with a non-planar structure. A large third-order molecular polarizability is achieved thanks to a lower excited state energy obtained due to donor-acceptor substitution. We determined the influence of variations in the donor-acceptor substitution pattern and relate them to the nonlinear response by modeling the molecular properties computationally, and by experimentally determining the rotational average of their third-order polarizability by degenerate four-wave mixing. We found that the best molecules are extremely efficient both in relation to their size and to the fundamental quantum limit. These molecules show great potential for applications where the molecules are combined into dense supramolecular solid state assemblies in the form of high optical quality thin films obtained by molecular beam deposition.

¹Lehigh University

²ETH Zurich

³ETH Zurich

10:36AM V36.00014 Organic molecular crystals: materials with competing orders, GIANLUCA GIOVANNETTI, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Via Bonomea 265, 34136 Trieste, Italy, SANJEEV KUMAR, Indian Institute of Science Education and Research Mohali, MGSIPAP Complex, Sector 26, Chandigarh 160 019, India, JEAN-PAUL POUGET, Laboratoire de Physique des Solides, Université Paris Sud, CNRS, UMR 8502, 91405 Orsay, France, MASSIMO CAPONE, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Via Bonomea 265, 34136 Trieste, Italy — The search for multiferroics has become an important research topic in the last few years. Almost all newly discovered multiferroics are transition metal compounds where spin, lattice and charge degrees of freedom are strongly entangled. The possibility of finding organic multiferroics can open up a new area of research where new mechanisms, different from those active in standard transition metal oxide multiferroics, may have a role for the simultaneous occurrence of magnetic and ferroelectric order. By means of ab-initio and model calculations, we show an instability towards multiferroicity in the organic molecular crystal TMTTF₂-PF₆. Coexistence of charge ordering with a structural dimerization results in a ferroelectric phase with the tendency to the dimerization magnetically driven. The Multiferroicity is induced by competing orders: charge distribution and lattice distortions coupled with the magnetic state.

10:48AM V36.00015 Energy Transport in Quantum Systems with Discrete Spectrum¹, GEORGE LEVIN, WESLEY JONES, KAMIL WALCZAK, KIRK YERKES, Air Force Research laboratory, THERMAL MANAGEMENT TEAM — Energy transport in quantum system driven by stochastic perturbations is examined. One of the goals of this study is to determine how the Landauer channels can be defined in a system with discrete energy spectrum. A model describes a particle trapped in a confining potential and subjected to a stochastic perturbation localized off-center of the potential well. The perturbation pumps energy into the system which results in non-zero average energy flux between different regions of the confining potential. The energy flux can be defined in terms of quantum advection modes, where each mode is associated with an off-diagonal element of the density matrix and carries a finite, quantized amount of energy per unit of the probability flux. Statistical correlations between different modes and the net energy flux will be discussed.

¹This work was supported by Air Force Office of Scientific Research contract.

Thursday, March 1, 2012 8:00AM - 11:00AM —

Session V37 DCMF: Topological Insulators: Magnetoelectric Effect, Control, and Dynamics

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8:00AM V37.00001 A thermodynamic measure of the Magento-electric coupling in the 3D topological insulator¹, DORON BERGMAN, GIL REFAEL, California Institute of Technology — We show that the magneto-electric coupling in 3D (strong) topological insulators is related to a second derivative of the bulk magnetization. The formula we derive is the non-linear response analog of the Streda formula for Hall conductivity (P. Streda, J. Phys. C: Solid State Physics, 15, 22 (1982)), which relates the Hall conductivity to the derivative of the magnetization with respect to chemical potential. Our finding allows one to extract the magneto-electric coefficient by measuring the magnetization, while varying the chemical potential and one more perturbing field. Such an experimental setup could circumvent many of the current difficulties with measuring the magneto-electric response in 3D topological insulators. The relation we find also makes transparent the effect of disorder, contained entirely in the density of states, and changing nothing as long as the system is gapped.

¹DLB is supported by the Sherman Fairchild foundation.

8:12AM V37.00002 Magnetoelectric response of a topological surface under the conditions of an imperfect quantum Hall effect¹, ALLAN MACDONALD, DMYTRO PESIN, The University of Texas at Austin, Austin, TX — An effective magnetic monopole is induced by an external charge in a topological insulator, and in an ordinary insulator covered by a graphene sheet or another two-dimensional electron system, when it has a perfect surface quantum Hall effect [X.-L. Qi, R. Li, J. Zang, and S.-C. Zhang, Science **323**, 1184 (2009)]. We discuss the observability of this magnetoelectric response under the realistic conditions of a quantum Hall effect that is imperfect because of finite temperature, disorder, or unintended doping. By generalizing the surface electrodynamics to allow for a finite longitudinal conductivity, we analyze the transient behavior which occurs as the potential from a suddenly introduced external charge is screened. Screening severely limits the experimental time scales on which observation of magnetic-monopole-related phenomena is possible. We estimate the longitudinal conductivity values that are necessary for the monopole to survive for an extended period of time and discuss implications of our findings for other transport properties of the surface.

¹This work was supported by DOE Division of Materials Sciences and Engineering grant DE-FG03-02ER45958.

8:24AM V37.00003 Magnetoelectric effect in topological insulator/magnetic layer nanostructure, YURIY SEMENOV, KI WOOK KIM, North Carolina State University — The topological insulator (TI) surface band structure can be modified by contacting ferromagnetic layers due to the proximity exchange interaction. When the magnetization $\mathbf{M}$ is in the in-plane direction, the proximate exchange interaction results in a shift of the Dirac cone in the momentum space, whereas an energy gap can be generated for out-of-plane orientation culminating the maximum value at perpendicular to plane direction. Such opening of energy gap lowers the valence electron energy that can be only partially compensated by increase of the conduction electron energies depending on chemical potential μ . Such correlation of electronic energy and magnetization direction open up a new way toward the electrical manipulation of $\mathbf{M}$. To quantitative estimation of this effect, we provide the thermodynamic potential calculation of the TI surface electrons interacted with proximate ferromagnetic insulator as a function of $\mathbf{M}$ rotation by angle θ about in-plane axis x . The result can be described as an additive magnetic energy $E = K_{eff}(\mu)\sin^2\theta$ in the form of uniaxial anisotropy, which is induced by interaction with TI surface electrons. In the case of TI Bi_2Se_3 , the numerical estimations predict the $K_{eff}(\mu)$ variation in the range of 1 meV/nm² if μ vary over 100 meV. The possible applications of the effect (memory and logic) are discussed.

8:36AM V37.00004 Magnetoelectric and thermoelectric transport in graphene and helical metal: Effect of applied electric field¹, SUNG-PO CHAO, HUAZHOU WEI, VIVEK AJI, University of California at Riverside — We report on the electrical and thermoelectric transport properties of the surface state of the 3D topological insulator (TI) and graphene in a quantizing magnetic field. An unique feature of these systems is the evolution of the Landau level spectrum as a function of applied in plane electric field. We bench mark out results at small fields by computing conductivity and thermopower within linear response. We find that the universal values of thermopower in the clean limit depend on the gyromagnetic ratio in TIs, providing a clear distinction from graphene. In large electric fields we find an oscillation of conductivity as a function of applied electric field for fixed chemical potential, but not for fixed particle density. Signatures of the Landau level dependence on electric fields are also found in thermopower. These results are suggested as possible probes, in transport measurements of topological surface states.

¹The authors' research is supported by University of California at Riverside under the initial complement for Vivek Aji.

8:48AM V37.00005 Noninvasive Probe of Charge Fractionalization in Quantum Spin-Hall Insulators, ION GARATE, KARYN LE HUR, Yale University — When an electron with well-defined momentum tunnels into a nonchiral Luttinger liquid, it breaks up into two separate wave packets that carry fractional charges and move in opposite directions. Observing this phenomenon has proven difficult, in part due to single-particle and plasmon backscattering caused by measurement probes. In this talk we propose a topological insulator RC circuit that might be ideally suited for detecting fractional charges directly and in a noninvasive fashion.

9:00AM V37.00006 Topological charge pumping effect by the magnetization dynamics on the Surface of Three-Dimensional Topological Insulators, HIROAKI UEDA, AKIHITO TAKEUCHI, GEN TATARA, Tokyo Metropolitan University, TAKEHITO YOKOYAMA, Tokyo Institute of Technology — We discuss a current dynamics on the surface of a 3-dimensional topological insulator induced by magnetization precession of a ferromagnet attached. It is found that the magnetization dynamics generates a direct charge current when the precession axis is within the surface plane. This rectification effect is due to a quantum anomaly (parity anomaly) and is topologically protected. The robustness of the rectification effect against first-varying exchange field is confirmed by the explicit calculation, where we adopt the dimensional regularization to remove the divergence which is inevitable in the study on the electromagnetic response of the Dirac system.

9:12AM V37.00007 ABSTRACT WITHDRAWN —

9:24AM V37.00008 Electric tuning of topological insulator states and their surface scattering, MICHAEL POVOLOTSKYI, TILLMANN KUBIS, GERHARD KLIMECK, Purdue University — Materials that show the topological insulating (TI) properties have been extensively studied both experimentally and theoretically in recent years, but an application of those materials for electronic devices is still a challenge. In this study we explored a possibility to switch electric conductance of a surface TI states in a Bi_2Te_3 thin film. In such films there are two surfaces that have TI states located at them. We have done a theoretical study of the surface states using atomistic description within an empirical tight binding approximation. It was found that applying electric field perpendicular to the surface one can affect spin polarization of the TI states. Analysis of the scattering rates for electrons that occupy TI states close to the Fermi level shows that: a) the surface states are spin polarized under an applied electric field; b) the electron scattering between two surface states depends on whether they occupy the same surface and have parallel spins; c) by varying strength of an applied electric field it is possible to modulate the scattering rate, because at small fields the states are not spin-polarized, while at higher fields the states become spin-polarized, and at very high fields the surface states are significantly coupled to the bulk states.

9:36AM V37.00009 Electrical control of the Kondo effect in a helical edge liquid, ERIK ERIKSSON, ANDERS STRÖM, University of Gothenburg, Sweden, GIRISH SHARMA, Ecole Polytechnique, France, HENRIK JOHANNESSON, University of Gothenburg, Sweden — Magnetic impurities affect the transport properties of the helical edge states of quantum spin Hall insulators by allowing single-electron backscattering. We study such a system in the presence of a Rashba spin-orbit interaction induced by an external electric field, showing that this can be used to control the Kondo temperature, as well as the correction to the electrical conductivity due to the impurity. In particular, the impurity contribution to the dc conductivity can be switched on and off by properly adjusting the strength of the Rashba coupling.

9:48AM V37.00010 Nonlinear spectroscopy of non-Abelian Berry curvature¹, FAN YANG, REN-BAO LIU, Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong, China — We propose a general scheme to measure the Berry curvatures of energy bands in insulators by standard nonlinear optical spectroscopy. Our method employs optical and terahertz lights to produce a signal. A general calculation shows that the third order response of the solid is directly related to the Berry curvatures of the energy bands. In particular, for a time-reversal invariant system, we get a nonzero effect compared with the linear response methods, which provides information about the underlying non-Abelian Berry curvature. For insulators with rotational symmetry, the response is proportional to the Berry curvature flux of the iso-energy surface, which enables people to determine the topological properties of the energy bands explicitly. The method is applied to the eight-band model of III-V compound semiconductors and gives a quantized susceptibility with some global coefficients.

¹This work is supported by Hong Kong RGC/GRF CUHK401011.

10:00AM V37.00011 The Shockley-model description of the edge states in topological insulators, VICTOR YAKOVENKO, SERGEY PERSHOGUBA, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park, Maryland 20742-4111 — We show that the edge states in topological insulators can be understood based on the well-known Shockley model, a 1D tight-binding model with two atoms per elementary cell connected via alternating tunneling amplitudes. We generalize the model to a 3D Shockley-like model corresponding to the sequence of layers connected via the tunneling amplitudes dependent on the in-plane momentum $\mathbf{p} = (p_x, p_y)$. The Hamiltonian of the model is a 2×2 matrix with the complex off-diagonal matrix element $t(k, \mathbf{p})$ dependent on both $\mathbf{p}$ and the out-of-plane momentum k . The equation $t(k, \mathbf{p}) = 0$ defines vortex lines in the 3D momentum space. We show that the projection of the vortex lines on the 2D momentum space defines a boundary between the regions of $\mathbf{p}$ where the edge states exist or do not exist. The vorticity of the vortex lines determines the crystal sublattice on which the edge states are localized. We illustrate how our approach works for the well-established topological insulator model by Fu, Kane, and Mele. We find that different configurations of the vortex contours are responsible for the topological insulator phases with even or odd numbers of the surface Dirac cones. We discuss how real materials, such as Bi_2Se_3 , can be described by this model.

10:12AM V37.00012 Thermoelectric efficiency of holey topological insulators¹, ARTEM ABANOV, OLEG TRETIKOV, JAIRO SINOVA, Texas A&M University — We study the thermoelectric properties of three-dimensional topological insulators with many holes (or pores) in the bulk. We show that at high density of these holes the thermoelectric figure of merit, ZT , can be large due to the contribution of the conducting surfaces and the suppressed phonon thermal conductivity. The maximum efficiency can be tuned by an induced gap in the surface states dispersion through tunneling or external magnetic fields. The large values of ZT , much higher than unity for reasonable parameters, make this system a strong candidate for applications in heat management of nanodevices, especially at low temperatures.

¹This work was supported by NSF under Grant No. DMR-0547875, No. 0757992, NSF-MRSEC DMR-0820414, ONR-N000141110780, SWAN, and by the Welch Foundation (A-1678).

10:24AM V37.00013 Spin-charge Dynamics On Surface States of Topological Insulators and 2DEG, XIN LIU, JAIRO SINOVA, Department of Physics, Texas A&M University — We study the spin-charge dynamics on the surface of a topological insulator and spin-orbit coupled two dimensional electron gas. A new approach is developed to study the spin-charge dynamics even valid in the very strong spin-orbit coupling regime where the spin splitting energy due to SOIs is at the same order to the Fermi energy. The effects of Coulomb interaction and external field are also considered. We predict the fast oscillation of spin polarization perpendicular and parallel to the surface. Based on our theory, we provide a scheme to measure the transport property of the surface state isolated from the bulk contribution.

10:36AM V37.00014 Ultrastrong coupling cavity QED of the magnetic cyclotron transition in a 2D electron gas: massive versus Dirac fermions, DAVID HAGENMÜLLER, SIMONE DE LIBERATO, CRISTIANO CIUTI, Laboratoire Matériaux et Phénomènes Quantiques, Université Paris Diderot-Paris 7 and CNRS, 75205 Paris Cedex 13, France — We show that the cyclotron transition of a two-dimensional electron gas can be ultrastrongly coupled to a cavity photon mode. The ratio between the vacuum Rabi frequency Ω_0 and the cyclotron frequency ω_0 can be much larger than 1 for large filling factor ν of the Landau levels (the normalized coupling Ω_0/ω_0 scales as $\sqrt{\alpha n_{QW} \nu}$, where α is the fine structure constant and n_{QW} is the number of quantum wells). We present a comprehensive cavity QED theory both for semiconductors with massive electrons[?, ?] and graphene with Dirac fermions[?]. We show the dramatic impact on the quantum ground state and excitation properties, drawing the comparison between the two different types of 2D electron gas.

[1] D. Hagenmüller, S. De Liberato, and C. Ciuti, Phys. Rev. B 81, 235303 (2010) and references therein.

[2] Experiments demonstrating ultrastrong coupling of the cyclotron transition in a GaAs-system in the THz regime have been reported, see G. Scalari *et al.*, submitted.

[3] D. Hagenmüller and C. Ciuti, submitted.

10:48AM V37.00015 Topological Floquet Spectrum in Three Dimensions via a Two-Photon Resonance , NETANEL LINDNER, DORON BERGMAN, GIL REFAEL, California Institute of Technology, VICTOR GALITSKI, University of Maryland — A recent theoretical work [Nature Phys., 7, 490 (2011)] has demonstrated that external non-equilibrium perturbations may be used to convert a two-dimensional semiconductor, initially in a topologically trivial state, into a Floquet topological insulator. Here, we develop a non-trivial extension of these ideas to three-dimensional systems. In this case, we show that a two-photon resonance may provide the necessary twist needed to transform an initially unremarkable band structure into a topological Floquet spectrum. We provide both an intuitive, geometrical, picture of this phenomenon and also support it by an exact solution of a realistic lattice model that upon irradiation features single topological Dirac modes at the two-dimensional boundary of the system. It is shown that the surface spectrum can be controlled by choosing the polarization and frequency of the driving electromagnetic field. Specific experimental realizations of a three-dimensional Floquet topological insulator are proposed.

Thursday, March 1, 2012 8:00AM - 11:00AM –
Session V40 DBIO DPOLY DCOMP: Focus Session: Single Molecule Biological Physics - Proteins 156A

8:00AM V40.00001 From single molecule to single tubules , CHIN-LIN GUO, California Institute of Technology — Biological systems often make decisions upon conformational changes and assembly of single molecules. *In vivo*, epithelial cells (such as the mammary gland cells) can respond to extracellular matrix (ECM) molecules, type I collagen (COL), and switch their morphology from a lobular lumen (100-200 micron) to a tubular lumen (1mm-1cm). However, how cells make such a morphogenetic decision through interactions with each other and with COL is unclear. Using a temporal control of cell-ECM interaction, we find that epithelial cells, in response to a fine-tuned percentage of type I collagen (COL) in ECM, develop various linear patterns. Remarkably, these patterns allow cells to self-assemble into a tubule of length ~ 1 cm and diameter ~ 400 micron in the liquid phase (i.e., scaffold-free conditions). In contrast with conventional thought, the linear patterns arise through bi-directional transmission of traction force, but not through diffusible biochemical factors secreted by cells. In turn, the transmission of force evokes a long-range (~ 600 micron) intercellular mechanical interaction. A feedback effect is encountered when the mechanical interaction modifies cell positioning and COL alignment. Micro-patterning experiments further reveal that such a feedback is a novel cell-number-dependent, rich-get-richer process, which allows cells to integrate mechanical interactions into long-range (> 1 mm) linear coordination. Our results suggest a mechanism cells can use to form and coordinate long-range tubular patterns, independent of those controlled by diffusible biochemical factors, and provide a new strategy to engineer/regenerate epithelial organs using scaffold-free self-assembly methods.

8:36AM V40.00002 Studying spatial gradients of signaling proteins in mitotic spindles with time-integrated multipoint moment analysis , DOOGIE OH, DANIEL NEEDLEMAN, Harvard University — The organization of the mitotic spindle is orchestrated by the activities of multiple signaling proteins, such as the GTPase Ran. It has been proposed that the Ran pathway produces a cascade of events which gives rise to spatial gradients in the behavior of soluble proteins, which in turn produce spatial gradients in microtubule behaviors important for spindle assembly. Previous experiments have directly demonstrated the existence of gradients around the spindle in the upstream components of the Ran pathway, but it is still unclear if there are significant gradients in the downstream soluble components in this pathway. We recently developed a method, TIMMA, time-integrated multipoint moment analysis, a multipoint form of fluorescence fluctuation spectroscopy capable of quantitatively measuring the concentration, diffusion coefficient, and molecular brightness of soluble proteins throughout live cells. We are using TIMMA to characterize the behaviors of the upstream and downstream components of the Ran pathway in live mitotic cell to test the validity of the Ran gradient model.

8:48AM V40.00003 New chemical kinetics for description of chemical noise in small, heterogeneous biological systems: Beyond the paradigm of the rate constant concept¹ , JAEYOUNG SUNG, Chung-Ang University — We introduce a novel chemical kinetics for quantitative description of chemical fluctuations in a small, heterogeneous biological reaction system. At first, we discuss the recently proposed renewal chemical kinetics, and its application to quantitative interpretation of the randomness in fluctuating enzymatic turnover times of α -galactosidase. From the analysis of the randomness parameter data of the single enzyme reaction, one can extract valuable quantitative information about the enzyme reaction system, beyond the reach of the conventional Michaelis-Menten analysis. Next, we discuss a new universal behavior in the time dependence of the chemical fluctuation of product density for a small, heterogeneous reaction system, which is predicted from an exact analytic study for a general reaction model and confirmed by stochastic simulation results. We also discuss the dependence of the chemical noise on substrate concentrations for a heterogeneous enzyme reaction system, which turns out qualitatively different from that for a homogeneous enzyme reaction system.

¹Nation Research Foundation of Korea

9:00AM V40.00004 Generalized Michaelis-Menten equation for conformation-modulated monomeric enzyme catalysis¹ , JIANLAN WU, Physics Department, Zhejiang University, China, JIANSHU CAO, MIT — The conformational fluctuations induce complex enzymatic catalytic behaviors, which can be investigated by single-molecule experiments. We introduce a kinetic network model to describe conformation-modulated monomeric enzyme catalysis and formulate a generalized Michaelis-Menten (MM) rate equation for non-equilibrium steady-state turnover reactions. Using the flux balance method, we map the original kinetic network to a flux network with unbalanced population currents and derive the general substrate concentration dependence for the average turnover rate of non-equilibrium steady-state enzymatic reactions. In addition to the standard MM term, the generalized MM equation includes non-MM correction terms, which share the same functional form of substrate-dependence. Each non-MM correction term corresponds to a non-equilibrium unbalanced population current induced by conformational fluctuations. Under detailed balance conditions without population currents, non-MM terms vanish and the classical MM equation is recovered. With non-MM terms, the generalized MM equation provides a systematic approach to investigate non-MM behavior and predicts cooperativity, inhibition, and multiple-stability.

¹This work was supported by NSF under grant CHE0806266, ARO under grant W911NF-09-1-0480 and Singapore-MIT Alliance for Research and Technology (SMART).

9:12AM V40.00005 Conformational-Modulated Enzyme Catalysis: Generalized Michaelis-Menten Equation and Single Molecule Measurements, JIANSHU CAO, Massachusetts Institute of Technology — The Michaelis-Menten (MM) equation is a basic rate equation to describe the substrate-dependence of enzymatic reactions; therefore, it is important to establish the validity of the MM-equation for complex enzymatic reactions and derive the correction terms when the MM equation fails. Indeed, single molecule experiments reveal complex catalytic behaviors induced by conformational dynamics and possible deviations from the MM rate equation. To model such complex catalytic reactions, we construct a generic kinetic network model characterized by multiple intermediates and multiple conformational sub-states and, by solving for the turnover rate of this network, we extend the MM equation into a general form. The generalized MM equation predicts that (i) the MM equation holds under detailed balance and (ii) the correction to the MM expression depends on the unbalanced conformational currents. Using these predictions, we can establish a relationship between the substrate-dependence of the turnover rate and the connectivity of the enzymatic network. To confirm these predictions, we propose several single molecule indicators to test the violations of detailed balance. However, these single molecule indicators may be difficult to resolve from noisy single molecule data. To address these issues, we propose information theory based data analysis methods to process single molecule time series, and apply the Bayesian technique to analyze a single protein fluctuation experiment.

- [1] Jianlan Wu and Jianshu Cao, "Generalized Michaelis-Menten equation for conformation modulated monomeric enzymes," in Adv. Chem. Phys. (2011)
- [2] Jianshu Cao, "Michaelis-Menten Equation and Detailed Balance in Enzymatic Networks," JPC B, P5493 (2001)
- [3] Jianshu Cao and Rob Silbey, "Generic models of single molecule kinetics: self-consistent solutions," JPC B, 112, p12876 (2008) feature article
- [4] Jim Witkoskie and Jianshu Cao, "Analysis of the entire sequence of a single photon experiment on a Flavin Protein," JPC B, 112, p5988-5991 (2008)

9:48AM V40.00006 Probing short-lived protein ligand interactions with single-molecule force spectroscopy, OZGUR SAHIN, Columbia University, MINGDONG DONG, Interdisciplinary Nanoscience Center, iNano, Aarhus, Denmark — Hydrogen bonding plays an important role in stabilizing biomolecular complexes. Although life time of individual bonds can be extremely short, cooperativity among many interactions increase the overall life time of the complex. To probe short-lived individual interactions, we have employed a recently developed atomic force microscopy technique that can carry out single-molecule force spectroscopy experiments on the microsecond timescale. Our loading-rate dependent measurements provide experimental evidence for an additional energy barrier in the biotin-streptavidin complex. The width of this barrier, estimated from the measurements, is both close to theoretical predictions based on steered molecular dynamics simulations and to the characteristic width of individual hydrogen bonds. We will present our experimental methodology and analysis of the results on biotin-streptavidin complex.

10:00AM V40.00007 Using Surface Curvature to Control the Dimerization of a Surface-Active Protein, MARTIN KURYLOWICZ, MAXIMILIANO GIULIANI, JOHN DUTCHER, University of Guelph — Understanding the influence of surface geometry on adsorbed proteins promises new possibilities in biophysics, such as topographical catalysis, molecular recognition of geometric cues, and modulations of oligomerization or ligand binding. We have created nano-textured hydrophobic surfaces that are stable in buffer by spin coating polystyrene (PS) nanoparticles (NPs) to form patchy NP monolayers on a PS substrate, yielding flat and highly curved areas on the same sample. Moreover, we have separated surface chemistry from texture by floating a 10 nm thick film of monodisperse PS onto the NP-functionalized surface. Using Single Molecule Force Spectroscopy we have compared *in situ* the distribution of detachment lengths for proteins on curved surfaces to that measured on flat surfaces. We have shown that β -Lactoglobulin (β -LG), a surface-active protein which helps to stabilize oil droplets in milk, forms dimers on both flat PS surfaces and surfaces with a radius of curvature of 100 nm, whereas β -LG monomers exist for more highly curved surfaces with radii of curvature of 25 and 40 nm. It is surprising that rather large radii of curvature have such a strong influence on proteins whose radius is only ~ 2 nm. Furthermore, the transition from dimer to monomer with changes in surface curvature offers promising applications for proteins whose function can be modified by their oligomerization state.

10:12AM V40.00008 Ligand Binding Stability and Site Specific Chemical Potentials in the Anisotropic Network Model¹, RAHMI OZISIK, OSMAN BURAK OKAN, Rensselaer Polytechnic Institute, ARAVIND RAMMOHAN, Corning Research Center — Anisotropic network model (ANM) is a quadratic elastic model based on local force balance around each constituent material point. In ANM the potential energy functional is system specific and is built up from the connectivity and spatial distribution of elastic contacts (Atilgan et al., Biophysical J 2001, 80, 505). Because the potential energy functional is readily available in closed form, it becomes possible to derive exact expressions for energetics of the system. Recently, a simple analytical identity has been derived for free energy change associated with bond addition/removal for the Gaussian Network Model (GNM), which is one dimensional analog of ANM (Hamacher, Phys. Rev. E 2011, 84, 016703). In the current work, we generalize this formulation to ANM, and for an arbitrary potential functional which might have an acting force distribution on its constituents. Our formulation gives a complete characterization of site specific chemical potential under an arbitrary time independent force distribution. We correlate the chemical potentials with bond orientational order parameters evaluated at each site. Our results are validated on all-heavy atom networks for 15 ligand bound/unbound protein pairs, and show the decisive role of coordination geometry around each node. We show that local chemical potential is predominantly governed by changes in the bond orientational order.

¹Partial support was provided by NSF Grant No. 1003574 and RPI.

10:24AM V40.00009 Watching Single Enzymes and Fluorescent Proteins in Action in Solution Using a Microfluidic Trap, RANDALL GOLDSMITH, University of Wisconsin, Madison — Observation of dynamics of single biomolecules over a prolonged time without altering the biomolecule via immobilization is achieved with a specialized microfluidic device. This device, the Anti-Brownian Electrokinetic (ABEL) Trap, uses real-time electrokinetic feedback to cancel Brownian motion of single objects in solution. First, we use the ABEL Trap to study Allophycocyanin (APC), a photosynthetic antenna-protein and popular fluorescent probe. A complex relationship between fluorescence intensity and lifetime is observed, suggesting light-induced conformational changes and radiative and non-radiative rate fluctuations. Second, we apply the ABEL Trap to single molecules of the multi-copper enzyme blue Nitrite Reductase where a fluorescent label reports on the oxidation state of the Type I Copper. Redox cycling is observed and kinetic analysis allows extraction of the microscopic rate constants in the kinetic scheme. Evidence of a substrate-induced shift of the intramolecular electron transfer rate is seen. Taken together, these observations provide windows of unprecedented detail into the dynamics of solution-phase biomolecules.

Thursday, March 1, 2012 8:00AM - 10:48AM —

Session V41 DBIO DPOLY: Focus Session: Physics of Proteins I: Dynamics and Function 156B

8:00AM V41.00001 Two tyrosyl radicals stabilize high oxidation states in cytochrome c oxidase for efficient energy conservation and proton translocation¹, DENIS ROUSSEAU, Albert Einstein College of Medicine — The reaction of hydrogen peroxide (H₂O₂) with oxidized bovine cytochrome c oxidase (bCcO) was studied by electron paramagnetic resonance (EPR) to determine the properties of radical intermediates. Two distinct radicals with widths of 12 and 46 G are directly observed by X-band CW-EPR in the reaction of bCcO with H₂O₂ at pH 6 and pH 8. High-frequency EPR (D-band) provides assignments to tyrosine for both radicals based on well-resolved *g*-tensors. The 46 G wide radical has extensive hyperfine structure and can be fit with parameters consistent with Y129. However, the 12 G wide radical has minimal hyperfine structure and can be fit using parameters unique to the post-translationally modified Y244 in CcO. The results are supported by mixed quantum mechanics and molecular mechanics calculations. This study reports spectroscopic evidence of a radical formed on the modified tyrosine in CcO and resolves the much debated controversy of whether the wide radical seen at low pH in the bovine system is a tyrosine or tryptophan. A model is presented showing how radical formation and migration may play an essential role in proton translocation. This work was done in collaboration with Michelle A. Yu, Tsuyoshi Egawa, Syun-Ru Yeh and Gary J. Gerfen from Albert Einstein College of Medicine; Kyoko Shinzawa-Itoh and Shinya Yoshikawa from the University of Hyogo; and Victor Guallar from the Barcelona Supercomputing Center.

¹This work was supported by NIH Grants GM074982 and GM098799 to DLR.

8:36AM V41.00002 Structural and electronic properties of copper-containing nitrite reductase (CuNiR): elucidating the mechanism of nitrite reduction at the T₂Cu center, YAN LI, MIROSLAV HODAK, JERRY BERNHOLC, North Carolina State University — Copper-containing nitrite reductases (CuNiRs) play an important role in catalyzing the reduction of NO₂⁻ to NO during the bacterial denitrification process. Experimental studies have provided the structures of various states of CuNiR in the catalytic reaction, but many important aspects of the initial and intermediate attachments as well as the mechanism of the enzyme function remain unclear. We present a density-functional-theory-based study of the structural and electronic properties of different coordination forms at the T₂Cu center. The nudged elastic band (NEB) method is used to examine the activation energy barriers and to determine the minimum energy pathways (MEP) of the reaction processes. Our results reveal the role of the Asp⁹⁸ residue in the enzymatic function of CuNiR and also address the transformation from the initial O-coordinated binding of NO₂⁻ to the N-coordinated attachment of the NO during the enzymatic reaction.

8:48AM V41.00003 Nanometer Scale Distance Measurements for Biological Systems using Gd³⁺-based Spin Probes at High Magnetic Fields, DEVIN EDWARDS, Department of Physics, University of California, Santa Barbara, DANIELLA GOLDFARB, Department of Chemical Physics, Weizmann Institute of Science, Israel, SONGI HAN, Department of Chemistry, University of California, Santa Barbara, MARK SHERWIN, Department of Physics, University of California, Santa Barbara — Determination of nanometer-scale distances is critical for understanding structure and dynamics of proteins. Electron Paramagnetic Resonance (EPR), primarily below 1 T, is used to complement other structural techniques by quantifying sparse distances up to 8 nm in biomolecules labeled with nitroxide-based radicals. EPR becomes more powerful with increasing magnetic fields and frequencies. At 95 GHz (3.5 T), Gd³⁺ ions have shown clear advantages over nitroxide probes (Potapov, JACS 2010). We show that these advantages are even more dramatic at 240 GHz (8.5 T). The width of Gd³⁺'s central EPR transition narrows with increasing average distance between Gd³⁺ ions out to distances as long as 5 nm. This doubles the distances accessible with nitroxides in continuous wave measurements, which can be carried out above the 200K protein-glass transition and with broad distance distributions. Temperature-dependent measurements of the phase memory times at 8.5 T and low temperatures show distance dependence out to 10 nm. Measurements of Gd³⁺ labeled Proteorhodopsin confirm that phase memory times remain long enough to observe distance dependence in a spin-labeled protein. This work is supported by the National Science Foundation and the Binational Science Foundation.

9:00AM V41.00004 Metal-like transport in proteins: A new paradigm for biological electron transfer¹, NIKHIL MALVANKAR, MADELINE VARGAS, MARK TUOMINEN, DEREK LOVLEY, University of Massachusetts, Amherst — Electron flow in biologically proteins generally occurs via tunneling or hopping and the possibility of electron delocalization has long been discounted. Here we report metal-like transport in protein nanofilaments, pili, of bacteria *Geobacter sulfurreducens* that challenges this long-standing belief [1]. Pili exhibit conductivities comparable to synthetic organic metallic nanostructures. The temperature, magnetic field and gate-voltage dependence of pili conductivity is akin to that of quasi-1D disordered metals, suggesting a metal-insulator transition. Magnetoresistance (MR) data provide evidence for quantum interference and weak localization at room temperature, as well as a temperature and field-induced crossover from negative to positive MR. Furthermore, pili can be doped with protons. Structural studies suggest the possibility of molecular pi stacking in pili, causing electron delocalization. Reducing the disorder increases the metallic nature of pili. These electronically functional proteins are a new class of electrically conductive biological proteins that can be used to generate future generation of inexpensive and environmentally-sustainable nanomaterials and nanoelectronic devices such as transistors and supercapacitors. [1] Malvankar et al. Nature Nanotechnology, 6, 573-579 (2011)

¹Funded by Office of Naval Research (grant no. N00014-10-1-0084), office of Science (BER), US Department of Energy (award no. DE-SC0004114, Cooperative Agreement no. DE-FC02-02ER63446) and NSF Center for Hierarchical Manufacturing (grant no. CMMI-102502).

9:12AM V41.00005 Behind the Scene Role of Conserved Threonine in Intein Splicing, ALBERT DEARDEN, Rensselaer Polytechnic Institute, BRIAN CALLAHAN, MARLENE BELFORT, University at Albany, SAROJ NAYAK, Rensselaer Polytechnic Institute — Protein splicing is an autocatalytic process where an "intein" self-cleaves from a precursor protein and catalyzes ligation of the flanking fragments. Inteins occur in all domains of life and have myriad uses in biotechnology. While reaction steps of intein splicing are known, mechanistic details remain incomplete. Here, we investigate the possible role of a highly conserved active-site Threonine residue in bringing about the initial step of splicing: peptide bond rearrangement at a conserved Glycine-Cysteine motif. We report that although not part of the active transition state in this reaction, Threonine plays an important role in reducing the energy barrier through charge screening of active residues in the transition state. Interestingly, Threonine-Glycine hydrogen bonding makes sulfur of the attacking Cysteine less nucleophilic, thereby minimizing Coulomb repulsion in the transition state. These non-intuitive results are obtained through a combination of crystal structure, quantum mechanical simulations, and mutagenesis data. Our results further predict that the sluggish reaction rates observed with intein mutants harboring Threonine-Alanine substitutions can be accelerated in the presence of non-aqueous solvents.

9:24AM V41.00006 Coherent Oscillations in Hemoglobin and Myoglobin Ligand Complexes and their Dynamical Connection to Global Protein Motion and Gas Discrimination, JACOB JANTZI, University of Pittsburgh, KRISTINA WOODS, Carnegie Mellon University — THz spectroscopy and Molecular Dynamics (MD) simulations are used to investigate the coherent oscillations in the heme group of two heme proteins (hemoglobin and myoglobin) and the affect of the heme dynamics on the collective fluctuations taking place in the proteins. Preliminary experiments have confirmed that the deoxy state (no gas in the active site) of both proteins do not possess a 40 cm^{-1} mode in their THz spectra. The 40 cm^{-1} mode has been observed in both experimental and theoretical investigations of myoglobin dynamics. The low-frequency mode at 40 cm^{-1} has been hypothesized to be connected with energy transport between the active site and the protein-solvent interface. Once a gas is introduced into the ligand, both proteins contain the 40 cm^{-1} mode in their experimental spectra. But both the shape and intensity of the myoglobin peak differs from that of hemoglobin. Additionally, we observe a number of collective protein fluctuations ($\leq 100 \text{ cm}^{-1}$) that are altered in the myoglobin spectrum but remain unchanged in the hemoglobin spectrum when a gas is introduced into the protein active site. We will present experimental data of both proteins that have been exposed to a number of different gases. The reaction of the protein collective motions in the gas is linked with the difference in the coupling of the coherent oscillations of the heme group with the protein global modes but also with the mechanism of protein relaxation that controls ligand migration.

9:36AM V41.00007 Vibrational Dynamics of Ferric MbCN-A Revisit by Resonance Raman and Vibrational Coherence Spectroscopy¹, WEIQIAO ZENG, YUHAN SUN, ABDELKRIM BENABBAS, PAUL M. CHAMPION, Department of Physics and Center for Interdisciplinary Research on Complex Systems, Northeastern University, Boston, MA 02115 — Ultrafast pump-probe spectroscopy has indicated that there exists a photoproduct state following the excitation of ferric MbCN^{[1][2]}. This excited state decays with a time constant of 3.6 ps^[1]. Previous studies on this system have suggested that in this photoproduct state, the heme is either (i) still six-coordinated but vibrationally hot in the electronic ground state^[1] or (ii) the proximal histidine residue (His93) is transiently dissociated, while CN⁻ is still bound^[2]. Recent resonance Raman measurements on ferric MbCN in static solution yield spectra that are very similar to ferric myoglobin, which has His93 and a water molecule as axial ligands. This indicates that a water molecule replaces CN⁻ in ferric MbCN under continuous laser excitation. Photolysis of CN⁻ from the heme iron is necessary to make this happen, which is not consistent with the above two suggestions. In this presentation we will revisit the dynamics of ferric MbCN with resonance Raman and vibrational coherence spectroscopy and try to explain how a water molecule competes with CN⁻ in binding to the heme under photo excitation^[3]. References: [1]Helbing J. et al., Biophys J, vol 87, 1881(2004) [2]Gruia F. et al., Biophys J, vol 94, 2252(2008) [3]Cao W. et al., Biochemistry, vol 40, 5728(2001)

¹This work is supported by grants from the NIH (DK35090) and the NSF(MCB-0744738).

9:48AM V41.00008 Effect of DNA binding on geminate CO recombination kinetics in CooA¹, ABDELKRIM BENABBAS, VENUGOPAL KARUNAKARAN, Northeastern University, HWAN YOUN, California State University, THOMAS POULOS, University of California, Irvine, PAUL CHAMPION, Northeastern University — CooA proteins are heme-based CO-sensing transcription factors. Here we study the ultrafast dynamics of geminate CO rebinding to RrCooA. The effects of DNA binding and the truncation of the DNA binding domain on the CO geminate recombination kinetics were investigated. The CO rebinding kinetics in these CooA complexes takes place on ultrafast timescales but remains non-exponential over many decades in time. We show that this non-exponential kinetic response is due to a quenched enthalpic barrier distribution resulting from a distribution of heme geometries that is frozen or slowly evolving on the timescale of CO rebinding. We also show that, upon CO binding, the distal pocket of the heme in RrCooA relaxes to form a very efficient hydrophobic trap for CO. DNA binding further tightens the narrow distal pocket and slightly weakens the iron-proximal histidine bond. Analysis of our data reveals that the uncomplexed and inherently flexible DNA binding domain adds additional structural heterogeneity to the heme doming coordinate. When CooA forms a complex with DNA, the flexibility of the DNA-binding domain decreases and the distribution of the conformations available in the heme domain becomes restricted.

¹This work is supported by grants from the NIH DK35090 to P.M.C and GM42614 to T.L.P, and the NSF (MCB-0744738) to P.M.C.

10:00AM V41.00009 Physical control of carrier-mediated ion-transporters by entrainment of their turnover rate¹, WEI CHEN, CLAUSELL MATHIS, ZHIHUI FANG, JASON MAST, KARIM HAMIDI, PATRICK KELLY, University of South Florida, MAX EVE, Massachusetts College of Liberal Arts — In the past, tremendous efforts have been made to physically activate carrier-mediated ion-transporters, such as Na/K pumps. However, the outcome is not significant. Recently, we developed a new technique which can effectively and efficiently control the pumping rate by introducing a concept of an electronic synchrotron accelerator to the biological system. The approach consists of two steps. First, a specially designed oscillating electric field is used to force or synchronize individual pump molecules to run at the same turnover rate and phase as the field oscillation frequency. Then, by gradually changing the field frequency and carefully keeping the pump synchronization we can entrain the pump molecules so that their pumping rate can be progressively modulated, either decelerated or accelerated, following the field frequency to a defined value. Based on theoretical analysis of the underlying mechanisms involved in the technique, computer simulation of the entrainment process, and intensive experimental studies we have realized significant activation of the Na/K pumping rate up to ten-folds quickly in less than ten seconds.

¹Supported by NIH grant, 2R01 NIGM 50785, and NSF grant, PHY515787.

10:12AM V41.00010 Molecular dynamics simulation studies of dielectric response and vibrational energy relaxation in photoactive yellow protein and green fluorescent protein, YAO XU, RAMACHANDRAN GNANASEKARAN, DAVID LEITNER, University of Nevada, Reno — The first step in the photocycle of many proteins involves conformational change of a chromophore or a charge transfer reaction following photoexcitation. To explore the response of the protein and solvent environment to photoexcitation of the chromophore in photoactive yellow protein (PYP) and green fluorescent protein (GFP) we carried out molecular dynamics simulations of the dielectric response and vibrational energy relaxation (VER) from the chromophore to the protein and solvent. In PYP the time scale of the protein response, mainly contributed by Tyr42 and Glu46, to photoexcitation appears prominently between 0.1 and 0.3 picoseconds. The frequency-dependent VER rate also reveals dynamic coupling between the chromophore and residues that hydrogen bond to it. Resonances in the VER rate appear at frequencies comparable to the oscillations observed in recent fluorescence decay studies. In GFP, which undergoes excited state proton transfer about 10 ps following photoexcitation that may be assisted by specific chromophore vibrations, both the protein and water molecules inside the β -barrel surrounding the chromophore mediate the dielectric response.

10:24AM V41.00011 Employing Solution X-Ray Scattering to Investigate Conformational Changes of Proteins, MUSTAFA TEKPINAR, WENJUN ZHENG, Department of Physics, University at Buffalo — Many proteins undergo global conformational changes to perform their functions. Small/Wide Angle Solution X-Ray Scattering (S/WAXS) is an increasingly used experimental technique to probe conformational changes of proteins in aqueous environment. We have developed a new modeling method to reconstruct coarse-grained and atomistic 3D models from S/WAXS data. The method has been applied to a variety of proteins including the R-T transition of hemoglobin.

10:36AM V41.00012 Near-Field Orientation Sensitive Terahertz Micro-Spectroscopy of Single Crystals, GHEORGHE ACBAS, ROHIT SINGH, Department of Physics, University at Buffalo, SUNY, Buffalo, NY, EDWARD SNELL, Department of Structural Biology, SUNY Buffalo, Buffalo, NY and Hauptman-Woodward Medical Research Institute, Buffalo, NY, ANDREA MARKELZ, Department of Physics, University at Buffalo, SUNY, Buffalo, NY — We present spectroscopic imaging studies of molecular crystals. These measurements examine the anisotropy of the intra and inter-molecular vibrational modes of single crystals at terahertz frequencies. The method is based on the technique developed in [1-2] for sub-wavelength resolution time domain terahertz spectroscopy (THz TDS), with added polarization orientation dependent measurements and hydration control. This method allows us to study the spectroscopic properties of small single crystals with sizes down to 20 micrometers. In addition, mapping the spectroscopic information at such small spatial scales allows us to reduce the water absorption and interference artifacts that usually affect protein THz TDS measurements. We show the polarization sensitive terahertz absorption spectra in the (0.3-3THz) range of sucrose, oxalic acid and lysozyme protein crystals.

1. M. A. Seo, et. al., Opt. Express, 15(19):11781–11789, 09 (2007)
2. J. R Knab, et. al., App. Phys. Lett., 97, 031115 (2010)

Thursday, March 1, 2012 8:00AM - 11:00AM – Session V42 DBIO: Focus Session: Systems Biology - Stochastic Gene Expression 156C

8:00AM V42.00001 Mapping the environmental fitness landscape: Lessons from a noisy synthetic gene circuit¹, GABOR BALAZSI, The University of Texas MD Anderson Cancer Center — Gene expression actualizes the organismal phenotypes encoded within the genome in an environment-dependent manner. Among all encoded phenotypes, cell population growth rate (cell population fitness) is perhaps the most important, since it determines how well-adapted a genotype is in various environments. Currently it remains unclear how a cell population's growth rate and its subpopulation fractions in specific environments emerge from the stochastic molecular-level kinetics of gene networks and the division rates of single cells. To address this question we developed and quantitatively characterized synthetic a gene circuit controlling the expression of a bifunctional antibiotic resistance gene in *Saccharomyces cerevisiae*. We found that knowing the cell division rates and nongenetic (cellular) memory of gene expression states were necessary for predicting the overall fitness of cell populations in specific antibiotic- and inducer-containing environments. We validated these predictions experimentally and identified environmental conditions that determined a “sweet spot” of drug resistance.

¹This research was supported by the NIH Director's New Innovator Award Program [1DP2 OD006481-01].

8:36AM V42.00002 Stochastic description of birth and death processes governed by a mixture of exponential and non-exponential waiting times, STEPHAN EULE, Max Planck Institute for Dynamics and Self-Organization, Goettingen — The dynamics of complex systems is significantly influenced by fluctuations originating from intrinsic as well as extrinsic sources. In general, the discrete nature of individual events, such as the birth and death of an individual in a population or the production and degradation of a molecule in a chemical reaction, is the main source of intrinsic noise. The occurrence of such events is usually modeled by Poissonian statistics, implying that the probability per unit time for an event to happen is assumed to be constant. Many complex systems however exhibit deviations from elementary Poissonian statistics. Such deviations can arise for example in coarse-grained stochastic models of gene expression, where the waiting time distribution can be more general than the simple exponential distribution. In this contribution we consider birth and death processes which are governed by both, exponential as well as non-exponential waiting times. We derive the corresponding master equation and present methods to approach this equation analytically. As an example we consider a reaction where the production of molecules is governed by a non-exponential waiting time distribution and the degradation follows regular Poissonian statistics.

8:48AM V42.00003 Mechanistic basis for transcriptional bursting of ribosomal genes in E. coli, SANDEEP CHOUBEY, Graduate program in Physics, Brandeis University, ALVARO SANCHEZ, Graduate program in Biophysics, Brandeis University, JANE KONDEV, Professor of Physics, Brandeis University — Upon adding more ribosomal genes to the E. coli cell, it adjusts the overall transcription of these genes by reducing the average transcription rate per gene, so as to keep constant the level of ribosomal RNA in the cell. It was observed that this reduction in the average transcription level per gene is accompanied by the generation of transcriptional bursts. The biophysical mechanism responsible for this type of transcriptional control is not yet known. We consider three possible mechanisms suggested in the literature: proximal pausing by RNA polymerase, cooperative recruitment of RNA polymerase by DNA supercoiling, and competition between RNA polymerase and a transcription factor for binding to regulatory DNA. We compute the expected statistical properties of transcription initiation for each one of these models, and compare our predictions with published distributions of distances between the polymerases transcribing the ribosomal genes, obtained from electron micrographs. We use this data to estimate the rates of transcription initiation, which are found to be in good agreement with independent measurements. We also show that the three mechanisms considered here can be discriminated by comparing their predictions for the mean and the variance of interpolymerase distances.

9:00AM V42.00004 Decreasing the stochasticity of mammalian gene expression by a synthetic gene circuit¹, DMITRY NEVOZHAY, Department of Systems Biology, The University of Texas MD Anderson Cancer Center, TOMASZ ZAL, Department of Immunology, The University of Texas MD Anderson Cancer Center, GABOR BALAZSI, Department of Systems Biology, The University of Texas MD Anderson Cancer Center — Gene therapy and functional genetic studies usually require precisely controlled and uniform gene expression in a population of cells for reliable level of protein production. Due to this requirement, stochastic gene expression is perceived as undesirable in these fields and ideally has to be minimized. The number of approaches for decreasing gene expression stochasticity in mammalian cells is limited. This creates an unmet need to develop new gene expression systems for this purpose. Based on earlier synthetic constructs in yeast, we developed and assessed a negative feedback-based mammalian gene circuit, with uniform and low level of stochasticity in gene expression at different levels of induction. In addition, this new synthetic construct enables highly precise gene expression control in mammalian cells, due to the linear dependence of gene expression on the inducer concentration applied to the system. This mammalian gene expression circuit has potential applicability for the development of new treatment modalities in gene therapy and research tools in functional genetics. In addition, this work creates a roadmap for moving synthetic gene circuits from microbes into mammalian cells.

¹This research was supported by the NIH Director's New Innovator Award Program [1DP2 OD006481-01] and a UT MD Anderson Cancer Center Institutional Research Grant [ORA 30026230] to Gabor Balazsi

9:12AM V42.00005 Applications of queueing theory to stochastic models of gene expression¹

, RAHUL KULKARNI, Department of Physics, Virginia Tech — The intrinsic stochasticity of cellular processes implies that analysis of fluctuations ('noise') is often essential for quantitative modeling of gene expression. Recent single-cell experiments have carried out such analysis to characterize moments and entire probability distributions for quantities of interest, e.g. mRNA and protein levels across a population of cells. Correspondingly, there is a need to develop general analytical tools for modeling and interpretation of data obtained from such single-cell experiments. One such approach involves the mapping between models of stochastic gene expression and systems analyzed in queueing theory. The talk will provide an overview of this approach and discuss how theorems from queueing theory (e.g. Little's Law) can be used to derive exact results for general stochastic models of gene expression. In the limit that gene expression occurs in bursts, analytical results can be obtained which provide insight into the effects of different regulatory mechanisms on the noise in protein steady-state distributions. In particular, the approach can be used to analyze the effect of post-transcriptional regulation by non-coding RNAs leading to new insights and experimentally testable predictions.

¹Supported by NSF PHY-0957430

9:48AM V42.00006 Cross-talk and interference can enhance information capacity of a signaling pathway

, SAHAND HORMOZ, Kavli Institute for Theoretical Physics, University of California Santa Barbara — A recurring theme in gene regulatory networks is transcription factors (TFs) that regulate each other, and then bind to overlapping sites on DNA, where they interact and synergistically control transcription of a target gene. TF binding is inherently a noisy process due to thermal fluctuations and the small number of molecules involved. A consequence of multiple TFs interacting at the binding site through competition or cooperativity is that their binding noise becomes correlated. Using concepts from information theory, we show that a correlated-noise channel can enhance its capacity if the TFs are no longer independent but regulating each other. Essentially, the frequency of observing each TF at a given concentration is no longer separable, but "entangled." The form of this entanglement elucidates the upstream TF cross-regulation (cross-talk). We demonstrate these ideas using a cartoon model of two TFs competing for the same binding site. Surprisingly, competition can enhance the information transmission rate. We suggest that this mechanism explains the motif of a coherent feed-forward loop terminating in overlapping binding sites commonly found in developmental networks, and discuss specific examples.

10:00AM V42.00007 Exact results for integral thresholds in models of stochastic oscillatory gene expression

, SRIVIDYA IYER BISWAS, NORBERT SCHERER, AARON DINNER, James Franck Institute, University of Chicago — Oscillatory stochastic gene expression is often combined with threshold regulation to ensure periodic occurrence of some cellular activity, such as cell division. In this work we first demonstrate the virtue of implementing such regulation using an integral threshold, rather than a step threshold, in the fluctuating numbers of the regulator. We then develop a general theoretical framework using which we derive a model independent result that relates the stochastic distribution of the time oscillating regulator numbers to the distribution of event (cell division) times, regardless of the underlying mechanism that generates a specific form of oscillations in the regulator copy numbers. We then use this result in conjunction with a simple model of stochastically oscillating gene expression to show how the shape of the division time distribution can be used to make deductions about the underlying stochastic dynamics of the oscillating regulator. Specifically, we show that bimodal division time distributions can occur, even in the absence of any bistability in the underlying model, and connect that observation to general features of the underlying stochastic model. Finally, we discuss connections to ongoing single cell experimental studies of *Caulobacter* cell-cycle division times.

10:12AM V42.00008 Fitness Effects of Network Non-Linearity Induced by Gene Expression Noise¹

, CHRISTIAN RAY, The University of Texas M.D. Anderson Cancer Center, TIM COOPER, University of Houston, GABOR BALAZSI, The University of Texas M.D. Anderson Cancer Center — In the non-equilibrium dynamics of growing microbial cells, metabolic enzymes can create non-linearities in metabolite concentration because of non-linear degradation (utilization): an enzyme can saturate in the process of metabolite utilization. Increasing metabolite production past the saturation point then results in an ultrasensitive metabolite response. If the production rate of a metabolite depends on a second enzyme or other protein-mediated process, uncorrelated gene expression noise can thus cause transient metabolite concentration bursts. Such bursts are physiologically unnecessary and may represent a source of selection against the ultrasensitive switch, especially if the fluctuating metabolic intermediate is toxic. Selection may therefore favor correlated gene expression fluctuations for enzymes in the same pathway, such as by same-operon membership in bacteria. Using a modified experimental *lac* operon system, we are undertaking a combined theoretical-experimental approach to demonstrate that (i) the *lac* operon has an implicit ultrasensitive switch that we predict is avoided by gene expression correlations induced by same-operon membership; (ii) bacterial growth rates are sensitive to crossing the ultrasensitive threshold. Our results suggest that correlations in intrinsic gene expression noise are exploited by evolution to ameliorate the detrimental effects of nonlinearities in metabolite concentrations.

¹Supported by NSF grant BIO IOS 1021675 to TFC & GB.

10:24AM V42.00009 Stochastic Gene Expression in Networks of Post-transcriptional Regulators

, CHARLES BAKER, TAO JIA, HODJAT PENDAR, RAHUL KULKARNI, Virginia Polytechnic Institute and State University — Post-transcriptional regulators, such as small RNAs and microRNAs, are critical elements of diverse cellular pathways. It has been postulated that, in several important cases, the role of these regulators is to modulate the noise in gene expression for the regulated target. Correspondingly, general stochastic models have been developed, and results obtained, for the case in which a single sRNA regulates a single mRNA target. We generalize these results to networks containing a single mRNA regulated by multiple sRNAs and to networks containing multiple mRNAs regulated by a single sRNA. For these systems, we obtain exact expressions relating the mean levels of the sRNAs to the mean levels of the mRNAs. Additionally, we consider the convergence of the original model to an approximate model which considers sRNA concentrations to be high; for the latter model we derive an analytic form for the generating function of the protein distribution. Finally, we discuss potential experimental protocols which, in combination with the derived results, can be used to infer the underlying gene expression parameters.

10:36AM V42.00010 Accurate analytical distributions for stochastic gene expression

, HODJAT PENDAR, Engineering Science and Mechanics Department, Virginia Tech, RAHUL KULKARNI, Department of Physics, Virginia Tech — Gene expression is significantly stochastic process that can give rise to phenotypic heterogeneity across a population of genetically identical cells. Gene expression variability is generally characterized by the mean and variance of associated distributions, however the entire distributions are often not adequately characterized by the first two moments. For stochastic models of gene expression, exact analytic results for protein steady-state distributions have been obtained only for the simplest case. In this talk, we show how to obtain approximate but accurate representations of protein steady-state distributions for a broad class of models of stochastic gene expression. We first present a procedure to obtain analytical solutions in two limiting cases as the ratio of mRNA to protein lifetimes is varied. We then propose a general strategy for constructing an analytical distribution that interpolates these limits while reproducing the exact mean and variance. The corresponding analytical distributions show excellent agreement with results from stochastic simulations throughout parameter space.

10:48AM V42.00011 Stochastic Hopf bifurcation in transcription networks with delayed feedback, JOHN WENTWORTH, Harvey Mudd College, MATHIEU GAUDREAU, McGill University, JORGE VINALS, University of Minnesota — We study the oscillatory instabilities of two model systems that rely on delayed negative feedback to induce oscillation: a single gene auto repressor system, and a dimer negative autoregulation system. We focus on fluctuations of intrinsic origin in the range of low copy number. The bifurcation diagram is obtained for these stochastic models, and shown to differ significantly from that of a macroscopic description that neglects fluctuations. Bifurcation lines remain sharp under fluctuations, but their location is a function of the relative size of the fluctuations. Shifts in the stability threshold of the oscillators can be traced back to the interplay between statistical correlations and delayed feedback. We finally show that there results cannot be captured by weak noise approximations (the diffusion limit), but instead result from strong fluctuations associated with low copy numbers.

Thursday, March 1, 2012 8:00AM - 11:00AM —
Session V43 FEd FGSA: Invited Session: Entrepreneurship - The Quest for Start-Up Success Based on Research Advances 157AB

8:00AM V43.00001 Start-ups for Dummies, LAWRENCE BOCK, USA Science & Engineering Festival — I will present the best practices I have learned from founding, co-founding or seeding the early stage growth of 50 high technology and life sciences companies.

8:36AM V43.00002 Pushing a physics discovery towards commercial impact, ERIC MAZUR, Department of Physics, Harvard University — In 1997 my research group discovered that shining intense, ultrashort laser pulses on the surface of a crystalline silicon wafer drastically changes the optical, material and electronic properties of the wafer. The resulting textured surface is highly absorbing and looks black to the eye, making this 'black silicon' useful for a wide range of commercial devices, from highly-sensitive detectors to improved photovoltaics. Over the following ten years we investigated this material and developed a prototype detector. The prototype gave us the confidence to commercialize black silicon. Together with a graduate student, I founded SiOnyx. The company, based in Beverly, MA, is in the process of manufacturing the first commercial products based on black silicon.

9:12AM V43.00003 How a Venture Capitalist Approaches an Investment Decision, DANIEL COLBERT, Rockport Capital Partners —

9:48AM V43.00004 Having your cake and eating it too; effective engagement in start-ups from an academic seat, CHAD MIRKIN, Northwestern University — In order for scientific advances to have a positive impact on society, they must be successfully transitioned from conceptually fundamental endeavors in academic research laboratories to valuable enabling technologies at start-up companies. Nanosphere, Nanolnk, and AuraSense are three start-up companies that have been spun out of Northwestern based on research initiated in my laboratory. These companies are focused on commercializing nanotechnology-based applications in the life science and semiconductor industries and have turned discoveries from my lab into viable commercial products. For example, several of the systems developed at these start-ups are in the clinical trial phase, with one already approved by the FDA, and they are poised to have a positive world-wide impact. Herein, I discuss the challenges associated with identifying commercial value in academic research projects, securing intellectual property, forming a company as a legal entity, and locating sources of start-up funds. Further, I will discuss the rewards of venturing into such enterprises and the ways of ensuring a start-up company's long-term success, while juggling the numerous responsibilities of an academic seat. I argue that these two activities are done not in competition, but rather are integral for driving the type of high-level, synergistic scientific research that is being done today.

10:24AM V43.00005 An entrepreneurial physics method and its experimental test¹, ROBERT BROWN, Case Western Reserve University — As faculty in a master's program for entrepreneurial physics and in an applied physics PhD program, I have advised upwards of 40 master and doctoral theses in industrial physics. I have been closely involved with four robust start-up manufacturing companies focused on physics high-technology and I have spent 30 years collaborating with industrial physicists on research and development. Thus I am in a position to reflect on many articles and advice columns centered on entrepreneurship. What about the goals, strategies, resources, skills, and the 10,000 hours needed to be an entrepreneur? What about business plans, partners, financing, patents, networking, salesmanship and regulatory affairs? What about learning new technology, how to solve problems and, in fact, learning innovation itself? At this point, I have my own method to propose to physicists in academia for incorporating entrepreneurship into their research lives. With this method, we do not start with a major invention or discovery, or even with a search for one. The method is based on the training we have, and the teaching we do (even quantum electrodynamics!), as physicists. It is based on the networking we build by 1) providing courses of continuing education for people working in industry and 2) through our undergraduate as well as graduate students who have gone on to work in industry. In fact, if we were to be limited to two words to describe the method, they are "former students." Data from local and international medical imaging manufacturing industry are presented.

¹I am grateful for research support from more than a dozen high-tech industrial companies.

Thursday, March 1, 2012 8:00AM - 11:00AM —
Session V44 DPOLY: Focus Session: Interparticle Interactions in Polymer Nanocomposites - Surface Interactions 157C

8:00AM V44.00001 The synthesis of metal nanoparticulate catalysts within functional microgel particles¹, MARIA KALIVA, ELENI PAVLOPOULOU, KONSTANTINOS CHRISTODOULAKIS, MARIA VAMVAKAKI, SPIROS H. ANASTASIADIS, Foundation for Research and Technology-Hellas and Univ. of Crete, Heraklion Crete, Greece — Electrostatically and sterically stabilized polymer microgel particles have been prepared containing either amino (poly(2-(diethylamino)ethyl methacrylate), PDEA) or carboxylic acid (poly(acrylic acid), PAA; poly(methacrylic acid), PMMA) functional groups. The PDEA, PAA and PMAA particles can be used for the incorporation of a large variety of metal nanoparticulate catalysts due to their functional amine and carboxylic acid groups; Pd, Ru and Ni nanoparticles have been synthesized. The more polar PAA microgels were designed as the nanocatalyst carrier system in aqueous reaction media while the less polar PMAA particles were prepared as the metal nanoparticle template for use in catalytic reactions that take place in organic solvents. The sterically and electrostatically stabilized microgel particles possess surface functional groups that can potentially interact with the microchannel walls of microfluidic catalytic reactors.

¹Sponsored by the EU (POLYCAT; CP-IP 246095-2)

8:12AM V44.00002 The role of nanoparticle synergies in modifying the thermal properties of biodegradable polymer blends¹ , KAI YANG, SHAN HE, SUNY-Stony Brook, RACHEL DAVIS², Smithtown High School East, MIRIAM RAFAILOVICH, SUNY-Stony Brook, TAKASHI KASHIWAGI, National Institute of Standards and Technology — Most of thermoplastic polymers are brittle, when sufficient amounts are added to get flame retardant properties. Furthermore, melt-blending starch with other biodegradable polymers is difficult since very few polymers are compatible with starches. We have developed a new nanoparticles where resorcinol diphenyl phosphates (RDP) is used to modify the surface energy, allowing the particles to be dispersed within polymer. When multiple types of particles share the same coating, they can be melt blended simultaneously and synergies can be achieved, imparting properties to the nanocomposite, which cannot be achieved by any single additive. Here we show that RDP modified starch, can be extruded together with the biodegradable polymers, Ecoflex and polylactic acid, to produce flame retardant nanocomposites which can pass the UL-94-V0 test. TEM images of the blend show that the RDP-coated starch particles were well dispersed within the polymer matrix providing the flame retardant properties, while the RDP clays are reducing the interfacial tension and contributing to compatibilization. Nanomechanical measurements of the chars remaining after cone calorimetric measurements indicate that maintaining flexibility of the chars may be an additional factor in achieving good flame retardant properties.

¹Supported by NSF-DMR-MRSEC program and The Morin Foundation.

²High school student who works in Garcia Center at Stony Brook

8:24AM V44.00003 ABSTRACT WITHDRAWN —

8:36AM V44.00004 Supramolecular Assembly in a Polymer Nanocomposite , RICK BEYER, AARON JACKSON, SAMUEL PRICE, CHRISTOPHER GOLD, Army Research Laboratory, ANDREW DUNCAN, E. I. du Pont de Nemours and Company — Overcoming the inherent tendency of nanoparticles to aggregate is critical and has typically been the main focus of research on the fabrication of polymer nanocomposites. Developing specific or organized arrangements of nanoparticles is even more technically challenging, but also more appealing due to the possibility of creating nanocomposites with desired optical, electrical, or magnetic properties. Successful approaches in this area often rely on the polymer matrix to organize the nanoparticle additive, but are limited when one considers the high-throughput processing procedures used industrially. In this presentation, the preliminary findings of a research effort to use the strong, reversible, interparticle or intermolecular interactions found in supramolecular assembly to promote synergistic organization of the polymer matrix and dispersion of nanoparticles in a polymer nanocomposite will be described. Here, the effect of incorporating functionalized metal nanoparticles into a supramolecularly assembling metallopolymer based on reversible bonds formed between a metal atom (such as Zn^{2+}) and the “mebip” ligand (2,6-bis(19-methylbenzimidazolyl)pyridine) will be discussed.

8:48AM V44.00005 Stabilizing nanotube films with thin polymer layers: Mitigating van der Waals forces through excluded-volume interactions , MATTHEW R. SEMLER, JOHN M. HARRIS, ERIK K. HOBBIE, North Dakota State University — Thin membranes of single-wall carbon nanotubes (SWCNTs) on elastic polymer substrates show considerable promise for flexible electronics applications, but the modulus and conductivity of these films decrease dramatically in response to applied strains. This softening arises from the strong van der Waals interactions between contacted nanotubes, which favor the parallel coarsening of SWCNT bundles in response to even very small external forces. By capping the SWCNT membranes with a thin layer of glassy polymer, we demonstrate a dramatic improvement in the mechanical response of the strained films. We link this behavior to the stabilizing influence of excluded-volume interactions mediated by the glassy polymer layer.

9:00AM V44.00006 SANS Studies of DNA-Templated Silver Nanoclusters , HONGYU GUO, SUNIL SINHA, University of California, San Diego, JASWINDER SHARMA, JENNIFER MARTINEZ, ANDREW SHREVE, Los Alamos National Laboratory — DNA-templated silver nanoclusters have received significant attention due to their useful properties, including high molar absorptivities, good quantum yields and photostability, and small size. Their potential use may range from biology to nanoscience. For example, they are promising biological fluorescence probes due to their fluorescence properties dependence to DNA template sequence. However, some basic features, like the structure of the DNA/Ag complex, are still unclear. We have conducted Small Angle Neutron Scattering (SANS) experiments to investigate the formation of the Nanoclusters. By comparing the SANS data from conjugated samples, pure DNA and DNA/Ag complex, we can characterize the size and position of the Ag clusters along the DNA strand. The time evolution of the DNA/Ag complex can also be studied since such aging process is kind slow. We found that the formation and aging of the Ag Nanoclusters are also strongly dependent on the DNA template sequence.

9:12AM V44.00007 Theory of the Structure and Miscibility of Soft Filler Polymer Nanocomposites , JIAN YANG, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — A new hybrid theory for soft filler polymer nanocomposites is constructed based on combining integral equation methods and small scale Monte Carlo simulation. The consequences of nanoparticle softness (surface fluctuations) and corrugation (discrete roughness) on the equilibrium behavior is investigated in the dilute filler limit. Under athermal (entropic) conditions, the monomer-particle pair correlations exhibit qualitatively different features relative to hard smooth spheres. Polymer-mediated depletion attractions in the particle potential-of-mean-force (PMF) are qualitatively modified by surface corrugation and/or fluctuations. With increasing particle softness, monomer-scale PMF oscillations are destroyed, and the interparticle separation and effective maximum attraction strength depend sensitively on surface fluctuation amplitude and monomer-nanoparticle size ratio. Second virial coefficient calculations are performed to estimate how particle softness/roughness modifies miscibility, and a mechanism is identified for entropically stabilizing rough nanofillers in the absence of a cohesive interface. Surface corrugation and softness is also found to significantly modify the bridging and sterically stabilized states associated with adsorbing polymers.

9:24AM V44.00008 Self-assembly of Nano-rods in Photosensitive Phase Separation , YA LIU, OLGA KUKSENOK, EGOR MARESOV, ANNA BALAZS, University of Pittsburgh — Computer simulations reveal how photo-induced chemical reactions in polymeric mixtures can be exploited to create long-range order in materials whose features range from the sub-micron to the nanoscale. The process is initiated by shining a spatially uniform light on a photosensitive AB binary blend, which thereby undergoes both a reversible chemical reaction and phase separation. When a well-collimated, higher intensity light is rastered over the sample, the system forms defect-free, spatially periodic structures. We now build on this approach by introducing nanorods that have a preferential affinity for one the phases in a binary mixture. By rastering over the sample with the higher intensity light, we can create ordered arrays of rods within periodically ordered materials in essentially one processing step.

9:36AM V44.00009 Dynamic mechanical properties of hydroxyapatite/polyethylene oxide nanocomposites: characterizing isotropic and post-processing microstructures , MEISHA SHOFNER, JI HOON LEE, Georgia Institute of Technology — Compatible component interfaces in polymer nanocomposites can be used to facilitate a dispersed morphology and improved physical properties as has been shown extensively in experimental results concerning amorphous matrix nanocomposites. In this research, a block copolymer compatibilized interface is employed in a semi-crystalline matrix to prevent large scale nanoparticle clustering and enable microstructure construction with post-processing drawing. The specific materials used are hydroxyapatite nanoparticles coated with a polyethylene oxide-b-polymethacrylic acid block copolymer and a polyethylene oxide matrix. Two particle shapes are used: spherical and needle-shaped. Characterization of the dynamic mechanical properties indicated that the two nanoparticle systems provided similar levels of reinforcement to the matrix. For the needle-shaped nanoparticles, the post-processing step increased matrix crystallinity and changed the thermomechanical reinforcement trends. These results will be used to further refine the post-processing parameters to achieve a nanocomposite microstructure with triangulated arrays of nanoparticles.

9:48AM V44.00010 Thermodynamic Interactions in Polymer Nanocomposites towards Controlled Nanoparticle Dispersion, ALISYN NEDOMA, RAJEEV DATTANI, JOAO CABRAL, Imperial College London, CENTRE FOR PLASTIC ELECTRONICS TEAM — Thermodynamic interactions in polymer/nanoparticle blends can be used to control the dispersion of nanoparticles. Here we introduce the use of polymer blends comprising immiscible A and B homopolymers, an A-B diblock copolymer “surfactant,” and nanoparticles. Upon thermal annealing, the composites self-assemble into equilibrium morphologies with well-dispersed nanoparticles. Polystyrene (PS), polymethyl methacrylate (PMMA), and a PS-PMMA diblock were chosen as the model polymers; C₆₀ fullerene was the model nanoparticle. Blends were prepared for C₆₀ loadings from 0.1 to 2 mass% for blends with symmetric homopolymers and a symmetric diblock copolymer. The molecular weight of the matched homopolymers was varied as 2, 20, and 40 kDa whilst the same 60-60 kDa diblock copolymer was used. Samples were studied using small angle neutron scattering, and the resulting morphologies were found to be lamellar for all C₆₀ loadings. Ongoing work is exploring the effects of polymer asymmetry on the nanostructure of the composites.

10:00AM V44.00011 Effect of competing monomer-monomer and monomer-particle interactions on the assembly of copolymer grafted nanoparticles¹, TYLER MARTIN, ARTHI JAYARAMAN, University of Colorado at Boulder — Functionalizing nanoparticles with copolymer ligands is an attractive method to tailor the assembly of the nanoparticles. In this talk we present simulation results that show the effect of competing monomer-monomer and monomer-particle interactions on assembly of nanoparticles grafted with AB copolymers with diblock or alternating sequence. We vary strengths of like-monomer (A-A and/or B-B) attractive interactions in the presence of strong or negligible monomer A- particle (A-P) attraction or monomer B- particle (B-P) interaction. At a constant particle size and graft length, the competing interactions and copolymer sequence dictate the amount of inter-grafted particle monomer aggregation, inter- and intra-graft monomer aggregation within the same grafted particle. The resulting monomer aggregation on/near the particle surface imparts an effective patchiness to the particle. For e.g., in case of particles grafted with AB diblock copolymer (with A block closer to the surface) the presence of strong B-P and B-B attractions leads to smaller attractive patches that extend from the surface, and in turn lead to anisotropic assembly, while presence of strong A-P and A-A attractions lead to larger attractive patches closer to the particle surface and in turn isotropic assembly.

¹NSF 0930940

10:12AM V44.00012 Dielectric Breakdown in Filled Silicone Elastomers at the Particle/Matrix Interface¹, ROGER DIEBOLD, School of Engineering and Applied Sciences, Harvard University; Materials Department, University of California, Santa Barbara, MICHAEL GORDON, Chemical Engineering Department, University of California, Santa Barbara, DAVID CLARKE, School of Engineering and Applied Sciences, Harvard University — Silicone elastomers, widely used as electrical insulators and potting agents, are typically filled with large amounts of fumed silica nanoparticles to enhance their mechanical strength and toughness. It is well known that as the filler particle diameter decreases to the nanometer length scale, the interfacial surface area to volume ratio increases dramatically, consequently determining many of the physical properties of the macroscopic composite. Thus, to understand electrical breakdown in these materials, it is imperative to investigate the interface between the filler particle and the bulk elastomer. In order to eliminate some of the complexities of studying dielectric breakdown at the filler/matrix interface, it is necessary to remove particle-particle interactions. In this paper, the authors will present ‘creep’ (surface) and ‘strike’ (through-thickness) dielectric breakdown results at idealized oxide/polymer interfaces which closely emulate those found in filled elastomer systems. Weibull and I-V curve analysis will be used to describe the effects of silane coupling agent functionalization on dielectric breakdown, and in particular, how different chemical moieties play a role in high-field interfacial electronic transport.

¹Funding: MRSEC program under NSF award no. DMR-0820484. Nanofabrication facilities: CNS (Harvard) and UCSB, part of the NNIN network, supported under NSF award no. DMR-0820484.

10:24AM V44.00013 The Development of Filler Structure in Colloidal Silica – Polymer Nanocomposites, JEFFREY METH, E.I. Dupont de Nemours & Co., Inc. — The realization of the full potential for polymeric nanocomposites to manifest their entitled property improvements relies, for some properties, on the ability to achieve maximum particle-matrix interfacial area. Well-dispersed nanocomposites incorporating colloidal silica as the filler can be realized in both polystyrene and poly(methylmethacrylate) matrices by exploiting the charge stabilized nature of silica in nonaqueous solvents which act as Bronsted bases. We demonstrate that dispersions of colloidal silica in dimethylformamide are charge stabilized, regardless of organosilyl surface functionalization. When formulated with polymer solutions, the charge stabilized structure is maintained during drying until the charged double layer collapses. Although particles are free to diffuse and cluster after this neutralization, increased matrix viscosity retards the kinetics. We demonstrate how high molecular weight polymers assist in immobilizing the structure of the silica to produce well-dispersed composites. The glass transition temperatures of these composites do not vary, even at loadings up to 50 v%.

Thursday, March 1, 2012 8:00AM - 10:24AM –

Session V45 DPOLY DBIO: Soft Matter Physics of Heterogeneous Membranes - Experiments

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8:00AM V45.00001 Structure and mechanics of biological fiber-laden membranes¹, YOGESH KUMAR MURUGESAN, ALEJANDRO REY, Department of Chemical Engineering, McGill University, DAMIANO PASINI, Department of Mechanical Engineering, McGill University — We present a mechanical model of the plant cell wall viewed as anisotropic 2D soft matter, where a dilute dispersion of cellulose fibrils of variable orientations is on a curved deformable viscoelastic membrane. The model integrates the elastic energy of the curved membrane, the nematic fiber orientation energy, and competing curvophilic and curvophobic interactions mediated by the membrane geometry and the fibrils' orientation. The selected membrane geometry is a straight cylinder, whose cross-sectional shape varies from a circle to a super-ellipse as in many plant species, and its size increases as in plant cell wall during growth. Model predictions indicate that due to curvature-orientation couplings, the fiber orientation displays three modes: axial (at large curvature), helical and transverse (at small curvature). The high curvature also promotes the order of the fibrils. The predicted fiber structure is validated with that in the cell wall of tracheids. To gain insight into the role of fiber structure on the elasticity of fiber-laden membranes, the effect of fiber orientation and order on the effective bending modulus of the fiber-laden membrane cross-section is investigated. The structure-property relations for super-elliptical membranes are established.

¹Financial support for this research was provided by Le Fonds Quebecois de la Recherche sur la Nature et les Technologies (FQNRT)

8:12AM V45.00002 From a single molecule to a membrane of structured ionic polymers: A molecular dynamic simulation study, DIPAK ARYAL, DVORA PERAHIA, Clemson University, GARY S. GREEST, Sandia National Laboratories — The association of an A-B-C-B-A co-polymer with an ionizable center and a bulky end block has been investigated using molecular dynamic simulations. The center block consists of a randomly sulfonated polystyrene connected to a flexible poly (ethylene-r-propylene) bridge and end capped with poly (t-butyl styrene). Tailoring the nature of individual segments within a block co-polymer is a potential design tool to form membranes with desired properties. The association mode and the dynamics of the segments control the overall characteristics. The membranes with three sulfonation level for the center block were made by evaporating a common solvent for all blocks. The local structure including size and distribution of the ionic blocks and the continuity of the styrene phase as well as long range correlations were identified at 300 and 500K. The initial membrane structure is affected by the structure in solution. Studies on changes that take place above the glass transition temperature for each of the blocks will also be presented.

8:24AM V45.00003 Investigation of the elastic properties of a lipid bilayer by fluorescence interferometry, DONG GUI, HSIANG-KU LIN, EHSAN NORUZIFAR, LEONID PRYADKO, ROYA ZANDI, UMAR MOHIDEEN, University of California, Riverside — Freestanding curved lipid bilayers were formed on micron diameter wells fabricated on a silicon chip. The height profile of the lipid bilayers was measured using fluorescence interference contrast microscopy. Dark and bright rings resulted from the interference of emission from the fluorophores in the lipid bilayers with the same light reflected from the bottom surface of the well. By changing the osmotic pressure difference across the bilayers, the relationship between the pressure and the membrane curvature was studied. By using Helfrich theory, the surface tension of the bilayer was extracted. The influence of detergents and antibiotics on the elastic property of lipid bilayers was also investigated.

8:36AM V45.00004 Regulating the Size and Stabilization of Lipid Raft-Like Domains and Using Calcium Ions as Their Probe, URI RAVIV, OR SZEKELY, The Hebrew University of Jerusalem — In this paper, we apply means to probe, stabilize and control the size of lipid raft-like domains in vitro. In biomembranes the size of lipid rafts is ca. 10 - 30 nm. In vitro, mixing saturated and unsaturated lipids results in micro-domains, which are unstable and coalesce. Using solution X-ray scattering, we studied the structure of binary and ternary lipid mixtures in the presence of calcium ions. Three lipids were used: saturated, unsaturated and a hybrid (1-saturated-2-unsaturated) lipid that is predominant in the phospholipids of cellular membranes. Only membranes composed of the saturated lipid can adsorb calcium ions, become charged and therefore considerably swell. The selective calcium affinity was used to show that binary mixtures, containing the saturated lipid, phase separated into large-scale domains. Our data suggests that by introducing the hybrid lipid to a mixture of the saturated and unsaturated lipids, the size of the domains decreased with the concentration of the hybrid lipid, until the three lipids could completely mix. We attribute this behavior to the tendency of the hybrid lipid to act as a line-active co-surfactant that can easily reside at the interface between the saturated and the unsaturated lipids and reduce the line-tension between them.

8:48AM V45.00005 Floret-shaped solid domains on giant fluid lipid vesicles induced by pH¹, STAVROULA SOFOU, AMEY BANDEKAR, Rutgers University — Lateral lipid phase separation and domain formation induced by changes in pH is significant in liposome-based drug delivery: environmentally responsive lipid heterogeneities can be tuned to alter collective membrane properties such as drug release and drug carrier reactivity impacting, therefore, the therapeutic outcomes. At the micron-meter scale, fluorescence microscopy on Giant Unilamellar fluid Vesicles (GUVs) shows that lowering pH (from 7.0 to 5.0) promotes the condensation of titratable PS or PA lipids into beautiful floret-shaped solid domains in which lipids are tightly packed via H-bonding and VdWs interactions. Solid domains phenomenologically comprise a circular “core” cap beyond which interfacial instabilities emerge resembling leaf-like stripes of almost vanishing Gaussian curvature independent of GUVs’ preparation path and in agreement with a general condensation mechanism. Increasing *incompressibility* of domains is strongly correlated with larger number of thinner stripes per domain, and increasing *relative rigidity* of domains with smaller core cap areas. Line tension drives domain ripening, however the final domain shape is a result of enhanced incompressibility and rigidity maximized by domain coupling across the bilayer. Introduction of a transmembrane osmotic gradient (hyperosmotic on the outer lipid leaflet) allows the domain condensation process to reach its maximum extent which, however, is limited by the minimal expansivity of the continuous fluid membrane.

¹DMR-0820341 through NYU-MRSEC

9:00AM V45.00006 The influence of membrane stress on phase separation and domain shape in phospholipid vesicles, DONG CHEN, Physics Department of University of Massachusetts Amherst, MARIA SANTORE, Polymer Sci. & Eng. Department of University of Massachusetts Amherst — Phase separation of mixed phospholipid bilayers is of interest due to the potential role of phospholipid rafts in cell adhesion and signaling. Studies of membrane dynamics and the phase diagram itself typically neglect the role of tension, though it is expected that imposition of moderate membrane tensions might mildly shift the phase separation temperature, as anticipated by Clausius Clapeyron. We show here, using a simple binary system (DOPC/DPPC), a more dramatic effect: The tension imposed on giant unilamellar phospholipid vesicles can alter the phase and the domain shape, completely changing the composition of the liquid and solid phases, their proportions, and the transition temperature. The example in this talk demonstrates how striped or patchy hexagonal phases can develop, depending on thermal history and tension. Different incorporation of tracers into the ordered phases suggests fundamental differences in their structure at the molecular level. Rapid quenching and low tensions favor hexagonal patches while increased tension and slower quenching favors a striped phase. For this reason it is believed that the patches contain corrugations such that the structure of the ordered phase is metastable.

9:12AM V45.00007 Membrane fluctuations alter the fluidity of clathrin protein lattices¹, ANDREW SPAKOWITZ, NICHOLAS CORDELLA, Department of Chemical Engineering, Stanford University, SHAFIGH MEHRAEEN, School of Biochemistry and Chemistry, Georgia Tech — Clathrin is a protein that plays a major role in the creation of membrane-bound transport vesicles in cells. The pinwheel subunits of clathrin assemble into closed, nanoscale assemblies with various shapes and sizes. We develop a model for clathrin, facilitating the study of membrane, surface, and bulk assembly. The clathrin are modeled as pinwheels that form leg-leg associations and resist bending and stretching deformations. Invoking theories of dislocation-mediated melting in two dimensions, we discuss the phase behavior for clathrin. We demonstrate that the generation of defects resembles creation of two dislocations, and we use orientational- and translational-order correlation functions to predict the crystalline-hexatic and hexatic-liquid phase transitions. Accounting for membrane fluctuations, we address the phase behavior of clathrin on a membrane surface. Membrane fluctuations act to soften the elastic coupling between defects in the clathrin lattice, altering the conditions for the crystalline-hexatic phase transition. This effect offers a mechanism for altering the fluidity of protein or polymer films. Furthermore, these results illustrate the pivotal role that molecular elasticity plays in the physical behavior of self-assembling and self-healing materials.

¹We acknowledge support from the Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under contract DE-AC02-76SF00515

9:24AM V45.00008 The structure of unsupported, self-assembled phospholipid bilayers on an artificially nano-patterned surface, GREGORY SMITH, SEUNG-YONG JUNG, JAMES BROWNING, JONG KEUM, NICKOLAY LAVRIK, PAT COLLIER, Oak Ridge National Laboratory — We present neutron reflectivity measurements of the in-situ microscopic architecture of phospholipid molecules at the interface between a regularly nano-patterned surface and an aqueous sub-phase using neutron reflectometry. 1,2-dilauroyl-sn-glycero-3-phosphocholine (DLPC) single bilayers were deposited on a patterned silicon substrate. The substrate was patterned with a rectangular array of nano-scaled holes using e-beam nano-lithographic techniques. The goal of these experiments is to produce a set of small freely-suspended bilayers spanning the nanostructured surface. We compare results for films deposited by vesicle adsorption or by the Langmuir–Shafer (L-S) technique. Initial data analysis shows that there are well formed bilayers on the surface. Detailed analysis of the reflectivity curves will be presented to confirm details of the architecture of these bilayer films. Bilayers prepared in this way may serve as model single bilayer systems with freely suspended areas for the study of membrane functionality in biological and biomimetic materials and systems.

9:36AM V45.00009 Peptide-induced Asymmetric Distribution of Charged Lipids in a Vesicle Bilayer Revealed by Small-Angle Neutron Scattering¹, WILLIAM HELLER, SHUO QIAN, Oak Ridge National Laboratory — Cellular membranes are complex mixtures of lipids, proteins and other small molecules that provide functional, dynamic barriers between the cell and its environment, as well as between environments within the cell. The lipid composition of the membrane is highly specific and controlled in terms of both content and lipid localization. Here, small-angle neutron scattering and selective deuterium labeling were used to probe the impact of the membrane-active peptides melittin and alamethicin on the structure of lipid bilayers composed of a mixture of the lipids dimyristoyl phosphatidylglycerol (DMPG) and chain-perdeuterated dimyristoyl phosphatidylcholine (DMPC). We found that both peptides enriched the outer leaflet of the bilayer with the negatively charged DMPG, creating an asymmetric distribution of lipids. The level of enrichment is peptide concentration-dependent and is stronger for melittin than alamethicin. The enrichment between the inner and outer bilayer leaflets occurs at very low peptide concentrations, and increases with peptide concentration, including when the peptide adopts a membrane-spanning, pore-forming state.

¹This research at Oak Ridge National Laboratory's Center for Structural Molecular Biology (DOE-BER project ERKP291) used facilities supported by the U.S. Department of Energy, managed by UT-Battelle, LLC under Contract DE-AC05-00OR22725.

9:48AM V45.00010 Cooperative assembly in targeted drug delivery, DEBRA AUGUSTE, Harvard University — Described as cell analogues, liposomes are self-assembled lipid bilayer spheres that encapsulate aqueous volumes. Liposomes offer several drug delivery advantages due to their structural versatility related to size, composition, bilayer fluidity, and ability to encapsulate a large variety of compounds non-covalently. However, liposomes lack the structural information embedded within cell membranes. Partitioning of unsaturated and saturated lipids into liquid crystalline ($L\alpha$) and gel phase ($L\beta$) domains, respectively, affects local molecular diffusion and elasticity. Liposome microdomains may be used to pattern molecules, such as antibodies, on the liposome surface to create concentrated, segregated binding regions. We have synthesized, characterized, and evaluated a series of homogeneous and heterogeneous liposomal vehicles that target inflamed endothelium. These drug delivery vehicles are designed to complement the heterogeneous presentation of lipids and receptors on endothelial cells (ECs). EC surfaces are dynamic; they segregate receptors within saturated lipid microdomains on the cell surface to regulate binding and signaling events. We have demonstrated that cooperative binding of two antibodies enhances targeting by multiple fold. Further, we have shown that organization of these antibodies on the surface can further enhance cell uptake. The data suggest that EC targeting may be enhanced by designing liposomes that mirror the segregated structure of lipid and receptor molecules involved in neutrophil-EC adhesion. This strategy is employed in an atherosclerotic mouse model in vivo.

10:00AM V45.00011 Polymer-Protein interaction at air/liquid interfaces: X-ray reflectivity and surface spectroscopy studies, WENJIE WANG, NATHANIEL ANDERSON, Ames laboratory, Iowa State University, SANJEEVA MURTHY, New Jersey Center for Biomaterials, Rutgers University, DAVID VAKNIN, Ames laboratory, Iowa State University — Adsorption of proteins onto a substrate is the first and a critical step that determines the cellular response of substrates. To understand the adsorption and distribution of proteins on surfaces, we employ surface sensitive X-ray scattering and spectroscopic techniques to monitor the adsorption of plasma proteins (fibrinogen) onto surfaces of polymers, poly(DTE carbonate), on aqueous surfaces. Our X-ray measurements provide the density profiles of the polymers-proteins systems on aqueous surfaces, with details on the interactions between the polymers and the protein, and distribution of the protein within and on the polymer surface. The hydrophobic and hydrophilic behaviors of these polymers are modified by incorporating poly(ethylene glycol) (PEG) and by iodinating the tyrosine rings. Our results confirm the inhibition of the adsorption of fibrinogen onto polymer surfaces by PEG, and the counteraction of this influence when the polymers are iodinated.

10:12AM V45.00012 Microporous device for local electric recordings on lipid bilayers, THERESA KAUFELD, CHRISTOPHER BATTLE, Drittes Physikalisches Institut, Georg August Universitaet Goettingen, CONRAD WEICHBRODT, CLAUDIA STEINEM, Fakultae fuer Chemie, Georg August Universitaet Goettingen, CHRISTOPH SCHMIDT, Drittes Physikalisches Institut, Georg August Universitaet Goettingen — Many methods for artificial membrane formation are available. We focus on the reconstitution of lipid bilayers on porous substrates combining the stability of solid supports and the accessibility of both sides of the bilayer of the classical BLM which is necessary for low noise electric experiments. Most commercially available porous substrates however are not suitable for electric experiments or a combination of several measuring techniques. Therefore, we designed a microporous substrate, which meets several demands: We wanted to have the possibility to perform multiple experiments in one, so we chose to divide the device into several individually addressable arrays of pores with separate electrolyte compartments and integrated electronic connections. Also, to perform electrical and fluorescence experiments at the same time, we designed a PDMS sample chamber so that the substrate is accessible to a microscope objective. By having separated electrolyte compartments, we are also able to exchange solutions or introduce chemicals throughout the experiment. Bilayer formation can be probed by impedance spectroscopy and fluorescence microscopy. The function of inserted ion channels can be measured by current recordings.

Thursday, March 1, 2012 8:00AM - 11:00AM –
Session V46 DPOLY DBIO: Invited Session: Active Matter and Dynamical Systems 160AB

8:00AM V46.00001 From filamentous bundles to active random flows, ZVONIMIR DOGIC, Department of Physics, Brandeis University, Waltham MA, USA — The cytoskeleton has a number of highly unusual material properties which are essential for the reproduction and survival of the cell. However, the extraordinary structural complexity of the cytoskeleton, which contains hundreds of different proteins, presents a particular challenge to any study of its material properties. I will outline experiments whose goal is to reconstitute certain material properties of the cytoskeleton using a few well-defined biochemical components. The long term goal is to understand the behavior of the resulting materials at all levels of hierarchy. For this reason, I will first describe experiments that probe the behavior of equilibrium filamentous bundles and their dependence on the properties of the constituent filaments and their interactions. Subsequently, I will describe the emergent dynamical patterns that form when molecular motors drive an assembly of filamentous bundles to highly out of equilibrium steady states.

8:36AM V46.00002 Spindle Assembly and Architecture: From Laser Ablation to Microtubule

, DANIEL NEEDLEMAN, Applied Physics & Molecular and Cellular Biology, Harvard University — The spindle is a dynamic steady-state structure composed of microtubules and a wide range of factors which control microtubule nucleation, growth, and motion. While many of the individual components of the spindle have been studied in detail, it is still unclear how these molecular constituents self-organize into this structure. Crucially, the extent to which microtubule behaviors are spatially regulated is not known. Here I describe how we are using laser ablation experiments to obtain detailed structural information in spindles: the location of microtubule plus ends, microtubule minus ends, and the length distribution of microtubules in different regions. All of our data can be explained by a very simple model which provides surprising insight into how the regulation of microtubule nucleation and stability gives rise to spindle architecture.

9:12AM V46.00003 Synchronization of eukaryotic flagella *in vivo*: from two to thousands¹

, RAYMOND E. GOLDSTEIN, Department of Applied Mathematics and Theoretical Physics, University of Cambridge — From unicellular organisms as small as a few microns to the largest vertebrates on Earth, we find groups of beating flagella or cilia that exhibit striking spatiotemporal organization. This may take the form of precise frequency and phase locking, as frequently found in the swimming of green algae, or beating with long-wavelength phase modulations known as metachronal waves, seen in ciliates such as *Paramecium* and in our own respiratory systems. The remarkable similarity in the underlying molecular structure of flagella across the whole eukaryotic world leads naturally to the hypothesis that a similarly universal mechanism might be responsible for synchronization. Although this mechanism is poorly understood, one appealing hypothesis is that it results from hydrodynamic interactions between flagella. This talk will summarize recent work using the unicellular alga *Chlamydomonas reinhardtii* and its multicellular cousin *Volvox carteri* to study in detail the nature of flagellar synchronization and its possible hydrodynamic origins.

¹Supported by the EPSRC, BBSRC, and a European Research Council Advanced Investigator Grant.

9:48AM V46.00004 Dynamic Patterns in Active Fluids

, FRANK JÜLICHER, Max Planck Institute for the Physics of Complex Systems, Noethnitzer Strasse 38, 01187 Dresden, Germany — Biological matter is inherently dynamic and exhibits active properties. A key example is the force generation by molecular motors in the cell cytoskeleton. Such active processes give rise to the generation of active mechanical stresses and spontaneous flows in gel-like cytoskeletal networks. Active material behaviors play a key role for the dynamics of cellular processes such as cell locomotion and cell division. We will discuss intracellular flow patterns that are created by active processes in the cell cortex. By combining theory with quantitative experiments we show that observed flow patterns result from profiles of active stress generation in the system. We will also consider the situation where active stress is regulated by a diffusing molecular species. In this case, spatial concentration patterns are generated by the interplay of stress regulation and self-generated flow fields.

10:24AM V46.00005 Order and instabilities in dense bacterial colonies¹

, LEV TSIMRING, University of California, San Diego — The structure of cell colonies is governed by the interplay of many physical and biological factors, ranging from properties of surrounding media to cell-cell communication and gene expression in individual cells. The biomechanical interactions arising from the growth and division of individual cells in confined environments are ubiquitous, yet little work has focused on this fundamental aspect of colony formation. By combining experimental observations of growing monolayers of non-motile strain of bacteria *Escherichia coli* in a shallow microfluidic chemostat with discrete-element simulations and continuous theory, we demonstrate that expansion of a dense colony leads to rapid orientational alignment of rod-like cells. However, in larger colonies, anisotropic compression may lead to buckling instability which breaks perfect nematic order. Furthermore, we found that in shallow cavities feedback between cell growth and mobility in a confined environment leads to a novel cell streaming instability. Joint work with W. Mather, D. Volfson, O. Mondragón-Palomino, T. Danino, S. Cookson, and J. Hasty (UCSD) and D. Boyer, S. Orozco-Fuentes (UNAM, Mexico).

¹Supported by NIH and UC MEXUS/CONACYT.

Thursday, March 1, 2012 8:00AM - 11:00AM — Session V47 DPOLY: Focus Session: Heterogeneous Colloids II 160C

8:00AM V47.00001 Self Assembly of Soft Matter Quasicrystals and Their Approximants¹

, CHRISTOPHER IACOVELLA, AARON KEYS, SHARON GLOTZER, University of Michigan Chemical Engineering Dept — The discovery of soft-matter quasicrystals (QCs) and their approximants [1-4] hints at a unique thermodynamic mechanism underlying their stability. In the past, specific interaction potentials have been contrived to stabilize QCs and their approximants in computer simulations, but such interactions are difficult to achieve in colloidal systems. Here, we use molecular simulation to demonstrate an alternative approach for assembling dodecagonal QCs and their approximants based solely on particle functionalization and shape [5]. Our approach replaces complex energetic interactions with simpler-to-achieve bonded and excluded-volume interactions, encouraging the formation of structures with low surface contact area, including non-close-packed and polytetrahedral structures. We argue that this mechanism can be widely exploited to assemble QCs and approximants in colloidal systems, and may further elucidate the formation of soft matter QCs in experiment [1-4].

[1] G. Ungar, et al., Science 299 (2003)

[2] X. Zeng, et al., Nature 428, (2004)

[3] S. Lee, M.J. Bluemle, F.S. Bates, Science, 330 (2010)

[4] S. Fischer, et al. Proc. Natl. Acad. Sci., 108, (2011)

[5] C.R. Iacovella, A.S. Keys, S.C. Glotzer, Proc. Natl. Acad. Sci., in press (2011) arXiv:1102.5589

¹DOE-BES # DE- FG02-02ER46000, NSF CHE 0624807, DOD/DDRE NSSEFF No. N00244-09-1-0062

8:12AM V47.00002 ABSTRACT WITHDRAWN —

8:24AM V47.00003 Self-assembly of anisotropic colloidal particles under confinement

, CARLOS AVENDANO JIMENEZ, FERNANDO ESCOBEDO, Cornell University — We perform molecular simulations of two novel anisotropic colloidal particles under confinement. The first is an ensemble of hard-hemispheres (mimicking mushroom cap colloids [1]) confined between two parallel walls separated by a distance H. We simulated: a) Low values of H that restrict the rotation of the particles (in a monolayer) where three main dense crystal structures are found: buckled phase, square, and triangular structures. (b) Large values of H where the particles are able to fully rotate; here parallel (spheres-like) or anti-parallel (column-like) dimers are observed which form ordered structures with triangular and rectangular symmetries at high densities. The second system is a model of hard-square particles with rounded corners. Recently, Zhao et. al. have reported the phase behaviour of monolayers of polymeric squares platelets with rounded corners, assembled at the bottom of the container [2]. This system exhibits the formation of a hexagonal rotator phase and the rhombic crystal phase that were not observed in earlier simulations of squares [3] which found instead a tetratic and square crystal phases. By interpolating between hard discs and hard squares, we map out the phase diagram as a function of the roundness of the particles and resolve the discrepancies of the earlier studies. [1] Riley and Liddell, Langmuir 26, 11648 (2010). [2] Zhao, Bruinsma, and Mason, PNAS 108, 2684 (2011). [3] Wojciechowski and Frenkel, Comp. Met. Sci. Technol. 10, 235 (2004).

8:36AM V47.00004 Towards Structural Complexity with Colloids¹ , MICHAEL ENGEL, University of Michigan

— Colloids rather easily assemble into simple crystal structures like the face-centered cubic lattice or the body-centered cubic lattice. More complex phases are harder to achieve, but have recently been reported using a number of approaches. Yet, assembling complex structures often results from trial-and-error and is not well understood. In this presentation, we show how novel crystals, quasicrystals, and liquid crystals can be achieved with colloidal building blocks by varying the interactions and the shapes of the building blocks. Using computer simulations, we demonstrate the formation of unusually ordered phases both with isotropic pair potentials, as well as with faceted shapes like polyhedra. We describe new tools we have developed to perform complex structural analysis on simulated systems and show how they may be used to analyze real space images from colloid experiments. We also compare the assembled structures with densest packings of the building blocks and show that good packings can often be distinct from what is observed to assemble from the disordered state. This suggests that dense packings may not be illustrative of what is achievable in colloid experiments.

¹Supported by Deutsche Forschungsgemeinschaft, AFOSR (FA9550-06-1-0337), and DOD-DDRE (N00244-09-1-0062).

9:12AM V47.00005 Novel Non-Close-Packed Structures Assembled by Spherical Colloids with Anisotropic Interactions under Electric Field , FUDUO MA, NING WU, Colorado School of Mines

— Spherical colloids with isotropic properties have been used as building blocks to assemble a variety of 2D and 3D structures in past, such as FCC, HCP, and BCT crystals. We recently, however, have observed new type of two-dimensional structures under the influence of electric field at the liquid-solid interface. This is primarily due to anisotropic interactions arising from electric field on both particles and aqueous solution. At low concentrations and low frequencies of the electric field, the isotropic spheres can form a series of colloidal clusters, ranging from 3 to 10. The analysis of cluster distributions shows non-trivial peaks for trimer, tetramer, hexamer, and nanomer. Those clusters can change bond angles freely while maintaining the overall structures intact. At high concentrations, those colloidal clusters with flexible bond angles can further assemble and connect themselves into a good variety of two-dimensional non-close-packed networks that have not been observed before. By precisely controlling the electric field strength, frequency, volume fraction of colloids, and ionic strength, we have made diversified non-close-packed structures that have potential applications in photonic crystal, catalysis, or filtration.

9:24AM V47.00006 Self-assembly of polydisperse nanoparticles into monodisperse supraparticles: a computer simulation study , TRUNG D. NGUYEN, University of Michigan, YUNSHENG XIA, National Center for Nanoscience and Technology, BYEONGDU LEE, Argonne National Laboratory, MING YANG, AARON SANTOS, University of Michigan, PAUL PODSIADLO, Argonne National Laboratory, ZHIYONG TANG, National Center for Nanoscience and Technology, SHARON C. GLOTZER, NICHOLAS A. KOTOV, University of Michigan

— Experiments have shown that polydisperse inorganic nanoparticles such as CdSe, CdS and PbS self-assemble into highly uniform supraparticles with a core-shell morphology[1]. The self-assembly process is believed to be self-limiting as indicated by the time evolution of the measured surface potential and supraparticle size distribution. We performed molecular dynamics simulations to demonstrate that the balance between van der Waals attraction and Coulombic repulsion leads to the self-limiting growth of the supraparticles[2-4]. That the uniform supraparticles are stable over a wide range of density indicates that they are thermodynamically stable, rather than consequences of limited diffusion. Our simulation results further reveal that the broad nanoparticle polydispersity leads to the core-shell morphology of the supraparticles. The generic nature of the governing interactions suggests great versatility in the composition, size and shape of the constituent building blocks, and allows for a large family of hierarchical self-assembled structures, including colloidal crystals. References 1. Y. Xia et al, Nat. Nano. 6, 580, 2011. 2. Gonzalez-Mozuelos et al, J. Chem. Phys. 103, 3145, 1995. 3. Van Hyning et al, Langmuir 17, 3120, 2001. 4. J. Ramsden, Proc. R. Soc. Lond. A 413, 407, 1987

9:36AM V47.00007 Particle dynamics in colloidal glasses with short-range attraction¹ , PIOTR

HABDAS, Department of Physics, Saint Joseph's University, KE CHEN, Department of Physics & Astronomy, University of Pennsylvania, MARTIN IWANICKI, DANIEL FLYNN, JOHN MICHAEL DEVANY, LISA MARIANI, Department of Physics, Saint Joseph's University, ARJUN G. YODH, Department of Physics & Astronomy, University of Pennsylvania — We study colloidal particle dynamics of a model glass system using confocal microscopy as the sample evolves from a repulsive glass towards an attractive glass. Short-range depletion forces induce the transition from a repulsive glass to the attractive glass. We identify particles which exhibit substantial motional events and characterize the transition using the properties of these motional events. It appears that number of particles that exhibit motional events doesn't change as the system is brought from a repulsive glass towards the attractive glass. Also, we investigate vibrational properties of these dense colloidal suspensions. Our preliminary results show that the boson peak for an attractive glass is lower than that for a repulsive system and it is shifted towards higher frequencies. To our knowledge, this is the first experimental investigation of the evolution of vibrational modes in colloidal glasses when particle interaction potential changes from repulsive to attractive.

¹P.H., M.I., D.F., J.M.D, L.M. acknowledge support of HHMI and Sigma Xi. L.M. acknowledges support of McNulty Scholars Program. A.G.Y. acknowledges financial support of the NSF Grants No. DMR-0804881, PENN MRSEC No. DMR11-20901, and NASA Grant NNX08AO0G

9:48AM V47.00008 Self-assembly of colloidal surfactants , WILLEM KEGEL, Utrecht University, Utrecht

— We developed colloidal dumbbells with a rough and a smooth part, based on a method reported in Ref. [1]. Specific attraction between the smooth parts occurs upon addition of non-adsorbing polymers of appropriate size. We present the first results in terms of the assemblies that emerge in these systems.

[1] D.J. Kraft, W.S. Vlug, C.M. van Kats, A. van Blaaderen, A. Imhof and W.K. Kegel, *Self-assembly of colloids with liquid protrusions*, J. Am. Chem. Soc. 131, 1182, (2009)

10:24AM V47.00009 The Structure of Dipolar Colloidal Gels in the Dilute Regime , VERONICA

I. MARCONI, FaMAF and Ifeg-Conicet, National University of Cordoba, Argentina, MARCELO A. CARIGNANO, Department of Biomedical Engineering, Northwestern University and Chemistry of Life Processes Institute, Evanston, IL, USA. — Dipolar colloidal systems are one of the simpler material presenting anisotropic interactions and are highly relevant for designing new soft materials easy to control. Using stochastic dynamics simulations we investigate the gelation process in a high dilute system of dipolar colloidal particles immerse in an implicit dielectric solvent. This system self assembles in a rich variety of structures, from open percolated networks or gels to short chains of particles that self cross. We perform simulations using a "continues model" for the dipolar particles interactions and we present a phase diagram, density vs temperature. Each phase is characterized in detail as a function of the spatial correlation (clusters) and response. Interestingly at this low density regime, it is possible to find, characterize and follow the dynamics of a clear and huge variety of short strings configurations (cross loops, triple pointed chains, bundles), mainly at very low temperature. In addition, studying the dynamics of gelation in detail we observe an increasing gelation time while density is decreased in good agreement with previous simulations and experiments on colloidal systems with directional interactions.

10:36AM V47.00010 Two-Dimensional Crystals of Icosahedral Viruses at Liquid interfaces, MASAFUMI FUKUTO, LIN YANG, ANTONIO CHECCO, Brookhaven National Laboratory, IVAN KUZMENKO, Argonne National Laboratory, QUYEN NGUYEN, NICK MANK, QIAN WANG, University of South Carolina — Two-dimensional (2D) assembly of turnip yellow mosaic virus (TYMV) on cationic lipid monolayers is investigated at the air-water interface. TYMV, an icosahedral virus with a diameter of 28 nm, exhibits well-defined roughness, charge distribution, and hydrophilic/hydrophobic patches on its surface. The electrostatic attraction to the lipid-coated aqueous interface provides means to impose a specific virus orientation and hence reduce the number of possible inter-particle interactions. The 2D geometry is particularly advantageous in dissecting the role of anisotropy in aqueous-media assembly, which involves various types of similarly weak interactions. We show that the assembly approach used not only facilitates crystallization but also provides insights on how complex anisotropic interactions can be exploited to generate long-range order. Specifically, we report an *in situ* x-ray scattering observation of novel 2D crystal forms of TYMV that reflect the virus' icosahedral symmetry. The symmetry, shape, and surface heterogeneities of TYMV suggest a mechanism by which these crystals are stabilized by a combination of hydrophobic, electrostatic, and steric interactions.

10:48AM V47.00011 Active colloids at liquid-liquid interfaces: dynamic self-assembly and functionality, ALEXEY SNEZHKO, IGOR ARANSON, Argonne National Laboratory — Self-assembled materials must actively consume energy and remain out of equilibrium in order to support structural complexity and functional diversity. Colloids of interacting particles suspended at liquid-liquid interfaces and maintained out of equilibrium by external alternating electromagnetic fields develop nontrivial collective dynamics and self-assembly. We use ferromagnetic colloidal micro-particles (so the magnetic moment is fixed in each particle and interactions between colloids is highly anisotropic and directional) suspended over an interface of two immiscible liquids and energized by vertical alternating magnetic fields to demonstrate novel dynamic and active self-assembled structures ("asters") which are not accessible through thermodynamic assembly. Structures are attributed to the interplay between surface waves, generated at the liquid/liquid interface by the collective response of magnetic microparticles to the alternating magnetic field, and hydrodynamic fields induced in the boundary layers of *both* liquids forming the interface. Two types of magnetic order are reported. We demonstrate that asters develop self-propulsion in the presence of a small in-plane dc magnetic field. We show that asters can capture, transport, and position target microparticles.

Thursday, March 1, 2012 8:00AM - 10:48AM —
Session V48 DPOLY DBIO: Focus Session: Advanced Optical Probes of Soft Matter - Forces, Imaging, Excitons 161

8:00AM V48.00001 TBD —

8:36AM V48.00002 Brownian vortex circulation due to spin orbit conversion in a circularly polarized optical tweezer, DAVID RUFFNER, DAVID G. GRIER, New York University, DEPARTMENT OF PHYSICS AND CENTER FOR SOFT MATTER RESEARCH TEAM — Strong focusing of circularly polarized beams converts spin angular momentum into orbital angular momentum. We describe this process in terms of a generalized vector potential, involving the amplitude, phase, and polarization of the light. This gives a more general understanding of this force in terms of experimentally accessible parameters. In addition, this formalism provides a framework for understanding other polarization induced forces, which arise from the curl of the spin angular momentum density. Experimentally we demonstrate deterministic polarization-induced circulation with trapped clusters of $1\mu\text{m}$ polystyrene spheres, and Brownian vortex circulation for a single sphere trapped in elliptically polarized optical tweezers.

8:48AM V48.00003 Pulling Particles Backward Using a Forward Propagating Beam, JACK NG, The Hong Kong University of Science and Technology, JUN CHEN, ZHIFANG LIN, Fudan University, CHE TING CHAN, The Hong Kong University of Science and Technology, FUDAN UNIVERSITY COLLABORATION, THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY COLLABORATION — Can the scattering force of a forward propagating beam pull a particle backward? A photon carries a momentum of $\hbar k$, so one may expect light will push against any object standing in its path. However, light can indeed "attract" in some cases. For example, if light is focused to a spot, small particles will be attracted towards it due to the gradient force. But it is probably more appropriate to say that the gradient force "grabs" rather than "pulls", as the particle will remain stable in the trap after being drawn to the focus. Here, we discuss another possibility—a backward scattering force which is always opposite to the propagation direction of the beam so that the beam keeps on pulling an object towards the source without an equilibrium point. In the absence of intensity gradient, using a light beam to pull a particle backwards is counter intuitive. The underlining physics is the maximization of forward scattering via interference of the radiation multipoles. We show explicitly that the necessary condition to realize a pulling force is the simultaneous excitation of multipoles in the particle and if the projection of the total photon momentum along the propagation direction is small, attractive optical force is possible.

9:00AM V48.00004 Lateral optical binding forces between two colloidal Mie particles, MING-TZO WEI, Lehigh University, JACK NG, C.T. CHAN, Hong Kong University of Science and Technology, H. DANIEL OU-YANG, Lehigh University — Micro particles in an intense optical field can self-organize into an array with well defined structure. This phenomenon, first reported by Burns et al., as optical binding, was believed to be caused by the optical gradient force. In spite of many attempts to calculate the binding forces and the colloidal structures, there has been a lack of experiments directly measuring the forces between the particles. Positioning two micron-sized polystyrene particles, each held by a tightly focused laser beam from a single coherence laser source, we found the lateral optical binding force oscillates with the inter particle separation, as well as the relative phase between the beams due to retardation. By independently changing the polarization directions at each optical trap, we examined the periodicity and magnitude of the forces. Our research indicates the forces under such conditions require a model beyond dipole approximation. In addition, an accurate calculation based on Mie theory with consideration of high focusing compare well with our experimental findings.

9:12AM V48.00005 Super-Resolution Imaging Using Randomly Diffusing Probes, ANNA LABNO, HU CANG, CHRISTOPHER GLADDEN, XIANG ZHANG, University of California at Berkeley — Recent advances in super-resolution microscopy allow imaging of biological tissues labeled with fluorescent dyes with unprecedented resolution. These techniques often rely on the fact that single emitters can be localized with nm accuracy. When multiple emitters reside within a diffraction-limited spot they are serially photo-switched to ensure that they emit one at a time. This approach has not been applied to other imaging modalities, for example imaging local electromagnetic field enhancement, mainly because photo-switching would be infeasible. Here we present a super-resolution imaging technique which circumvents the requirement for serial photoswitching by using the random motion of single dye molecules to scan the surface in a stochastic manner. This technique allowed us to image electromagnetic field enhancement of a single spot formed on thin metallic film with 1.2nm accuracy and gain insight into the mechanism for generating field enhancement.

9:24AM V48.00006 Three-dimensional thermal noise images of single biopolymer filaments allows to determine their orientation and quantify their mechanical properties, MARTIN KOCHANZYK, TOBIAS BARTSCH, PINYU THRASHER, ERNST-LUDWIG FLORIN, The University of Texas at Austin — Intracellular biopolymer networks perform many essential functions for living cells. Most of these networks show a highly nonlinear mechanical response that is well-studied on the macroscopic scale. While much work has been done to connect the macroscopic responses of networks to specific network properties, such as filament persistence length, cross-linking geometry and pore size, there is a lack of experimental techniques that can simultaneously determine the structure and the mechanical properties of a network in situ on the single filament level. Thermal Noise Imaging is a scanning probe technique that utilizes the confined thermal motion of an optically trapped particle as a three-dimensional, noninvasive scanner for soft, biological material. It achieves nanometer precision in probe position detection at MHz bandwidth. Thermal noise imaging visualizes single biopolymer filaments as nanoscale tunnels and allows for the quantification of their mechanical properties from their transversal fluctuations. The experiments presented here pave the way for investigating force distributions inside biopolymer networks on the single filament level, as well as establish thermal noise imaging as a quantitative tool for studying biological material on the nanometer scale.

9:36AM V48.00007 Microscopy method for the characterization of structural color on a single wing scale of Morpho butterfly¹, BEOM-JIN YOON, MATIJA CRNE, JUNG OK PARK, MOHAN SRINIVASARAO, School of Materials Science and Engineering, Georgia Institute of Technology — The structural color and the iridescence of Morpho rhetenor were investigated using an optical microscope and a digital camera. Incoherent white light source was used for both spatial and spectral analysis. The scattering pattern from the micrometer sized single scale in the back focal plane of the objective lens was observed with Bertrand lens equipped in the optical microscope. We precisely controlled incident angle of the light using common components typically embedded in most optical microscope; aligning aperture stop at the center or off-center. Wide range of the angular scattering pattern from a single scale was measured and the iridescence of Morpho rhetenor was measured quantitatively. The single scale of Morpho rhetenor diffusively reflected the normally illuminated light, while blue band was more effectively reflected than green and red band. We retrieved the raw intensity data generated at the imaging sensor of the digital camera and quantitatively analyzed the spatial distribution of the scattered light. The reflectivity measured by the digital camera was comparable to the result from microspectrometer reported earlier.

¹This work was partially supported by NSF funding (DMR-0907529).

9:48AM V48.00008 High Fidelity Detection of Defects in Polymer Films using Surface-Modified Nanoparticles, CHAITANYA PRATIWADA, SINDHUJA CHARI, JOLANTA MARSZALEK, MATTHEW BECKER, ALAMGIR KARIM, University of Akron — Defects are ubiquitous to materials and material surfaces. As we push the thresholds of length scale producing defect free materials, surfaces and interfaces, it becomes increasingly difficult to detect their presence over multiple length scales. The ideal example is the semiconductor industry where the driving force is higher performance and lower cost devices with material interfaces. In this regard, Chemical mechanical planarization, CMP, emerged as the premier method for achieving ultra flat surfaces below the 0.35 micron technology node, enabling many of the advanced electronic devices currently in production. The interactions between numerous process settings and output metrics are difficult to predict and often lead to defects. Failure analysis (FA) is critical and the current methods involve advanced imaging methods such as SEM. We design a cost effective method to detect physico-chemical defects at multiple length scales through Polymer-Nanoparticles (NPs) interactions in relatively shorter period of time (time of imaging is reduced 50 fold). This method can be used in conjunction with the traditional imaging methods to pin point location of these defects, which can be further analyzed.

10:00AM V48.00009 A Study of the Polarizability of Single-Walled Carbon Nanotubes in an Optical Field, JINGYU WANG, H. DANIEL OU-YANG, Lehigh University — Whereas the behavior of single-walled carbon nanotubes (SWCNT) in an electric field has been extensively studied, the polarizability of SWCNTs at optical frequencies remains unclear due to the difficulty in direct detection. It was demonstrated by utilizing Raman spectroscopy as a characterization means, optical tweezers could selectively aggregate SWCNTs. While it was commonly believed that the trapping effect due to the large optical field gradient caused the strong response of tubes to the laser beam, we expect the aligning effect due to the optical polarization also has a considerable contribution. To quantify these two possible effects experienced by an ensemble of individual DNA-SWCNTs of different chiralities, and address the issue of tube-tube interaction, We design an experiment by applying optical tweezers with variable polarization states and inspecting resonance Raman excitation for sensitive detection. Specifically, we measure the radial breathing mode signal of SWCNTs as a function of laser power and the direction of polarization for different tube types and concentrations. The research may lead to a more complete understanding of sorting phenomenon of individual SWCNTs in an optical field at microscopic level.

10:12AM V48.00010 Dynamics of Aerial Tower Formation in Bacillus subtilis Biofilms, NAVEEN SINHA, AGNESE SEMINARA, JAMES WILKING, MICHAEL BRENNER, DAVE WEITZ, Harvard University — Biofilms are highly-organized colonies of bacteria that form on surfaces. These colonies form sophisticated structures which make them robust and difficult to remove from environments such as catheters, where they pose serious infection problems. Previous work has shown that sub-mm sized aerial towers form on the surface of Bacillus subtilis colony biofilms. Spore-formation is located preferentially at the tops of these towers, known as fruiting bodies, which aid in the dispersal and propagation of the colony to new sites. The formation of towers is strongly affected by the quorum-sensing molecule surfactin and the cannibalism pathway of the bacteria. In the present work, we use confocal fluorescence microscopy to study the development of individual fruiting bodies, allowing us to visualize the time-dependent spatial distribution of matrix-forming and sporulating bacteria within the towers. With this information, we investigate the physical mechanisms, such as surface tension and polymer concentration gradients, that drive the formation of these structures.

10:24AM V48.00011 The Orientation of Luminescent Excitons in Layered Organic Nanomaterials, JON SCHULLER, Columbia University, SINAN KARAVELLI, Brown University, KELIANG HE, Case Western Reserve University, SHYUAN YANG, Columbia University, JIE SHAN, Case Western Reserve University, JOHN KYMISSIS, Columbia University, RASHID ZIA, Brown University — A fundamental understanding of optoelectronics in organic semiconductors is complicated by the diversity of excitons which can exist within a single material system. Measurements that distinguish between different exciton types are crucial for a complete understanding of organic materials. By fitting experimental curves of angle-, polarization-, and energy-dependent PL to analytical Purcell calculations we quantify the relative dipole moments for in-plane and out-of-plane oriented excitons in organic and inorganic layered nanomaterials. In mono- and bi-layers of Molybdenum Disulfide (MoS₂) and Graphene Oxide the luminescence arises only from in-plane oriented excitons. In the perylene derivative PTCDA, however, we show that PL arises from both in-plane and out-of-plane excitons. We observe a difference in emission frequency between the dipole orientations which indicates the existence of two distinct exciton species: an in-plane oriented Frenkel exciton and an out-of-plane oriented Charge Transfer exciton. Based on these results we devise and implement a method for isolating luminescence from either exciton species. We observe different temporal dynamics for the two distinct excitons, highlighting the power of this technique for fundamental studies of organic materials.

10:36AM V48.00012 Accessing exciton transport in light-harvesting structures with plasmonic nanotip, SEMION K. SAIKIN, Department of Chemistry and Chemical Biology, Harvard University, JOHANNES FEIST, ITAMP, Harvard-Smithsonian Center for Astrophysics, Harvard University, M.T. HOMER REID, Research Laboratory of Electronics, Massachusetts Institute of Technology, MIKHAIL D. LUKIN, Department of Physics, Harvard University, ALAN ASPURU-GUZIK, Department of Chemistry and Chemical Biology, Harvard University — Natural light-harvesting complexes, such as that of plant cells or photosynthetic bacteria, are considered as possible prototypes for artificially designed solar cell materials. In these structures the energy of light absorbed by a peripheral antenna is transmitted very efficiently in a form of excitons to a reaction center. Usually, information about the exciton transport is obtained from time-resolved nonlinear optical experiments where the frequencies of a pump and a probe fields select particular electronic transitions in the light-harvesting complex. We explore a complimentary setup utilizing a plasmonic nanotip as a local sub-wavelength probe of excitation dynamics. As specific examples we consider an LHII complex involved in the light-harvesting process of purple bacteria and a Fenna-Matthews-Olson pigment-protein complex of green-sulphur bacteria.

Thursday, March 1, 2012 8:00AM - 11:00AM –
Session V49 DMP DPOLY: Focus Session: Organic Electronics and Photonics - Solar Cells and Light Emitting Devices 162A

8:00AM V49.00001 Frequency dependence of magnetoresistance in MEH-PPV, THADDEE KAMDEM DJIDJOU, THO NGUYEN, Z. VALY VARDENY, ANDREY ROGACHEV, University of Utah — The organic magnetoresistance (OMAR) in organic light emitting diodes (OLED) made of MEH-PPV was investigated by means of DC transport and the admittance spectroscopy in the range of 1 Hz to 10 MHz at room temperature. The measurements were carried out on unipolar and bipolar OLEDs made of pristine MEH-PPV as well as MEH-PPV with traps introduced by the UV light irradiation. We found that in bipolar, UV-exposed OLEDs, the magnitude of magnetoresistance effect in real part of admittance increases with DC bias, reaches very high value of 35 % (in the field 30mT) at bias 4.8 V and decreases at higher bias voltages. Also, we observed that the cutoff frequency of OMAR effect monotonically increases with DC bias voltage. The cutoff has extrinsic origin and is likely caused by a dissipative process related to the reorientation of permanent dipoles. At the highest tested bias voltage 6.7 V, we were able to detect the OMAR at the highest frequency of our system, 10 MHz. We have found that imaginary part of the admittance is also affected by magnetic field. The effect of magnetic field on dynamical capacitance of the device at low frequencies is very strong and opens up a possibility of using these devices as magnetic field sensors.

8:12AM V49.00002 Graphene-Based Polymer Bulk Heterojunction Solar Cells, FEI YU, VIKRAM KUPPA, University of Cincinnati — The requirement of exciton dissociation in organic photovoltaics necessitates the presence of a large-area interface accessible to the interior of the active layer. Traditionally, such bulk heterojunctions (BHJ) have been spin-coated from a blend of conjugated polymer and functionalized fullerene molecules. We propose and demonstrate BHJs that utilize chemically modified graphene nanoparticles in order to facilitate charge transfer in polymeric solar cells. Devices based on P3HT:PCBM:graphene were fabricated on patterned ITO glass, and the effect of graphene on performance was investigated. Various device parameters including short-circuit current density, open-circuit voltage, fill factor, power conversion efficiency, and external quantum efficiency are compared with traditional BHJs. Results are discussed in the context of the morphology of the active layer, and the distribution and orientation of graphene platelets, as characterized by SEM, AFM and TEM.

8:24AM V49.00003 Planar Organic Photovoltaics for more Opportunities of Efficiency Enhancement and Parameters Controlling¹, FERAS G. ALZUBI, Nanoscience Technology Center, Department of Physics, University of Central Florida, SAIFUL I. KHONDAKER, Nanoscience Technology Center, Department of Physics, School of Electrical Engineering and Computer Science, University of Central Florida — Organic photovoltaics have been intensively studied as a cheap, easy processed and reliable source of energy that will eventually substitute the inorganic photovoltaics. Commonly, PV devices are made in vertical geometry where the BHJ active material is sandwiched between two electrodes one of them must be transparent to shine the light through. This vertical geometry created some challenges such as requirement of transparent ITO electrode as well as tying up the active material film thickness and electrodes separation. As an approach to overcome these challenges, we utilize the planar geometry to fabricate PV device where the poly (3-hexylthiophene) and [6,6]-phenyl C61-butyric acid methylester (P3HT/PCBM) blend is deposited between two asymmetric metallic electrodes. We investigated the PV behavior for different metal electrodes which is an advantage provided by planar structure. Also, we discuss the behavior of the power conversion efficiency (PCE) with independently varying the active material film thickness and electrodes separation.

¹This work is supported by U.S. National Science Foundation under Grant No. ECCS 0801924.

8:36AM V49.00004 Low band gap polymer bulk heterojunction solar cell on a co-planar digitated electrodes structure, ABRAR QUADERY, FERAS ALZUBI, Nanoscience Technology Center, Department of Physics, University of Central Florida, SIMON TANG, ANDRE J. GESQUIERE, Nanoscience Technology Center, Department of Chemistry, University of Central Florida, SAIFUL KHONDAKER, Nanoscience Technology Center, Department of Physics, University of Central Florida — Usage of additive in a bulk heterojunction organic solar (BHJ) cell to enhance absorption of solar spectrum in the NIR range is attracting significant research interest. At present, the BHJ solar cells are fabricated in a vertical geometry where a transparent electrode is necessary limiting the choice to mostly ITO. This may create a significant challenge as the performance of organic solar cell is dependent on the work function matching of active materials and the electrode. In order to address this challenge, we fabricated solar cell by dropcasting a ternary blend of P3HT:PC₆₀BM: PCPDTBT on a simple structure comprising of co-planar digitated electrodes with different work functions. We will discuss the performance of our device and its implication.

8:48AM V49.00005 Charge Accumulation and Internal Photovoltaic Processes in Organic Solar Cells, HUIDONG ZANG, YU-CHE HSIAO, QING LIU, University of Tennessee, ILIA IVANOV, Oak Ridge National Laboratory, BIN HU, University of Tennessee — The accumulation of dissociated charge carriers plays an important role in reducing the loss occurring in open-circuit voltage (Voc), short-circuit photocurrent (Isc), fill factor (FF) in organic solar cells. We found from light-assisted capacitance measurements that the charge accumulation inevitably occurs at device interfaces in bulk-heterojunction ITO/PEDOT/P3HT:PCBM/Ca/Al solar cells. Our experimental studies have indicated that the charge accumulation can reduce the Voc through charge injection, Isc through charge collection, and FF through charge transport. Furthermore, our light-assisted capacitance measurements reveal that using a dielectric thin film of TiOx can decrease charge accumulation in the ITO/PEDOT/P3HT:PCBM/TiOx/Ca/Al solar cell. In particular, we find that decreasing the charge accumulation can reduce the loss occurring in Voc, Isc, and FF. Clearly, controlling charge accumulation presents a new mechanism to improve photovoltaic performance in organic solar cells.

9:00AM V49.00006 Photocurrent noise in organic bulk heterojunction solar cells, N.S. VIDHYADHIRAJA, MONOJIT BAG, K.S. NARAYAN, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India — We report the first electrical noise measurements from illuminated bulk heterojunction polymer based solar cells. The dependence of photocurrent fluctuations on temperature, light intensity and device conditions was analyzed. We find flicker noise of the form $1/f^\alpha$ at low frequencies (<1 kHz). An unusual log-normal feature in the noise power spectrum is observed in the frequency regime > 5 kHz. We develop a theoretical description employing kinetic Monte-Carlo simulations that points to the importance of a mobility edge in the understanding of fluctuations in the low frequency regime, while also capturing the temperature dependence of the noise amplitude. We find that a Gaussian disorder model with uncorrelated traps is not sufficient to describe the log-normal feature, thus highlighting the significance of spatial and/or energetic correlations among the trap states.

9:12AM V49.00007 Relating charge transport and performance in single-layer graded-composition organic light-emitting devices, RUSSELL HOLMES, University of Minnesota — Organic light-emitting devices (OLEDs) continue to receive interest for application in displays and as solid-state lighting sources. While OLEDs can exhibit high external quantum and luminous power efficiencies, high performance often requires the use of complex, multilayer architectures. Consequently, there has been interest in the development of OLED architectures containing fewer device active layers or perhaps, a single active layer. Here, we describe an approach to realize efficient electroluminescence from a single active layer through the use of engineered composition gradients. Graded-emissive layer (G-EML) devices contain a single layer consisting of nearly 100% hole-transporting material (HTM) at the anode and nearly 100% electron-transport material (ETM) at the cathode, and having a continuously varying HTM:ETM composition across the active layer. Electroluminescence originates from a phosphorescent guest that is uniformly doped throughout the G-EML. For red-, green-, and blue-emitting phosphors, efficiencies are realized that rival those of more complex, multilayer structures. The G-EML balances electron and hole injection and transport leading to effective charge carrier confinement and exciton formation. This talk will examine how charge confinement in the G-EML is realized through a spatial variation in the carrier mobility across the active layer. In addition, separate measurements of the G-EML exciton recombination zone show that it is substantially broader than that of conventional, abrupt heterojunction OLEDs, a feature which may help to reduce bimolecular exciton quenching in these structures.

9:48AM V49.00008 Sources of high photo-current in inverted organic solar cells¹, ABAY GADISA, Department of Chemistry and Astronomy, UNC- Chapel Hill, YINGCHI LIU, RENE LOPEZ, Department of Physics and Astronomy, UNC- Chapel Hill, EDWARD SAMULSKI, Department of Chemistry, UNC- Chapel Hill, SOLAR UNC TEAM — Inverted organic solar cells have been proved to render exceptional environmental stability compared to the conventional solar cell architecture. On the other hand, polymer/fullerene based inverted solar cells produce more photo-current compared to conventional cells comprising the same active layer thickness. The origin of this current has never been clearly stated so far. We have investigated the photovoltaic properties of inverted solar cells comprising a bulk heterojunction layer of poly(3-hexylthiophene) (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM). The blend layer was formed by spin casting the blend solution on ITO substrate, covered with an Al doped zinc-oxide layer (ZnO-Al) deposited through pulsed laser deposition technique. The inverted solar cells show over 15% increase in photo-current yield compared to conventional solar cells. We have discovered that the inverted solar cells produce additional photo-current through dissociation of excited electron-hole pairs near the polymer/ZnO-Al interfaces. Since ZnO-Al is a good electron conductor, the electrons generated at the polymer/ZnO-Al interface are more efficiently collected compared to photo-current produced in the bulk of the active film. External quantum efficiency exceeding 70% was recorded in the ZnO-Al based inverted solar cells. In general, ZnO-Al is not only characterized by its high electron conductivity, and transparency but also serves as electron acceptor.

¹This project is supported by the NSF-SOLAR program DMR-0934433.

10:00AM V49.00009 ABSTRACT WITHDRAWN —

10:12AM V49.00010 Near-Infrared Photodetector Consisting of J-Aggregating Cyanine Dye and Metal Oxide Thin Films, TIMOTHY OSEDACH, Harvard University, ANTONIO IACCHETTI, Politecnico di Milano, RICHARD LUNT, Michigan State University, TRISHA ANDREW, PATRICK BROWN, GLEB AKSELROD, VLADIMIR BULOVIC, MIT — We demonstrate a photodetector structure that employs metal-oxide charge transport layers and that is sensitized at near-infrared wavelengths by a thin film of a J-aggregating cyanine dye. The high absorption coefficient of the J-aggregate film, combined with the use of a reflective anode and optical spacer layer, enables an external quantum efficiency (EQE) of $16.1 \pm 0.1\%$ ($\lambda = 756$ nm) to be achieved at zero-bias in a device consisting of an 8.1 ± 0.3 nm-thick dye film. The specific detectivity (D^*) and response speed (f_{3dB}) of the fully-optimized device are measured to be $(4.3 \pm 0.1) \times 10^{11}$ cm Hz^{1/2} W⁻¹ and 91.5 kHz, respectively. Modeling of our structure reveals that the photocurrent is limited by the diffusion of photo-generated excitons to the metal oxide/J-aggregate hetero-interface and we determine the exciton diffusion length in the J-aggregate film to be $L_D = 2.0 \pm 0.4$ nm. This work provides insights relevant to the use of J-aggregating cyanine dyes in photodetector and photovoltaic applications and highlights the importance of engineering the optical field profile within such structures in order to maximize performance.

10:24AM V49.00011 Electrical Stability Tests of Polymer Light Emitting Devices¹, JACOB COX, ZAC BARCIKOWSKI, MARIAN TZOLOV, Lock Haven University of Pennsylvania — The degradation of polymer light emitting devices (PLEDs) is a main concern influencing the commercial production of functioning devices. There are various sources of degradation related to the polymer film, the interfaces, and the cathodes. The fundamental understanding of these processes helps to develop strategies for fabrication of devices with longer lifetimes. We are reporting on devices in which delamination of the metal cathode is the dominating degradation mechanism. We have performed stability tests at constant current and constant voltage accompanied by current-voltage characteristics. The results indicate initial improvement of functionality followed by degradation. The change in the current-voltage characteristics indicates modifications of the electron and hole transport through the polymer layer in addition to the delamination. The delamination appears only if the current is above a certain threshold value. We have studied the kinetics of the delamination which gradually increased with time. Several types of semitransparent anodes were used to clarify the origin of the observed delamination, e.g. gold, platinum, and ZnO:Al. The devices were also exposed to thermal stress tests to verify if the evolution of volatile molecules is involved in the observed degradation.

¹This work was partly supported by the NSF grant # 0923047.

10:36AM V49.00012 Rational design of charge transport molecules for blue organic light emitting devices, ASANGA PADMAPERUMA, LELIA COSIMBESCU, PHILLIP KOECH, EVGUENI POLIKARPOV, JAMES SWENSEN, DANIEL GASPAR, PNNL, PACIFIC NORTHWEST NATIONAL LABORATORY TEAM — The efficiency and stability of blue OLEDs continue to be the primary roadblock to developing organic solid-state white lighting as well as power efficient displays. It is generally accepted that such high quantum efficiency can be achieved with the use of organometallic phosphor doped OLEDs. The transport layers can be designed to increase the carrier density as a way to reduce the drive voltage. We have developed a comprehensive library of charge transporting molecules using combination of theoretical modeling and experimental evidence. Our work focuses on using chemical structure design and computational methods to develop host, transport, emitter, and blocking materials for high efficiency blue OLEDs, along with device architectures to take advantage of these new materials. Through chemical modification of materials we are able to influence both the charge balance and emission efficiency of OLEDs, and understand the influence of the location of photon emission in OLEDs as a function of minor chemical modifications of host and electron transport materials. Design rules, structure-property relationships and results from state of the art OLEDs will be presented.

10:48AM V49.00013 Transient Capacitance of Light-Emitting Electrochemical Cells¹, NANCY HAEGEL, YEVTTE DAVIS, PETER CROOKER, Naval Postgraduate School, J. DEVIN MACKENZIE, YUKA YOSHIOKA, Add-Vision, Inc. — Although the steady-state behavior of light-emitting electrochemical cells (LECs) has been addressed theoretically, the transient properties of LECs have yet to be studied in detail. We present time- and frequency-dependent measurements of the capacitance, current, and optical emission of LECs as a constant voltage bias is applied and removed. We find that the capacitance increases more rapidly than the light or current and, unlike the light and current behavior, can be oscillatory and even negative at lower frequencies. Variable temperature experiments were performed to enable observation of a range of transient phenomena that cannot be fully explored at room temperature. The transient behavior suggests that the capacitance is determined by a combination of ion distribution, free carrier screening, and junction width. We interpret our data by qualitatively extending the ideas of existing steady-state theory.

¹Supported by NSF Grant 0804527 and DOD Rapid Reaction Office

Thursday, March 1, 2012 8:00AM - 11:00AM – Session V50 DPOLY: Structure and Properties of Copolymers 162B

8:00AM V50.00001 Designing 100 K Glass Transition Breadths in Bulk Polymer Systems: Effects of Architecture in Homopolymers, Copolymers, and Copolymer Blends, STEPHEN MARROU, SEAN WUNDROW, JOHN TORKELOSON, Northwestern University — Gradient copolymers have attracted interest as vibration or acoustic damping materials due to their extremely broad, tunable glass transition temperature (T_g) responses, up to 100 K in breadth. This behavior is caused by large compositional heterogeneity resulting from sinusoidal composition profiles in nanophase-separated systems. We have also found that some homopolymers and random copolymers exhibit large T_g breadths caused by incompatible main- and side-chain interactions. For example, the T_g response broadens with increasing side-chain length in the poly(n-alkyl methacrylate) series by more than a factor of 2 in going from poly(methyl methacrylate) to poly(n-hexyl methacrylate). We have also blended weakly-segregating styrene/n-butyl acrylate random copolymers of different compositions to allow for tunable T_g breadths over a 100 K temperature range. Finally, we have shown that blending a selective plasticizer into a styrene/4-vinylpyridine gradient copolymer results in a dramatic shift in the T_g response of a single nanophase region, increasing the T_g breadth above 100 K.

8:12AM V50.00002 Structure and Mechanical Behavior of Elastomeric Multiblock Terpolymers Containing Glassy, Rubbery, and Semicrystalline Blocks, FENG ZUO, University of Minnesota, C. GUILLERMO ALFONZO, The Dow Chemical Company, FRANK BATES, University of Minnesota — Multiblock terpolymers containing poly(cyclohexylethylene) (C), poly(ethylene-*alt*-propylene) (P), and poly(ethylene) (E) were synthesized. The CECPEC (denoted XPX) and CECP (XP) each contain 50 v% P and equal amounts of C and E. These materials have been studied by DSC, DMS, TEM, SAXS, WAXS, and tensile deformation to characterize the morphology, phase behavior, and mechanical properties. Microphase separation is induced by crystallization of E and/or chemical incompatibility between the three blocks, leading to a morphology which contains continuous region of P and continuous region of microphase separated X, resulting in mechanically resilient materials. High M_w block copolymers microphase separate with two different length scales associated with segregation between C and E, and X and P. These structural features produce a non-classical scaling relationship for the C-E domain spacing, $d \sim N^{0.31}$. The role of semicrystalline E domains during uniaxial deformation has been exposed with WAXS experiments, which support a two-step mechanism involving recoverable and non-recoverable deformation to different extents. Strain hardening is observed in double-anchored XPX, but not in single-anchored XP, at large tensile strains.

8:24AM V50.00003 Energy Storage and Dissipation in Random Copolymers during Biaxial Loading, HANSOHL CHO, MARY BOYCE, Massachusetts Institute of Technology, MASSACHUSETTS INSTITUTE OF TECHNOLOGY TEAM — Random copolymers composed of hard and soft segments in a glassy and rubbery state at the ambient conditions exhibit phase-separated morphologies which can be tailored to provide hybrid mechanical behaviors of the constituents. Here, phase-separated copolymers with hard and soft contents which form co-continuous structures are explored through experiments and modeling. The mechanics of the highly dissipative yet resilient behavior of an exemplar polyurea are studied under biaxial loading. The hard phase governs the initially stiff response followed by a highly dissipative viscoplasticity where dissipation arises from viscous relaxation as well as structural breakdown in the network structure that still provides energy storage resulting in the shape recovery. The soft phase provides additional energy storage that drives the resilience in high strain rate events. Biaxial experiments reveal the anisotropy and loading history dependence of energy storage and dissipation, validating the three-dimensional predictive capabilities of the microstructurally-based constitutive model. The combination of a highly dissipative and resilient behavior provides a versatile material for a myriad of applications ranging from self-healing microcapsules to ballistic protective coatings.

8:36AM V50.00004 X-ray scattering studies of ordered block copolymer melts during uniaxial extensional flow, WESLEY BURGHARDT, RUINAN MAO, ERICA MCCREADY, Northwestern University — We present the design and implementation of a new apparatus for in situ x-ray scattering studies of polymer melts during homogenous uniaxial extensional flow. The instrument is based on the commercial SER extensional flow fixture, which employs counter-rotating drums to deform a strip of polymer melt, which is incorporated into a custom-built convection oven designed to facilitate x-ray access to the sample and operation in a synchrotron environment. Here we report measurements of extensional flow-induced structural changes in a cylindrically ordered styrene-ethylene butylene-styrene triblock copolymer melt. At early stages, SAXS data reveal that the ordered microstructure deforms affinely until Hencky strains of ~ 0.2 . A global re-orientation process leads to alignment of microdomains predominantly along the stretching direction after Hencky strains of ~ 1 . Further stretching does not lead to further qualitative changes in 2-D SAXS patterns. Relaxation of both microdomain orientation and d-spacing is observed following cessation of extensional flow, albeit with different characteristic time scales. In situ x-ray scattering data are compared with off-line measurements of transient extensional viscosity, performed using the SER fixture in a rotational rheometer.

8:48AM V50.00005 ABSTRACT WITHDRAWN —

9:00AM V50.00006 Understanding the Dynamics of Magnetic Field Alignment for Rod-Coil Block Copolymers, BRYAN MCCULLOCH, University of California - Berkeley, GIUSEPPE PORTALE, WIM BRAS, ESRF, DUBBLE CRG, ALEXANDER HEXEMER, Advanced Light Source, LBNL, RACHEL A. SEGALMAN, University of California - Berkeley — Alignment of semiconducting block copolymer nanostructures is crucial to optimize charge transport in these materials. Magnetic fields can act on the liquid crystalline conjugated polymers, inducing alignment in rod-coil block copolymers. By using a combination of small angle x-ray scattering (SAXS) and transmission electron microscopy (TEM) we have studied the magnetic field alignment of poly(alkoxy phenylene vinylene-*b*-isoprene) (PPV-PI) rod-coil block copolymers. In situ measurements have also shown the magnetic field leads to a stabilization of the ordered phase. Furthermore, there appear to be two distinct timescales for alignment: at short times the alignment of these materials is fast likely caused by preferential growth of aligned domains, and at long times alignment increases by the very slow process of defect annihilation. Further, there is an optimum temperature where the kinetics and thermodynamic driving forces for alignment are balanced, producing very highly aligned samples. Understanding the mechanisms by which alignment occurs has lead to knowledge helping to rationally optimize the magnetic alignment of rod-coil block copolymers.

9:12AM V50.00007 In-situ SAXS observation of magnetic field effects on block copolymer ordering and alignment¹, CHINEDUM OSUJI, MANESH GOPINADHAN, PAWEŁ MAJEVSKI, Dept. of Chemical and Environmental Engineering, Yale University — The use of external fields to direct block copolymer self-assembly is well documented. Magnetic fields offer particular promise due to their space-pervasive nature and the ability to produce arbitrary alignments over truly macroscopic length scales in appropriate systems. We present here the results of in-situ SAXS studies of side-chain liquid crystalline diblock copolymers ordering under high magnetic fields and ex-situ GISAXS data on thin films. Despite the coincidence of the block copolymer order-disorder transition (ODT) and the LC clearing temperature in these weakly segregated materials, there is no measurable effect of the field on the ODT of the system, up to 6 T. This is in line with rough estimates based simply on the magnitudes of the relevant energy scales - the free energy of field interaction and the enthalpy of the isotropic-LC transition. We show that the alignment of the system is critically limited by the viscosity of the mesophase such that alignment can only be advanced by residence in a small temperature window near T_{ODT} . This residence produces a weakly aligned system which thereafter transitions to a strongly aligned state on cooling even in the absence of the field.

¹NSF support under DMR-0847534 is gratefully acknowledged.

9:24AM V50.00008 Characterizing Mesoporous Block Copolymers by Resonant Soft X-ray Scattering¹, DAVID WONG, KEITH BEERS, UC Berkeley and Lawrence Berkeley National Lab, CHENG WANG, Advanced Light Source, Lawrence Berkeley National Lab, JEFFREY KORTRIGHT, Lawrence Berkeley National Lab, NITASH BALSARA, UC Berkeley and Lawrence Berkeley National Lab — Mesoporous block copolymers membranes can be used as water filtration membranes and battery separators. In these applications, it is often advantageous to generate a structure where one block serves as a structural component, and the second block lines the pores. The membrane thus has 3 components: the two blocks and vacuum (or air). Small Angle X-ray Scattering (SAXS), which relies on electron density for contrast, only distinguishes between vacuum and polymer. This is because the scattering contrast between the two blocks is much less than that between the polymer and vacuum. Resonant Soft X-ray Scattering (RSoXS) experiments can be used to adjust the contrast between block copolymer phases by tuning the energy of the incident x-ray beam. We have studied mesoporous poly(styrene-block-ethylene-block-polystyrene) (SES) films, where the semicrystalline polyethylene serves as a structural phase, and the polystyrene lines the pores. At a particular energy, the scattering contrast between PS and vacuum becomes negligible, while contrast between PS and PE is enhanced. We present RSoXS data at different x-ray energies to demonstrate this contrast enhancement.

¹This work was supported by the Asst. Secretary for Energy Efficiency and Renewable Energy, Office of Vehicle Technologies of the U.S. DOE under the Batteries for Advanced Transportation Technologies Program.

9:36AM V50.00009 Self-assembly Morphology and Crystallinity Control of Di-block Copolymer Inspired by Spider Silk¹, WENWEN HUANG, SREEVIDHYA KRISHNAJI, DAVID KAPLAN, PEGGY CEBE, Tufts University — To obtain a fuller understanding of the origin of self-assembly behavior, and thus be able to control the morphology of biomaterials with well defined amino acid sequences for tissue regeneration and drug delivery, we created a family of synthetic silk-based block copolymers inspired by the genetic sequences found in spider dragline, HABn and HBAn ($n=1,2,3,6$), where B = hydrophilic block, A = hydrophobic block, and H is a histidine tag. We assessed the secondary structure of water cast films by Fourier transform infrared spectroscopy (FTIR). The crystallinity was determined by Fourier self-deconvolution of amide I spectra and confirmed by wide angle X-ray diffraction (WAXD). Results indicate that we can control the self-assembled morphology and the crystallinity by varying the block length, and a minimum of 3 A-blocks are required to form beta sheet crystalline regions in water-cast spider silk block copolymers. The morphology and crystallinity can also be tuned by annealing. Thermal properties of water cast films and films annealed at 120 C were determined by differential scanning calorimetry and thermogravimetry. The sample films were also treated with 1,1,1,3,3,3-Hexafluoro-2-propanol (HFIP) to obtain wholly amorphous samples, and crystallized by exposure to methanol. Using scanning and transmission electron microscopies, we observe that fibrillar networks and hollow micelles are formed in water cast and methanol cast samples, but not in samples cast from HFIP.

¹Support was provided from the NSF CBET-0828028 and the MRI Program under DMR-0520655 for thermal analysis instrumentation.

9:48AM V50.00010 The Effects of Blockiness on the Chemical Composition Distribution of Partially Functionalized Polystyrene, WAYNE POWERS, Rensselaer Polytechnic Institute, JAN GENZER, North Carolina State University, CHANG Y. RYU, Rensselaer Polytechnic Institute, RENSSELAER POLYTECHNIC INSTITUTE COLLABORATION, NORTH CAROLINA STATE UNIVERSITY COLLABORATION — Monodisperse polystyrene has been functionalized chemically to make random copolymers with controlled sequence distribution of the unmodified and modified styrene segments. The sequence blockiness of the resulting random copolymers can be controlled via the temperature of reaction, with a high temperature reaction resulting in a "truly random" copolymer, and a low temperature resulting in a "random blocky" copolymer. Interaction chromatography has been employed to estimate the chemical composition distribution of these partially functionalized polystyrenes. Two different chemical systems will be discussed; i.e., the brominated and borylated polystyrene systems. The results of our analysis reveal that the chemical composition distribution of "random blocky" copolymers is narrower than that of the corresponding "truly random" copolymers. The chemical composition of the two systems will be compared directly, and the influence of "chain conformation inversion" will be discussed.

10:00AM V50.00011 Large Scale Purification and Characterization of Model Poly(isopropyl methacrylate)-block-Poly(styrene) Diblock Copolymers, ASEM ABDULAHAD, Rensselaer Polytechnic Institute, DU YEOL RYU, Yonsei University, CHANG YEOL RYU, Rensselaer Polytechnic Institute — The development of purification techniques of block copolymers is vital for overcoming the synthetic difficulty of preparing well-defined block copolymers using various living polymerization techniques. A large scale separation technique would lead us to obtaining sufficient amounts of homopolymer-free block copolymers for subsequent physical characterization. This can potentially aid in the elucidation of the role of chemical heterogeneity on the thermodynamic transitions and viscoelastic properties of block copolymer materials. Employing an acute understanding of polymer adsorption/desorption onto nanoporous silica during solvent gradient interaction chromatography, we demonstrate the large scale purification of anionic polymerized poly(isopropyl methacrylate)-block-poly(styrene) diblock copolymers with narrow molecular weight distribution. Additionally, we address the impact of removing early-terminated poly(styrene) homopolymers on the viscoelasticity of these model diblock copolymers, as well as their impact on block copolymer assembly as analyzed by small-angle X-ray scattering.

10:12AM V50.00012 Quantifying Fluctuation Effects on the Order-Disorder Transition of Symmetric Diblock Copolymers, JING ZONG, QIANG (DAVID) WANG, Department of Chemical and Biological Engineering Colorado State University — How fluctuations change the order-disorder transition (ODT) of symmetric diblock copolymers is a classic yet unsolved problem in polymer physics.¹ Here we unambiguously quantify the fluctuation effects by direct comparisons between fast off-lattice Monte Carlo (FOMC) simulations² and mean-field theory using exactly the same model system (Hamiltonian), thus without any parameter-fitting. The symmetric diblock copolymers are modeled as discrete Gaussian chains with soft, finite-range repulsions as commonly used in dissipative-particle dynamics simulations. The effects of chain discretization and finite-range interactions on ODT are properly accounted for in our mean-field theory.³ Our FOMC simulations are performed in a canonical ensemble with variable box lengths to eliminate the adverse effects of fixed box sizes on ODT.⁴ Furthermore, with a new order parameter for the lamellar phase, we use replica exchange and multiple histogram reweighting to accurately locate ODT in our simulations.

¹L. Leibler, *Macromolecules*, **13**, 1602 (1980); G. H. Fredrickson and E. Helfand, *J. Chem. Phys.*, **87**, 697 (1987).

²Q. Wang and Y. Yin, *J. Chem. Phys.*, **130**, 104903 (2009).

³Q. Wang, *J. Chem. Phys.*, **129**, 054904 (2008); **131**, 234903 (2009).

⁴Q. Wang et al., *J. Chem. Phys.*, **112**, 450 (2000).

10:24AM V50.00013 Simulation of micelle lattice ordering via nucleation from disorder in a diblock copolymer melt, RUSSELL SPENCER, ROBERT WICKHAM, University of Guelph — We examine the dynamics of the order-disorder transition (ODT) in diblock copolymer melts by simulating the nucleation of the BCC phase of spherical micelles out of the disordered phase, using the time-dependent Landau-Brazovskii model. Questions about the description of the disordered phase as a phase of disordered micelles, and the role of intermediate close-packed structures suggest a rich dynamics for this ordering transition. For a copolymer composition $f = 0.39$, we find that above a critical size, which diverges at the ODT, a spherical nucleus of the BCC micelle phase grows, forming the BCC phase directly. The growth rate varies linearly with undercooling. We also examine the growth of nuclei of the close-packed phases. For more asymmetric copolymers, $f = 0.35$ and $f = 0.3$, a region of disordered micelles surrounds a core of the BCC phase in the growing nucleus, suggesting that, for asymmetric copolymers, the ODT proceeds via a two-step mechanism.

10:36AM V50.00014 Order-to-order Transition in Closed-loop type Block Copolymer, HYUNGJU AHN, HOYEON LEE, SUNGMIN PARK, DU YEOL RYU, Yonsei University — Recently, the complex morphologies such as gyroid (GYR), hexagonally perforated layer (HPL) and non-cubic network phase (Fd $\bar{d}$) observed in block copolymer (BCP) melts. In this study, we investigated the unique and unusual OOT behavior of asymmetric deuterated polystyrene-block-poly(n-pentyl methacrylate) copolymers, denoted as dPS-b-PnPMA at narrow range of volume fraction. Scattering results and transmission electron microscopy show that dPS-b-PnPMA exhibits an unusual OOT phase behavior of GYR $\rightarrow$ HPL and GYR $\rightarrow$ HPL $\rightarrow$ GYR, whereas a general morphological transition occurs from HPL to GYR with increasing temperature. The OOT process found in this work provides a physical insight into a new type of morphological transition in diblock copolymer system.

10:48AM V50.00015 Self-assembly Behavior of Poly(3-alkylthiophene)-*block*-poly(methyl methacrylate) Block Copolymers Prepared by Anionic Coupling Reaction, JIN KON KIM, HONG CHUL MOON¹, Pohang University of Science and Technology — We synthesized rod-coil block copolymers composed of regioregular poly(3-alkylthiophene) (P3AT) and poly(methyl methacrylate) (PMMA) via anionic coupling reaction. For poly(3-hexylthiophene)-b-PMMA, the morphology was mainly determined by self-crystallization of P3HT moieties due to strong rod-rod interaction. On the other hand, poly(3-decylthiophene) (P3DDT)-b-PMMA, the self-crystallization was effectively suppressed. Detail phase behaviors were investigated at temperatures higher melting point (T_m) of P3DDT using small-angle x-ray scattering (SAXS), wide-angle x-ray scattering (WAXS) and transmission electron microscopy (TEM).

¹presenting author

Thursday, March 1, 2012 8:00AM - 11:00AM –
Session V52 GSNP DFD: Focus Session: Extreme Mechanics - Biological Systems and Structures 153C

8:00AM V52.00001 Micro-actuation through swelling and tissue engineering, NICHOLAS FANG, MIT
— No abstract available.

8:36AM V52.00002 Plant tendrils: Nature's hygroscopic springs, SHARON GERBODE, Harvey Mudd College, JOSHUA PUZEY, ANDREW MCCORMICK, L. MAHADEVAN, Harvard University — Plant tendrils are specialized climbing organs that have fascinated biologists and physicists alike for centuries. Initially straight tendrils attach at the tip to an elevated rigid support and then winch the plant upward by coiling into a helical morphology characterized by two helices of opposite handedness connected by a helical perversion. In his renowned treatise on twining and tendril-bearing plants, Charles Darwin surmised that coiled tendrils serve as soft, springy attachments for the climbing plant. Yet, the true effect of the perverted helical shape of a coiled plant tendril has not been fully revealed. Using a combination of experiments on Cucurbitaceae tendrils, physical models constructed from strained rubber sheets, and numerical models of helical perversions, we have uncovered that tendril coiling occurs via anisotropic shrinkage of a strip of specialized cells in the interior of the tendril. Furthermore, variations in the mechanical behavior of tendrils as they become drier and “woodier” adds a new twist to the story of tendril coiling.

8:48AM V52.00003 Radial force development during root growth measured by photoelasticity, EVELYNE KOLB, PMMH-UMR 7636 ESPCI, 10 rue Vauquelin, 75231 Paris Cedex 5, France; Université Pierre et Marie Curie - Paris 6, 75230 Paris cedex 05, France, CHRISTIAN HARTMANN, IRD-UMR 211 “BIOEMCO,” 46 rue d'Ulm, 75230 Paris cedex 05, France, PATRICIA GENET, CNRS-UMR 7618, 46 rue d'Ulm, 75230 Paris cedex 05, France; Université Paris Diderot - Paris 7, 75205 Paris cedex 13, France — The mechanical and topological properties of a soil like the global porosity and the distribution of void sizes greatly affect the development of a plant root, which in turn affects the shoot development. In particular, plant roots growing in heterogeneous medium like sandy soils or cracked substrates have to adapt their morphology and exert radial forces depending on the pore size in which they penetrate. We propose a model experiment in which a pivot root (chick-pea seeds) of millimetric diameter has to grow in a size-controlled gap δ (δ ranging 0.5-2.3 mm) between two photoelastic grains. By time-lapse imaging, we continuously monitored the root growth and the development of optical fringes in the photoelastic neighbouring grains when the root enters the gap. Thus we measured simultaneously and in situ the root morphological changes (length and diameter growth rates, circumnutation) as well as the radial forces the root exerts. Radial forces were increasing in relation with gap constriction and experiment duration but a levelling of the force was not observed, even after 5 days and for narrow gaps. The inferred mechanical stress was consistent with the turgor pressure of compressed cells. Therefore our set-up could be a basis for testing mechanical models of cellular growth.

9:00AM V52.00004 Digging Like Plants: Flexible Intruders in Granular Materials, DAWN WENDELL, KATHARINE LUGINBUHL, MIT, DIEGO SOLANO, Northeastern University, PEKO HOSOI, MIT — Inspired by plant root growth in granular media, we report on the effects of flexibility on the mechanical work required to dig through granular systems. In the case where the digger is significantly thinner than the grain diameter, increased flexibility in one-dimension leads to savings of nearly 50%. A simple numerical model based solely on the variability of forces in the granular substrate and the flexibility of the digger gives similar results to those observed in experiments.

9:12AM V52.00005 Helical Buckling of Plant Roots: Mechanics and Morphology, JESSE SILVERBERG, Department of Physics, Cornell University, ROSLYN NOAR, Department of Plant Pathology, North Carolina State University, MICHAEL PACKER, Department of Physics, Cornell University, MARIA HARRISON, Boyce Thompson Institute, Cornell University, CHRIS HENLEY, ITAI COHEN, Department of Physics, Cornell University, SHARON GERBODE, School of Engineering and Applied Sciences, Harvard University — How do plant roots respond to heterogeneities in their environment as they grow? Using a simple model system consisting of a layered hydrogel, we present a controlled mechanical barrier to the roots allowing us to perturb their growth. Interestingly, we find a localized helical root morphology which forms prior to the root passing through the gel layer interface. We interpret this geometry as a combination of a purely mechanical buckling caused by continued root elongation modified by the growth medium and a simultaneous twisting near the root tip. We study the morphology of the helical deformation as the modulus of the gel is varied using 3D time-lapse imaging and demonstrate that its shape scales with gel stiffness as expected by a simple model based on the theory of buckled rods. Our results demonstrate that mechanics is sufficient to account for the shape and its variations. In addition, we hypothesize that the twisted growth near the root tip arises from a touch-activated growth response that we call thigmotorsion.

9:24AM V52.00006 Dislocations and Grain Boundaries in Optimally-Packed, Twisted Filament Bundles, AMIR AZADI, Department of Physics, University of Massachusetts, Amherst, GREGORY GRASON, Department of Polymer Science and Engineering, University of Massachusetts, Amherst — From the collagen fiber to the parallel-actin bundle, twisted and rope-like assemblies of filamentous molecules are common and vital structural elements in cells and tissue of living organisms. We study the intrinsic frustration occurring in these materials between the two-dimensional organization of filaments in cross-section and out-of-plane interfilament twist in bundles based on the non-linear continuum elasticity theory of columnar materials. We find that interfilament twist generates in-plane stresses that couple favorably to the presence of topological defects, edge dislocations, in the cross-sectional packing, thereby restructuring the ground state filament packing of twisted bundles. The stability of dislocations increases with increases in both the degree of twist and lateral bundle size. We show that in ground states of large bundles, multiple dislocations pile up into linear arrays, radial grain boundaries, whose number and length grows with bundle twist. Remarkably, the “polycrystalline” texture of these optimal packings of twisted bundles show a striking similarity to models of the “almost crystalline” cross-section of collagen fibers.

9:36AM V52.00007 Mechanical Behavior of Bio-inspired Model Suture Joints, YANING LI, Department of Mechanical Engineering, ERICA LIN, CHRISTINE ORTIZ, Department of Materials Science and Engineering, MARY BOYCE, Department of Mechanical Engineering, BOYCE GROUP/MIT COLLABORATION, ORTIZ GROUP/MIT COLLABORATION — Suture joints of varying degrees of geometric complexity are prevalent throughout nature as a means of joining structural elements while providing locally tailored mechanical performance. Here, micromechanical models of general trapezoidal waveforms of varying hierarchy are formulated to reveal the role of geometric complexity in governing stiffness, strength, toughness and corresponding deformation and failure mechanisms. Physical constructs of model composite suture systems are fabricated via multi-material 3D printing (Object Connex500). Tensile tests are conducted on samples covering a range in geometry, thus providing quantitative measures of stiffness, strength, and failure. The experiments include direct visualization of the deformation and failure mechanisms and their progression, as well as their dependence on suture geometry, showing the interplay between shear and tension/compression of the interfacial layers and tension of the skeletal teeth and the transition in failure modes with geometry. The results provide quantitative guidelines for the design and tailoring of suture geometry to achieve the desired mechanical properties and also facilitate understanding of suture growth and fusion, and evolutionary phenotype.

9:48AM V52.00008 Morphogenesis of protrusions from confined lipid bilayers mediated by mechanics, MARINO ARROYO, Universitat Politècnica de Catalunya-BarcelonaTech, MARGARITA STAYKOVA, Princeton University, MOHAMMAD RAHIMI, Universitat Politècnica de Catalunya-BarcelonaTech, HOWARD A STONE, Princeton University — Biological membranes adopt a wide range of shapes that structure and give functionality to cells, compartmentalizing the cytosol, forming organelles, or regulating their area. The formation, stabilization, and remodeling of these structures is generally attributed to localized forces or to biochemical processes (insertion of proteins, active compositional regulation). Noting that in the crowded intra and extra-cellular environments membranes are highly constrained, we explore to what extent can mechanics explain the shape of protrusions out of confined membranes. For this purpose, we developed an in-vitro system coupling a lipid bilayer to the strain-controlled deformation of an elastic sheet (Staykova et al, PNAS 108, 2011). We show that upon contracting the elastic support, tubular or spherical protrusions grow out of the adhered membrane, which can be reversibly controlled with strain and osmolarity without resorting to localized forces or chemical alterations of the bilayer. The morphologies produced by our minimal system are ubiquitous in cells, suggesting mechanics may be a simple and generic organizing principle. We can understand most of our observations in terms of a phase diagram accounting for elasticity, adhesion, and the limited amount of area and volume available.

10:00AM V52.00009 Thin-shell model for faceting of multicomponent elastic vesicles, RASTKO SKNEPNEK, MONICA OLVERA DE LA CRUZ, Northwestern University — We use a discretized version of a thin elastic shell model to show that a two-component elastic vesicle can lower its energy by faceting into a wide variety of polyhedral shapes. The elastic shell model allows us to completely remove effects of the topological defects necessarily present in spherical topology. Therefore, we show that the faceting mechanism of multicomponent elastic vesicles is fundamentally different than the familiar defect-driven buckling into icosahedra. We present a detailed gallery of faceted shapes and discuss how the interplay between bending and stretching energies leads to faceting. Present work extends our recent study of the faceting of a two-component shell in the presence of topological defects [1]. [1] G. Vernizzi, R. Sknepnek, M. Olvera de la Cruz, Proc. Natl. Acad. Sci. USA 108, 4292 (2011).

10:12AM V52.00010 Charge Effects on Mechanical Properties of Elastomeric Proteins, RAVI KAPPIYOR, Department of Engineering Science and Mechanics, Virginia Tech, Blacksburg, VA 24061, USA, GANESH BALASUBRAMANIAN, Eduard-Zintl-Institute für Anorganische und Physikalische Chemie, Technische Universität Darmstadt, 64287 Darmstadt, Germany, DANIEL DUDEK, ISHWAR PURI, Department of Engineering Science and Mechanics, Virginia Tech, Blacksburg, VA 24061, USA — Several biological molecules of nanoscale dimensions, such as elastin and resilin, are capable of performing diverse tasks with minimal energy loss. These molecules are efficient in that the ratio of energy output to energy consumed is very close to unity. This is in stark contrast to some of the best synthetic materials that have been created. For example, it is known that resilin found in dragonflies has a hysteresis loss of only 0.8% of the energy input while the best synthetic rubber made to date, polybutadiene, has a loss of roughly 20%. We simulate tensile tests of naturally occurring motifs found in resilin (a highly hydrophilic protein), as well as similar simulations found in reduced-polarity counterparts (i.e. the same motif with the charge on each individual atom set to half the natural value, the same motif with the charge on each individual atom set to zero, and a motif in which all the polar amino acids have been replaced with nonpolar amino acids). The results show a strong correlation between charge and extensibility. In order to further understand the effect of properties such as charge on the system, we will run simulations of elastomeric proteins such as resilin in different solvents.

10:24AM V52.00011 Denaturation of Circular DNA: Supercoils, overtwist and condensation¹

, ALKAN KABAKCIOGLU, Koc University, AMIR BAR, DAVID MUKAMEL, Weizmann Institute of Science — The statistical mechanics of DNA denaturation under fixed linking number is qualitatively different from that of the unconstrained DNA. Past work suggests that the nature of this constrained melting transition is sensitive to the mechanism that relaxes the torsional stress induced on the bound portions by the loops. Quantitatively different melting scenarios are reached from two alternative assumptions, namely, that the denatured loops are formed in expense of 1) overtwist, 2) supercoils. Recent work has shown that the supercoiling mechanism results in a BEC-like picture where a macroscopic loop appears at T_c and grows steadily with temperature while no such phenomenon has been reported for the overtwisting case. By extending an earlier result, we show here that a macroscopic loop appears in the overtwisting scenario as well. We calculate its size as a function of temperature and show that the fraction of the total sum of microscopic loops decreases above T_c , with a cusp at the critical point.

¹Supported by TUBITAK through the grant TBAG-110T618

10:36AM V52.00012 Mechanics of short rod-like molecules in tension , PRASHANT PUROHIT, University of

Pennsylvania — Rod like macromolecules such as actin, DNA etc., are most commonly stretched using optical tweezers or fluid flow. In this presentation we will describe the mechanics of short rod like molecules in tension. The mechanics is dominated by the competition between tensile forces (exerted by fluid flow, or by a device, such as, optical tweezers) and the thermal fluctuations of the molecule. For molecules whose contour length is comparable to the persistence length we show that the boundary conditions play major role in determining the mechanical behavior. We use the equipartition theorem of statistical mechanics to obtain expressions for the amplitude of the transverse fluctuations of the molecule and its force-extension relation for various boundary conditions. We then apply our theory to an experiment on short fluctuating actin filaments trapped by various means. We estimate the tension in these filaments by fitting our theory to the measured values of transverse fluctuations as a function of the position along the filament.

10:48AM V52.00013 Turning by buckling: a cheap evolutionary strategy for turning among

marine bacteria , KWANGMIN SON, JEFFREY GUASTO, ROMAN STOCKER, MIT — Marine bacteria have long been known to swim forward and backward ('run and reverse') by controlling the rotational direction of a 20 nm helical flagellum. Recent detailed observations have shown that these bacteria can also make sharp, $\sim 90^\circ$ turns, an astounding feature for a micron-scale organism with just one degree of freedom under its control. We demonstrate that a buckling instability originating from the flexible linkage ('hook') between the body and the flagellum is responsible for the reorientation. Using high-magnification (40~100X) observations based on high-speed video microscopy (420~1000 fps), we captured the extreme deformation of the flagellum and the hook involved in this process. The mechanical properties of the hook are finely tuned to the hydrodynamic loads experienced by the cell: the hook becomes unstable only when the compressive load during the onset of forward swimming exceeds the threshold for Euler buckling. Combining the data with a model of buckling of thin structures, we show that bacteria take advantage of the flexibility of the flagellum and the hook to generate a turn, which may represent the evolutionarily cheapest bacterial strategy to actively change direction.

Thursday, March 1, 2012 8:00AM - 11:00AM –

Session V53 GSNP: Wet and Cohesive Granular Materials 153B

8:00AM V53.00001 An analytical framework for aeolian saltation , MEREDITH REITZ, DOUGLAS JEROLMACK,

University of Pennsylvania — We construct an analytical framework for steady state aeolian saltation, using experimentally-derived splash function relationships and the additional constraint of a threshold height, above which the wind velocity is strong enough to carry a grain from reptation into saltation. This threshold height rises as the wind profile magnitude is lowered by the increasing number of saltating grains being accelerated by the wind, until the number of grains being demoted below this threshold due to loss of energy to collisions with the bed equals the number being promoted. The balance of these populations at steady state determines both the flux of grains in saltation and the saturated wind velocity profile, while the approach to this balance describes the transient evolution to this state. We also formulate the difference between the critical impact Shields stress, defined as the stress below which transport ceases, and the higher critical fluid Shields stress, at which transport is initiated. Finally, we test the dependence of grain flux and trajectory lengths and speeds on the erodibility of the bed, and compare these results with observed differences in scaling. We also compare our results to findings for saltation under water.

8:12AM V53.00002 X-Ray Fluoroscopy of Sedimentation in Elastic Fluids , T.A. BRZINSKI, R. KARUNA-

MUNI, A.D.A. MAIDMENT, P.E. ARRATIA, D.J. DURIAN, University of Pennsylvania — Dispersions of spheres in a Newtonian fluid will sediment until all grains form a packing. While the system approaches its final configuration, the dispersion is roughly homogenous in space and time except at two well-defined interfaces: a dispersion-supernatant interface, and an interface below the dispersion at which grains stack to form a packing. In order to better understand this packing process we perturb the dynamics at the lower interface by adding a flexible, high molecular weight polymer that enhances fluid elasticity. The fluid strain-rate between spheres has an extensional component that is inversely proportional to grain separation, so elasticity dominates the fluid forces as the grain separation becomes small, thus frustrating the packing process. In order to observe the effect of this perturbation, we utilize x-ray fluoroscopy. In the case of a system without polymer we observe settling rates in accordance with a typical Stokes' model until all grains have settled into a random packing. In the polymeric case we see that, alongside the Newtonian-like settling, there's a time- and depth-dependent compression of the disperse phase, resulting in a smooth transition between dispersion and packing rather than the sharp interface observed in the Newtonian case.

8:24AM V53.00003 Three dimensional imaging of soft sphere packings under shear¹ , JOSHUA

DIJKSMAN, HU ZHENG, ROBERT BEHRINGER, Duke University — The (microscopic) flow of three dimensional disordered athermal granular packings remains poorly understood. However, experimentally studying flow and deformations in a three dimensional packing of grains is challenging due to the opacity of such packings. We use refractive index matched scanning with hydrogel spheres to image such flows. Hydrogel is soft and has low friction, which allows for the study of contact forces via contact deformations. We look at how force networks develop in sheared packings close to the onset of mechanical rigidity.

¹Support from NSF-DMR0906908 and ARO-W911NF-11-1-0110 is gratefully acknowledged

8:36AM V53.00004 Fluidization of wet granulates under hydrodynamic shear - experiments¹

, CHRISTOPH GÖGELEIN, ILENIA BATTIATO, MATTHIAS SCHRÖTER, STEPHAN HERMINGHAUS, JÜRGEN VOLLMER, Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany — Very recently, the fluidization threshold of a wet granular bed under hydrodynamic shear forces were predicted theoretically [1]. This theory described the flow through a wet granular bed by a continuum model and provides analytical expressions for the averaged drag force on a single particle. Moreover, the theory predicts the stability of the granular bed in dependence of the strength of the capillary and buoyancy forces. These theoretical predictions are tested in the present study by a newly designed flow channel. We will present our first experimental results for the fluidization onset of granular beds.

[1] I. Battiato, and J. Vollmer, "Fluidization of wet granulates under hydrodynamic shear," submitted for publication.

¹We all thank the BP Explore Program for generous funding.

8:48AM V53.00005 Building designed granular towers one drop at a time, JULIEN CHOPIN, ARSHAD KUDROLLI, Clark University — The impact of a drop on a surface leads to beautiful dynamical shapes that result from a subtle interplay between inertial effects, fluid properties and substrate characteristics. In this talk, we will present an experiment where the successive impacts of drops lead to surprisingly slender mechanically stable structures that we called granular towers. They are created by dripping a dense granular suspension on a liquid absorbing surface such as a blotter paper or a dry granular bed. These towers formed by rapid solidification of the drop upon impact are analogous to many natural structures found in nature including frozen lava flows, icicles and stalagmites. We find that the height can be determined by balancing the excess liquid flux and the drainage through the granular tower. The velocity impact, the free fall time and the density of the suspension are found to control the tower width and its detailed morphology. We show that these facts can be manipulated to obtain various symmetric, smooth, corrugated, zigzag, and chiral structures. Further, the shape of the tower can be used as a quick diagnostic tool to characterize the rheology of a granular suspension. [J. Chopin and A. Kudrolli, Phys. Rev. Lett. 107, 208304 (2011)]

9:00AM V53.00006 Dynamics of failure in cohesive granular packings¹, JENNIFER RIESER, University of Pennsylvania, WENBIN LI, JU LI, Massachusetts Institute of Technology, JERRY GOLLUB, University of Pennsylvania and Haverford College, DOUGLAS DURIAN, University of Pennsylvania — We explore the grain-scale interactions that precede large-scale deformations and mark the onset of mechanical failure in two-dimensional disordered granular packings. The two-dimensionality of the system allows for direct observation of all particle dynamics during the compression of a pillar. The grains are cohesive, with an attraction governed by tunable capillary forces induced through an interstitial fluid. For our analysis, we focus on the evolution of local rearrangements into shear bands within the pillar, quantifying the structural differences within the packing due to the presence of cohesion. We observe that cohesion results in greater spatial heterogeneity within the packing during compression. We also compare the compression of ordered and disordered packings.

¹DMR05-1120901

9:12AM V53.00007 Cohesive granular aggregates under punching: theory and experiments, ALEXEI PERELET, TAPAN SABUWALA, GUSTAVO GIOIA, Department of Mechanical Science and Engineering - University of Illinois, Urbana-Champaign — When poured into a container, cohesive granular materials form low-density, open granular aggregates. If put under compression, these aggregates densify by particle rearrangement. We seek experimental evidence that particle rearrangement occurs in the form of a phase transition between two configurational phases of the aggregate (G. Gioia, A. M. Cuitiño, S. Zheng, and T. Uribe, PRL 88, 204302, 2002). We use a simple model to show that when an open granular aggregate with two configurational phases is penetrated by a punch that lacks a characteristic length scale, the functional relation between the punching force and the penetration of the punch depends solely on the dimensionality of the punch: for a two-dimensional, wedge-shaped punch the force-penetration curve is linear whereas for a three-dimensional, conical punch the force-penetration curve is quadratic. To test these predictions we carry out experiments with open granular aggregates of a fine powder. The experimental measurements are in accord with the theoretical predictions.

9:24AM V53.00008 Discrete Particle Dynamics Simulations of Adhesive Systems with Thermostatting¹, FLINT PIERCE, JEREMY LECHMAN, JOHN HEWSON, Sandia National Laboratories — Aggregation/coagulation/flocculation processes are ubiquitous in modern industry from fields as diverse as waste water treatment, the food industry, algae biofuel production, and materials processing where control of the size and morphology of aggregates is paramount to the application of interest. Population balance models have historically been used with success in predicting aggregation kinetics and size distributions for these processes. However, even the most robust population balance schemes can lack an exact description of the underlying physical processes governing attractive or adhesive particulate matter suspended in a background medium, including finite aggregate strength and yield stress, restructuring length and time scales, and response to hydrodynamic forces. In order to elucidate these phenomena, We develop and use a JKR type model for simulating adhesive particulate matter in a background medium varying from dilute gas to liquid. We evaluate the time and length scales for restructuring/fragmentation that result from this model as a function of aggregate size and fractal dimension. We additionally introduce a method for pairwise thermostatting of the adhesive potential and discuss the applicability of this model to various adhesive systems.

¹Supported by LDRD program at Sandia National Laboratories

9:36AM V53.00009 Normal Mode Spectrum of Finite Sized Granular Systems: The Effects of Fluid Viscosity at the Grain Contacts, JOHN VALENZA, DAVID JOHNSON, Schlumberger-Doll Research — We investigate the effects of adsorbed films on the attenuative properties of loose granular media occupying a finite sized rigid container, which is open on the top. We measure the effective mass, $\bar{M}(\omega)$, of loose tungsten particles prepared under two different sets of conditions: 1) We lightly coat tungsten grains with a fixed volume fraction of silicone oil (PDMS), where the liquid viscosity is varied for individual realizations. 2) In the other set of experiments we vary the humidity. On a theoretical level we are able to decompose the effective mass into a sum over the contributions from each of the normal modes of the granular medium. Our results indicate that increasing either the PDMS viscosity or the humidity, as the case may be, does markedly increase the damping rate of each normal mode relevant to our measurements. However, there is appreciable damping even in the absence of any macroscopic film. With a notable exception in the case of the highest humidity in the humidity controlled experiments, all the relevant modes are weakly damped in the sense of a microscopic theory based on damped contact forces between rigid particles.

9:48AM V53.00010 Influence of liquid bridges on the macroscopic properties of granular assemblies, GEOFFROY LUMAY, University of Liege, JORGE FISCINA, Universität des Saarlandes, FRANCOIS LUDEWIG, NICOLAS VANDEWALLE, University of Liege — We present the results of two experimental studies concerning the compaction dynamics of cohesive granular materials. In the first study, the cohesion between neighboring grains is induced by capillary bridges in a wet granular material. The cohesiveness is tuned using different liquids having specific surface tension values. The second study concerns initially dry granular materials surrounded by a well controlled air humidity. Then, the cohesion inside the packing is controlled through the relative humidity which influence both triboelectric and capillary effects. For both cases, the evolution of the parameters extracted from the compaction curves (the compaction characteristic time τ , the initial and final packing fractions) have been analyzed as a function of the cohesiveness. A model, based on free volume kinetic equations and the presence of a capillary energy barrier, is able to reproduce quantitatively the experimental results (Phys. Rev. Lett. 105, 048001 (2010)).

10:00AM V53.00011 Wetting and packing effects on evaporation out of a porous medium, CESARE MIKHAIL CEJAS, BERTRAND SELVA, RAPHAEL BEAUFRET, LARRY HOUGH, CNRS UMI 3254 Complex Assemblies of Soft Matter COMPASS, CHRISTIAN FRETIGNY, CNRS UMR7615 Physico-chimie des Polymères et des Milieux Dispersés (PPMD) - ESPCI Paris, REMI DREYFUS, CNRS UMI 3254 Complex Assemblies of Soft Matter COMPASS, COMPASS TEAM — Evaporation through granular media involves complex fluid transport and exhibits two regimes: (1) a capillary-supported regime maintaining hydraulic continuity to the surface and vapor exchange with the atmosphere followed by (2) a diffusion-limited regime through the medium. A well-defined intermediate partially saturated zone (PSZ) has already been observed in the past. It is evidently seen from our experimental investigations using a 2D model soil of glass beads. The PSZ is the region identified above the interface formed by the drying front, which separates the PSZ from the fully-saturated wet region. This intermediate zone is filled with a dynamic mixture of vapor and liquid. The existence of this zone is of significant importance as it sets the kinetics of the evaporation process. Here we will present how wetting and packing effects influence the size of this partially saturated zone and we will show how a simple model based on geometrical considerations can explain our observations.

10:12AM V53.00012 A coupled deformation-diffusion theory for fluid-saturated porous solids, DAVID HENANN, KEN KAMRIN, LALLIT ANAND, Department of Mechanical Engineering, MIT — Fluid-saturated porous materials are important in several familiar applications, such as the response of soils in geomechanics, food processing, pharmaceuticals, and the biomechanics of living bone tissue. An appropriate constitutive theory describing the coupling of the mechanical behavior of the porous solid with the transport of the fluid is a crucial ingredient towards understanding the material behavior in these varied applications. In this work, we formulate and numerically implement in a finite-element framework a large-deformation theory for coupled deformation-diffusion in isotropic, fluid-saturated porous solids. The theory synthesizes the classical Biot theory of linear poroelasticity and the more-recent Coussy theory of poroplasticity in a large deformation framework. In this talk, we highlight several salient features of our theory and discuss representative examples of the application of our numerical simulation capability to problems of consolidation as well as deformation localization in granular materials.

10:24AM V53.00013 Water Retention of Sandy Soil with Hydrogel Particle Additives under Steady Rain, YULI WEI, 1. Department of Physics and Astronomy, University of Pennsylvania ; 2. Complex Assemblies of Soft Matter, CNRS-Rhodia-UPenn UMI 3254, DOUGLAS DURIAN, Department of Physics and Astronomy, University of Pennsylvania — We probe the water retention behavior of a dry model sandy soil with hydrogel particle additives under a steady rain using a self-built raindrop impingement set-up. The 0.4mm dry hydrogel particles are sent into a dry model sandy soil, 1mm glass beads, in different methods and a steady rain is created to irrigate the soil packing. The mass of the retained water in the packing is measured as a function of rain time. The influences of packing height, gel concentration, and gel location are examined respectively. For the model sandy soil alone, the packing height has little effect on the results. Rain water wets a shallow top region and flows out through a narrow path in the packing. With hydrogel particles uniformly mixed into the top region of a model sandy soil packing, the retained water increases as the gel number ratio increases or when the hydrogel particles are concentrated into the wet top region. A better way is to place hydrogel particles in a layer at certain depths under soil surface. The wet gel layers formed during the rain not only lock water inside but also clog the water path and force rain water to wet other dry soil regions. The clogging efficiency is determined by the wet gel layer number and the soil confinement.

10:36AM V53.00014 Period tripling causes rotating spirals in agitated wet granular matter, KAI HUANG, INGO REHBERG, Experimentalphysik V, Universitaet Bayreuth, 95440 Bayreuth, Germany — Pattern formation of a thin layer of vertically agitated wet granular matter is investigated experimentally. Due to the strong cohesion arising from the capillary bridges formed between adjacent particles, agitated wet granular matter exhibits a different scenario as its dry counter-part. Rotating spirals with three arms, which correspond to the kinks between regions with different colliding phases, are the dominating pattern. This preferred number of arms corresponds to period tripling of the agitated granular layer, unlike predominantly subharmonic Faraday crispations in dry granular matter. The chirality of the spatiotemporal pattern corresponds to the rotation direction of the spirals. Understanding this well traceable instability could pave a way for testifying elaborate theories on dense flow of wet granular matter.

10:48AM V53.00015 The melting of an ice blok assembly¹, STEPHANE DORBOLO, FRS-FNRS, Universite de Liege, NICOLAS VANDEWALLE, Universite de Liege, CLAUDE LAROCHE, Private Laboratory, GRASP TEAM, PRIVATE LABORATORY TEAM — The melting of an assembly of ice blocks under an unidirectional controlled load was investigated. The volume occupied by the ice blocks and the volume of ice were simultaneously measured. While the ice volume continuously decreases, sudden breakdown of the total volume was observed suggesting large reorganization of the whole assembly. The waiting-times between two successive collapses and the magnitudes of the collapse have been correlated. The pile structure was studied using a x-ray tomography before and after a collapse. The arch network re-organization is responsible for the melting dynamics as the pile becomes more and more ordered during the melting.

¹F.R.S-FNRS is thank for financial support

Thursday, March 1, 2012 8:00AM - 11:00AM –
Session V54 DCMP: Superconductivity: Magnetic Field Effects Including Vortex Related Phenomena (Theory) 152

8:00AM V54.00001 Vortex Dynamics in Ferromagnetic Superconductors: Excitations of Domain Walls and Enhanced Viscosity, SHIZENG LIN, LEV BULAEVSKII, CRISTIAN BATISTA, Theoretical division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545 — As more and more superconductors with coexisting magnetic order are found in the last decades, understanding of the vortex dynamics in these superconductors becomes a relevant issue [1, 2]. We investigate vortex dynamics in ferromagnetic superconductors both numerically and analytically. Driven by the Lorentz force, the vortices perturb the magnetic moments and excite magnons. At some velocities, the motion of vortices is resonant with magnetic moments, and the amplitude of magnon excitation is enhanced. When the relaxation rate of magnon is smaller than the pumping rate, the magnon becomes unstable and domain walls are created. The domain walls interact strongly with vortices motion and greatly enhance the viscosity of vortices. Depending on the density of vortices, the vortex configuration may be modulated by the magnetic system. The underlying dynamics of the vortices and magnetic moments can be probed by transport measurement.

[1] L. N. Bulaevskii, A. I. Buzdin, M. L. Kubic, and S. V. Panjukov, Adv. Phys. 34, 175 (1985).

[2] A. Shekhter, L. N. Bulaevskii, and C. D. Batista, Phys. Rev. Lett. 106, 037001 (2011).

8:12AM V54.00002 The effect of impurities on the Superheating field of Type II superconductors¹, FAREH PEI-JEN LIN, ALEXANDER GUREVICH, Department of Physics, Old Dominion University — We calculate the superheating field $H_s(T)$, the maximum field at which the Meissner state exists, for a type-II, single band s-wave superconductor with nonmagnetic and magnetic impurities. $H_s(T)$ was calculated for the entire temperature region $0 < T < T_c$ and arbitrary impurity concentrations by solving the Eilenberger equations for the large Ginzburg-Landau parameter. We show that, although the effect of nonmagnetic impurities on H_s is relatively weak, they give rise to a maximum in $H_s(T, c)$ at a concentration c corresponding to a moderately clean limit. Impurities significantly affect the density of states at $H = H_s$: in the clean limit the superheating field corresponds to a gapless state, but above a critical concentration $c > c_g$, the quasiparticle gap $E_g(c)$ appears at $H = H_s$ so that $E_g \sim 0.410\Delta$ in the dirty limit. This feature can be important for the nonlinear surface resistance at strong rf fields $H \sim H_s$.

¹This work is supported by Argonne National Laboratory 1F-31461

8:24AM V54.00003 Gap structure probed by field-angle resolved thermal oscillations in Ce-CoIn₅ superconductor¹, MATTHIAS J. GRAF, TANMOY DAS, Los Alamos National Laboratory, ANTON B. VORONTSOV, Montana State Univ., ILYA VEKHTER, Louisiana State Univ. — We calculate the angle-resolved oscillations of the specific heat and thermal conductivity in a rotating in-plane magnetic field in the multiband superconductor CeCoIn₅ using realistic tight-binding Fermi surfaces. We find that an electron pocket at the M point and a hole pocket at the Γ point of the Brillouin zone yield sufficiently large Fermi surface anisotropies to produce fourfold oscillations not only for d -wave pairing, but also for s -wave pairing in the regime where our approximations are valid for both nodal and isotropic gap, namely near the upper critical field H_{c2} and down to fields of order $H_{c2}/2$. More importantly, in this region we find a sign reversal in the oscillations as a function of temperature and fixed field for all gap symmetries investigated. We compare our results with available data on CeCoIn₅ and CeIrIn₅ and discuss how Fermi surface anisotropies affect the identification of gap structures and symmetries.

¹Supported by the U.S. DOE under Contract No. DE-AC52-06NA25396.

8:36AM V54.00004 Pnictide Half-Dirac Nodal Quasiparticle Scaling Properties in Vortex State, IMAM MAKHFUDZ, Johns Hopkins University — We investigate the scaling properties of quasiparticles of Pnictide with “half-Dirac” node under magnetic field in vortex state. By computing the density of states, we aim to find in vortex state the form of non-Simon-Lee scaling predicted for such system by several recent works in non-vortex state. We find by exact diagonalization of the BdG Hamiltonian and finite size scaling a $N(E) \sim \sqrt{E}$ power law in the case without magnetic field which agrees with analytical prediction. We consider the vortex state by first studying the hypothetical situation of uniform magnetic field without vortices and then we properly treat the magnetic field-induced vortex lattice by expressing the BdG Hamiltonian in terms of superfluid velocity and Berry's gauge field. The two calculations are shown to agree with each other. We then analyze quantitatively, the effects of anisotropic dispersion to the quasiparticles scaling properties in vortices. A very crucial prediction is also made on an upper bound to the value of “anomalous dimension” δ of density of states scaling with magnetic field, a quantity that can be measured experimentally.

8:48AM V54.00005 Vortex-assisted photon counts and their magnetic field dependence in superconducting nano-wire single-photon detectors, LEV BULAEVSKII¹, MATTHIAS GRAF, SHIZENG LIN, Los Alamos National Laboratory, VLADIMIR KOGAN², Ames National Laboratory — We argue that photon counts in a superconducting nano-wire single-photon detector (SNSPD) are caused by the transition from a current-biased metastable superconducting state into the normal state. Such a transition is triggered by photons with the frequency ω above the critical frequency ω_c or by photons with the frequency $\omega < \omega_c$ and subsequent vortex crossing from one edge of the superconducting strip to the other. The vortex is pushed across the strip due to the Lorentz force in the presence of the bias current I . We calculate the efficiency of photon counts as a function of ω , I , bath temperature, and the strip geometry. We derive the dependence of the rate of vortex-assisted photon counts on the bias current at given ω and strip geometry. The resulting photon count rate has a plateau at high currents, close to the critical current, and drops as a power-law with high exponent at lower currents. While a magnetic field applied perpendicular to the superconducting strip does not affect the formation of hot spots by photons, it increases the rate of vortex crossings (with and without photons). We show that by applying a magnetic field one may identify the origin of dark and photon-assisted counts.

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²Ames National Laboratory, Ames, Iowa, 50011, USA

9:00AM V54.00006 Type-1.5 superconductivity: effects of interband interactions and Semi-Meissner State¹, EGOR BABAEV, UMass Amherst and KTH Stockholm, JOHAN CARLSTROM, KTH Stockholm and UMass Amherst, JULIEN GARAUD, UMass Amherst — A conventional superconductor is described by a single complex order parameter field which has two fundamental length scales, the magnetic field penetration depth λ and the coherence length ξ . Their ratio κ determines the response of a superconductor to an external field, sorting them into two categories as follows; type-I when $\kappa < 1/\sqrt{2}$ and type-II when $\kappa > 1/\sqrt{2}$. Multicomponent systems can possess three or more fundamental length scales and allow a separate “type-1.5” superconducting state when $\xi_1 < \sqrt{2}\lambda < \xi_2$. In that state, as a consequence of the extra fundamental length scale vortices attract one another at long range but repel at shorter ranges. As a consequence the system should form an additional Semi-Meissner state. In that state vortices form clusters in low magnetic fields. In the vortex clusters the component with larger coherence length is depleted and consequently its current is mostly concentrated on the boundaries of the vortex cluster, thus resembling the screening currents in type-I superconductors. We discuss how the vortex clusters and type-1.5 regimes are affected by various interband couplings in multiband superconductors.

¹Supported by NSF CAREER Award No. DMR-0955902, Swedish Research Council, and by the Knut and Alice Wallenberg Foundation through the Royal Swedish Academy of Sciences fellowship.

9:12AM V54.00007 Length scales, collective modes, and type-1.5 regimes in three-band superconductors¹, JOHAN CARLSTROM, KTH Stockholm, UMass Amherst, JULIEN GARAUD, UMass Amherst, EGOR BABAEV, KTH Stockholm, UMass Amherst — The recent discovery of iron pnictide superconductors has resulted in a rapidly growing interest in multiband models with more than two bands. We derive normal modes and characteristic length scales in the conventional $U(1)$ three-band Ginzburg-Landau model as well as in its time-reversal symmetry-broken counterpart with $U(1) \times Z_2$ symmetry. We show that, in the latter case, the collective modes are associated with the mixed phase-density modes and thus are different from the Leggett modes in two band superconductors. Next we show that gradients of densities and phase differences can be inextricably intertwined in vortex excitations in three-band models. This can lead to very long-range attractive intervortex interactions and the appearance of type-1.5 regimes even when the intercomponent Josephson coupling is large. We next show that field-induced vortices can lead to a change of broken symmetry from $U(1)$ to $U(1) \times Z_2$ in the system. In the type-1.5 regime, it results in a semi-Meissner state where the system has a macroscopic phase separation in domains with broken $U(1)$ and $U(1) \times Z_2$ symmetries.

¹Supported by the Swedish Research Council, the Knut and Alice Wallenberg Foundation through the Royal Swedish Academy of Sciences fellowship and by NSF CAREER Award No. DMR-0955902.

9:24AM V54.00008 Molecular Dynamics of Type-1.5 Superconductors, QINGZE WANG, CHRISTOPHER VARNEY, University of Massachusetts, Amherst, HANS FANGOHR, University of Southampton, EGOR BABAEV, University of Massachusetts, Amherst — In multi-component superconductors and structures of interlaced layered type-I type-II layers there exists a range of parameters where inter-vortex interaction is repulsive at short ranges and attractive at long range. Such regimes were termed “type-1.5 superconductivity” recently. This vortex interaction leads to a microscopic phase separation in Meissner and vortex droplets. In this talk, we utilize molecular dynamics to investigate the magnetic response of such superconductors in the type-1.5 regimes.

9:36AM V54.00009 Stabilization of a vortex-antivortex lattice created by a magnetic-field pulse, V.N. GLADILIN, TQC, University of Antwerp and INPAC-University of Leuven, Belgium, J. TEMPERE, J.T. DEVREESE, TQC, University of Antwerp, Belgium, V.V. MOSHCHALOV, INPAC-University of Leuven, Belgium — Using the time-dependent Ginzburg-Landau approach, we theoretically investigate the formation and evolution of vortex-antivortex patterns, which are created in a thin superconducting film by a single pulse of an inhomogeneous magnetic field. The field pulse is induced by a periodic square array of current loops, where the current direction is either the same for all the loops or changes from one loop to another in the checkerboard order. In an ideally homogeneous superconductor film, the vortices and antivortices, generated by an applied magnetic field pulse, fully recombine within a relatively short time interval after switching off the current in the loops. We demonstrate that in the presence of even relatively weak pinning centers the vortex-antivortex distributions, induced by a short magnetic-field pulse, can eventually evolve into vortex-antivortex lattices, which remain stable for an arbitrarily long time. This work was supported by the Methusalem Funding of the Flemish Government, the NES-ESF program, the Belgian IAP, the Fund for Scientific Research-Flanders (FWO- Vlaanderen).

9:48AM V54.00010 Topological solitons in three-band superconductors with broken time reversal symmetry, JULIEN GARAUD, UMass Amherst and KTH Stockholm, JOHAN CARLSTROM, KTH Stockholm and UMass Amherst, EGOR BABAEV, UMass Amherst and KTH Stockholm — We report that three-band superconductors with Broken Time Reversal Symmetry allow magnetic field-induced topological solitons. When time reversal symmetry is broken, ground state exhibits $U(1) \times Z_2$ symmetry. Domain-wall, are natural solutions when theories exhibit such a discrete symmetry. Closed domain-walls are unstable to collapse because of their line tension. We show that closed domain-walls can be stabilized by confining vortices. The resulting topological solitons are stable and can be induced by fluctuations or quenching the system through a phase transition. This new kind of solitons can provide an experimental signature of the Time Reversal Symmetry Breakdown. Based on: J. Garaud, J. Carlström, and E. Babaev, Phys. Rev. Lett. 107, 197001 (Nov 2011).

10:00AM V54.00011 Vortex dynamics in Superconducting Corbino Disks: Molecular Dynamics and Heat Transport Simulations¹, MASARU KATO, DAVID FUJIBAYASHI, Department of Mathematical Sciences, Osaka Prefecture University — Understanding vortex dynamics is important for application of superconductivity, because vortex motion causes resistive state of superconductors and controlling vortex motion is useful for superconducting devices. Also vortex dynamics shows much variety of phenomena. In a corbino disk geometry, where electric current is injected at the center of the disk and flows toward the perimeter of the disk, vortex moves circular by the Lorentz force from this current. But the Lorentz force depend on the distance from the center as $1/r$, and therefore the vortex velocity faster in the center region than those in the perimeter region. Then vortex motion generates heat and causes non-uniform temperature distribution. Non-uniform temperature distribution causes further vortex motion. Therefore in the superconducting corbino disk, vortex dynamics is not a simple problem. In order to investigate this vortex dynamics, we combine the molecular dynamics and the heat transport simulations. Our simulation results show that dynamical structure of vortices depends on the heat resistance between the superconductor and a substrate as well as the heat capacity and heat conductance of superconductors. Especially there is a transition from laminar flow to the spiral or non-uniform flow.

¹This work is partly supported by “The Faculty Innovation Research Project” of Osaka Prefecture University.

10:12AM V54.00012 Φ_0 as a smallest unit of the intermediate state of a type-I superconductor: Revelation through nonlinear dynamics, GOLIBJON BERDIYOROV, Departement Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium, ALEXANDER HERNANDEZ-NIEVES, Centro Atómico Bariloche, 8400 San Carlos de Bariloche, Rio Negro, Argentina, FRANCOIS PEETERS, Departement Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium, DANIEL DOMINGUEZ, Centro Atómico Bariloche, 8400 San Carlos de Bariloche, Rio Negro, Argentina, MILORAD MILOSEVIC, Departement Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium — We study by time-dependent Ginzburg-Landau simulations the nonlinear dynamics of the intermediate state in a current-carrying type-I superconductor. The stray magnetic field of the current induces the intermediate state, where nucleation of flux domains is *discretized to a single fluxoid at a time*, while their final shape (tubular or laminar), size and nucleation rate depend on applied current and edge conditions. The current induces opposite flux domains on opposite sides of the sample, and subsequently drives them to annihilation – which is *also discretized*, as a sequence of vortex-antivortex pairs. Discretization of both nucleation and annihilation leave measurable traces in the voltage signal across the sample. These dynamic phenomena provide an unambiguous proof of a flux quantum being the smallest building block of the intermediate state in type-I superconductors.

10:24AM V54.00013 Nucleation and development of dendritic flux avalanches in superconducting films, JØRN INGE VESTGÅRDEN, DANIIL SHANTSEV, YURI GALPERIN, TOM HENNING JOHANSEN, Department of Physics, University of Oslo, Norway — The stability of superconducting films is threatened by thermomagnetic runaways commonly observed as abrupt dendritic flux avalanches. We report numerical simulations of the electrodynamics and thermal behavior of superconducting films, where the gradual flux penetration is interrupted by such avalanches. The simulation formalism is based on an efficient method for treating the nonlinear and nonlocal electrodynamics, and it handles both the slow flux creep dynamics prior to the avalanches and the transition to the many orders of magnitude faster instability regime. Then the temperature rises quickly above the critical temperature, and the avalanche develops fully in less than 100 nanoseconds, with an initial velocity of approximately 100 km/s. Both the morphology and speed of the avalanches are in excellent agreement with results from magneto-optical imaging experiments. The sample is seeded with randomly distributed disorder, which results in a significantly reduced threshold for onset of avalanches. Interaction with the material disorder also contributes to branching and irreproducibility of the flux structures. However, disorder is not the main mechanism behind branching and dendritic structures are also found to develop in completely uniform samples.

10:36AM V54.00014 Josephson and pancake vortices in Bi-2212 with anti-dots array, KAZUTO HIRATA, SHUICHI OOI, TAKASHI MOCHIKU, National Institute for Materials Science — Josephson and pancake vortices in Bi-2212 with anti-dots (holes) array have been studied with measuring the flow-resistance and the c-axis resistance. The samples for the measurements were prepared by a focused ion-beam milling with a diameter of 200 nm and 1000 nm pitch hole-array and in the in-line structure. Angular dependence of the flow-resistance does not show lock-in phenomenon as usually observed in the behaviors of Josephson vortices in Bi-2212. Instead, there are several peaks observed in the flow-resistance. A couple of peak can be explained with the matching field effect of pancake vortices to the array, but the others not. The c-axis transport measurements show characteristic transitions near the matching fields and between them in the c-axis resistance with the perpendicular field to the superconducting layers. This is related to the accommodation rate of pancake vortices into the holes and to the interaction between/among the vortices outside the holes and the trapped vortices.

10:48AM V54.00015 Effect of pinning force on critical current using molecular dynamic simulation, ABDALLA OBEIDAT, HADEEL ABU LAHIM, Jordan University of Science and Technology — Molecular dynamics have been used to study the effect of pinning force on the critical current at different temperatures. Our simulation is built on assuming a two dimensional periodic arrays of vortices and pins at different sites. The critical current density has been studied at different temperatures by solving the over damped equation of vortex motion taking into account the vortex-vortex interaction, the thermal force, the vortex-pinning interaction as well as the driving Lorentz force. The results show a second phase transition at specific low temperature at all pinning forces with a definite pinning size.

Thursday, March 1, 2012 11:15AM - 1:51PM – Session W1 DAMOP: Photonic Systems and Entanglement Generation 203

11:15AM W1.00001 Efficient quantum computing using coherent photon conversion, NATHAN K. LANGFORD, University of Vienna, Austrian Academy of Sciences, University of Oxford, SVEN RAMELOW, University of Vienna, Austrian Academy of Sciences, ROBERT PREVEDEL, University of Vienna, University of Waterloo, WILLIAM J. MUNRO, NII and NTT Basic Research Laboratories, GERARD J. MILBURN, University of Queensland, University of Vienna, ANTON ZEILINGER, University of Vienna, Austrian Academy of Sciences — Single photons make very good quantum information carriers, but current schemes for photonic quantum information processing (QIP) are inefficient. We describe a new scheme, *coherent photon conversion (CPC)*, using classically pumped nonlinearities to generate and process complex multiqumata states¹. One example based on four-wave mixing provides a full suite of QIP tools for scalable quantum computing from a single, versatile process, including: deterministic multiqubit entanglement gates based on a novel photon-photon interaction, high-quality heralded multiphoton states without higher-order imperfections, and robust, high-efficiency detection. Using photonic crystal fibres, we present observations of quantum correlations from a four-colour nonlinear process suitable for CPC and study the feasibility of reaching the deterministic regime with current technology. The scheme could also be implemented in optomechanical, electromechanical and superconducting systems.

¹Published in Nature **478**, 360 (2011)

11:27AM W1.00002 Dephasing of multiparticle Rydberg excitations for fast entanglement generation¹, F. BARIANI, Y.O. DUDIN, T.A.B KENNEDY, A. KUZMICH, School of Physics, Georgia Institute of Technology, Atlanta, GA, 30332-0430, USA — We propose an approach to fast entanglement generation based on Rydberg dephasing of collective excitations (spin waves) in large, optically thick atomic ensembles. Rather than trying to prevent multiple excitations via the Rydberg blockade mechanism, our idea is to allow multiple Rydberg level excitations to self-interact and dephase. The strong interaction required to dephase multiple excitations is induced by mixing adjacent, opposite-parity Rydberg levels with a microwave field. These levels experience resonant $1/r^3$ dipole-dipole interactions ($ns + n'p \rightarrow n'p + ns$) that extend over the whole ensemble in contrast to the weaker, short range $1/r^6$ Van der Waals coupling due to non-resonant processes ($ns + ns \rightarrow np + (n-1)p$). The interaction-induced phase shifts suppress the contribution of multiply excited states in phase matched optical retrieval. The dephasing mechanism therefore permits isolation and manipulation of individual spin wave excitations. High quality single photons can be created with $1/e$ maximum efficiency in few microseconds. The dephasing mechanism is shown to have favorable, approximately exponential, scaling. Required long coherence times are achieved via four-photon excitation and read-out of long wavelength spin waves.

¹We acknowledge financial support from NSF and AFOSR.

11:39AM W1.00003 Unconventional ultra-efficient photon blockade and single-photon emitters from weakly nonlinear systems based on coupled cavities, MOTOAKI BAMBA, CRISTIANO CIUTI, Laboratory MPQ, University Paris Diderot - Paris 7 and CNRS — Single photons are usually generated by non-resonant excitation of single (artificial) atoms or by resonant excitation of Kerr systems with a giant nonlinear interaction much larger than the losses of the system (standard photon blockade). Here, we present a general class of destructive quantum interference effects [1,2], which provide a robust protocol to achieve strong photon antibunching and single-photon emission in a double cavity system, where one resonantly driven cavity is coupled to an auxiliary nonlinear cavity. An original scheme [2] shows the single-photon emission can be also produced by the auxiliary cavity with orthogonal polarization with respect to the pump beam, hence providing a direct way to get spatial and polarization selection.

[1] M. Bamba, A. Imamoglu, I. Carusotto, C. Ciuti, *Origin of strong photon antibunching in weakly nonlinear photonic molecules*, Phys. Rev. A **83**, 021802 (2011) and references therein.

[2] M. Bamba, C. Ciuti, *Counter-polarized single-photon generation from the auxiliary cavity of a weakly nonlinear photonic molecule*, Appl. Phys. Lett. **99**, 171111 (2011).

11:51AM W1.00004 Anomalous Stokes scattering by an atomic ensemble: detection of entanglement and vector metrology of field gradient¹, WANG YAO, HONGYI YU, Department of Physics and Center for Theoretical and Computational Physics, The University of Hong Kong — We investigate the collective Stokes scattering by a typical atomic cloud, i.e. with size much larger than the light wavelength and with density much lower than that required for Dicke superradiance. We show that the diffraction pattern of the Stokes photon can be used to detect entanglement in the atomic ensemble. When the atomic cloud is placed in a static magnetic field or electric field, the change of diffraction pattern by the evolution in the field can also provide sensitive vector metrology of the spatial gradient of the field.

¹The work was supported by the Research Grant Council of Hong Kong under Grant No. HKU 706711P.

12:03PM W1.00005 Unique Properties and Prospects: Quantum Theory of the Orbital Angular Momentum of Ince-Gauss Beams¹, WILLIAM PLICK, MARIO KRENN, ROBERT FICKLER, SVEN RAMELOW, ANTON ZEILINGER, Institute for Quantum Optics and Quantum Information — The Ince-Gauss modes represent a new addition to the standard solutions to the paraxial wave equation. Parametrized by the ellipticity of the beam, they span the solution space between the Hermite-Gauss and the Laguerre-Gauss modes. These beams may be decomposed in either basis, and single photons in the Ince-Gauss modes exist naturally as superpositions of either Laguerre-Gauss or Hermite-Gauss modes. We present the fully quantum theory of the orbital angular momentum of these beams. Interesting features that arise are: stable beams with fractional orbital angular momentum, non-monotonic behavior of the OAM with respect to ellipticity, and the possibility of orthogonal modes possessing the same OAM. We believe that these modes may open up a fully new parameter space for quantum informatics and communication, and thus are worthy of thorough study.

¹Austrian Academy of Sciences

12:15PM W1.00006 Entanglement of Ince-Gauss Modes of Photons¹, MARIO KRENN, ROBERT FICKLER, WILLIAM PLICK, RADEK LAPKIEWICZ, SVEN RAMELOW, ANTON ZEILINGER, University of Vienna, Faculty of Physics, IQOQI Vienna, Austrian Academy of Sciences, Austria — Ince-Gauss modes are solutions of the paraxial wave equation in elliptical coordinates [1]. They are natural generalizations both of Laguerre-Gauss and of Hermite-Gauss modes, which have been used extensively in quantum optics and quantum information processing over the last decade [2]. Ince-Gauss modes are described by one additional real parameter – ellipticity. For each value of ellipticity, a discrete infinite-dimensional Hilbert space exists. This conceptually new degree of freedom could open up exciting possibilities for higher-dimensional quantum optical experiments. We present the first entanglement of non-trivial Ince-Gauss Modes. In our setup, we take advantage of a spontaneous parametric down-conversion process in a non-linear crystal to create entangled photon pairs. Spatial light modulators (SLMs) are used as analyzers. [1] Miguel A. Bandres and Julio C. Gutiérrez-Vega “Ince Gaussian beams”, Optics Letters, Vol. 29, Issue 2, 144-146 (2004) [2] Adetunmise C. Dada, Jonathan Leach, Gerald S. Buller, Miles J. Padgett, and Erika Andersson, “Experimental high-dimensional two-photon entanglement and violations of generalized Bell inequalities”, Nature Physics 7, 677-680 (2011)

¹Supported by ERC (Advanced Grant QIT4QAD) and the Austrian Science Fund (SFB F4007, CoQuS).

12:27PM W1.00007 Entangling two spatially separated qubits via interaction with nonclassical radiation¹, EYOB SETE, Department of Physics and Astronomy, Texas A&M University, SUMANTA DAS, Max-Planck-Institute fur Kernphysik — We propose a scheme for entangling two spatially separated noninteracting qubits using two-mode squeezed light in a cavity. Unlike other methods that typically require dipolar coupling for creating entanglement, our proposal relies solely on the interaction of the qubits with the squeezed cavity field. The squeezed field induces exchange of correlated photons which leads to transfer of entanglement from the field to discrete entanglement between qubits. Our scheme exhibits substantial steady-state entanglement which is robust against decoherence under the strong squeezing condition. In addition, we find that the entanglement generated between two asymmetric qubits is stronger than that generated by identical ones and crucially depends on the degree of squeezing.

¹E. A. S. is supported by the Herman F. Heep and Minnie Belle Heep Texas A&M University Endowed Fund held and administered by the Texas A&M Foundation.

12:39PM W1.00008 Generating coherent states of entangled spins¹, HONGYI YU, YU LUO, WANG YAO, Department of Physics and Center of Theoretical and Computational Physics, The University of Hong Kong, Hong Kong, China — A coherent state of many spins contains quantum entanglement, which increases with the decrease of the collective spin value. We present a scheme to engineer this class of pure state based on incoherent spin pumping with several collective raising and lowering operators. In a pumping scenario aimed for maximum entanglement, the N -qubit steady state realizes the ideal resource for the $1 \rightarrow N/2$ quantum telecloning. We show how the scheme can be implemented in the cold atomic system in an optical lattice. Error analysis shows that high-fidelity state engineering is possible for $N \sim O(100)$ spins in the presence of decoherence. The scheme can also prepare the large-scale Affleck-Kennedy-Lieb-Tasaki state.

¹The work was supported by the Research Grant Council of Hong Kong under Grant No. HKU 706711P.

12:51PM W1.00009 Non-destructively probing matter-photon correlations described by the Dicke-Hubbard Lattice model¹, SARA RAJARAM, NANDINI TRIVEDI, The Ohio State University — The Dicke-Hubbard Lattice (DHL) Hamiltonian is a prototypical system to study photon matter entanglement across a symmetry breaking quantum phase transition in the matter subsystem. The model describes a cavity containing a periodic lattice, with a single mode photon field delocalized across the cavity. Like the Bose-Hubbard model, the Hamiltonian includes on-site repulsion between atoms and nearest neighbor hopping of an atom from one site to another. In addition, matter-light coupling in the DHL model can excite an atom to a higher band by absorbing a photon and the reverse process. We focus on the DHL model in a region of parameter space in which light is “superradiant” and matter is either a Mott-insulator or superfluid of both bands. Through mean field, exact diagonalization, and quantum Monte Carlo calculations we examine photon statistics across the matter quantum phase transition in order to elucidate how the photon statistics reflect the matter correlations. Doing so provides a novel technique to non-destructively probe the Mott-insulator to superfluid phase transition.

¹We acknowledge support from ARO W911NF-08-1-0338 (SR) and NSF DMR-0907275 (NT).

1:03PM W1.00010 The Impact of Geometry on the TM PBGs of Photonic Crystals and Quasicrystals, LIN JIA, MIT, ION BITA, Qualcomm MEMS Technologies, EDWIN THOMAS, Rice University — Here we demonstrate a novel quantitative procedure to pursue statistical studies on the geometric properties of photonic crystals and photonic quasicrystals (PQCs) which consist of separate dielectric particles. The geometric properties are quantified and correlated to the size of the photonic band gap (PBG) for wide permittivity range using three characteristic parameters: shape anisotropy, size distribution, and feature-feature distribution. Our concept brings statistical analysis to the photonic crystal research and offers the possibility to predict the PBG from a morphological analysis.

1:15PM W1.00011 A low-dimensional population-competition model for analyzing transverse optical patterns¹, Y.C. TSE, M.H. LUK, Physics Department, Chinese University of Hong Kong, N.H. KWONG, College of Optical Sciences, University of Arizona, P.T. LEUNG, Physics Department, Chinese University of Hong Kong, S. SCHUMACHER, Physics Department and Center for Optoelectronics and Photonics Paderborn, University of Paderborn, R. BINDER, College of Optical Sciences and Department of Physics, University of Arizona — Under favorable conditions, laser beams passing through a nonlinear medium (e.g. atomic vapors) can undergo directional instabilities, generating transverse optical patterns in the far field. In particular, a low intensity all-optical switching scheme using these transverse patterns in semiconductor quantum well microcavities was numerically demonstrated. Trying to understand the switching mechanism through the simulation results has turned out to be a complicated task. In this Contribution, we present a low-dimensional “population-competition” model that (i) exhibits nearly all the pattern selection and switching behaviors and (ii) is simple enough to allow a comprehensive analysis of its solution structure in the relevant region of parameter space. We will explain the relation between this simple model and the realistic theory. Using elementary methods in Catastrophe Theory, we analyze the “phase diagrams” of our model’s steady state solutions in parameter space, with the help of which we construct an organized picture of the behaviors of the realistic simulation results.

¹S. S. acknowledges financial support from the Deutsche Forschungsgemeinschaft

1:27PM W1.00012 Phonon effects on analog quantum simulation with ultracold ions in a linear Paul trap, C.-C. JOSEPH WANG, JAMES FREERICKS, Georgetown University — Linear Paul traps have been used to simulate the transverse field Ising model with long-range spin couplings. Here, we study the effects of phonon creation on the spin state probability and spin entanglement. The effective spin models are created by applying a spin-dependent force with a laser that couples the spin state to the phonons of the ion crystal. Adiabatically removing the phonons creates an action described by a static spin Hamiltonian plus additional quantum time-dependent phases. In appropriate limits, the system is described predominantly by the static spin Hamiltonian. Here, we solve for the evolution of the coupled spin-phonon system exactly using exact diagonalization and examine the effect of phonon creation during the simulation on the probabilities of different spin states and on their entanglement. In particular, we examine phonon effects on the possibility for seeing the kink transition when the laser is detuned between the two phonon modes that lie below the COM mode.

1:39PM W1.00013 Entanglement Effects in Highly Dense Systems, SAMINA MASOOD, University of Houston-Clear Lake — We study the effect of entanglement in Jaynes-Cummings model using Neumann Entropy in the highly dense systems. We study a highly dense system such as neutron star as a good application of our results.

Thursday, March 1, 2012 11:15AM - 2:15PM –

Session W2 GIMS GERA: Invited Session: Instrumentation and Measurement Science for Energy Research: PV and Batteries 204AB

11:15AM W2.00001 Using Deep Level Transient Spectroscopy (DLTS) to characterize defects in semiconductor devices, DAVID LANG, Materials Physics Consultant — Deep Level Transient Spectroscopy (DLTS) is a member of the class of instrumentation methods that utilizes the detection of trapped electronic charge to characterize defects in solids. Such methods detect this charge either directly, e.g. via capacitance measurements, or indirectly, e.g. via the current associated with the release of trapped charge. These types of instrumentation have been widely used since the dawn of solid-state physics, particularly for nonradiative defects in semiconductors and insulators. In the case of semiconductor devices, the highly sensitive capacitive detection of trapped charge in the junction depletion layer makes these methods particularly powerful. The DLTS method introduced the concept of time-domain filtering (the so-called “rate window”) to create a defect spectrum from the transient response of the device versus temperature. This talk will give an overview of DLTS, with particular emphasis on the correlation between defects and device performance.

11:51AM W2.00002 Role of Defects and Their Analysis in Photovoltaics, ROBERT OPILA, University of Delaware — Defects are intrinsically related to the performance of solar cells. In solar cells the generation and collection of charge carriers determines their efficiency. Effective transport of charge carriers across interfaces and minimization of their recombination in the bulk or at surfaces and interfaces is of utmost importance. In this talk we will discuss the role of surface and bulk defects. First, the role of surface passivation is very important in limiting the rate of carrier of recombination. Here we will combine spectroscopic evaluation of the surface of a Si device with electrical lifetime measurements to ascertain what factors determine the quality of a solar cell passivation. We have also utilized time-resolved photoluminescence (TRPL) to assess the quality of materials grown under varying conditions. TRPL decay is best fit by a biexponential model that includes both the minority carrier lifetime and the rate of trap filling. At low laser powers the trap state recombination dominates and decay times are very short. At higher laser powers the trap states become saturated and we can extract the minority carrier lifetime. By evaluating the relative contributions of the trap-filling and minority carrier lifetimes we can assess the density of traps (defects) as a function of the growth conditions and guide refinement of growth recipes to improve material quality.

12:27PM W2.00003 The Integration of Scanning Electron Microscopy, Scanning Probe Microscopy, and Luminescence Spectroscopy in one Platform: New Opportunities and Applications in Photovoltaics, MANUEL ROMERO, National Renewable Energy Laboratory — We have recently integrated scanning tunneling microscopy (STM), atomic force microscopy (AFM), and near-field scanning optical microscopy (NSOM) onto the mechanical stage of a scanning electron microscope compatible with operation under high vacuum and the use of cryogenics. This instrument is unique in the sense that is not just the assembly of different microscopes but an integrated platform in which both the electron beam and the ultrasharp tip of the AFM/STM/NSOM can be controlled simultaneously and independently as excitation or sensing elements, providing innovative modes of operation and access to optoelectronic properties in the micro and nanoscale not accessible before. Furthermore, this instrument is equipped with focused laser illumination of the tip and detection of luminescence and can be used to measure cathodoluminescence, scanning tunneling luminescence, photoluminescence, and electroluminescence, all with high resolution. In this contribution, we review the application of these techniques to the development of second- and third-generation photovoltaics (PV) beyond those commercially available today. Among these applications, we present the luminescence and electron transport across single grain boundaries in chalcopyrite and kesterite compounds, the detection of single molecule species using plasmonics, the nanoscale imaging of the exciton transport in organic semiconductors, and the *in situ* manipulation and measurement of nanowires.

1:03PM W2.00004 Li ion nanowire batteries and their *in situ* characterization in the TEM, DMITRY RUZMETOV, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD, USA — The ability to measure the morphological, chemical, and transport characteristics with nanoscale resolution in electrochemical energy storage devices is critical for understanding the complex interfacial reactions and phase transformation that accompany cycling of secondary batteries. In this talk I will describe the use of an all-nanowire Li ion battery for *in situ* characterization of charge and discharge reactions. The nanowire batteries (NWBs) consist of a metalized core, a LiCoO₂ cathode, LiPON solid electrolyte, and a thin film Si anode. Measuring several micrometers in length and several hundred nanometers in diameter, the NWBs can be readily imaged and analyzed in transmission electron microscopes (TEM, STEM). We use focused ion beam milling and electron beam induced deposition to separate the cathode and anode and fabricate Pt contacts to a NWB. *In situ* electrical cycling of NWBs in TEM reveals that the most of the structural changes due to cycling happens in the electrolyte layer especially near the cathode/electrolyte interface. Electrical response from a single NWB was measured in the sub-pA range. For NWBs with the thinnest electrolyte, approximately 100 nm, we observe rapid self-discharge, along with void formation at the electrode/electrolyte interface, indicating electrical and chemical breakdown. The analysis of the NWB's electrical characteristics reveals space-charge limited electronic conduction, which effectively shorts the anode and cathode electrodes. When the electrolyte thickness is increased, the self-discharge rate is reduced substantially and the NWBs maintain a potential above 2 V. Our study illustrates that at reduced dimensions the increase in the electric field can lead to large electronic current in the electrolyte effectively shorting the battery even when the electrolyte layer is uniform and pinhole free. The scaling of this phenomenon provides useful guidelines for design of 3D Li ion batteries.

1:39PM W2.00005 In-Situ TEM Electrochemistry of Individual Nanowire and Nanoparticle Electrodes in a Li-Ion Cell, JIANYU HUANG, Sandia National Lab. — Recently, we created the first Li-ion electrochemical cell inside a transmission electron microscope (TEM) and observed, in real time with atomic scale resolution, the lithiation/delithiation processes. This experiment opened the door for a suite of experimental studies involving in-situ TEM characterization of Li-ion battery materials. In this presentation, I'll first review our latest progress of using the in-situ electrochemical cell setup inside the TEM to reveal the intrinsic electrochemistry of several high energy density anode materials such as SnO₂, ZnO, Si, Ge, Al nanowires, Si nanoparticles, carbon nanotubes, and graphene. Several electrochemical mechanisms were observed and characterized in real-time, including lithiation induced stress, volume changes, phase transformations, pulverization, cracking, embrittlement, and mechanical failure in anode materials. These results indicate the strong material, size and crystallographic orientation dependent electrochemical behavior and degradation mechanisms that occur in Li-ion battery anodes. In the future, we will need further advancements in in-situ characterization for understanding important processes in Li-ion batteries. For example, liquid cells are required in order to examine the electrochemical reactions between battery materials and the standard battery electrolytes, which are ethylene carbonate-based. Furthermore, in-situ studies need to be correlated with electrochemical studies performed on bulk electrodes. I will present a comparison between our in-situ results and electrochemical studies on conventional battery electrodes and highlight how in-situ studies can have important impact on the design of Li-ion batteries. Finally I will discuss outstanding challenging issues and opportunities in the field of Li-ion battery research.

References: **Science** 330, 1515 (2010); 330, 1485 (2010); **Nano Lett.** Doi: 10.1021/nl200412p, 10.1021/nl2024118, 10.1021/nl201684d, 10.1021/nl202088h, **ACS Nano**, doi: 10.1021/nn200770p, 10.1021/nn202071y; **PRL** 106, 248302 (2011); **Eng. Env. Sci.** doi: 10.1039/c1ee01918j

Thursday, March 1, 2012 11:15AM - 2:15PM – Session W3 DCMF: Invited Session: Fractional Topological Insulators 205AB

11:15AM W3.00001 Fractional Topological Insulators in 2 and 3 dimensions, F.J. BURNELL, Oxford University — I will present a family of exactly solvable models whose low energy physics is that of a 3D topological band insulator of fractionally charged fermions. When time reversal is broken at the surface, these insulators display a fractional magnetoelectric effect, leading to fractional quantum Hall surface states. Further, some – but not all – of them can be shown to be genuine topological insulators, whose gapless surface states are protected by time reversal. This gives an explicit construction of fractional topological insulators in 3D. This work has been done in collaboration with Michael Levin (University of Maryland), Maciej Koch-Janusz (Weizmann Institute), and Ady Stern (Weizmann Institute).

11:51AM W3.00002 Composite fermions for fractionally filled Chern bands¹, R. SHANKAR², Yale Physics — We consider fractionally filled bands with a non-zero Chern index that exhibit the Fractional Quantum Hall Effect in zero external field³ a possibility supported by numerical work.⁴ Analytic treatments are complicated by a non-constant Berry flux and the absence of Composite Fermions (CF), which would not only single out preferred fractions, but also allow us compute numerous response functions at nonzero frequencies, wavelengths and temperature using either Chern-Simons field theory or our Hamiltonian formalism.⁵ We describe a way to introduce CF's by embedding the Chern band in an auxiliary problem involving Landau levels. The embedded band can be designed to approximate a prescribed Chern density in k space which determines the commutation relations of the charge densities and hence preserve all dynamical and algebraic aspects of the original problem. We find some states for which the filling fraction and dimensionless Hall conductance are not equal. The approach extends to two-dimensional time-reversal invariant topological insulators and to composite bosons.

¹We thank the NSF for grants DMR-0703992 and PHY-0970069 (GM), DMR-0103639 (RS).

²In collaboration with G. Murthy, University of Kentucky

³R. Roy and S. Sondhi, *Physics* **4**, 46 (2011) and papers reviewed therein.

⁴Ibid.

⁵G. Murthy and R. Shankar, *Rev. Mod. Phys.*, **75**, 1101, (2003)

12:27PM W3.00003 Fractional Topological Insulators¹, CLAUDIO CHAMON, Boston University — The prediction and experimental discovery of topological band insulators and topological superconductors are recent examples of how topology can characterize phases of matter. In these examples, electronic interactions do not play a fundamental role. In this talk I shall discuss cases where interactions lead to new phases of matter of topological character. Specifically, I shall discuss fractional topological states in lattice models which occur when interacting electrons propagate on flattened Bloch bands with non-zero Chern number. Topologically ordered many-particle states can emerge when these bands are partially filled, including a possible realization of the fractional quantum Hall effect without external magnetic fields. I shall also ponder on the possible practical applications, beyond metrology, that the quantized charge Hall effect might have if it could be realized at high temperatures and without external magnetic fields in strongly correlated materials.

¹Work supported by DOE Grant DEFG02-06ER46316

1:03PM W3.00004 Generic Wavefunction Description of Fractional Quantum Anomalous Hall States and Fractional Topological Insulators, XIAO-LIANG QI, Stanford University — No abstract available.

1:39PM W3.00005 Correlated topological insulators and the fractional magnetoelectric effect¹, BRIAN SWINGLE, Harvard University — I will describe the recent theoretical construction of electronic phases in 3d that combine the physics of electron fractionalization with that of topological insulators. Called fractional topological insulators, these states of matter host protected surface states and fractionally charged quasiparticle excitations. I will then discuss the emergent gauge theory description of these phases with an emphasis on the crucial role of deconfinement at low energies. I will also describe a wide variety of experimental signatures of fractional topological insulators as well as suggesting directions for experimental searches.

¹This work is supported by a Simons Fellowship. Collaborators: M. Barkeshli, J. McGreevy, and T. Senthil.

Thursday, March 1, 2012 11:15AM - 1:51PM – Session W4 DAMOP: Strongly Interacting Fermi Gases 205C

11:15AM W4.00001 Revealing the Superfluid Lambda Transition in the Universal Thermodynamics of a Unitary Fermi Gas¹, MARK KU, ARIEL SOMMER, LAWRENCE CHEUK, MARTIN ZWIERLEIN, Department of Physics, MIT-Harvard Center for Ultracold Atoms, and Research Laboratory of Electronics, MIT, Cambridge, Massachusetts 02139, USA — We have observed the superfluid phase transition in a strongly interacting Fermi gas via high-precision measurements of the local compressibility, density and pressure down to near-zero entropy. We perform the measurements by in-situ imaging of ultracold ⁶Li at a Feshbach resonance. Our data completely determine the universal thermodynamics of strongly interacting fermions without any fit or external thermometer. The onset of superfluidity is observed in the compressibility, the chemical potential, the entropy, and the heat capacity. In particular, the heat capacity displays a characteristic lambda-like feature at the critical temperature of $T_c/T_F = 0.167(13)$. This is the first clear thermodynamic signature of the superfluid transition in a spin-balanced atomic Fermi gas. We provide a new value of the Bertsch parameter ξ_S . The experimental results are compared to recent Monte-Carlo calculations. Our measurements provide a benchmark for many-body theories on strongly interacting fermions, relevant for problems ranging from high-temperature superconductivity to the equation of state of neutron stars.

¹This work was supported by the NSF, AFOSR-MURI, ARO-MURI, ONR, DARPA YFA, a grant from the Army Research Office with funding from the DARPA OLE program, an AFOSR PECASE, the David and Lucile Packard Foundation, and the Alfred P. Sloan Foundation.

11:27AM W4.00002 Probing upper branch physics in strongly interacting Fermi gases¹, SHIZHONG ZHANG, The Ohio State University, EDWARD TAYLOR, McMaster University, WILLIAM SCHNEIDER, MOHIT RANDERIA, The Ohio State University — Motivated by a recent experiment at MIT, we consider the collision of two clouds of spin-polarized atomic Fermi gases close to a Feshbach resonance. We explain why two dilute gas clouds, with attractive interactions between its constituents, bounce off each other as if they were billiard balls. Our hydrodynamic analysis, in excellent agreement with experiment, gives strong evidence for a novel metastable many-body state, the so-called upper branch, with repulsive effective interactions. We also propose another experiment, measuring spin decoherence rates, to study the physics of the upper branch.

¹Supported by NSF-DMR 0706203, NSF-DMR 0907366, and ARO W911NF-08-1-0338, and NSERC.

11:39AM W4.00003 Strongly interacting atomic Fermi gases in a trap with mass and population imbalances at finite temperature¹, JIBIAO WANG, Zhejiang University, HAO GUO, Hong Kong University, QIJIN CHEN, Zhejiang University — A great advantage of studying atomic Fermi gases is the easy tunability of multiple physical parameters, including interaction strength, mass and population imbalances, as well as species dependent trapping potential. Indeed, the mixture of ⁶Li and ⁴⁰K gases has been of great interest, with and without population imbalance. In this talk, we will address the finite temperature phase diagrams of two component atomic Fermi gases with both mass and population imbalances in a trap, using a pairing fluctuation theory. We show that in certain parameter ranges, there exist intermediate temperature superfluids as well as phase separation with exotic sandwich-like shell structure with superfluid or pseudogapped normal state in the middle. We consider pairing strength over the entire range of BCS-BEC crossover. Our result is relevant to future experiment on mixtures of ⁶Li and ⁴⁰K and possibly other Fermi atoms. References: H. Guo, C.-C. Chien, Q.J. Chen, Y. He, and K. Levin, Phys. Rev. A 80, 011601(R) (2009); C.-C. Chien, Q.J. Chen, Y. He, and K. Levin, Phys. Rev. Lett. 98, 110404 (2007); C.-C. Chien, Q.J. Chen, Y. He, and K. Levin, Phys. Rev. Lett. 97, 090402 (2006); Q.J. Chen, I. Kosztin, B. Janko, and K. Levin, Phys. Rev. Lett. 81, 4708 (1998).

¹Supported by NSF, MOE and MOST of China

11:51AM W4.00004 Two-particle current from Superfluid Fermi Gases in the BCS-BEC Crossover, EMIKO ARAHATA, Department of Basic Science, The University of Tokyo, TETSURO NIKUNI, Department of Physics, Faculty of Science, Tokyo University of Science — In recent years, the crossover from the BCS-type superfluid to the Bose-Einstein condensation (BEC) of tightly-bound molecules has been realized in ultracold atomic Fermi gases using a tunable pairing interaction associated with a Feshbach resonance. In the BCS-BEC crossover it will be important to reveal the nature of fermion pairs. In this paper, we propose that two-particle (double photoemission) current (DPE current) is a powerful technique to provide direct insight into the pair-correlations. The DPE from superconductors has been studied both theoretically and experimentally, where a pair of electrons is emitted from the system upon the absorption of one photon. In this study, we consider an analogous situation in ultracold atomic gases, and derive a general expression for DPE current from superfluid Fermi gases in the BCS-BEC crossover. We show DPE current as a function of energy and momentum transfers, and identify the contributions of the condensed pair components and uncorrelated pair states, and discuss the possibility of distinguishing between weakly-bound Cooper pairs and tightly-bound molecules.

12:03PM W4.00005 Feshbach resonances and BCS-BEC crossover in optical lattices, ZHAOCHUAN SHEN, LEO RADZIHOVSKY, VICTOR GURARIE, Department of Physics, University of Colorado — In this talk we study Feshbach resonances of fermionic atoms placed in a periodic potential. We investigate the criteria when such a system can be described by a Hubbard model with variable interaction strength in case of broad resonance, or by a tight binding model of atoms and molecules which can convert into each other on sites of the lattice in case of narrow resonances. Assuming the applicability of these models, we first study the BCS-BEC crossover for broad resonance. We find that while below half filling the system undergoes the conventional crossover from a BCS superconductor to a Bose condensate of molecules, above half filling the nature of the BEC phase changes to that of a condensate of molecules made of holes. Switching our attention to the case of narrow resonance, we find that the crossover takes the system from a BCS to hole-BEC regime, then back to BCS, and finally to a conventional BEC of atomic molecules. In the latter crossover, we find that the size of Cooper pairs/molecules changes non-monotonously, being larger in the BCS and smaller in the BEC regimes. Finally, at a unity filling we find a quantum phase transition from a band insulator to a BCS-BEC superfluid replacing the crossover.

12:15PM W4.00006 Resonant enhancement of the FFLO state in 3D by an optical potential¹, JEROEN DEVREESE, SERGHEI KLIMIN, MICHEL WOUTERS, JACQUES TEMPERE, Universiteit Antwerpen, TQC (THEORIE VAN KWANTUMSYSTEMEN EN COMPLEXE SYSTEMEN) TEAM — In a two component Fermi gas, spin-imbalance leads to a competition between Cooper-pairing with zero momentum and with nonzero momentum. The latter gives rise to the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state. Hitherto this state has not been observed in a 3D Fermi gas. We propose a new way to enhance the presence of the FFLO state, by adding a 1D periodic potential. To investigate the effect of this potential, we study the ground state properties of the system, starting from the partition sum of an imbalanced Fermi gas in path-integral representation. To describe the FFLO state, a saddle point is chosen in which the pairs can have nonzero momentum. Minimizing the resulting free energy leads to the phase diagram of the system. The stability region of the FFLO state is found to be greatly enlarged due to the presence of the periodic potential, compared to the ordinary 3D case. We find that the FFLO state can exist at higher spin imbalance if the wavelength of the optical potential becomes smaller. We propose that this concept can be used experimentally to enhance the FFLO state.

[1] Jeroen P.A. Devreese, S.N. Klimin, and J. Tempere, Phys. Rev. A 83, 013606 (2011).

[2] Jeroen P.A. Devreese, M. Wouters, and J. Tempere, J. Phys. B 44, 115302 (2011); Phys. Rev. A 84, 043623 (2011).

¹JPAD acknowledges a Ph. D. fellowship of the Research Foundation - Flanders (FWO-V).

12:27PM W4.00007 Single magnetic impurity in a spin-imbalanced superfluid Fermi gas¹, JIAN LI, CHIN-SEN TING, Texas Center for Superconductivity and Department of Physics, University of Houston, TEXAS CENTER FOR SUPERCONDUCTIVITY AND DEPARTMENT OF PHYSICS, UNIVERSITY OF HOUSTON TEAM — A spin-imbalanced superfluid Fermi gas harmonically trapped in a two-dimensional optical lattice with a single classical magnetic impurity is investigated by Bogoliubov-de Gennes equations. In spin-balanced and weak spin-imbalanced case, we show that a strong magnetic impurity can change sign of the pairing order parameter. The amplitude of the sign-changed order parameter caused by impurity is affected by the strength of impurity potential, temperature and particle density. Compared to spin-balanced case, we find that an additional in-gap bound state can be induced by a strong magnetic impurity in weak spin-imbalanced case. In strong spin-imbalanced case where the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state is established as the ground state, the impurity induces wide spatial oscillations of pairing order parameters and can enhance the order parameters by suppressing the local spin-imbalance. Our results can be used to create and manipulate the FFLO state with magnetic impurities in spin-imbalanced Fermi gases.

¹This work was supported by the Texas Center for Superconductivity at the University of Houston and by the Robert A. Welch Foundation under Grant No. E-1146.

12:39PM W4.00008 Proposal for interferometric detection of the topological character of modulated superfluidity in ultracold Fermi gases¹, MASON SWANSON, The Ohio State University, YEN LEE LOH, The University of North Dakota, NANDINI TRIVEDI, The Ohio State University — A system with unequal populations of up and down fermions may exhibit a Larkin-Ovchinnikov (LO) phase characterized by periodic domain walls across which the order parameter changes sign and the excess polarization is localized. Despite fifty years of theoretical and experimental work, there has so far been no unambiguous observation of an LO phase. We propose an experiment in which two fermion clouds, prepared with unequal population imbalances, are allowed to expand and interfere. We show that a pattern of staggered fringes in the interference is unequivocal evidence of LO physics. The resilience of these interference signatures against thermal and quantum fluctuations is also discussed, and our results are supported with time-of-flight simulations of the experiment. Y.-L. Loh and N. Trivedi, Phys. Rev. Lett. 104, 165302 (2010). M. Swanson et al., arXiv:1106.3908

¹We acknowledge support from the NSF Graduate Research Fellowship Program and ARO grant no. W911NF-08-1-0338 and DARPA grant no. 6002534

12:51PM W4.00009 A single impurity atom in a two-dimensional Fermi gas, JESPER LEVINSEN, University of Cambridge, MEERA PARISH, University College London — We consider a single impurity atom immersed in a Fermi gas in two dimensions and interacting via an attractive, short-range potential. Using variational wave functions for polarons, molecules, trimers, and quadruplets, we arrive at the ground state phase diagram as a function of mass ratio and interaction strength. We show that the phase diagram includes a Fulde-Ferrell-Larkin-Ovchinnikov phase for experimentally relevant mass ratios.

1:03PM W4.00010 Realization of a Resonant Fermi Gas with a Large Effective Range, ERIC HAZLETT, YI ZHANG, RON STITES, KEN O'HARA, The Pennsylvania State University — We have measured the interaction energy and three-body recombination rate for a two-component Fermi gas near a narrow Feshbach resonance and found both to be strongly energy dependent. Even for deBroglie wavelengths greatly exceeding the van der Waals length scale, the behavior of the interaction energy as a function of temperature cannot be described by atoms interacting via a contact potential. Rather, energy-dependent corrections beyond the scattering length approximation are required, indicating a resonance with an anomalously large effective range. For fields where the molecular state is above threshold, the rate of three-body recombination is enhanced by a sharp, two-body resonance arising from the closed-channel molecular state which can be magnetically tuned through the continuum. This narrow resonance can be used to study strongly correlated Fermi gases that simultaneously have a sizeable effective range and a large scattering length.

1:15PM W4.00011 Anomalous Dimers in Quantum Mixtures near Broad Resonances:Pauli Blocking, Fermi Surface Dynamics and Implications¹, JUNLIANG SONG, Institute of Quantum Optics and Quantum Information of Austrian Academy of Sciences, FEI ZHOU, University of British Columbia — We study the energetics and dispersion of anomalous dimers that are induced by the Pauli blocking effect in a quantum Fermi gas of majority atoms near interspecies resonances. Unlike in vacuum, we find that both the sign and magnitude of the dimer masses are tunable via Feshbach resonances. We also investigate the effects of particle-hole fluctuations on the dispersion of dimers and demonstrate that the particle-hole fluctuations near a Fermi surface (with Fermi momentum $\hbar k_F$) generally reduce the effective two-body interactions and the binding energy of dimers. Furthermore, in the limit of light minority atoms the particle-hole fluctuations disfavor the formation of dimers with a total momentum $\hbar k_F$, because near $\hbar k_F$ the modes where the dominating particle-hole fluctuations appear are the softest. Our calculation suggests that near broad interspecies resonances when the minority-majority mass ratio m_B/m_F is smaller than a critical value (estimated to be 0.136), dimers in a finite-momentum channel are energetically favored over dimers in the zero-momentum channel. We apply our theory to quantum gases of $^6\text{Li}^{40}\text{K}$, $^6\text{Li}^{87}\text{Rb}$, $^{40}\text{K}^{87}\text{Rb}$ and $^6\text{Li}^{23}\text{Na}$ near broad interspecies resonances, and discuss the implications.

¹Austrian Science Fund FWF FOCUS

1:27PM W4.00012 Unpolarized Fermi gas in squeezed anisotropic harmonic trap by Quantum Monte Carlo methods, XIN LI, LUBOS MITAS, Physics Department, North Carolina State University — Using diffusion Monte Carlo (DMC) method, we calculate the ground state properties of unpolarized Fermi gas at unitarity regime in both isotropic and anisotropic harmonic potentials. We study the effects of anisotropy by increasing the frequency in z direction ω_z of the harmonic potential while keeping the frequency in x and y direction unchanged. The true unitarity regime is obtained by extrapolating the interaction range to zero and the calculations are done using the fixed-node diffusion Monte Carlo method. The trial function is of the BCS form with the pairing function expanded in appropriate linear combinations of the anisotropic oscillator eigenstates. We evaluate the binding energies for varying particle numbers and we estimate its behavior in the limit of large number of atoms. We estimate dependence of projected density profile and momentum distribution on the X-Y plane with respect to ω_z . Our results can be readily used as a benchmark for the cold atom experiment with similar experimental set-up. Supported by ARO and NSF.

1:39PM W4.00013 A Theory for Normal Fermi Gases at Unitarity, ERIK WEILER, THEJA DE SILVA, Binghamton University — In this study, we will develop a simple, yet accurate, mean-field-like theory for the normal phase of a unitarity Fermi gas. First, we derive a self-consistent equation for the self-energy using a momentum-dependent coupling constant. Using zero temperature Monte Carlo results as a starting point, we then derive an analytical expression for the momentum-dependent self-energy within one-step iteration. Lastly, we determine the validity of our analytical self-energy by comparing it to fully numerical calculations. Our theory shows excellent agreement with pressure measurements made by Nascimbene, *et al.* in a recent experiment performed by the ENS group.

Thursday, March 1, 2012 11:15AM - 2:03PM —
Session W5 DCMP: Thin Film Growth and Processing 206A

11:15AM W5.00001 Etch induced losses in high Q-value superconducting resonators, MARTIN SANDBERG, MICHAEL VISSERS, JEFF KLINE, MARTIN WEIDES, JIANSONG GAO, National Institute of Standards and Technology, Boulder, CO 80305, DAVID WISEBEY, Saint Louis University, St. Louis, Missouri 63103, DAVID PAPPAS, National Institute of Standards and Technology, Boulder, CO 80305 — We have investigated how the microwave loss in coplanar wave-guide titanium nitride resonators fabricated on Si wafers is affected by the choice of etch method used to pattern the resonators. Three different etches has been investigated, one fluorine based reactive etch, one chlorine based reactive ion etch, and one argon ion mill. At high microwave probe powers, the two different reactive etches show low internal loss whereas the milled samples show dramatically higher loss. At single photon powers we observe that the fluorine etch resonators exhibit substantially lower loss than the chlorine etched resonators. In the single photon limit we observe loss tangents of $1 \cdot 10^{-6}$ for the fluorine etched, $4 \cdot 10^{-6}$ to $5.5 \cdot 10^{-6}$ for the chlorine etch and $1.4 \cdot 10^{-4}$ for the argon ion mill. We compare these results to numerically calculated filling factors and find that the chlorine etch Si surface has a higher loss tangent than the fluorine etched surface. We also find that re-deposition of Silicon onto the titanium nitride surfaces is the probable cause of the high loss observed for argon ion milled resonators.

11:27AM W5.00002 ABSTRACT WITHDRAWN —

11:39AM W5.00003 Atomic Layer Deposition Films as Diffusion Barriers for Silver Artifacts¹

, AMY MARQUARDT, Department of Materials Science and Engineering, University of Maryland, College Park, MD, 20742, ERIC BREITUNG, Library of Congress, Washington D.C., TERRY DRAYMAN-WEISSER, GLENN GATES, Walters Art Museum, Baltimore, MD, GARY W. RUBLOFF, RAY J. PHANEUF, Department of Materials Science and Engineering, University of Maryland, College Park, MD, 20742 — Atomic layer deposition (ALD) was investigated as a means to create transparent oxide diffusion barrier coatings to reduce the rate of tarnishing for silver objects in museum collections. Accelerated aging by heating various thicknesses (5 to 100nm) of ALD alumina (Al_2O_3) thin films on sterling and fine silver was used to determine the effectiveness of alumina as a barrier to silver oxidation. The effect of aging temperature on the thickness of the tarnish layer (Ag_2S) created at the interface of the ALD coating and the bulk silver substrate was determined by reflectance spectroscopy and X-Ray Photoelectric Spectroscopy (XPS). Reflectance spectroscopy was an effective rapid screening tool to determine tarnishing rates and the coating's visual impact. X-Ray Photoelectric Spectroscopy (XPS), and Time of Flight Secondary Ion Mass Spectroscopy (ToF-SIMS) analysis showed a phase transformation in the Ag_2S tarnish layer at 177 °C and saturation in the thickness of the silver sulfide layer, indicating possible self-passivation of the tarnish layer.

¹Work supported by the NSF under SCIART collaborative research grant #DMR1041809.

11:51AM W5.00004 ABSTRACT WITHDRAWN —

12:03PM W5.00005 Normal versus anomalous roughening of electrodeposited Prussian Blue layers, ANDRE PASA, MARILIA ALAMINI, RENE DA SILVA, VINICIUS ZOLDAN, EDUARDO ISOPPO, Laboratorio de Filmes Finos e Superfícies, Departamento de Física, Universidade Federal de Santa Catarina, 88.040-900 Florianópolis, SC, Brazil, UBIRAJARA RODRIGUES-FILHO, Instituto de Química de São Carlos, USP, 13.564-970 São Carlos, SP, Brazil, FABIO AARAO REIS, Instituto de Física, Universidade Federal Fluminense, Av. Litorânea s/n, Niterói, RJ, 24210-340, Brazil, ALOISIO KLEIN, Laboratorio de Materiais, UFSC, C.P. 476, Florianópolis, SC, Brazil. — Electrochemically deposited Prussian Blue films on gold over silicon substrates are studied by various microscopy methods. Film surface features and roughness scaling suggest faceted anomalous roughening. However, accounting for the time increase of adsorption rate, which reduces surface diffusion lengths as the film grows, a scenario of diffusion-dominated growth (Mullins-Herring class) emerges. A significant effect of the diffusion-to-deposition ratio on the roughness scaling is found, consistently with the close packed surface morphology and formation of a film with single crystalline grains. That effect also explains the striking difference of exponents obtained from the anomalous and normal scaling interpretations.

12:15PM W5.00006 ABSTRACT WITHDRAWN —

12:27PM W5.00007 ABSTRACT HAS BEEN MOVED TO X50.00007 —

12:39PM W5.00008 Continuum Description of Atomistics for Nanomechanics of Grain Boundary Embrittlement in FCC Metals, K.-S. KIM, C.-K. WANG, M.-H. CHA, H. B. CHEW, School of Engineering, Brown University — A nonlinear field projection method has been developed to study nanometer scale mechanical properties of grain boundaries in nanocrystalline FCC metals [1]. The nonlinear field projection is based on the principle of virtual work, for virtual variations of atomic positions in equilibrium through nonlocal interatomic interactions such as EAM potential interaction, to get field-projected subatomic-resolution traction distributions on various grain boundaries. The analyses show that the field projected traction produces periodic concentrated compression sites on the grain boundary, which act as crack trapping or dislocation nucleation sites. The field projection was also used to assess the nanometer scale failure processes of Cu $\Sigma 5$ and $\Sigma 9$ grain boundaries doped with Pb. It was revealed that the most significant atomic rearrangement is dislocation emission which requires local GB slip, and some Pb locks the local GB slip and in turn, embrittles the GB. Reference: [1] C.-K. Wang, et al., 2011, *MRS Proceedings*, Vol. 1297, DOI: 10.1557/opl.2011.678.

12:51PM W5.00009 Coherent Surface X-ray Scattering: Observation of Pt (001) Step-Flow Motion, MICHAEL PIERCE, Department of Physics, Rochester Institute of Technology, DANIEL HENNESSY, KEE-CHUL CHANG, Materials Science Division, Argonne National Laboratory, VLADIMIR KOMANICKY, Faculty of Science, Safarik University, JOSEPH STRZALKA, ALEC SANDY, Advanced Photon Source, Argonne National Laboratory, ANDI BARBOUR, HOYDOO YOU, Materials Science Division, Argonne National Laboratory — We recently [1] observed oscillations of speckle intensities from the Pt (001) surface at high temperatures ($T > 1620\text{K}$), persisting for tens of minutes. Using a model of hex-reconstructed terraces we showed that the observed oscillations come from surface dynamics due to sublimation induced step-flow motion. Our results demonstrate the possibility that coherent surface x-ray scattering (CSXS) can be applied to monitor the real-time evolution of surfaces. Hopefully CSXS can be extended further to in-situ “real-world” environments. This work and the use of the Advanced Photon Source were supported by the U.S. DOE, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357. The work at Safarik University was supported by VEGA 1/0138/10 and VVCE-0058-007.

[1] M.S. Pierce, et al., *Appl. Phys. Lett.* 99, 121910 (2011).

1:03PM W5.00010 Study of Electrode Surface Dynamics Using Coherent Surface X-ray Scattering¹, HOYDOO YOU, Argonne National Laboratory, MICHAEL PIERCE, Rochester Institute of Technology, VLADIMIR KOMANICKY, Safarik University — We present successful efforts to develop a new surface x-ray scattering technique that allows in-situ measurements of surface dynamics in electrochemical systems. The technique, sensitive to the microstates of the system, can measure the transient dynamics of phase relaxation from one phase to another upon changing electrochemical conditions, as well as the equilibrium dynamics of microstates even if the electrode macroscopic state appears static. We will discuss the underlying physics of surface x-ray speckle correlation spectroscopy and present our recent study of Au (100) surface in vacuum, water, and electrolytes.

¹This work and the use of the Advanced Photon Source was supported by the U.S. DOE, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357. The work at Safarik University was supported by VEGA 1/0138/10 and VVCE-0058-007.

1:15PM W5.00011 Effect of tensile misfit dislocation on diffusion of Ni adatom on Ni/Cu(111): a Molecular Dynamics study¹, OLEG TRUSHIN, Yaroslavl Branch of the Institute of Physics and Technology of RAS, Yaroslavl, Russia, MARAL AMINPOUR, TALAT S. RAHMAN, Physics Department, University of Central Florida — We apply molecular dynamics and molecular static methods to calculate the effect of tensile misfit dislocation on Ni adatom diffusion for Ni/Cu(111) system and compare the results with those calculated previously for Cu adatom on the Cu/Ni(111) system [1] which has compressive dislocation. Our Ni/Cu(111) substrate model system consists of 5 layers of Ni on top of a 7-layer Cu(111) slab which after energy minimization displays an isolated misfit dislocation buried at the Cu-Ni interface, causing the Ni film to be under tensile stress. In contrast to the isotropic trajectory that emerges on a defect-free surface, in this tensile stressed system we find that presence of the defect under the surface strongly affects the adatom trajectory, introducing anisotropy in atomic diffusion similar to compressive system, but with the difference: tensile misfit dislocation enhances diffusion in the direction perpendicular to the misfit dislocation line and decreases it in the direction parallel to it, whereas compressive dislocation induces the opposite behavior. We present the calculated energy barriers for the adatom and compare them with adatom diffusion on defect – free and on the surface containing compressive dislocation.

[1] M. Aminpour, O. Trushin, and T. S. Rahman, Physical Review B, 84, 035455 (2011).

¹The work was supported in part by DOE grant No. FG0203ER46354.

1:27PM W5.00012 Enhancement of Ag Cluster Mobility on Ag(111) Surface by clustering with Chlorine¹, YU-NING WU, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida, USA, NOUARI KEBAILI, ALBERT MASSON, CATHERINE BRÉCHIGNAC, Laboratoire Aimé Cotton, CNRS-Université Paris Sud 11, France — Chlorine is observed to accelerate the fragmentation of Ag nanostructures deposited on graphite. To understand the role of chlorine in the stability of Ag nanostructures, we have studied the formation and diffusion of Ag_n and Ag_nCl_m (n = 1 to 4) clusters on Ag(111) surface, using density functional theory (DFT) with generalized gradient approximations (GGA) and the projector-augmented wave method. Our calculation shows that the formation energies and diffusion barriers of Ag_n clusters are both lowered by clustering with chlorine when n=1, 3 and 4, indicating the enhancement of mass transport on Ag(111) surface. (AgCl)_n clusters (n=1, 3 and 4) are good candidates for surface mass transport units. We have also studied a chloridized Ag₅₅ cluster and an Ag₅₅-Ag₅₅ neck structure. Chlorine is found to loosen the Ag₅₅ structure and weaken the binding between the Ag₅₅ bulbs in the neck structure.

¹US/DOE/BES/DE-FG02-02ER45995, DOE/NERSC and UF/HPC

1:39PM W5.00013 Growth and Characterization of Metal Oxides Layers on CVD Graphene, A. MATSUBAYASHI, J. ABEL, D.P. SINHA, J.U. LEE, V.P. LABELLA, College of Nanoscale Science and Engineering, University at Albany, State University of New York — Thin metal oxide layers deposited on graphene can be utilized as dielectric barriers between ferromagnetic metals and graphene to help overcome conductivity mismatch between the metal and graphene. Furthermore, these layers have been shown to increase the spin relaxation time measured utilizing non local detection and spin precession measurements. However, simply depositing metal oxide layers such as aluminum oxide on graphene results in non uniform film lowering the quality of the interface barrier. This presentation will show our work growing uniform aluminum oxide layers on graphene under ultra high vacuum conditions utilizing a Ti seed layer. The surface roughness of the films was measured with atomic force microscopy with and without titanium seed layers. The results show titanium seed layers reduced the surface roughness by a factor of 4 indicating a more uniform film. In addition, X-ray photoelectron spectroscopy results will be presented to confirm the stoichiometry of the films.

1:51PM W5.00014 Ab-initio study on stabilized ZnO (0001) polar surface with graphene substrate, GUO-HONG CHEN, HONG-JUN XIANG, XIN-GAO GONG, Fudan University — First-principles calculations have been performed on interfaces between zinc oxide (0001) surfaces and graphene layer. By modifying the initial interface configurations we have found the energetically stable interface structure. Results indicate that the unstable polar ZnO (0001) surface could be stabilized by the graphene layer. Further analyses show that the structure stabilization could be well understood by the charge transfer between the carbon atoms and oxygen atoms. This suggests that polar ZnO (0001) surfaces can be obtained in experiments by growing them on graphene substrates.

Thursday, March 1, 2012 11:15AM - 2:03PM –

Session W6 DMP: Focus Session: Carbon Nanotube Synthesis, Structure and Defects 206B

11:15AM W6.00001 Chirality selective growth of carbon nanotubes from one-dimensional fusion of aromatic compounds, HONG EN LIM, YASUMITSU MIYATA, RYO KITAURA, Nagoya University, HIROMICHI KATAURA, AIST, JST-CREST, HISANORI SHINOHARA, Nagoya University — We have investigated the formation of carbon nanotubes (CNTs) from one-dimensional coalescence of various polyaromatic compounds with different edge structures within an outer tube template. Transformation of the filled precursors into an inner tube was confirmed upon high-temperature thermal annealing. These newly formed inner tubes were then extracted through ultrasonication, as reported in our previous study [1]. High resolution transmission electron microscope observations of the samples together with the photoluminescence analyses of the extracted dispersions reveal that the chirality of the inner tubes generated were greatly affected not only by the edge structures but also by the intermediates formed. In particular, graphene nanoribbon-like intermediates obtained from perylene-derivative can be preferentially converted into near-zigzag CNTs with (8,1) chirality. The present method may provide the controlled growth of chiral-specific CNTs, which has been difficult to achieve using ordinary synthesis approaches.

[1] Y. Miyata, et al., ACS Nano 2010, 4, 5807.

11:27AM W6.00002 Hierarchical 3D microstructures from pyrolysis of epoxy resin, MICHAEL DE VOLDER, DOMINIEK REYNAERTS, KULeuven, CHRIS VAN HOOFF, IMEC, A. JOHN HART, University of Michigan — Nature is replete with examples of microscale dendrites connected to tree-like backbones ranging from the overall structures of trees to vascular networks. These branched structures have emerged as a result of an optimization between the maximization of a surface area and the minimization of transport losses. Elucidating these sophisticated designs proposed by nature is of paramount importance for the creation of higher-efficiency materials. The fabrication of such structures is however particularly challenging at small scale. In this paper, we focus on amorphous carbon microstructures, which provide a wide electrochemical stability window, excellent bio-compatibility, and cost-effective fabrication. However, relatively few methods have been developed for the fabrication of hierarchical amorphous carbon microstructures. Here we show that novel anisotropic microarchitectures comprising vertically aligned amorphous carbon nanowires CNWs can be made by oxygen plasma treatment of epoxy resins, followed by pyrolysis. Interestingly, these structures can also be shaped into deterministic three-dimensional (3D) hierarchical structures where nanowires are anchored to a micro-sized solid carbon core. These structures could play a key role in the development of new electrodes for micro-sensors, bioprobes, batteries, and fuel cells.

11:39AM W6.00003 Semiconducting nanotube dominant chemical vapor deposition synthesis of isopropanol carbon feedstock, YUCHI CHE, CHUAN WANG, JIA LIU, XUE LIN, University of Southern California, H.-S. PHILIP WONG, Stanford University, CHONGWU ZHOU, University of Southern California — The development of guided chemical vapor deposition (CVD) growth of single wall carbon nanotubes provides great platform for wafer-scale integration of aligned nanotube into circuits and systems. However, the co-existence of the metallic and semiconducting nanotubes is still a major problem for the development of carbon nanotube based nanoelectronics. To address this limitation, we developed a method to get semiconducting dominant nanotube by using isopropanol carbon feedstock. We achieved a purity of 87% of semiconducting nanotube growth, which was verified by measuring single nanotube transistors fabricated from aligned nanotube arrays. Besides, Raman spectrum was characterized to confirm the enhanced fraction of semiconducting nanotube as well. To further understand chemical mechanism of synthesis at atomic level, we performed the mass spectrum study and compared the measurement results from different carbon source. Furthermore, to discuss the future application of this synthesis method, we fabricated thin-film transistor from as-grown nanotube network. Transistor with on/off ratio over 104 and mobility up to 116 cm²/v•s was achieved, which shows great potential for thin-film transistor applications.

11:51AM W6.00004 Synthesis and Characterization of Carbon Nanotubes Produced From Thermal Decomposition of Nickelocene, HERBERT VINSON, BALEESWARAIAH MUCHHARLA, X. ZHANG, Southern Illinois University, Carbondale, AMÉLIA CHURCH, Rice University, Houston, VAIVA KRUNGLEVICIUTE, Southern Illinois University, Carbondale, S. KAR, Northeastern University, Boston, ALDO MIGONE, SAIKAT TALAPATRA, Southern Illinois University, Carbondale, SOUTHERN ILLINOIS UNIVERSITY, CARBONDALE COLLABORATION, NORTHEASTERN UNIVERSITY, BOSTON COLLABORATION — We have employed a direct thermal deposition technique, which used Nickelocene both as the catalyst as well as the carbon source, to grow films of carbon nanotubes (CNT). The CNT films obtained using this procedure were characterized using Transmission Electron Microscopy which indicated the presence of thin diameter carbon nanotubes as well as single walled CNT ropes. Volumetric adsorption measurements were performed to determine the porosity and specific surface areas of these samples. Electrical transport measurements performed on long ropes of CNTs extracted from these bulk films will be presented and will be discussed in the framework of transport theories of quasi-one dimensional systems.

12:03PM W6.00005 Covalently Functionalized Carbon Nanotubes for Electronics¹, DELPHINE BOUILLY, JANIE CABANA, FRANÇOIS MEUNIER, FRANÇOIS LAPOINTE, FRANCIS L. LAROCHE, MATTHIEU PAILLET, RICHARD MARTEL, Université de Montréal, MAXIME DESJARDINS-CARRIÈRE, PHILIPPE GAGNON, ELYSE ADAM, Ecole Polytechnique de Montréal, REGROUPEMENT QUÉBÉCOIS SUR LES MATÉRIAUX DE POINTE (RQMP) TEAM — Covalent chemistry on carbon nanotubes generates useful and stable functionalities, but it also generally damages their electronic properties, which is a critical drawback for device applications. Here we present two approaches to achieve covalent functionalization of carbon nanotubes without compromising on their electronic properties. For each case, we demonstrate the fabrication of functional carbon nanotube devices. First, double-walled carbon nanotubes (DWNTs) are functionalized using a monovalent reaction with aryldiazonium salts. Absorption and Raman spectroscopy along with electrical measurements show that the functionalization occurs strictly on the outer wall and preserves the optical and transport properties of the inner wall. Functionalized-DWNT devices are operated with similar characteristics as pristine single-walled carbon nanotube (SWNT) devices [1]. Second, SWNTs are functionalized with different addends using a divalent carbene reaction. For both metallic and semiconducting species, electrical measurements of numerous functionalized and unfunctionalized SWNT devices show identical characteristics. Ref: [1] Bouilly D. et al. ACS Nano, 5 (6), 4927 (2011)

¹NSERC Vanier Scholarship and Canada Research Chairs (CRC) funding is acknowledged.

12:15PM W6.00006 Mechanocapillary forming of carbon nanotube microstructures, A. JOHN HART, University of Michigan — The hierarchical structure and organization of filaments within both natural and synthetic materials can determine a wide variety of collective chemical and physical functionalities. Carbon nanotubes (CNTs) are known for their record properties, and densely packed CNTs are therefore expected to enable new materials having outstanding multifunctional performance. However, it remains a significant challenge to build highly ordered assemblies of CNTs, and this challenge has largely limited the design and properties of macroscale CNT yarns and sheets, and CNT-based surfaces and interfaces. We have created a versatile technique called *capillary forming* to manipulate patterned vertically aligned (VA-) CNTs into diverse 3D microarchitectures, and to enable their integration in applications ranging from microsystems to macroscale functional films. Capillary forming relies on shape-directed capillary rise during solvent condensation, followed by evaporation-induced shrinkage. Three-dimensional transformations result from shrinkage of the vapor-liquid-solid interface and the resulting heterogeneous strain distribution in the microstructures. A portfolio of microscale CNT assemblies with highly ordered internal structure and freeform geometries including straight, bent, folded and helical profiles, are fabricated using capillary forming. The mechanical stiffness and electrical conductivity of capillary formed CNT micropillars are 5 GPa and 10⁴ S/m respectively. These values are at least hundred-fold higher than as-grown CNT forests and exceed the properties of typical microfabrication polymers. Finally, the potential applications of these structures are demonstrated as vertical microsprings with geometrically tunable compliance, and hydrogel-driven microtransducers.

12:51PM W6.00007 *Ab initio* studies of defects in carbon nanofoam structures¹, DAVID TOMANEK, ZHEN ZHU, Michigan State University, ARKADY KRASHENINNIKOV, University of Helsinki — We combine *ab initio* density functional and GW calculations to study the stability, electronic and elastic properties of hypothetical cellular foam-like carbon nanostructures. These systems with a mixed sp²/sp³ bonding character are structurally related to bundles of carbon nanotubes. The cross-sectional honeycomb structure may accommodate the same type of structural defects as the honeycomb lattice of graphene. The infinite 3D foam structure is a narrow-gap semiconductor, with the binding energy of atoms nearly 0.5 eV lower than graphene. Quasi-2D layered foam structures of finite thickness may be stabilized by terminating caps. When exposed to hydrostatic pressure, the unit cells of the foam deform significantly from their initially hexagonal shape.

¹Supported by the National Science Foundation Cooperative Agreement #EEC-0832785, titled “NSEC: Center for High-rate Nanomanufacturing”.

1:03PM W6.00008 Energetical Stability of Near-Armchair Carbon Nanotubes: A Systematic First-Principles Study, KOICHIRO KATO, TAKASHI KORETSUNE, SUSUMU SAITO, Department of Physics, Tokyo Institute of Technology — We perform the systematic first-principles study of 57 kinds of carbon nanotubes (CNTs) and investigate the energetical stability of so-called “near-armchair” CNTs. The density functional theory computational code which utilizes the helical symmetry and has been developed in our group is extensively used in the present work. Because the computational effort can be drastically reduced by using the helical symmetry of CNTs, the systematic study of fully-optimized CNTs including the experimentally abundant CNTs was finally achieved in this work. As a result, it is found that “near-armchair” CNTs including (6,5) and (7,5) CNTs are energetically more stable than other CNTs. This result corresponds well with the high abundance of these near-armchair CNTs experimentally reported so far. In addition, by performing the systematic analysis of CNT bond-lengths and angles, the presence of the geometrical family pattern after their structural optimizations has been revealed for the first time. It is also confirmed that the geometrical optimization plays a very important role in predicting electronic structures of chiral CNTs as well as achiral CNTs. The fundamental gap corrections associated with the geometrical optimizations are sizable even in one nm diameter CNTs.

1:15PM W6.00009 Diameter and Chiral Selective Purification of SWNT and DWNT Using CO₂, PHILIPPE GAGNON, MAXIME BIRON, MAXIME DESJARDINS-CARRIERE, Ecole Polytechnique de Montreal, EMMANUEL FLAHAUT, Université Paul Sabatier, PATRICK DESJARDINS, Ecole Polytechnique de Montreal, RICHARD MARTEL, Université de Montreal — Oxidation of carbon nanotubes in air is a well known method to eliminate carbonaceous impurities from raw material. Recently, it has also been used to selectively remove single-wall carbon nanotubes (SWNT) present in double-walled carbon nanotubes (DWNT) soot[1]. Here, we propose a more efficient purification process for both SWNT and DWNT based on a high temperature oxidation in a pure CO₂ gas flow. This treatment, combined with a standard reflux in nitric acid, provides fast oxidation of amorphous carbon and removal of other impurities without affecting the structure of the carbon nanotubes. Parameterization of the treatment allowed us to observe both diameter and chirality dependence of the nanotubes reaction rate with CO₂. This selective character was applied to produce thin films of clean and highly enriched DWNT and of semiconducting SWNT. Microscopy and spectroscopy analyses will be shown and reveal that those films are composed of very high quality carbon nanotubes (micrometers long, very low impurity and catalyst concentration, low Raman I_D/I_G ratios). Also, no significant nanotube shortening is observed following the different diameter or chirality enrichment treatments.

[1] K. Iakoubovskii et al., J. Phys. Chem. C, 112, 30 (2008)

1:27PM W6.00010 Radial Elasticity Measurement of Single-walled Carbon Nanotubes by Atomic Force Microscopy¹, YUEHAI YANG, WENZHI LI, Department of Physics, Florida International University, CONDENSED MATTER PHYSICS TEAM — By applying well-calibrated tapping mode and contact mode AFM upon horizontally aligned SWCNTs grown directly on quartz substrates, we have obtained effective radial modulus (E_{radial}) of SWCNTs with diameters less than 2 nm. The measured E_{radial} decreases from 57 to 9 GPa with the increase of the SWCNT diameter from 0.92 to 1.91 nm. Our experimental result is consistent with the computational data obtained using the modified molecular structure mechanics model. We have also compared our measurements with the reported experimental results obtained on SWCNTs with diameters from 2 to 3 nm. Our measurements of large diameter SWCNTs (diameter close to 2nm) are in agreement with the reported data and modeling. However, our measurements of SWCNTs with smaller diameters deviate from this previous study. This has been explained by the compressibility of the substrate and the AFM tip. By employing Hertzian theory, we specifically exploit the components of deformation of the AFM tip-SWCNT-substrate system. Further calculation using our measured E_{radial} indicates that under the same normal force the deformation of our quartz-SWCNT-silicon tip system can be as much as 96% more than the deformation of the SWCNT compressed between a rigid substrate and an AFM tip.

¹This work is supported by the National Science Foundation under grant DMR-0548061.

1:39PM W6.00011 ABSTRACT WITHDRAWN —

1:51PM W6.00012 Synthesis and high temperature stability of amorphous Si(B)CN-MWCNT composite nanowires, ROMIL BHANDAVAT, GURPREET SINGH, Kansas State University — We demonstrate synthesis of a hybrid nanowire structure consisting of an amorphous polymer-derived silicon boron-carbonitride (Si-B-C-N) shell with a multiwalled carbon nanotube core. This was achieved through a novel process involving preparation of a boron-modified liquid polymeric precursor through a reaction of trimethyl borate and polyureasilazane under atmospheric conditions; followed by conversion of polymer to glass-ceramic on carbon nanotube surfaces through controlled heating. Chemical structure of the polymer was studied by liquid-NMR while evolution of various ceramic phases was studied by Raman spectroscopy, solid-NMR, Fourier transform infrared and X-ray photoelectron spectroscopy. Electron microscopy and X-ray diffraction confirms presence of amorphous Si(B)CN coating on individual nanotubes for all specimen processed below 1400 degree C. Thermogravimetric analysis, followed by TEM revealed high temperature stability of the carbon nanotube core in flowing air up to 1300 degree C.

Thursday, March 1, 2012 11:15AM - 2:15PM —

Session W7 DMP: Focus Session: Graphene Devices - Mechanical Effects 207

11:15AM W7.00001 Nanomechanical Field-Effect Magnetometry in Graphene¹, JAMES HONE, Columbia University — This presentation will describe our studies of graphene nanomechanical resonators in the quantum Hall (QH) regime. We observe strong magneto-mechanical coupling to de Haas-van Alphen oscillations of magnetization, resulting in oscillatory frequency shifts of up to 1 MHz. This response is over two orders of magnitude larger than the expected response in a “standard” torque magnetometry framework. Instead, we find that the electric field-effect modulation of the magnetic energy provides a gradient force without a magnetic field gradient. Modeling of the effect produces excellent agreement with experiment, using only the disorder as a free parameter. We further use this novel mechanism to quantify the many-body exchange interaction of broken-symmetry QH states. This new mechanism may prove to be a useful tool for magnetic studies across low-dimensional materials and in sensing applications.

¹The author acknowledges support from Air Force Office of Scientific Research Grant No. MURI FA955009-1-0705

11:51AM W7.00002 High frequency graphene resonators¹, KEVIN FISCHER, BRITT BAUGHER, TCHEFOR NDUKUM, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — We study mechanical resonance properties of suspended graphene devices through radio frequency electromechanical downmixing techniques. Taking advantage of graphene's atomically thin nature, unusually large transconductance, and extremely high Young's Modulus, we have fabricated high-frequency suspended graphene resonators. Our global-gate devices have resonated at over 500MHz in a low temperature environment with reasonable quality factors. This research will pave the way for high-quality resonators in the GHz regime which will be used in high frequency applications such as ultra high sensitive mass, chemical and charge detectors.

¹MIT Center for Materials Science and Engineering, ONR, NSF

12:03PM W7.00003 Optical Detection of Vibrations and Mass Loading of Graphene Mechanical Resonators Compatible with TEM and AFM, BENJAMIN ALEMAN, MICHAEL ROUSSEAS, YISHENG YANG, WILL REGAN, FENG WANG, ALEX ZETTL, University of California, Berkeley — We produce arrays of exceptionally clean, suspended graphene mechanical resonators in high-yield using a simple, polymer-free procedure by transferring CVD-graphene to a flexible perforated substrate. The lack of a backing substrate facilitates Transmission Electron Microscopy (TEM) characterization, yet the membranes are still compatible with Atomic Force Microscopy (AFM) studies. We detect mechanical vibrations of resonators through optical interferometry and find excellent agreement with a theoretical model based on the 2D wave equation. We find quality factors of 1.25 μm diameter circular membranes to be as high as $Q \sim 800\text{--}1000$ at room temperature, and observe lifting of mode degeneracies in square membranes. TEM and AFM studies reveal graphene folding, nanoparticle contamination, holes, tears, and other defects that can lead to the observed degeneracy splitting in square membranes. Controlled mass loading is also explored to suppress certain vibrational modes and tune vibrational frequencies for possible high density archival memory applications. The graphene membrane devices reported here open up a host of new possibilities for correlating TEM and AFM studies of an individual graphene membrane to its performance and properties as a mechanical resonator.

12:15PM W7.00004 Graphene xylophone: Mechanical properties of graphene based nano resonators¹, SANG WOOK LEE, HAKSEONG KIM, HOYEOL YUN, JEONG-AH LEE, Konkuk University, YOUNGWOOK KIM, JUN SUNG KIM, POSTECH — Mechanical properties of graphene xylophone structure were investigated. The arrays of the graphene ribbon patterns were prepared using nano lithography and suspended graphene structure was realized on the pre-patterned trench by the micro contact transfer printing method. Xylophone like structure was prepared for studying length and thickness dependence of mechanical properties of graphene resonator. The various mechanical behaviors, such as frequency tuning, non-linearity and bistability of single, bi and multi layer graphene structure will be discussed in this presentation. The potential application of our graphene xylophone structure for RF component will be suggested in the end of this presentation.

¹This work was supported by NRF, WCU, and BK21

12:27PM W7.00005 Cavity Optomechanics with Graphene Resonators, ROBERT BARTON, ISAAC STORCH, VIVEKANANDA ADIGA, Cornell University, REYU SAKAKIBARA, University of California Berkeley, SI PING WANG, PEIJIE ONG, B. ILIC, Cornell University, PAUL MCEUEN, Kavli Institute, Cornell University, JEEVAK PARPIA, HAROLD CRAIGHEAD, Cornell University — Optical manipulation of micromechanical and nanomechanical resonators promises control of quantum states of macroscopic systems, among other applications. Because the spring constant of a resonator scales with its mass, there are advantages associated with using the lightest possible membranes as the mechanical elements. Here, we demonstrate that graphene, a one-atom-thick membrane, can be used as the mechanically active part of an optomechanical system. We show that a laser coupled to a Fabry-Perot cavity between a graphene resonator and a reflective backplane can both enhance and damp graphene motion. The enhancement of resonator motion is sufficient to induce self-oscillation, which is useful for applications in sensing and signal processing. These experiments demonstrate that graphene resonators are useful for optomechanical applications and show promise for resonator cooling toward the quantum ground state.

12:39PM W7.00006 Ultrathin circular membranes with high quality factors, VIVEKANANDA ADIGA, School of Applied and Engineering Physics, Cornell University, ROB ILIC, Cornell Nanofabrication Facility, ROB BARTON, School of Applied and Engineering Physics, Cornell University, JEEVAK PARPIA, Physics Department, Cornell University, HAROLD CRAIGHEAD, School of Applied and Engineering Physics, Cornell University — We have fabricated large ultrathin circular drum resonators from monolayer graphene (up to 90 μm in diameter) and silicon nitride ($\sim 15\text{ nm}$, up to 1mm in diameter). Resonant frequency, quality factor (Q) of different modes of these self tensioned graphene drums and high tensile stress ($\sim 1\text{ GPa}$) silicon nitride were measured using optical interferometric detection technique. We measured extremely high quality factors (up to 5,000 for graphene and up to 4,000,000 for ultrathin silicon nitride membranes) at room temperature. High quality factors observed in these resonators indicate dissipation mechanisms which differ from the conventional high surface to volume ratio resonators that show very low quality factors. The measured mechanical dissipation (Q^{-1}) shows a strong size and modal dependence, possibly indicating the influence of clamping losses in these tensioned membranes. These findings pave the way for identifying optimum size and modes for achieving high Q oscillators for applications in mass sensing and optomechanical coupling experiments which are underway.

12:51PM W7.00007 Novel Fabrication Techniques for Wafer-Scale Graphene Drum Nano-ElectroMechanical Resonators, SUNWOO LEE, CHANGYAO CHEN, VIKRAM V. DESHPANDE, GWAN HYOUNG LEE, Columbia University, ISAAC STORCH, Cornell University, CONGCHUN ZHANG, YOUNG-JUN YU, PHILIP KIM, Columbia University, PAUL MCEUEN, Cornell University, JAMES HONE, Columbia University — Graphene NanoElectroMechanical Systems (NEMS) have shown excellent mass sensitivity as well as resonant and oscillatory behaviors that are desirable in mass sensors and active elements in Radio Frequency Integrated Circuit (RFIC) design. Out of many structures proposed for graphene NEMS, it has been recently shown that a drum resonator exhibits higher Q-factor than other structures such as a bar resonator. However, fabricating a large array of drum graphene resonator has been problematic because liquid or gas can be trapped inside the drum. Such issues led to designs with a hole in the center of a drum or with a drainage trench, either at the cost of additional lithography step or lowered Q-factor. Here, we demonstrate two novel fabrication methods that are free of the trapping without any compromise in additional lithography step or Q-factor degradation. In one method, wafer scale graphene is dry-stamped on prefabricated leads, holes and local gates. In the other method, an resist strip with a circular hole at the center holds graphene underneath. I will discuss direct electrical readout and characterization of devices using these two methods. These drum structures may provide a practical way to achieve wafer scale high Q graphene NEMS.

1:03PM W7.00008 Graphene NanoElectroMechanical Oscillator, CHANGYAO CHEN, VIKRAM DESHPANDE, SUNWOO LEE, PHILIP KIM, JAMES HONE, Columbia University — Graphene based NanoElectroMechanical Systems (NEMS) working in Radio Frequency (RF) regime possess considerable advantages own to the remarkable electrical and mechanical properties of this atomic thin material. Here we demonstrated self-sustained nanoelectromechanical oscillator made from graphene. Our recent developed transduction scheme enables the direct conversion from mechanical motion to electrical domain, then subsequently being fed back to the system as excitation. The absence of extra RF actuation and the stable performance shows the possibility of practical application of graphene oscillator, for example, as signal filters, mass sensors or timing devices.

1:15PM W7.00009 Uniaxially Strained Graphene Resonators, HIRAM CONLEY, KIRILL BOLOTIN, Vanderbilt University — Strained graphene allows one to explore the connection between the mechanical and electrical properties of graphene. Exploring this interplay between the mechanical and electrical properties in graphene may enable tuning graphene's mechanical and electrical properties as well as opening up new exotic electronic states. We have developed a technique to fabricate uniaxial strained graphene transistors and mechanical resonators with strains as high as 0.5%. We demonstrate how strain perturbs both the mechanical and electrical properties of graphene, highlighted by the strain quenching of flexural phonons.

1:27PM W7.00010 Local Optical Probe of Motion and Stress in a NEMS, ANTOINE RESERBAT-PLANTEY, LAËTITIA MARTY, OLIVIER ARCIZET, NEDJMA BENDIAB, VINCENT BOUCHIAT, Institut Néel CNRS, DEP NANO TEAM — Nanoelectromechanical systems (NEMSs) are emerging nanoscale elements at the crossroads between mechanics, optics and electronics, with significant potential for actuation and sensing applications. The reduction of dimensions compared to their micronic counterparts brings new effects including sensitivity to very low mass, resonant frequencies in the radiofrequency range, mechanical non-linearities and observation of quantum mechanical effects. An important issue of NEMS is the understanding of fundamental physical properties conditioning dissipation mechanisms, known to limit mechanical quality factors and to induce aging due to material degradation. There is a need for detection methods tailored for these systems which allow probing motion and stress at the nanometer scale. Here, we show a non-invasive local optical probe for the quantitative measurement of motion and stress within a multilayer graphene NEMS provided by a combination of Fizeau interferences, Raman spectroscopy and electrostatically actuated mirror. Interferometry provides a calibrated measurement of the motion, resulting from an actuation ranging from a quasi-static load up to the mechanical resonance while Raman spectroscopy allows a purely spectral detection of mechanical resonance at the nanoscale. Such spectroscopic detection reveals the coupling between a strained nano-resonator and the energy of an inelastically scattered photon, and thus offers a new approach for optomechanics.

1:39PM W7.00011 Nonlinear Damping Mechanism in Mechanical Graphene Resonators. , ALEXANDER CROY, DANIEL MIDTVEDT, ANDREAS ISACSSON, JARI M. KINARET, Chalmers University of Technology — Based on a continuum mechanical model for single-layer graphene¹ we propose and analyze a microscopic mechanism for dissipation in nano-electromechanical graphene resonators. We find that coupling between flexural modes and in-plane phonons leads to linear and nonlinear damping of out-of-plane vibrations. By tuning external parameters, such as static gate voltage, one can cross over from a linear to a nonlinear-damping dominated regime. We discuss how the effective quality factor depends on parameters such as temperature, and compare our results with recent experiments.

¹J. Atalaya, A. Isacsson, and J. M. Kinaret, Nano Letters 8, 4196 (2008).

1:51PM W7.00012 Graphene Nanoelectromechanical Systems are Unique¹ , TCHEFOR NDUKUM, BRITT BAUGHER, KEVIN FISCHER, PABLO JARILLO-HERRERO, MIT — Graphene Nanoelectromechanical systems (GNEMS) with their light mass show a lot of interesting novel physics effects compared to conventional Nanoelectromechanical systems (NEMS). Superior gate tunability of the order of $>10\text{MHz/V}$ at room temperature as well as high quality factors of $\sim 10^5$ at mK temperatures for the fundamental mode have already been obtained. Studying their high frequency modes, we have observed for the first time avoided crossing between graphene modes as well as between graphene modes and their suspended contacts. In addition we have studied the atypical variation of the mode dispersion versus gating resulting from tensioning and electrostatic coupling to the gate. In particular, we measure an additional frequency shift near 0Vg which could be due to a strong electromechanical coupling near the Dirac Point.

¹NSF, ONR, CMSE

2:03PM W7.00013 Current-induced forces in graphene-based nanoelectromechanical systems , SILVIA VIOLA KUSMINSKIY, Dahlem Center for Complex Quantum Systems - Freie Universität Berlin — Transport currents have distinct effects on the vibrational dynamics of nanoelectromechanical systems. Recently, we have developed a comprehensive scattering-matrix approach to treat out-of-equilibrium current-induced forces [c.f. Phys. Rev. Lett. 107, 036804 (2011)]. We apply our method to the vibrational dynamics of a suspended graphene membrane, paying special attention to the different coupling mechanisms between Dirac fermions and flexural modes in graphene.

Thursday, March 1, 2012 11:15AM - 2:15PM – Session W8 DMP GMAG: Focus Session: Frustrated Magnetism - Pyrochlore lattice 208

11:15AM W8.00001 Topological phases in $\text{R}_2\text{Ir}_2\text{O}_7$, GANG CHEN, MICHAEL HERMELE, CU Boulder — We construct and analyze a theoretical model for the pyrochlore iridates $\text{R}_2\text{Ir}_2\text{O}_7$ with R ($= \text{Pr}, \text{Nd}, \text{Sm}, \text{Gd}, \text{Tb}, \text{Dy}, \text{Ho}, \text{Yb}$) magnetic. The electrons on trivalent rare earth ions R^{3+} form local Ising doublets due to the local crystal field. Based on a space group symmetry analysis, we write down the generic Kondo coupling between the Ising spin at R sites and the effective spin at Ir sites. Besides this interaction, we also include direct electron tunneling between Ir sites and indirect electron tunneling via intermediate oxygens for Ir-Ir coupling. This simple minimal model gives a rich phase diagram with broad regions of topological semi-metal and axion insulator phases. Based on these findings, we propose $\text{R}_2\text{Ir}_2\text{O}_7$ to be one of the most promising candidates to realize the topological semi-metal and axion insulator phases. Implications for existing and future experiments are discussed.

11:27AM W8.00002 Muon Spin Relaxation Studies of Pyrochlore Iridates $\text{R}_2\text{Ir}_2\text{O}_7$, ($\text{R} = \text{Y}, \text{Yb}$, and Nd) , STEVEN DISSELER, CHETAN DHITAL, STEPHEN WILSON, Boston College, SEAN GIBLIN, ISIS-RAL, ALEX AMATO, CHRIS BAINES, Paul Scherrer Institute, MICHAEL GRAF, Boston College — We report results for zero field muon spin relaxation measurements over the range $2\text{ K} < T < 220\text{ K}$ taken at the ISIS facility for three members of the pyrochlore iridate family, $\text{R}_2\text{Ir}_2\text{O}_7$, comprised of both magnetic ($\text{R} = \text{Yb}, \text{Nd}$) and non-magnetic ($\text{R} = \text{Y}$) species. The formation of a static internal field is detected via a loss of asymmetry below the bifurcation temperature observed in magnetic susceptibility for all three compounds. We will present results describing the nature of this internal field based on short time muon depolarization data taken at PSI. Longitudinal field measurements reveal the internal field is of order 1000 G for all three materials, and the existence of dynamic fluctuations at 2 K for $\text{R} = \text{Yb}, \text{Nd}$; the depolarization is quasistatic near 2 K for $\text{R} = \text{Y}$. We discuss these results as applied to understanding the unusual magnetic and transport properties observed in the iridate family, and the implications regarding long range magnetic order and the low temperature ground state.

11:39AM W8.00003 Chiral RKKY interaction in $\text{Pr}_2\text{Ir}_2\text{O}_7$, REBECCA FLINT, T. SENTHIL, Massachusetts Institute of Technology — $\text{Pr}_2\text{Ir}_2\text{O}_7$ experimentally realizes a chiral spin liquid selected out of a degenerate quantum spin-ice manifold. We propose that such a chiral state is selected by an analogue of the magnetic RKKY effect, whereby the chiral fluctuations of conducting Ir electrons close to a Mott transition promote correlations between the chirality of the local Pr moments. $\text{Pr}_2\text{Ir}_2\text{O}_7$ provides the perfect setting for such a *chiral RKKY* effect, as its spin ice manifold naturally contains chiral states, and chiral fluctuations in the Ir are enhanced by the proximity to the metal insulator transition between $\text{Pr}_2\text{Ir}_2\text{O}_7$ and $\text{Nd}_2\text{Ir}_2\text{O}_7$. We calculate the chiral susceptibility within a simplified model, showing that this chiral RKKY coupling can be ferro-chiral and estimating the magnitude.

11:51AM W8.00004 Emergent spin superstructures and degeneracy in models of itinerant magnets , SANJEEV KUMAR, Indian Institute of Science Education and Research (IISER) Mohali, Knowledge City, Sector 81, Mohali 140306 India, JOERN VENDERBOS, MARIA DAGHOFER, JEROEN VAN DEN BRINK, Institute for Theoretical Solid State Physics, IFW Dresden, 01171 Dresden, Germany — In recent years, there has been immense research interest in frustrated magnets with metallic character, such as the pyrochlores $\text{R}_2\text{Mo}_2\text{O}_7$, where R denotes a rare-earth element (Science **291**, 2573 (2001)). The frustration in magnetic sector in such systems can have interesting consequences for the electronic properties. More interestingly, the electronic degree of freedom can aid the system in selecting unconventional magnetic states. Motivated by these possibilities we investigate the double-exchange model with competing super-exchange interactions on various lattices. On a triangular lattice we find a novel chiral spin state to be the ground state at half filling (PRL **105**, 216405 (2010)). On checkerboard and Kagome lattices, the itinerant electrons play a crucial role in lifting the degeneracy of the magnetic sector and select specific ground states with intriguing superstructures. A very interesting effect takes place on a honeycomb lattice, where a Yafet-Kittel type magnetic structure emerges from the interplay between the super-exchange and double-exchange interactions (PRL **107**, 076405 (2011)). Some of these emergent spin states have a macroscopic degeneracy related to a symmetry which is intermediate between local and global.

12:03PM W8.00005 Resolving magnetic frustration in a Laves lattice , JIYANG WANG, University of Chicago, YEJUN FENG, Argonne National Laboratory, RAFAEL JARAMILLO, Harvard University, JASPER VAN WEZEL, Argonne National Laboratory, PAUL CANFIELD, Ames Laboratory, THOMAS ROSENBAUM, University of Chicago — CeFe_2 is a ferromagnet that exhibits antiferromagnetic fluctuations in its ground state. We use x-ray diffraction and diamond-anvil-cell techniques to directly measure the transition to antiferromagnetism in pure CeFe_2 at high pressure which couples to the change in the lattice symmetry. Numerical simulations are adopted to identify the magnetic structure of the ground states and to quantitatively illustrate effects of competing magnetic energy scales and geometrical frustration on the magnetic phase diagram. Comparison of phase transitions under both chemical substitution and applied pressure suggests a general solution to the physics of Laves phase magnets.

12:15PM W8.00006 Neutron Diffraction Investigation of Magnetic and Orbital Order in FeV_2O_4 , G.J. MACDOUGALL, A.A. ACZEL, V.O. GARLEA, Oak Ridge National Laboratory, Oak Ridge, TN, H.D. ZHOU, National High Magnetic Field Laboratory, Tallahassee, FL, S.E. NAGLER, Oak Ridge National Laboratory, Oak Ridge, TN — The vanadium spinels, AV_2O_4 , with divalent cations on the diamond sublattice are model magnetic systems for the study of interacting orbital, lattice and spin degrees of freedom. Studies of both systems with diamagnetic (e.g. Zn^{2+} , Cd^{2+} , Mg^{2+}) and spin-only (e.g. Mn^{2+}) cations on the A-site sublattice have revealed multiple phase transitions and ground state properties heavily influenced by V^{3+} orbital degrees-of-freedom. I will report on neutron powder diffraction measurements of another spinel system, FeV_2O_4 , which additionally has two-fold orbitally degenerate Fe^{2+} cations on the A-site sublattice. Previous x-ray and Mossbauer studies have reported four structural phase transitions in this material and at least one magnetic transition. Our data confirm the existence of three structural transitions and reveal distortions of local polyhedra with important implications for orbital order. We confirm the existence of hypothesized collinear antiferromagnetism below a temperature $T_{N1}=110\text{K}$ and further identify a second magnetic transition at $T_{N2}=60\text{K}$ where V^{3+} moments cant away from the Fe^{2+} spin direction to form a 2-in-2-out spin structure on the pyrochlore sublattice. I will discuss these observations in the context of recent predictions for orbital order in vanadate spinels.

12:27PM W8.00007 Universal exchange-driven phonon splitting, JOACHIM DEISENHOFER, Augsburg University, CHRISTIAN KANT, Technical University of Vienna, MICHAEL SCHMIDT, ZHE WANG, FRANZ MAYR, VLADIMIR TSURKAN, ALOIS LOIDL, Augsburg University — We report on a linear dependence of the phonon splitting on the non-dominant exchange coupling J_{nd} in the antiferromagnetic monoxides MnO , $\text{Fe}_{0.92}\text{O}$, CoO and NiO , and in the highly frustrated antiferromagnetic spinels CdCr_2O_4 , MgCr_2O_4 and ZnCr_2O_4 . For the monoxides our results directly confirm the theoretical prediction of a predominantly exchange induced splitting of the zone-centre optical phonon [1,2]. We find the linear relation $\hbar\Delta\omega = \beta J_{nd} S^2$ with slope $\beta = 3.7$. This relation also holds for a very different class of systems, namely the highly frustrated chromium spinels. Our finding suggests a universal dependence of the exchange-induced phonon splitting at the antiferromagnetic transition on the non-dominant exchange coupling [3].

[1] S. Massidda et al., Phys. Rev. Lett. 82, 430 (1999).

[2] W. Luo et al., Solid State Commun. 142, 504 (2007).

[3] Ch. Kant et al., arxiv:1109.4809.

12:39PM W8.00008 First-principles study of the structural and magnetic phase transition in CdCr_2O_4 , ANIL KUMAR, KARIN RABE, Rutgers University — We use first-principles calculations to investigate the mechanism for the paramagnetic (PM) cubic to an antiferromagnetic (AFM) tetragonal structural phase transition at 7.8 K in the spinel oxide compound CdCr_2O_4 . Because of the magnetic frustration associated with AFM interactions on the pyrochlore lattice formed by the Cr ions, we focus on the spin-lattice coupling, specifically (a) the forces on the atoms and resulting atomic displacements induced by the spin configuration and (b) the spin-phonon coupling. Using the linear response method, we determine the full phonon dispersion relations for the PM, FM and AFM orderings in cubic and tetragonal structures. We determine the strength of spin-phonon couplings using IFCs for various magnetic orderings and show that the spin-phonon couplings are large but do not lead to any unstable modes that could alone drive the structural transition at low temperatures. Instead, we find that it is the symmetry-lowering forces and stresses induced by AFM ordering that drive the cubic to tetragonal phase transition at low temperature. The results are compared with a recent experimental determination of the phonon dispersion in the cubic and tetragonal phases of CdCr_2O_4 and the implications for related compounds discussed.

12:51PM W8.00009 Frustration and Jahn-Teller ordering in magnetic spinel oxides, MOUREEN KEMEL, STEPHANIE MOFFITT, University of California, Santa Barbara, MATTHEW SUCHOMEL, DANIEL SHOEMAKER, Argonne National Laboratory, RAM SESHADRI, University of California, Santa Barbara — Geometrically frustrated magnetic systems have become extremely important for the study of novel phenomena often present in highly degenerate magnetic ground states. Extensive study of the canonically frustrated ZnCr_2O_4 and MgCr_2O_4 has increased the understanding of frustration in three-dimensional systems, however little is known about the structural effect of dilute magnetism on the A site. We present the effects on magneto-structural coupling of dilute magnetic cations on the diamagnetic A site of ZnCr_2O_4 and MgCr_2O_4 . In ZnCr_2O_4 and MgCr_2O_4 , a spin-driven structural distortion concomitant with the onset of long-range magnetic order resolves the large ground state degeneracy at temperatures far below the theoretical Curie-Weiss temperature. Employing variable temperature high-resolution synchrotron powder diffraction studies and magnetic susceptibility measurements, we show the changes in spin-lattice coupling in the solid solutions $\text{Zn}_{1-x}\text{Co}_x\text{Cr}_2\text{O}_4$, $\text{Zn}_{1-x}\text{Cu}_x\text{Cr}_2\text{O}_4$ and $\text{Mg}_{1-x}\text{Cu}_x\text{Cr}_2\text{O}_4$ for $x \leq 0.2$. These results highlight the effect of dilute A site magnetism on magnetic frustration as well as the role of dilute Jahn-Teller active Cu^{2+} on spin-lattice coupling in these frustrated systems.

1:03PM W8.00010 Ultrasound Velocity Measurements in the Geometrically Frustrated Spinel MgCr_2O_4 , TADATAKA WATANABE, Department of Physics, College of Science and Technology (CST), Nihon University, Chiyoda, Tokyo 101-8308, Japan, YUSUKE KOUSAKA, Department of Physics and Mathematics, Aoyama-Gakuin University, Sagami-hara, Kanagawa 229-8558, Japan, KEISUKE TOMIYASU, Department of Physics, Tohoku University, Aoba, Sendai 980-8578, Japan — Magnesium chromite spinel MgCr_2O_4 is a geometrically frustrated magnet with the Néel temperature $T_N \simeq 13\text{ K}$, and the Weiss temperature $\theta_W = -390\text{ K}$. Recent inelastic neutron scattering experiments provided a compelling evidence for the spin molecular ground states in not only the paramagnetic phase but also the antiferromagnetic phase. We performed ultrasound velocity measurements of MgCr_2O_4 in all the symmetrically independent elastic moduli of C_{11} , $(C_{11} - C_{12})/2$, and C_{44} . Temperature dependence of all of these elastic moduli exhibits a remarkable softening in the paramagnetic phase. Taking into account the absence of orbital degrees of freedom in Cr^{3+} ($3d^3$) in MgCr_2O_4 , the spin degrees of freedom should play a significant role for the elastic softening. The most probable origin for the elastic softening in the paramagnetic phase is the strong coupling of the acoustic phonons to the molecular spin fluctuations.

1:15PM W8.00011 Magnetic correlations and magnetic order in the pyrochlore $\text{Er}_2\text{Ti}_2\text{O}_7$, S.H. CURNOE, Memorial University of Newfoundland, P. DALMAS DE RÉOTIER, A. YAOUANC, Y. CHAPUIS, B. GRENIER, E. RESSOUCHE, C. MARIN, Institut Nanosciences et Cryogénie, SPMS, CEA and University Joseph Fourier, C. LAGO, Universidade del País Vasco, C. BAINES, Paul Scherrer Institute, S.R. GIBLIN, ISIS Facility, Rutherford Appleton Laboratory — We analyse short-range magnetic correlations in the pyrochlore magnet $\text{Er}_2\text{Ti}_2\text{O}_7$. Four unique nearest-neighbour exchange interactions are permitted by the space group symmetry of the pyrochlore lattice; the four corresponding nearest-neighbour exchange constants for $\text{Er}_2\text{Ti}_2\text{O}_7$ are extracted from diffuse neutron scattering maps. Low-temperature magnetic order in $\text{Er}_2\text{Ti}_2\text{O}_7$ is discussed in light of these results. The results are compared to recently published values for the sister compound $\text{Yb}_2\text{Ti}_2\text{O}_7$, which has similar features.

1:27PM W8.00012 Low Temperature Spin Structure of Gadolinium Titanate, BEHNAM JAVANPARAST, PAUL MCCLARTY, MICHEL GINGRAS, University of Waterloo — Many rare earth pyrochlore oxides exhibit exotic spin configurations at low temperatures due to frustration. The nearest neighbor coupling between spins on the corner-sharing tetrahedral network generate geometrical magnetic frustration. Among these materials, gadolinium titanate ($\text{Gd}_2\text{Ti}_2\text{O}_7$) is of particular interest. Its low temperature ordered phases are not yet understood theoretically. Bulk thermal measurements such as specific heat and magnetic susceptibility measurements find two phase transitions in zero external field, in agreement with simple mean field calculations. However, recent neutron scattering experiments suggest a so-called 4-k spin structure for intermediate phase and a so called canted 4-k structure for lower temperature phase that does not agree with either mean-field theory or Monte Carlo simulation which find the 1-k state and Palmer-Chalker state respectively as the lowest free energy configuration for those phases. In our work, we study the 4-k structure in detail and present a new phase diagram for dipolar Heisenberg spins on a pyrochlore lattice, certain portions of which describe gadolinium titanate.

1:39PM W8.00013 Elastic properties of the titanate pyrochlore $\text{Tb}_2\text{Ti}_2\text{O}_7$ ¹, V. KEPPENS, Y. LUAN, Department of Materials Science and Engineering, The University of Tennessee, Knoxville, TN, A. MIGLIORI, J. BETTS, National High Magnetic Field Laboratory, Los Alamos, NM, H.D. ZHOU, National High Magnetic Field Laboratory, Tallahassee, FL, H.A. DABKOWSKA, B.D. GAULIN, Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON — The presence of geometric frustration inhibits the formation of long-range spin ordering in $\text{Tb}_2\text{Ti}_2\text{O}_7$ even at very low temperatures, making this compound the prototype of a “spin liquid.” We have initiated a study of the elastic properties of $\text{Tb}_2\text{Ti}_2\text{O}_7$ as a function of temperature (0.5-300 K) and magnetic field (0-15T) using Resonant Ultrasound Spectroscopy (RUS). All three elastic constants show a pronounced softening below 50 K, indicative of a possible structural transition at very low temperatures. Application of a magnetic field partially suppresses the elastic softening in this compound, suggesting that the magnetoelastic coupling plays a significant role in the spin liquid physics of $\text{Tb}_2\text{Ti}_2\text{O}_7$ at low temperatures.

¹Work supported by NSF-DMR-0804719.

1:51PM W8.00014 Imaging Magnetic Order in Magnetostructural Phases of Mn_3O_4 ¹, XU WANG, MINJUNG KIM, S.L. COOPER, RAFFI BUDAKIAN, Department of Physics and Frederick Seitz Materials Research Laboratory University of Illinois at Urbana-Champaign, Urbana, IL 61801 — Frustration in A-site spinels due to the competition between complex structure and strong interactions has been the focus of many theoretical and experimental studies recently. Mn_3O_4 is one such material with a three way interplay between complex lattice geometry, strong spin-lattice coupling and magnetic interactions. Mn_3O_4 is known to have two distinct phases below the Neel temperature that differ in both structure and magnetic order, including a tetragonal phase with disordered spins, and at lower temperatures, an orthorhombic phase exhibiting long-range commensurate magnetic order. In this talk, we present a nanometer-scale imaging investigation of the transition between these two phases. With cryogenic magnetic force microscopy (MFM), we observe novel magnetic stripe patterns accompanying this phase transition. Complementary electron backscatter diffraction (EBSD) measurements indicate that the magnetic patterns are closely related to local crystalline orientation. The onset and spatial periodicity of the magnetic patterns show variations with temperature and external magnetic field. We will also discuss possible causes of this phenomenon and their implications.

¹Work supported by the U.S. Department of Energy under Award No. DE-FG02-07ER46453

2:03PM W8.00015 Spin state of Mn_3O_4 investigated by ^{55}Mn NMR, EUNA JO, KYONGMO AN, JEONGHYUN SHIM¹, CHANGSOO KIM, SOONCHIL LEE, Department of physics, KAIST, Daejeon 305-701, Korea, KAIST TEAM — The ^{55}Mn nuclear magnetic resonance spectrum for spinel oxide Mn_3O_4 was measured in the temperature range of 6 K - 30 K to investigate the spin structure in the ground state. The spectrum consists of three peaks in the frequency range of 250 - 265 MHz, which corresponds to the hyperfine field range of 24 - 25 T. The temperature dependence of the spectrum and the rf enhancement factor show that Mn^{3+} ions have two different magnetic moments, one of which is strongly related with the commensurate-incommensurate phase transition. This is consistent with the picture of two magnetic moments, R and S, claimed from the result of a neutron experiment. The dipolar hyperfine field was calculated to explain the splitting of two peaks coming from R and S and to estimate the magnetic moments. The spin-spin relaxation time has a frequency dependence that induces spectrum broadening and further splitting of the peak coming from S, indicating that the Suhl-Nakamura interaction is the major relaxation mechanism in Mn_3O_4 .

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Thursday, March 1, 2012 11:15AM - 2:15PM – Session W9 DMP GMAG: Focus Session: Complex Bulk Oxides: Multiferroics 209

11:15AM W9.00001 Evolution of spin wave excitations in $\text{Sr}_2\text{FeSi}_2\text{O}_7$ under an external magnetic field, KAZUKI IIDA, JOOSEOP LEE, NAOYUKI KATAYAMA, SUNGDAE JI, ISRAEL KLICH, SEUNGHUN LEE, University of Virginia, DUC LE, Helmholtz Zentrum, SUNG CHANG, NIST Center for Neutron Research, TAEHWAN JANG, YOONHEE JEONG, Pohang University of Science and Technology, SANGWOOK CHEONG, Rutgers University, UNIVERSITY OF VIRGINIA TEAM, HELMHOLTZ ZENTRUM COLLABORATION, NIST CENTER FOR NEUTRON RESEARCH COLLABORATION, POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY COLLABORATION, RUTGERS UNIVERSITY COLLABORATION — Evolution of static and dynamic spin correlations in a new multiferroic material $\text{Sr}_2\text{FeSi}_2\text{O}_7$ under an external magnetic field was investigated by elastic and inelastic neutron scattering techniques. An external magnetic field up to $B = 14$ Tesla induces four different magnetic and ferroelectric phases in $\text{Sr}_2\text{FeSi}_2\text{O}_7$. The static magneto-electric coupling can be understood as the spin-dependent metal-ligand hybridization proposed for a related material $\text{Ba}_2\text{CoGe}_2\text{O}_7$. By analyzing the inelastic neutron scattering data obtained from a single crystal of $\text{Sr}_2\text{FeSi}_2\text{O}_7$ without field, we have determined the effective spin Hamiltonian in this material that includes isotropic nearest neighbor exchange interaction in the two-dimensional Fe square plane and easy plane single ionic anisotropies. The spin wave excitations show interesting changes as upon ramping up the system enters the field-induced phases for $B > 6.5$ Tesla, which will also be discussed.

11:27AM W9.00002 THz spectroscopy of spin waves in multiferroic $\text{Ba}_2\text{CoGe}_2\text{O}_7$ in high magnetic fields¹, URMAS NAGEL, T. RÕÕM, NICPB, Tallinn, Estonia, S. BORDÁCS, D. SZALLER, I. KÉZSMÁRKI, Department of Physics, BUTE, Budapest, Hungary, H. ENGELKAMP, HFML, Radboud University Nijmegen, The Netherlands, J. ROMHÁNYI, K. PENC, MTA SzFKI, Budapest, Hungary, L. DEMKÓ, N. KIDA, H. MURAKAWA, Y. ONOSE, R. SHIMANO, S. MIYAHARA, N. FURUKAWA, Y. TOKURA, Multiferroics Project, ERATO, University of Tokyo, Japan — By applying external magnetic field the square-lattice antiferromagnet $\text{Ba}_2\text{CoGe}_2\text{O}_7$ can be transformed to a chiral form, evidenced by large optical activity when the light is in resonance with spin excitations at sub-terahertz frequencies. We found that the magnetochiral effect, the absorption difference for the light beams propagating parallel and anti-parallel to the applied magnetic field, has an exceptionally large amplitude close to 100% and persists to fields up to 30 T. All these features are ascribed to the magnetoelectric nature of spin excitations as they interact both with the electric and magnetic components of light. We observe a spin flop at 15 T, that is consistent with our theoretical calculations.

¹We acknowledge the support by the Estonian Ministry of Education and Research (SF0690029s09) and Estonian Science Foundation (ETF7011, ETF8170). Part of this work has been supported by EuroMagNET II under the EU contract number 228043.

11:39AM W9.00003 Ground State Properties and Magnetodielectric Coupling in $\text{Sm}_{0.5}\text{Nd}_{0.5}\text{Fe}_3(\text{BO}_3)_4$ ¹, C.S. NELSON, Brookhaven National Laboratory, Upton, NY, USA, R.P.S.M. LOBO, LPEM, ESPCI, CNRS, UPMC, Paris, France, L.N. BEZMATERNYKH, Kirensky Institute of Physics, Siberian Branch of RAS, Russia — We report x-ray scattering and polarized infrared reflectivity measurements of the substituted ferroborate $\text{Sm}_{0.5}\text{Nd}_{0.5}\text{Fe}_3(\text{BO}_3)_4$. Below $T_N = 33$ K, a new set of commensurate peaks with resonant enhancements at the rare earth L edges indicates a doubling of the magnetic structure along the c-axis and simultaneous ordering of the rare earth and iron ions. Rare earth spin polarizations decrease rapidly with increasing temperature, in contrast to that of the iron ions. Shell-specific measurements of the rare earth spin polarizations indicate similar behaviors of the Sm and Nd 5d states, while the Sm 4f and 5d states have different temperature dependences. Along the c-axis we observe negative thermal expansion below ~ 75 K and a strong phonon softening from room temperature down to T_N , at which it freezes in frequency. Also at T_N we observe the appearance of an electromagnon in the ab-plane that gets its spectral weight from the lowest frequency phonon. These results indicate a lattice instability linked to magnetism with a strong coupling between magnetic and elastic properties.

¹Use of the NSLS, BNL, was supported by the U.S. DOE, Office of Science, Office of BES, under Contract No. DE-AC02-98CH10886.

11:51AM W9.00004 Spin-driven ferroelectricity in ferroaxial crystals, LAURENT CHAPON, Institut Laue-Langevin, France — Spin-driven ferroelectricity in most non-collinear magnets, such as TbMnO_3 , is induced by the so-called inverse Dzyaloshinskii-Moriya mechanism and requires a cycloidal magnetic structure, an ordered magnetic state that is not truly chiral (or lacks helicity). Conversely, in a truly chiral magnetic state (proper helix), the pseudo-scalar helicity can not couple directly to the electric polarization, and therefore can't induce ferroelectric order. However, in systems of specific crystal symmetry, named here “ferroaxials,” the presence of collective structural rotations mediates an indirect coupling between magnetic helicity and ferroelectricity. I will review our recent experimental results for new compounds of this class, obtained by magnetic X-ray and neutron diffraction techniques, including a clear demonstration that the magnetic helicity can be controlled by an electric field.

12:27PM W9.00005 Multiferroic behavior in trimerized Mott insulators, YOSHITOMO KAMIYA, CRISTIAN BATISTA, Theoretical Division, Los Alamos National Laboratory — We demonstrate multiferroic behavior in trimerized Mott insulators through the interplay between spins and electric dipole moments resulting from electronic charge fluctuations in frustrated units [L. N. Bulaevskii, C. D. Batista, M. V. Mostovoy, and D. I. Khomskii, Phys. Rev. B 78, 024402 (2008)]. The model consists of stacked triangular layers of trimers with small inter-trimer exchange interactions J' and J'' . We construct a phase diagram using a semi-classical approach. Ferroelectric states coexist with ferro- or antiferromagnetic orderings depending on the value of the magnetic field H and the sign of the inter-layer exchange J'' . The electric polarization undergoes abrupt changes as a function of H .

12:39PM W9.00006 Electric field control of magnetic chiralities in ferroaxial multiferroic $\text{RbFe}(\text{MoO}_4)_2$ ¹, ALEXANDER J. HEARMON, FEDERICA FABRIZI, Clarendon Laboratory, Department of Physics, Oxford University, UK, LAURENT C. CHAPON, Institut Laue Langevin, Grenoble, France, ROGER JOHNSON, Clarendon Laboratory, Department of Physics, Oxford University, UK, P. JANE BROWN, Institut Laue Langevin, Grenoble, France, PAOLO G. RADAELLI, Clarendon Laboratory, Department of Physics, Oxford University — The onset of ferroelectric polarisation in high symmetry, proper-screw type multiferroic materials cannot be explained in terms of conventional microscopic mechanisms or symmetry analysis since the direction of the magnetic propagation vector is orthogonal to the plane of the spins. $\text{RbFe}(\text{MoO}_4)_2$ undergoes a structural distortion at $T_c = 190$ K in which the oxygen tetrahedra rotate, imposing an “axiality” to the crystal structure. We show that a simple symmetric-exchange driven coupling of this axiality with the magnetic chiralities below $T_N = 4$ K explains the appearance of a ferroelectric polarisation parallel to both the axial vector and direction of magnetic propagation. We present spherical neutron polarimetry data that are sensitive to both helical and triangular chiral domains of the magnetic structure. We are able to distinguish the magnetic order in the two axial domains that are present in equal proportions, and to demonstrate direct control of the magnetic structure by an applied electric field. The above formalism may be readily generalised to other ‘ferroaxial’ systems in which the magnetic ordering breaks the inversion symmetry in a point group supporting an axial vector.

¹This work is supported in part by EPSRC grant EP/J003557/1

12:51PM W9.00007 Electric field control of nonvolatile four-state magnetization at room temperature, SAE HWAN CHUN*, YI SHENG CHAI*, BYUNG-GU JEON, HYUNG JOON KIM, YOON SEOK OH, INGYU KIM, HANBIT KIM, BYEONG JO JEON, SO YOUNG HAAM, JU-YOUNG PARK, SUK HO LEE, KEE HOON KIM, CeNSCMR, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea, JAE-HO CHUNG, Department of Physics, Korea University, Seoul 136-713, Korea, JAE-HOON PARK, Department of Physics and Division of Advanced Materials Science, POSTECH, Pohang 790-784, Korea — We find the realization of large converse magnetoelectric (ME) effects at room temperature in a multiferroic hexaferrite $\text{Ba}_{0.52}\text{Sr}_{2.48}\text{Co}_2\text{Fe}_{24}\text{O}_{41}$ single crystal, in which rapid change of electric polarization in low magnetic fields (about 5 mT) is coined to a large ME susceptibility of 3200 ps/m. The modulation of magnetization then reaches up to $0.62 \mu_B/\text{f.u.}$ in an electric field of 1.14 MV/m. We find further that four ME states induced by different ME poling exhibit unique, nonvolatile magnetization versus electric field curves, which can be described by an effective free energy with a distinct set of ME coefficients. *These authors contributed equally to this work.

1:03PM W9.00008 Magnetoelectric Effects and Related Phenomena in Spin-spiral Hexaferrites, TSUYOSHI KIMURA, Division of Materials Physics, Graduate School of Engineering Science, Osaka University — Among various multiferroics, extensive studies of ferroelectrics originating from magnetic orders, i.e., *magnetically-induced ferroelectrics* in which the inversion symmetry breaking and resultant ferroelectricity are induced by complex magnetic orders, have been triggered almost a decade ago by the discovery of multiferroic nature in a perovskite-type rare-earth manganites TbMnO_3 . The magnetically-induced ferroelectrics often show giant magnetoelectric effects, remarkable changes in electric polarization in response to a magnetic field, since the origin of their ferroelectricity is driven by magnetism which sensitively responds to an applied magnetic field. Though a large number of new magnetically-induced ferroelectrics have been reported in the past decade, so far there has been no practical application employing the magnetoelectric effect of the magnetically-induced ferroelectrics. This is partly because none of the existing magnetically-induced ferroelectrics have combined large and robust electric and magnetic polarizations at room temperature until quite recently. The situation is changed by the discoveries of magnetoelectricity in hexagonal ferrites (*hexaferrites*) with spin-spiral structures.^{1,2,3} In this presentation, I show our recent studies on magnetoelectric effects and related phenomena in the new series of magnetically-induced ferroelectrics which are promising candidates for multiferroics operating at room temperature and low fields. This work has been done in collaboration with Y. Hiraoka, T. Ishikura, K. Okumura, Y. Kitagawa, H. Nakamura, Y. Wakabayashi, M. Soda, T. Asaka, and Y. Tanaka.

¹T. Kimura, G. Lawes, and A. P. Ramirez, Phys. Rev. Lett. 94, 137201 (2005).

²Y. Kitagawa *et al.*, Nature Mater. 9, 797 (2010).

³K. Okumura *et al.*, Appl. Phys. Lett. 98, 212504 (2011).

1:39PM W9.00009 Pressure-induced Polarization Reversal in Z-type Hexaferrite Single Crystal, BYUNG-GU JEON, SAE HWAN CHUN, KEE HOON KIM, CeNSCMR, Seoul National University — Multiferroic materials with a gigantic magnetoelectric (ME) coupling at room temperature have been searched for applications to novel devices. Recently, large direct and converse ME effects were realized at room temperature in the so-called Z-type hexaferrite ($\text{Ba,Sr}_3\text{Co}_2\text{Fe}_{24}\text{O}_{41}$) single crystals [1,2]. To obtain a new control parameter for realizing a sensitive ME tuning, we studied ME properties of the crystals under uniaxial pressure. Upon applying a tiny uniaxial pressure of about 0.6 GPa, magnetic field-driven electric polarization reversal and anomaly in a $M-H$ loop start to appear at 10 K and gradually disappear at higher temperature above 130 K. By comparing those results with longitudinal magnetostriction at ambient pressure, we propose the pressure-dependent variations of transverse conical spin configuration as well as its domain structure under small magnetic field bias, and point out the possibility of having two different physical origins of the ME coupling in this system. [1] Y. Kitagawa *et al.*, Nat. Mater. **9**, 797 (2010) [2] S. H. Chun *et al.*, submitted.

1:51PM W9.00010 The complex multiferroic phase diagram of $\text{Mn}_{1-x}\text{Co}_x\text{WO}_4$ ¹, B. LORENZ, K.-C. LIANG, TCSUH and Dept. of Physics, University of Houston, Y. Q. WANG, Y.Y. SUN, TCSUH, University of Houston, F. YE, J.A. FERNANDEZ-BACA², H.A. MOOK, Neutron Scattering Science Division, Oak Ridge National Laboratory, C.W. CHU³, TCSUH and Dept. of Physics, University of Houston — MnWO_4 is a classical multiferroic where ferroelectricity is induced by an inversion symmetry breaking helical spin order. The origin of the helical order is found in competing magnetic exchange interactions with strong uniaxial anisotropy, resulting in magnetic frustration. The microscopic parameters can be tuned by chemical substitution of Fe, Zn, or Co for Mn. The effects of Co substitution up to 30% on the magnetic structure and the ferroelectric (FE) phase are investigated. The multiferroic phase diagram of $\text{Mn}_{1-x}\text{Co}_x\text{WO}_4$ is completely resolved. At low Co content, the FE polarization is oriented along the b-axis and decreases with increasing x. At doping levels between 7.5% and 12% Co, the polarization points along the a-axis and it reaches a maximum value of 90 $\mu\text{C}/\text{m}^2$ at x=10%. With further increasing x, the FE polarization rotates back to the b-axis. Its magnitude decreases continuously and vanishes above 30% Co content. This complex behavior comes along with a delicate sequence of different magnetic phases which are explored by magnetization, heat capacity, and neutron scattering experiments.

¹Supported by the DOE, the AFOSR, the T.L.L. Temple Foundation, the J.J. and R. Moores Endowment, and the State of Texas (TCSUH)

²also at: Dept. of Physics and Astronomy, University of Tennessee

³also at: Lawrence Berkeley National Laboratory

2:03PM W9.00011 Spin flop transition in the multiferroic $\text{Mn}_{1-x}\text{Co}_x\text{WO}_4$ studied by neutron diffraction, FENG YE, SONGXUE CHI, HUIBO CAO, JAIME FERNANDEZ-BACA, Oak Ridge National Laboratory, BERND LORENZ, YAQI WANG, P.W. CHU, University of Houston — Elastic neutron diffraction is employed to investigate the ground state magnetic structure of the multiferroic $\text{Mn}_{1-x}\text{Co}_x\text{WO}_4$. Unlike the undoped MnWO_4 that has low- T collinear spin structure, the doped MnWO_4 exhibits complex evolution of magnetic structure. Samples at lower concentration ($x < 0.10$) have similar elliptical spiral structure as MnWO_4 in the multiferroic phase. With increasing x , the magnetic structure undergoes a sudden spin-flop transition which switches electric polarization from crystalline b -axis to a -axis. Polarized neutron scattering is also used to study the correlation between the bulk electricity and magnetic helicity.

Thursday, March 1, 2012 11:15AM - 2:15PM —

Session W10 DAMOP: Invited Session: Novel Bose-Einstein Condensates: Photons, Excitons, Magnons, Rydberg Atoms, and Polar Molecules 210A

11:15AM W10.00001 Bose-Einstein condensation of photons, MARTIN WEITZ, University of Bonn — Bose-Einstein condensation, the macroscopic ground state accumulation of particles with integer spin (bosons) at low temperature and high density, has been observed in several physical systems, including cold atomic gases and solid state physics quasiparticles. However, the most omnipresent Bose gas, blackbody radiation (radiation in thermal equilibrium with the cavity walls) does not show this phase transition. The photon number is not conserved when the temperature of the photon gas is varied (vanishing chemical potential), and at low temperatures photons disappear in the cavity walls instead of occupying the cavity ground state. Here I will describe an experiment observing a Bose-Einstein condensation of photons in a dye-filled optical microcavity [1]. The cavity mirrors provide both a confining potential and a non-vanishing effective photon mass, making the system formally equivalent to a two-dimensional gas of trapped, massive bosons. By multiple scattering of the dye molecules, the photons thermalize to the temperature of the dye solution. In my talk, I will begin with a general introduction and give an account of current work and future plans of the Bonn photon gas experiment.

[1] J. Klaers, J. Schmitt, F. Vewinger, and M. Weitz, Nature **468**, 545 (2010).

11:51AM W10.00002 Superfluid Phase Transition of Long-Lifetime Polaritons¹, DAVID SNOKE, University of Pittsburgh — Exciton-polaritons are quanta of electronic excitation which can have their properties tailored in semiconductor structures to have extremely light mass, about four orders of magnitude less than a free electron. One can think of them as photons dressed with an effective mass and an atom-like interaction. Because of their very light mass, exciton-polaritons show Bose quantum effects even at moderate densities and temperatures from tens of Kelvin up to room temperature. In the past five years, multiple experiments have shown effects of polaritons analogous to Bose condensation of cold atoms, such as a bimodal momentum distribution, quantized vortices, a Bogoliubov excitation spectrum, spatial condensation in a trap, and Josephson junction oscillations. In these experiments, though, the lifetime of the polaritons has been just a little longer than their thermalization time, which means that nonequilibrium effects play an important role; in particular, the transition to superfluidity has been smeared out rather than a sharp transition. In this talk I report new results with polaritons that have very long lifetime compared to their thermalization time. We see a discontinuous jump in the properties of the polariton gas indicative of a true phase transition, and we see ballistic transport over hundreds of microns. We also now have a way to use a laser to create a potential barrier for the polaritons.

¹This material is based upon work supported by the National Science Foundation under Grant No. 0706331.

12:27PM W10.00003 BEC of magnons at room temperature and spatio-temporal properties of magnon condensate, SERGEJ DEMOKRITOV, Institute for Applied Physics, University of Munster, Germany — No abstract available.

1:03PM W10.00004 An ultracold high-density sample of rovibronic ground-state molecules in an optical lattice, HANS-CHRISTOPH NAEGERL, University of Innsbruck — No abstract available.

1:39PM W10.00005 BEC of Rydberg atoms, MATTHIAS WEIDEMUELLER, Univ. Heidelberg — No abstract available.

Thursday, March 1, 2012 11:15AM - 2:15PM –

Session W11 DMP: Focus Session: Graphene Structure, Stacking, Interactions: Local Probes and Microscopy 210B

11:15AM W11.00001 Direct Imaging of a Two-Dimensional Silica Glass on Graphene, P.Y. HUANG, Cornell University, S. KURASCH, University of Ulm, A. SRIVASTAVA, V. SKAKALOVA, Max Planck Institute for Solid State Research, J. KOTAKOSKI, A.V. KRASHENINNIKOV, University of Helsinki, R.M. HOVDEN, Q. MAO, Cornell University, J.C. MEYER, University of Vienna, J. SMET, Max Planck Institute for Solid State Research, D.A. MULLER, Cornell University, U. KAISER, University of Ulm — Large-area graphene substrates [1] are a promising lab bench for synthesizing and characterizing novel low-dimensional materials such as two-dimensional (2D) glasses. Unlike 2D crystals such as graphene, 2D glasses are almost entirely unexplored—yet they have enormous applicability for understanding amorphous structures, which are difficult to probe in 3D. We report direct observations of the structure of an amorphous 2D silica supported on graphene. To our knowledge, these results represent the first discovery of an extended 2D glass. The 2D glass enables aberration-corrected scanning transmission electron microscopy and spectroscopy, producing the first atomically-resolved experimental images of a glass. The images strikingly resemble Zachariasen's seminal 1932 cartoons of a 2D continuous random network glass [2] and allow direct structural analyses not possible in 3D glassy materials. DFT calculations indicate that van der Waals interactions with graphene energetically favor the 2D structure over bulk SiO₂, suggesting that graphene can be instrumental in stabilizing new 2D materials. [1] J. C. Meyer et al., *Nature* **454**, 319–322 (2008). [2] W. H. Zachariasen, *J. Am. Chem. Soc.* **54**, 3841–3851 (1932).

11:27AM W11.00002 Imaging defects on epitaxial graphene/SiC(0001) using non-contact AFM with a Q-plus sensor¹, Y. LIU, L. LI, University of Wisconsin, Milwaukee — STM has been commonly used to study the atomic structures of resonant scatters such as vacancies and adsorbates on graphene, which are leading factors limiting its mobility. However, since STM probes primarily the local density of states, complex patterns are often observed when imaging defects on graphene, making it challenging to determine their atomic structures using STM alone. In this work, we carried out an integrated study of defects on epitaxial graphene/SiC(0001) using non-contact AFM with Q-plus sensors in addition to STM. With atomic resolution AFM imaging, straight forward identifications of single- and di-vacancy defects can be made. These results and their implications for understanding electron scattering in epitaxial graphene on SiC(0001) will be presented at the meeting.

¹Supported by DOE (DE-FG02-05ER46228).

11:39AM W11.00003 Direct Imaging of Charged Impurities in Substrates used for Graphene Devices, K.M. BURSON, Center for Nanophysics and Adv. Mat. (CNAM), U. of Maryland, College Park, C.R. DEAN, Dept. of Mech. Eng. and Dept. of Elec. Eng., Columbia U., New York, P. KIM, Dept. of Phys., Columbia U., New York, K. WATANABE, T. TANIGUCHI, Adv. Mat. Laboratory, Nat. Inst. for Materials Science, Tsukuba, Japan, S. ADAM, Center for Nanoscale Science and Tech., NIST, Gaithersburg, A.E. CURTIN, W.G. CULLEN, M.S. FUHRER, CNAM, U. of Maryland, College Park — The use of hexagonal boron nitride (h-BN) as a substrate for graphene led to approximately an order of magnitude improvement in electron mobility compared to graphene on SiO₂. One hypothesis for the improvement is a reduction in trapped charge density on the surface of h-BN compared to SiO₂. We address this directly by mapping local potential fluctuations above the bare substrates h-BN and SiO₂ using Kelvin probe microscopy in ultra-high vacuum. We compare the results to a model of randomly distributed charges in a 2D plane at the surface of an insulating substrate. For SiO₂, the results are well modeled by a 2D charge density of $\sim 2.5 \times 10^{11} \text{ cm}^{-2}$. Previous measurements of charged impurity scattering in graphene indicates that this density of substrate charges would limit graphene mobility to 20,000 cm²/Vs, in good agreement with the maximum values reported for graphene on SiO₂. h-BN displays potential fluctuations that are approximately an order of magnitude lower than SiO₂, consistent with an order of magnitude improvement in mobility in graphene/h-BN devices. This work was supported by the US ONR MURI program, and the U. of MD NSF-MRSEC under Grant No. DMR 05-20471.

11:51AM W11.00004 Self-Organized Graphene Nanoribbons on SiC(0001) Studied with Scanning Tunneling Microscopy¹, DAVID TORRANCE, BAIQIAN ZHANG, TIEN HOANG, PHILLIP FIRST, Georgia Institute of Technology — Graphene nanoribbons grown directly on nanofacets of SiC(0001) offer an attractive union of top-down and bottom-up fabrication techniques. Nanoribbons have been shown to form on the $\langle 1\bar{1}0n \rangle$ facets of templated silicon carbide substrates,² but also appear spontaneously along step-bunches on vicinal SiC(0001) miscut slightly towards $\langle 1\bar{1}00 \rangle$. These self-organized graphene nanoribbons were characterized with low-energy electron diffraction (LEED) and Auger electron spectroscopy (AES) in ultra-high vacuum. Our measurements indicate that the graphene forms a continuous “buffer layer” across the SiC(0001) terraces during nanoribbon formation, with the zigzag edge of the buffer layer aligned parallel to the step-bunched nanofacets. Scanning tunneling microscopy/spectroscopy (STM/STS) was used to characterize the topography and electrical characteristics of the graphene nanoribbons. These measurements indicate that the graphene nanoribbons are highly-crystalline with predominantly zigzag edges.

¹Work supported by the NSF and the NRI-INDEX

²Sprinkle et al., *Nat. Nanotech.* **5**, 727 (2010).

12:03PM W11.00005 Imaging epitaxial graphene on SiC(0001) using STM with functionalized W tips¹, S.H. RHIM², Y. QI, G.F. SUN, Y. LIU, M. WEINERT, L. LI, U. Wisconsin-Milwaukee — Epitaxial graphene on SiC(0001) is studied using scanning tunneling microscopy with W tips functionalized by transition-metal (Cr, Fe) coatings, enabling the imaging of states within a few meV of the Fermi level that are not accessible with conventional W tips. First-principles modeling of these tips as pyramidal structures on W(110) indicates that an apex atom is stable for the Cr/W(110) tip but not for the Fe/W(110) or W/W(110) tips. Further calculations of the tunneling current show that the Cr- and Fe-coated tips can get significantly closer to the substrate than a bare W tip at a given current, and that the Cr (Fe) tip states contributing to the tunneling at low bias are spatially more localized than the W tip states. These characteristics lead to increased resolution, making possible the selective imaging of the complex electronic properties of the epitaxial graphene on SiC(0001)^{1,2}.

¹DOE (DE-FG02-05ER46228)

²present: Northwestern University

12:15PM W11.00006 Scanned probe studies of dielectric screening and charge puddles in epitaxial graphene on SiC(0001) , A.E. CURTIN, A. IMTIAZ, T.M. WALLIS, P. KABOS, National Institute of Standards and Technology, Boulder, CO, R.L. MYERS-WARD, C.R. EDDY, JR., L.O. NYAKITI, V.D. WHEELER, D.K. GASKILL, U.S. Naval Research Laboratory, Code 6880, Washington, DC 20375 — Epitaxial growth of graphene on SiC(0001) produces wafer-scale monolayer films suitable for large scale device applications. However, the presence of the buffer layer beneath the graphene produces n-doping of 10^{12} - 10^{13} cm⁻² and limits mobility to $\sim 10^3$ cm²/Vs. Recently H intercalation has produced p-doped samples with similar carrier density and improved mobility. Transport measurements on processed devices show evidence of charge impurity scattering, but these measurements cannot show whether the transport behavior is due to top gate dielectrics or intrinsic to the as-grown graphene. Here we use scanning microwave microscopy to look at graphene samples and bare SiC substrates to extract information about the screening role of the buffer layer. This data is complemented by earlier results suggesting charge puddles due to random impurities to not exist in epitaxial samples.

12:27PM W11.00007 Scanning Tunneling Microscopy Study of Mechanically-Stacked Double Layer Graphene , HONGWOO BAEK, Seoul National University, JEONGHOON HA, National Institute for Standards and Technology, BEOMYONG HWANG, JEONGHOON KWON, Seoul National University, JOSEPH STROSCIO, National Institute for Standards and Technology, YOUNG KUK, Seoul National University — Bilayer graphene has drawn considerable attention due to deviation from Dirac Fermion picture such as anomalous quantum hall effect and a tunable band gap in their spectrum. While a pristine Bernal (AB) stacked bilayer graphene can be synthesized by mechanical exfoliation, growth on a SiC single crystal and epitaxial growth on metal substrates, separate control of the top and the bottom layers has seldom been performed. In this study, artificially modified 2D layers were demonstrated with individually stacked double layer graphene. Large-area graphene was grown on a Cu foil by chemical vapor deposition (CVD). CVD-grown graphene layers were transferred successively onto several insulating substrates with minimum chemical process for realizing bilayer graphene. Mechanically-stacked double layer graphene was mainly investigated using scanning tunneling microscopy and spectroscopy. The artificial bilayer graphene showed Moire patterns as determined by misalignment angle. In spatially resolved spectrums of local density of states, dependence on separation distance between two graphene layers and their corrugation was measured. In addition, we confirmed less charging effects of graphene on BN thin film than on SiO₂ or SiN.

12:39PM W11.00008 Scanning Tunneling Spectroscopy of Potassium on Graphene , DANIEL COR-MODE, BRIAN LEROY, MATTHEW YANKOWITZ, University of Arizona — We investigate the effect of charged impurities on the electronic properties of large single crystal CVD grown graphene using scanning tunneling microscopy. Mono- and multilayer crystals were prepared by transferring graphene from copper onto exfoliated boron nitride flakes on 300 nm SiO₂ substrates. The boron nitride provides an ultra flat surface for the graphene. Potassium atoms are controllably deposited on the graphene at low temperature by heating a nearby getter source. Scanning tunneling spectroscopy and transport measurements were performed in ultra high vacuum at 4.5 K. Transport measurements demonstrate the shifting of the Dirac point as the samples are doped, while STM measurements demonstrate the size, arrangement and local electronic influence of the potassium atoms.

12:51PM W11.00009 Nanoscale electronic and optical investigations of functionalized graphene¹ , OZGUN SUZER, JONGWEON CHO, JOSEPH SMERDON, LI GAO, NATHAN GUISINGER, JEFFREY GUEST, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439, USA — A rigorous understanding of light-matter interactions at the nanometer scale is pivotal in the development of nanoscale device applications. Graphene and its functionalized derivatives, due to their unique properties, promise unexpected capabilities as a platform for such devices, which has led to significant interest in graphene-based nano-optical, optoelectronic, and photovoltaic applications. Here, we will describe our efforts to resolve and understand the structural, electronic and optical properties of these systems. We will present a UHV STM study of the structural and electronic properties of C60 molecules deposited on graphene that was grown epitaxially on SiC(0001), which serves as a model system for the study of molecule-surface interactions. Our results indicate reduced coupling of the molecules to the graphene and underlying substrate, compared to those on metallic substrates, suggesting a path for developing molecular-scale electronic and optically active “devices” that are not dominated by the substrate. We will also discuss our efforts to correlate these STM studies with the optical properties of the system using a UHV STM that incorporates confocal optical microscopy and spectroscopy at the tip-sample junction with integrated high-numerical aperture optics.

¹This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357 and “SISGR” Contract No. DE-FG02-09ER16109.

1:03PM W11.00010 Three Different Translations Can Each Convert the Top Plane of Graphite to Graphene¹ , D. QI, P. XU, Y. YANG, M.L. ACKERMAN, S.D. BARBER, J.K. SCHOELZ, L. BELLAICHE, SALVADOR BARRAZA-LOPEZ, P.M. THIBADO, Department of Physics, University of Arkansas, IGOR A. KORNEV, Propriétés et Modélisation des Solides, France — The discovery of graphene, a unique two-dimensional electron system with extraordinary physical properties, has ignited tremendous research activity in both science and technology. Graphene can be obtained from graphite by moving its top layer until it becomes locally decoupled from the bulk. However, a detailed microscopic understanding of this process has yet to be completed. Here we present STM images of the top plane of graphite, which has been transformed into graphene. In addition, we also present STM images which reveal several intermediate stages in between pure graphene and pure graphite. Density functional theory was used to simulate STM images from a six-layer slab of graphite. We also moved the top layer of graphite incrementally in three different directions. Vertical movement of the top layer by about 0.1 nm created graphene. A continuous transition from pure graphite to pure graphene was observed with the simulations. Horizontal movement of the top layer can also create graphene in two ways. In one configuration, the carbon atoms perfectly align with the layer below, while in the second the carbon atoms have no vertical alignment with the layer below. Other significant details found between graphite and graphene will be discussed.

¹Support provided by ONR N00014-10-1-0181, N00014-08-1-0915, NSF 0855358, 0701558, DoE 46612

1:15PM W11.00011 Graphene on Ru(0001): The four hills in the 25 on 23 structure , THOMAS GREBER, Physik-Institut, University of Zurich, Switzerland, MARCELLA IANNUZZI, Physical Chemistry, University of Zurich, HAIFENG MA, Physik-Institut, University of Zurich, IRAKLI KALICHAHA, Swiss Light Source, Paul Scherrer Institut, HAITAO ZHOU, GENG LI, YI ZHAO, Institute of Physics, Chinese Academy of Sciences, Beijing, 100190, China, STEVEN LEAKE, OLIVER BUNK, Swiss Light Source, Paul Scherrer Institut, HONJUN GAO, Institute of Physics, Chinese Academy of Sciences, Beijing, JÜRIG HUTTER, Physik-Institut, University of Zurich, PHIL WILLMOTT, Swiss Light Source, Paul Scherrer Institut — A single layer of sp² hybridized carbon on Ru(0001) accommodates in a 23 on 25 superstructure with 625 carbon honeycombs as found by surface x-ray diffraction (SXRD) [1]. In a significant computational effort 25x25 unit cells of graphene were relaxed on 23x23 Ru(0001) unit cells with up to 6 substrate layers. The density functional theory calculations that take van der Waals interactions into account predict 4 protrusions, quantum dots [2] or “hills” in the unit cell with two kinds of hills: 3 Ω -type hills with a honeycomb around the summits, and one T-type hill with a single carbon atom on the summit. This prediction is confirmed by state of the art low temperature scanning tunneling microscopy and is in line with the SXRD data in Ref.[1].

[1] Martoccia et al. Phys. Rev. Lett. 101 (2008) 126102.

[2] Zhang et al. J. Phys.: Condens. Matter 22 (2010) 302001.

1:27PM W11.00012 Thickness Determination of Multilayer Graphene Using Transmission Electron Microscopy¹, BRIAN SHEVITSKI, MATTHEW MECKLENBURG, UCLA Department of Physics and Astronomy & CNSI, JONATHAN WASSEI, UCLA Department of Chemistry and Biochemistry, RICHARD KANER, UCLA Department of Chemistry and Biochemistry & CNSI, BRUCE WEILLER, The Aerospace Corporation, E.R. WHITE, UCLA Department of Physics and Astronomy & CNSI, BEN DAWSON, MASA ISHIGAMI, UCF, Department of Physics, B.C. REGAN, UCLA Department of Physics and Astronomy & CNSI — With dark field transmission electron microscopy and select area electron diffraction (SAED) crystallographic grain boundaries in graphene can be easily imaged. We present a complete, quantitative theoretical model of the SAED pattern that allows determination of the number of layers. Grain boundary maps of single and multilayer graphene grown by chemical vapor deposition will be shown.

¹Supported by NSF Award No. HRD00603239, NSF CAREER Award 0748880, and the EICN at UCLA.

1:39PM W11.00013 High resolution transmission electron microscopy of lattice dynamics of graphene, JIAN-HAO CHEN, NASIM ALEM, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, ABHAY GAUTAM, MARTIN LINCK, CHRISTIAN KISIELOWSKI, Nation Center for Electron Microscopy, Lawrence Berkeley National Laboratory, ALEX ZETTL, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — Lattice dynamics of carbon atoms in graphene was investigated by aberration corrected ultra-high resolution transmission electron microscopy near the holes and the grain boundaries. We studied in-situ formation of various unusual defect structures in graphene under various conditions. In this presentation we will show the stability and dynamics of the atoms at the holes, grain boundaries and the defects and discuss their formation mechanism. This work will also elaborate on the electronic properties of the defects in light of recent experimental and theoretical progress.

1:51PM W11.00014 High resolution transmission electron microscope Imaging and first-principles simulations of atomic-scale features in graphene membrane, WEI WANG, SAGAR BHANDARI, WEI YI, DAVID BELL, ROBERT WESTERVELT, EFTHIMIOS KAXIRAS, Harvard University, KAXIRAS TEAM, WESTERVELT TEAM — Ultra-thin membranes such as graphene[1] are of great importance for basic science and technology applications. Graphene sets the ultimate limit of thinness, demonstrating that a free-standing single atomic layer not only exists but can be extremely stable and strong [2–4]. However, both theory [5, 6] and experiments [3, 7] suggest that the existence of graphene relies on intrinsic ripples that suppress the long-wavelength thermal fluctuations which otherwise spontaneously destroy long range order in a two dimensional system. Here we show direct imaging of the atomic features in graphene including the ripples resolved using monochromatic aberration-corrected transmission electron microscopy (TEM). We compare the images observed in TEM with simulated images based on an accurate first-principles total potential. We show that these atomic scale features can be mapped through accurate first-principles simulations into high resolution TEM contrast. [1] Geim, A. K. & Novoselov, K. S. *Nat. Mater.* **6**, 183-191, (2007). [2] Novoselov, K. S. *et al. Science* **306**, 666-669, (2004). [3] Meyer, J. C. *et al. Nature* **446**, 60-63, (2007). [4] Lee, C., Wei, X. D., Kysar, J. W. & Hone, J. *Science* **321**, 385-388, (2008). [5] Nelson, D. R. & Peliti, L. *J Phys-Paris* **48**, 1085-1092, (1987). [6] Fasolino, A., Los, J. H. & Katsnelson, M. I. *Nat. Mater.* **6**, 858-861, (2007). [7] Meyer, J. C. *et al. Solid State Commun.* **143**, 101-109, (2007).

2:03PM W11.00015 Interference effects in electronic transport in mesoscopic graphene, LINGLI WANG, University of California, Riverside, VICTOR A. GOPAR, Universidad de Zaragoza, Spain, SHAN-WEN TSAI, University of California, Riverside — Graphene consists of a monolayer of carbon atoms arranged in a honeycomb lattice and has been intensively studied due to its fascinating physical properties. We study transport in mesoscopic graphene systems, in particular, conductance oscillations due to interference of the Dirac electrons in phase-coherent transport. Green's functions are calculated in the tight-binding model via *T*-matrix formalism, and the conductance is then obtained using the Landauer-Büttiker formalism. We consider a measurement set-up consisting of two STM tips, as well as transport from a contact and a STM tip. Regular Bloch oscillations are obtained, as well as richer structures when different types of isolated impurities are considered.

Thursday, March 1, 2012 11:15AM - 2:15PM –
Session W12 DMP: Focus Session: Graphene: Growth, Mechanical Exfoliation, and Properties - Exfoliation and Doping 210C

11:15AM W12.00001 Graphene Carrier Control and Band Gap Formation through Stacked Graphene Sheets, GLENN JERNIGAN¹, US Naval Research Laboratory — Graphene's use in RF transistors and frequency doublers is attractive since its high mobility and high saturation velocity translate into operation at high frequencies while utilizing little power. However, further graphene development for device applications is hindered by high metal contact resistance, poor control of channel conductivity, and the absence of a band gap. In this talk, I will present our efforts at NRL to address these challenges using two strategies: 1) substitutional insertion of group III-V atoms into graphene's lattice to control the carriers and 2) through a synthetic means to create bilayer graphene with a band gap. Substitutional incorporation of atoms into graphene can result in doping, if their concentration does not drastically affect the π -network. Using selective oxidation to remove C atoms from the graphene lattice, we are able to backfill the C vacancies using molecular beam deposition of dopants with controllable ultra-low fluxes. We will show that boron and phosphorus dopants can provide extra holes and electrons to the graphene π -network, respectively, modifying the carrier concentration in transport measurements. Bernal-stacked graphene bilayers have a relatively small band gap ($\sim$ few meV). However, if the symmetry of the system is broken by the application of a large applied electric field, the band gap can be increased ($\sim$ 250 meV). Alternatively, we find it is possible to obtain such large built-in electric fields when graphene sheets of opposite doping are stacked. By bonding a p-type, CVD-grown graphene monolayer transferred from Cu to an n-type, epitaxially grown graphene monolayer on SiC, we formed a p-n graphene bilayer. Transport measurements and modeling of the resulting electric field generated by opposite doping of the graphene sheets indicate the creation of a 100-300 meV band gap in the synthetic bilayer.

¹Electronics Science and Technology Division, Solid State Devices Branch Code 6812

11:51AM W12.00002 Atomic characterization of monolayer doped graphene sheets synthesized by chemical vapor deposition, R.T. LU, Department of Physics, The Pennsylvania State University, USA, Q. LI, Center for Nanophase Materials Sciences Division, Oak Ridge National Laboratory, USA, A. BOTELLO-MÉNDEZ, Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Belgium, J.C. CHARLIER, Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Belgium, B. WANG, A. BERKDEMIR, H.R. GUTIÉRREZ, J. ZHU, H. TERRONES, Department of Physics, The Pennsylvania State University, USA, M.H. PAN, Center for Nanophase Materials Sciences Division, Oak Ridge National Laboratory, USA, M. TERRONES, Department of Physics, The Pennsylvania State University, USA; Research Center for Exotic Nanocarbons, Shinshu University, Japan — Large-area, high-quality monolayer nitrogen (or boron)-doped graphene sheets were synthesized on copper foils by a modified chemical vapor deposition (CVD) apparatus. As-grown graphene sheets could be easily transferred from copper foils onto different substrates (e.g. silicon/silicon dioxide wafers). Compared with pristine graphene, nitrogen (or boron)-doped graphene shows strong D-band caused by doping and structural defects formed within the lattice. Scanning tunneling microscopy (STM) and spectroscopy (STS) reveal that the defects in the doped graphene samples arrange in different geometrical configurations. The localized states in the valence and conduction bands are in accordance with the type of dopant and bonding type. These experimental results are in agreement with first principles calculations of LDOS of doped graphene and STM image simulations.

12:03PM W12.00003 Graphene melting by molecular dynamics simulations, BRAD STEELE, ROMAIN PERRIOT, VASILY ZHAKHOVSKY, IVAN OLEYNIK, University of South Florida — Mechanisms of melting of graphene were studied by molecular dynamics (MD) using two different interatomic potentials: the Reactive Empirical Bond Order (REBO) and recently developed Screened Environment Dependent (SED)-REBO potentials. Melting was investigated in two-dimensional (2-D) and three-dimensional (3-D) coordinate space. It was shown that the loss of long-range order and melting proceeds through generation and in-plane aggregation of Stone-Wales (S-W) defects in REBO-graphene, followed by the formation of a complex 3D network of carbon chains. Although S-W defects are also formed in the SED-REBO-graphene, they do not cluster. Instead, the melting proceeds through the formation of dangling bonds and vacancies. The melting temperature of graphene using REBO was found to be 5,200 K, whereas for SED-REBO it is lower by ~800K. The melting in 2-D occurs at higher temperatures compared to 3-D because of in-plane geometrical constraints.

12:15PM W12.00004 Unexpected Structures for Intercalation of Sodium in Epitaxial SiC-Graphene Interfaces¹, ANDREAS SANDIN, North Carolina State University, THUSHARI JAYASEKERA, Southern Illinois University-Carbondale, J. E. (JACK) ROWE, KI-WOOK K, MARCO BUONGIORNO-NARDELLI, DANIEL B. DOUGHERTY, North Carolina State University — We show using scanning tunneling microscopy and spectroscopy and calculations from first principles that several different intercalation structures exist for Na in epitaxial graphene on SiC(0001). Intercalation takes place rapidly at room temperature and tunneling spectroscopy shows that it significantly electron dopes the graphene. Upon annealing above room temperature a quite different intercalation structure is formed which removes the carbon-rich interface layer and transforms this into a second graphene layer. In addition, we find that direct deposition of Na onto the carbon rich buffer layer graphene precursor decouples it from the SiC substrate leading to formation of a new sheet of graphene. This interface-layer decoupling is unambiguously demonstrated by transforming bare buffer layer to a graphene layer. Our observations show that intercalation in graphene is fundamentally different than in graphite and provides a very versatile approach to metal-graphene functionality and electronic-property control.

¹Work partially supported by NSF Center for Molecular Spintronics

12:27PM W12.00005 Electron phonon renormalization in N-doped graphene, RAMAKRISHNA PODILA, Department of Physics, Clemson University, PAOLA AYALA, University of Vienna, JOHN SPEAR, Department of Physics, Clemson University, THOMAS PICHLER, University of Vienna, APPARAO RAO, Department of Physics, Clemson University, CLEMSON UNIVERSITY TEAM, UNIVERSITY OF VIENNA COLLABORATION — Current research efforts are aimed at controlling the electronic properties graphene sheets using electron (or hole) doping for successful device fabrication. The presence of strong coupling between electronic and vibrational properties in graphene greatly assists Raman spectroscopy in probing the dopant-induced electronic energy changes. Previously, Raman spectroscopy was employed as a tool to probe the electron and phonon renormalization in doped single-walled carbon nanotubes (SWNT). It was found that the increase in electron velocity influences lattice vibrations locally near a negatively charged defect. These local renormalization effects were observed to result in a new effectively downshifted (up-shifted) Raman peak below the G' peak for n-doped (p-doped) SWNTs. In case of graphene, we find that the several Raman features for CVD grown N-doped graphene vary depending upon local dopant bonding environment. For instance, non-graphitic dopants (pyridinic, pyrrolic) were observed to result in highly intense D & D'-band unlike the graphitic dopants. We explain these results in terms of the zig-zag (armchair) edges formed by graphitic (non-graphitic) bonding environment of the dopant.

12:39PM W12.00006 Transport properties of pristine and doped graphene, POOJA PUNEET, RAMAKRISHNA PODILA, Department of Physics and Astronomy, Clemson University, Clemson SC 29634, LUCIANA OLIVEIRA, Department of Materials Science and Engineering, Clemson University, Clemson SC 29634, TERRY TRITT, APPARAO RAO, Department of Physics and Astronomy, Clemson University, Clemson SC 29634 — Graphene has attracted a lot of attention for various applications recently. Chemically exfoliated graphene is one of the best methods to prepare good quality and large amount of few-layer graphene sheets. We prepared pristine and doped graphene using chemical exfoliation through high energy tip sonication technique. The exfoliated graphene was later sintered for studying thermoelectric properties. The thermopower of these samples exhibits valleys, tentatively assigned to phonon drag, which shift towards higher temperature upon vacuum annealing and electron doping. Such a similar behavior was previously observed in doped carbon nanotubes. The effects of vacuum annealing and doping upon the fundamental behavior of thermoelectric power and thermal conduction of graphene will be presented.

12:51PM W12.00007 Experimental investigation of carrier quantum confinement in graphene quantum dots and nanoribbons, KIRAN LINGAM, RAMAKRISHNA PODILA, APPARAO RAO, Department of Physics and Astronomy, Clemson University, CLEMSON UNIVERSITY TEAM — Recently, Zhu *et al.* (Chem. Comm., 2011. 47(24), 6858) and Pan *et al.* (Adv. Mat., 2010. 22(6), 734) have successfully synthesized graphene quantum dots (width <10 nm). They probed the carrier quantum confinement in such GQDs using photoluminescence spectroscopy (PL). However, a self-consistent explanation for the observed PL spectra is lacking. Interestingly, we find that the organic reducing agents used for synthesizing GQDs have PL signature similar to the GQDs themselves. Thus, deconvoluting solvent effects is extremely important to achieve further progress in synthesis and application of GQDs. We studied the PL behavior of hydrothermally synthesized graphene nanoribbons (GNRs) and GQDs to understand the solvent effects and the underlying mechanism for the observed PL. We will discuss the effects of size, shape and morphology on the PL behavior of GQDs and GNRs.

1:03PM W12.00008 Scanned Probe Measurements of Graphene on Ferroelectrics, SCOTT SCHARFENBERG, RUIJUAN XU, CHRISTOPH BAEUMER, MOONSUB SHIM, LANE MARTIN, NADYA MASON, University of Illinois at Urbana-Champaign — We present results on scanned probe measurements of graphene and few-layer graphite (FLG) on ferroelectric thin films. The graphene was mechanically exfoliated onto the PbZr_{0.2}Ti_{0.8}O₃ and other ferroelectric films, and its topography and polarization were characterized using atomic force microscopy, Kelvin Probe (surface potential) Force Microscopy, and Piezoresponse Force Microscopy. We discuss how graphene can be used as a top electrode for ferroelectric materials, as changing the potential of the graphene can cause the ferroelectric region beneath it to switch polarization. We demonstrate that the change in polarization is reversible. We also show how the surface potential of FLG on PZT depends on the number of layers of graphene. *The authors acknowledge Grant DMR-1124696, Sub-Award 235743-3668.

1:15PM W12.00009 Can Structured Mixed Solvents be Used for Graphene Exfoliation?, ANDREW OYER, CHETAN HIRE, JAN-MICHAEL CARRILLO, ALEXANDRU ASANDEI, DOUGLAS ADAMSON, ANDREY DOBRYNIN, University of Connecticut — Using a combination of computational and experimental techniques we investigate graphene exfoliation and suspension in C₆H₆, C₆F₆ and their mixtures. Our MD simulations show that an equimolar mixture of C₆H₆/C₆F₆ has the highest affinity for graphene. This is manifested in the formation of translational and orientational order normal to the graphene surface, with no translational ordering parallel to the graphene surface. The solvent structure is driven by quadrupolar interactions and consists of stacks of alternating C₆H₆/C₆F₆ molecules rising from the surface of the graphene. These stacks give rise to density oscillations in registry with the graphene surface. The period of the density oscillations is on the order of 3.4 Å, corresponding to the van der Waals diameter of carbon and this ordered structure extends 30 Å from each side of the graphene sheet. To experimentally verify the results of the molecular dynamics simulations we use dynamic contact angle measurements. These measurements demonstrate an increase in solvent affinity for HOPG in the case of 1:1 mixtures in comparison with pure components. The quality of the exfoliated material and flakes after sonication is verified by AFM, SEM, and TEM techniques. The graphene sheets produced in the equimolar mixture can be freeze-dried at room temperature, (T=300K) producing sponge-like graphene structures held together entirely by graphene sheet interactions and reflecting the structure of the graphene sheets in solution.

1:27PM W12.00010 Fabrication and Characterization of folded Graphene on Graphite, DAVID COSTA MILAN, GIOVANNI SAENZ ARCE, University of Alicante, MOHAMMED MOAIED, University Autonoma of Madrid, MARIA JOSE CATURLA, University of Alicante, JUAN JOSE PALACIOS, University Autonoma of Madrid, CARLOS UNTIEDT, University of Alicante, LT-NANOLAB TEAM, COND. MATTER DEPT TEAM — Graphene is one of the most studied carbon compounds due to its electronic properties. Applying an electric pulse between a Graphite surface and STM tip the upper layer of a Graphite surface could be folded due to mechanical and electrostatic forces forming voids, bend, move, and decouple or transfer part of the tip to the surface. Ab-initio electrostatic calculations and MD thermal simulations support our experimental method. Due to the different new discovered and studies physical-effects in Graphene edges, which can significantly influence the overall electronic and magnetic properties of Graphene nanostructures, this results may be exploited as an method to obtain different structures. Here we study Graphene flakes obtained with this Method. Folded Graphene's structure and electronic properties are studied to determine its degree of coupling to the graphite substrate. Cross-sectional analysis of the fold shown reveals that it consists of a single sheet of graphite folded. Graphene edges and folded line reveals new electronic and magnetic properties. Among others the possibility of a multi folded Graphene sheet system gains importance due to the opportunity of getting a Semi-Carbon-Nanotube-Graphene device.

1:39PM W12.00011 Controlling desorption of H, O, atoms and OH group from graphene by pulse laser, YOSHIYUKI MIYAMOTO, Nanosystem Res. Ins., AIST, HONG ZHANG, College of Physical Science and Technology, Sichuan University — Possibilities of reduction of graphene oxide and one-side dehydrogenation of graphane (H-terminated graphene) with using ultra-short pulse (~ 2 fs) laser are discussed. We have performed molecular dynamics (MD) simulation of O-, H-, and OH-adsorbed graphene sheets induced by electronic excitation upon irradiation with laser pulse. The time-dependent density functional theory treating real-time propagation of electron wave functions combined with the Ehrenfest approximation for the MD was employed and FPSEID [1] code was used to check the energy conservation rule under dynamical external field [2]. We found asymmetric pulse shape as a function of time causes an efficient desorption of O atoms and OH groups from graphene which can be applicable for reduction of graphene oxide alternative to chemical and thermal treatment. Meanwhile, such asymmetric pulse shape is beneficial for one-side H-desorption from graphane that will trigger further structural changes such as spontaneous shrink/rippling or heterogeneous termination on side-by-side.

[1]O. Sugino, Y. Miyamoto, PRB**59**, 2579, (1999);B66, 089901(E) (2002)

[2]Y. Miyamoto, H. Zhang, PRB**77**, 165123 (2008)

1:51PM W12.00012 Graphene on Au-coated SiO_x substrate: Its visibility and intrinsic core-level photoemission, CHUNG-LIN WU, JHIH-WEI CHEN, CHIANG-LUN WANG, Department of Physics, National Cheng-Kung University, CHIA-HAO CHEN, National Synchrotron Radiation Research Center, YI-CHUN CHEN, Department of Physics, National Cheng-Kung University — With the motivation of precisely and intrinsically characterizing a exfoliated graphene using photoelectron spectroscopy, a conducting substrate having high optical contrast is greatly desired. Here, we demonstrate that exfoliated graphene can be optically visible on a thin 9-nm Au-coated SiO_x substrate, and can be easily conducted into scanning photoelectron microscopy/spectroscopy (SPEM/S) studies. Because of the elimination of charging effect, precisely core-level characterization of exfoliated graphene is presented with different numbers of layers. Consequently, the usage of Au-coated SiO_x substrate serves a simple but effective method to study pristine graphene by photoelectron spectroscopy and other electron-detection techniques.

2:03PM W12.00013 Stage-1 intercalation compounds of few graphene layers by anhydrous ferric chloride, PINGHENG TAN, WEIJIE ZHAO, JIAN LIU, SKLSM, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, PR China, ANDREA FERRARI, Engineering Department, University of Cambridge, Cambridge CB3 0FA, UK — Anhydrous ferric chloride (FeCl_3) was used to intercalate few graphene layers into stage-1 intercalation compounds. The intercalant, staging, stability, and doping of the resulting intercalation compounds are characterized by Raman scattering. The G peak of pure stage-1 compounds upshifts to $\sim 1626 \text{ cm}^{-1}$, which is similar to that of heavily-doped monolayer graphenes by 18M sulfuric acid. A single Lorentzian line shape for the 2D band of stage-1 compounds were observed, which indicates that each layer behaves as a decoupled heavily doped monolayer. By performing Raman measurements at different excitation energies, we show that, for a given doping level, the variation of the 2D intensity relative to the G peak with excitation energy allows one to assess the Fermi energy. This allows us to estimate a Fermi level shift of up to $\sim 0.85 \text{ eV}$, which agrees well with that estimated from the 2D/G intensity ratio and is close to $\sim 0.9 \text{ eV}$ measured in stage-1 GICs by electron energy loss spectroscopy. The stage-1 intercalation compound of few graphene layers is thus ideal test-beds for the physical and chemical properties of heavily doped graphenes.

Thursday, March 1, 2012 11:15AM - 2:15PM –

**Session W13 DMP GMAG: Focus Session: Low-Dimensional and Molecular Magnetism - Met-
allorganics and Spincrossover Molecular Magnets 211**

11:15AM W13.00001 Magnetic properties of selected Prussian Blue Analogs (PBAs), MANJITA SHRESTHA, SOURAV ADAK, HEINZ NAKOTTE, New Mexico State University, LUKE L. DAEMEN, MONIKA HARLT, VIVIEN ZAPF, Los Alamos National Laboratory — Prussian Blue Analogs consists of MC_6 and AN_6 octahedra connected by cyanide ligands (M, A= metals). They typically crystallize in cubic structures. We have studied temperature and field dependence of the magnetization and the susceptibility of selected Prussian Blue Analogs such as hexacyanocobaltates, -ferrates and -chromates. All compounds exhibit modified Curie –Weiss behavior in the paramagnetic region. The observed effective moments of those compounds were compared with the ones of the respective free-ion values. Furthermore, we find evidence that a few of the compounds exhibit a transition to long-range magnetic order at low temperatures.

11:27AM W13.00002 Persistent Photocontrolled Magnetism in Core-Shell Prussian Blue Analogues¹, ELISABETH S. KNOWLES, MATTHIEU F. DUMONT, MARCUS K. PEPRAH, MARK W. MEISEL, Dept. Phys. and NHMFL, Univ. Florida, CARISSA H. LI, DANIEL R. TALHAM, Dept. Chem., Univ. Florida — Cubic heterostructured (BA) particles of Prussian blue analogues, composed of shells of ferromagnetic $\text{K}_7\text{Ni}_6[\text{Cr}(\text{CN})_6]_4 \cdot n\text{H}_2\text{O}$ (A), $T_c \sim 70 \text{ K}$, surrounding bulk cores ($\sim 350 \text{ nm}$) of photoactive ferrimagnetic $\text{Rb}_6\text{Co}_6[\text{Fe}(\text{CN})_6]_4 \cdot m\text{H}_2\text{O}$ (B), $T_c \sim 20 \text{ K}$, have been studied. Below $T_c \sim 70 \text{ K}$, these samples exhibit a persistent photoinduced decrease in low-field magnetization, resembling results from previous core-shell particles² and analogous ABA films.³ This net decrease suggests that the photoinduced lattice expansion in the B layer generates a strain-induced decrease in the magnetization of the A layer, similar to a pressure-induced decrease observed by others in a pure A material⁴ and by us in the BA cubes. To quantify the length scale over which the photoinduced strain dissipates into the A layer, a series of B and BA cubes of varying shell thickness have been characterized.

¹We acknowledge early contributions to this work by D.M. Pajerowski. Supported by NSF DMR-0701400 (MWM), DMR-1005581 (DRT), DMR-0654118 (NHMFL), and the State of Florida.

²M.F. Dumont *et al.*, Inorg. Chem. **50** (2011) 4295.

³D.M. Pajerowski *et al.*, J. Am. Chem. Soc. **132** (2010) 4058.

⁴M. Zentková *et al.*, J. Phys.: Condens. Matter **19** (2007) 266217.

11:39AM W13.00003 Pressure-induced local lattice distortions in Co(dca)₂¹, J.L. MUSFELDT, University of Tennessee, Z. LIU, Carnegie Institute of Washington, A. LITVINCHUK, University of Houston, T.V. BRINZARI, University of Tennessee, G.L. CARR, Brookhaven National Laboratory, J.A. SCHLUETER, Argonne National Laboratory, J.L. MANSON, Eastern Washington University, M.-H. WHANGBO, North Carolina State University — We employed vibrational spectroscopy along with complementary lattice dynamics and spin density calculations to investigate local structure and magnetism through the series of pressure-induced transitions in Co(dca)₂. Analysis of several ligand bending modes reveals compression and distortion of molecular linkages and a major change in the crystal lattice through the 1 GPa transition, whereas a modified local structure (due to a change in molecular symmetry) but similar crystal lattice is anticipated above 3 GPa. We discuss our findings in terms of the competition between antiferromagnetic and ferromagnetic exchange interactions.

¹We thank the NSF for support of this work.

11:51AM W13.00004 Magnetotransport Properties of Switchable Valence Tautomer Films¹, WILLIAM RICE, FRANK TSUI, Physics, University of North Carolina at Chapel Hill, DANIEL STASIW, ROBERT SCHMIDT, DAVID SHULTZ, Chemistry, North Carolina State University, ROBERT BRUCE, WEI YOU, Chemistry, University of North Carolina at Chapel Hill — We report tunneling magnetoresistance (TMR) and spectroscopy results in trilayer stacks of spincoated molecular films sandwiched between two metallic thin film electrodes. The molecules, cobalt dioxolene complexes, exhibit switchable bistable paramagnetic states as a result of intramolecular electron transfer accompanied by a spin-crossover of the Co ion, the so-called valence tautomerism (VT). Temperature dependent differential conductance measurements show changes in the density of states that correspond to the temperature dependent VT transition. The observed electronic transition is shown to be switchable by light exposure, which correlates the counterpart in the magnetic susceptibility. In trilayers with two ferromagnetic electrodes, e.g. Permalloy and Co, spin valve effects have been observed above and below the VT transition, including room temperature. The dependence of the TMR effect on bias voltage, light exposure, and molecular film thickness has been examined systematically as a function of temperature, aimed at exploring the effects of spin dependent states in the VT molecules.

¹NSF Center for Chemical Innovation: Center for Molecular Spintronics (CHE-0943975)

12:03PM W13.00005 Computational studies of the Fe(II) spin crossover compound Fe[H₂B(pz)₂]₂(bpy)¹, YIFENG CHEN, MARCO BUONGIORNO NARDELLI, Department of Physics, North Carolina State University — Using calculations from first principles, we studied the electronic and transport properties of the Fe(II) spin crossover (SCO) compound Fe[H₂B(pz)₂]₂(bpy). The magnetic transition has been imposed by constrained magnetization calculations and the computed electronic structure agrees with available experimental data. Besides the characterization of the single molecule, we constructed a π -stacking molecular chain of the compound and evaluated electronic transport in the direction of the chain for both the low-spin and the high-spin configurations. We found the high-spin configuration to be more conductive than the low-spin case, in agreement with experimental measurements of corresponding currents through disordered thin films. Molecule-molecule interactions are taken into account by the London dispersion forces. The spin-switchable electronic transport properties of this kind of Fe(II) SCO compound systems provide viable proofs for future switchable molecular spintronic devices and applications.

¹NSF Center for Chemical Innovation: Center for Molecular Spintronics (CHE-0943975)

12:15PM W13.00006 ABSTRACT WITHDRAWN —

12:27PM W13.00007 Highly Unquenched Orbital Moment In Fe Phthalocyanine¹, JUAN BAR-TOLOME, Consejo Superior de Investigaciones Científicas — Metal-Phthalocyanine molecules (MPc) form a family of compounds with a wide range of commercial application such as catalysts or dyes, and more recently in thin film technology. In an early work we found that in the α -phase of FePc, where the FePc molecules are stacked in a herringbone structure, the Fe atoms are strongly magnetically coupled into ferromagnetic Ising chains with very weak antiferromagnetic interchain coupling. The chains achieve 3D long range ordering at $T_N=10$ K, and strong irreversibility (slow relaxation) below 5K. The Fe(II) is in a S=1 state and the hyperfine field in the ordered phase reaches a record value in Fe(II) of $B_{hf}=66.2$ T. This result is consistent with a large, unquenched orbital moment. It has been measured directly in a X-ray Magnetic Circular Dichroism (XMCD) spectroscopic study on FePc thin films deposited parallel on a Au surface predeposited on a Si substrate. The XMCD spectra at the L₃ and L₂ edges were measured as a function of incident angle γ . The orbital moment is $|m_L| = 0.53 \pm 0.04 \mu_B$ and the isotropic spin component is $m_S = 0.64 \pm 0.05 \mu_B$. The origin of this unusually high orbital moment is the incompletely filled e_g level lying close to the Fermi energy. The ferromagnetically coupled Fe moments show strong, in-plane anisotropy [1]. Angular dependent measurements at the Fe K-edge also show strong quadrupolar excitations associated to a strong orbital moment, confirming the above result of the existence of a large, unquenched orbital moment in this molecule. Submonolayer FePc thin films deposited on Au, recently studied my XAS and XMCD have shown that there is charge transfer from the substrate to the Fe atom, modifying the electronic structure and magnetic properties [2]

[1] J. Bartolomé et al., Phys. Rev. B 81, 195405 (2010)

[2] S. Stepanow et al., Phys. Rev. B 83, 220401(R) (2011).

¹Work supported by the us AFOSR.

1:03PM W13.00008 Theoretical modelling of exchange interactions in metal-phthalocyanines, WEI WU, Department of Materials, Imperial College London, ANDREW FISHER, Department of physics and astronomy, University College London, NIC HARRISON, Department of Chemistry, Imperial College London, MICHELE SERRI, ZHENLIN WU, SANDRINE HEUTZ, Department of Materials, Imperial College London, TIM JONES, Department of Chemistry, Warwick University, UK, GABRIEL AEPPLI, Department of physics and astronomy, University College London, ORGANIC SPINTRONICS TEAM — The theoretical understanding of exchange interactions in organics provides a key foundation for quantum molecular magnetism. Recent SQUID magnetometry of a well know organic semiconductor, copper-phthalocyanine [1,2] (CuPc) shows that it forms quasi-one-dimensional spin chains. Green's function perturbation theory calculation [3] is used to find the dominant exchange mechanism. Hybrid density functional theory simulations [4] give a quantitative insight to exchange interactions and electronic structures. Both calculations are performed for different stacking and sliding angles for lithium-Pc, cobalt-Pc, chromium-Pc, and copper-Pc. The exchange interactions depend strongly on stacking angles, but weakly on sliding angles. Our results qualitatively agree with the experiments, and remarkably α -cobalt-Pc has a very large exchange above liquid-Nitrogen temperature. Our theoretical predictions on the exchange interactions can guide experimentalists to design novel organic semiconductors.

[1] S. Heutz, et. al., Adv. Mat., 19, 3618 (2007) [2] Hai Wang, et. al., ACS Nano, 4, 3921 (2010) [3] Wei Wu, et. al., Phys. Rev. B 77, 184403 (2008) [4] Wei Wu, et. al., Phys. Rev. B 84, 024427 (2011)

1:15PM W13.00009 Magneto-optical spectroscopic studies of solid and solution-phase tetraphenyl porphyrin¹, JACOB WAHLEN-STROTHMAN, ZHEN WEN PAN, CODY LAMARCHE, LANE MANNING, NAVEEN RAWAT, University of Vermont, TAKAHISA TOKUMOTO, STEPHEN MCGILL, National High Magnetic Field Lab, MADALINA FURIS, KELVIN CHU, University of Vermont — Tetraphenylporphyrin (TPP) is a heterocyclic model system for porphyrins found in heme proteins, cytochromes and photosynthetic cofactors. TPP can accommodate a metal ion in the center; D-shell ion porphyrin complexes with a crystalline solid phase are of interest for magnetic studies because of the possibility of macroscopic long-range magnetic order of the ion spins. We have investigated the 5K magnetic properties of poly-crystalline thin films of TPP complexed with Zn, Mn and Cu and deposited through a room temperature capillary pen technique that produces grain size in the 100 micron to 1mm range. Our novel setup measures the UV/VIS, linear dichroism and MCD simultaneously and incorporates a photoelastic modulator and a microscopy superconducting magnet for high-field (5T) measurements. In addition, we present 25T data on samples from the new split magnet at NHMFL. We present solution and crystalline data on metal-complexed TPP; data are analyzed in terms of A and B-type MCD using a perimeter model. We find good agreement with previous solution data, and novel crystalline phase spectra that are correlated to the long range ordering of the solid state.

¹This work supported by NSF DMR-0821268, DUE-0942562 and EPS-0701410

1:27PM W13.00010 Spin exchange interaction in quasi-1D Cu-phthalocyanine crystalline thin film measured by Magnetic Circular Dichroism (MCD) spectroscopy, ZHENWEN PAN, NAVEEN RAWAT, CODY LAMARCHE, Material Science and Physics Dept., University of Vermont, TAKAHISA TOKUMOTO, National High Magnetic Field Laboratory, ANTHONY WETHERBY, RORY WATERMAN, Chemistry Dept., University of Vermont, RANDY HEADRICK, Material Science and Physics Dept., University of Vermont, STEVE MCGILL, National High Magnetic Field Laboratory, MADALINA FURIS, Material Science and Physics Dept., University of Vermont — Highly-oriented Cu-phthalocyanine (PC) pen-written crystalline thin films can be viewed as quasi-1D spin 1/2 magnetic chains. In order to reveal the nature of spin exchange between localized S=1/2 Cu spins, MCD spectroscopy was performed on films with millimeter-sized grains fabricated from a soluble CuPc derivative in magnetic fields up to 10 Tesla at temperatures ranging from 0.4 K to 77K. At T<2K and B<4T the MCD associated with transitions between Q-band π electron states exhibits a non-linear temperature-dependent Brillouin-like increase with magnetic field. For B>4T the MCD evolves linearly with magnetic field, as expected from diamagnetic carbon-based systems. Theoretical modeling¹ of electronic structure and exchange interactions in this system predicts an indirect exchange mechanism mediated by delocalized ligand states. Our MCD measurements identified the states responsible for this exchange.

¹W. Wu et. al., PRB 84,024427(2011)

1:39PM W13.00011 Introducing copper phthalocyanine as a qubit¹, MARC WARNER, London Centre for Nanotechnology, SALAHUD DIN, Imperial College London, London, UK, JULES GARDENER, Harvard University, GAVIN W. MORLEY, University of Warwick, UK, WEI WU, Imperial College London, UK, MARSHALL STONEHAM, ANDREW J. FISHER, University College London, UK, SANDRINE HEUTZ, Imperial College London, London, UK, CHRISTOPHER W. M. KAY, GABRIEL AEPPLI, University College London, UK — Quantum information processing (QIP) has been shown to solve certain useful problems faster than its classical counterpart. However finding a physical system upon which to execute these algorithms is a challenging task. One promising implementation is to use an electron spin in a magnetic field as the information bearing quantum system. Numerous options have been proposed along these lines. Here I discuss a new candidate qubit, copper phthalocyanine. The copper atom at the centre of the molecule carries an unpaired electron. Pulsed electron paramagnetic resonance measurements of relaxation times reveal that it has potential for QIP. We measure the spin-lattice and spin-spin relaxation times of this electron and demonstrate single qubit manipulations. Solid-state electronic devices can be built with this low cost material, which is optically active, and offers great opportunities for chemical and physical modification, leading to significant control of magnetic and other properties.

¹We thank the EPSRC for financial support through the Basic Technology Programme “Molecular Spintronics.”

1:51PM W13.00012 Structure-Controlled Coercivity of Low-Dimensional Metallo-Organic Thin Films¹, THOMAS GREDIG, MATTHEW BYRNE, BRIAN CACHA, JACOB KALMANIR, MATHEW WERBER, California State University Long Beach, CA — Metallo-organic thin films based on iron phthalocyanine were prepared to form self-assembled structures. Based on the substrate, the metal-ion chains can be grown perpendicular or parallel to the substrate. Individual iron chains are separated by 1.3 nm and interact weakly at low temperatures. The magnetic response of these structurally templated thin films is studied for a fixed film thickness and varied deposition temperatures. The magnetic hysteresis loops are wasp-shaped and mark long-range ferromagnetic interaction below a temperature of 4.5 K. The hysteresis loop coercivity can be correlated with the grain size of the iron phthalocyanine thin film. The enhanced coercivity is attributed to longer iron chains that are formed in larger grains.

¹This project is supported by National Science Foundation grant DMR-0847552.

2:03PM W13.00013 The Otto thermodynamic cycle using the magnetic molecule Ni₂, WOLFGANG HÜBNER, CHUANDING DONG, GEORGIOS LEFKIDIS, Dept. of Physics and Research Center OPTIMAS, University of Kaiserslautern — In order to design realistic molecular heat engines, the study of quantum thermodynamics is essential since classical thermodynamics does not apply in this extreme miniaturization limit [1,2]. Realizing a thermodynamic cycle on an existing magnetic molecule embodies a novel and unique approach to understand and exploit the thermodynamic properties of spin at the molecular level.

Here we propose an Otto cycle in the Ni₂ dimer based on a fully ab-initio calculation of the electronic states and the perturbative inclusion of spin-orbit coupling. A laser pulse, described by the time-dependent Schrödinger equation, is used to heat the Ni₂ dimer. The pulse not only excites the electrons to higher, many-body electronic states, but also influences the spin of the system due to spin-orbit coupling. Using a low-temperature thermal bath the system is cooled back to the ground state. The adiabatic work exchange between the Ni₂ and the environment is described by the quasi-static expansion or compression of the bond length of the dimer. The calculated efficiency of the cycle is up to 34%.

[1] T. D. Kieu, Phys. Rev. Lett. **93** 140403 (2004)

[2] H. T. Quan, Phys. Rev. E **79** 041129 (2009)

[3] T. Zhang et al., Phys. Rev. A **75** 062102 (2007)

Thursday, March 1, 2012 11:15AM - 2:15PM —
Session W14 GMAG DMP FIAP: Focus Session: Spins in Semiconductors - Ferromagnetism and Spin Dynamics in Semiconductors 212

11:15AM W14.00001 Spin Dynamics in Bi₂Se₃ / GaAs Heterostructures, ANDREW L. YEATS, PAUL V. KLIMOV, BOB B. BUCKLEY, Center for Spintronics and Quantum Computation, University of California, Santa Barbara CA 93106, ANTHONY RICHARDELLA, DUMING M. ZHANG, NITIN SAMARTH, Center for Nanoscale Science & Dept. of Physics, Penn State University, University Park PA 16802, MICHAEL E. FLATTE, Dept. of Physics, University of Iowa, Iowa City IA 52242, DAVID D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara CA 93106 — The narrow band gap semiconductor Bi₂Se₃ has been characterized as a topological insulator (TI), wherein strong spin-orbit coupling and time-reversal symmetry give rise to spin-polarized surface conduction states. Molecular beam epitaxy (MBE) of Bi₂Se₃ thin films onto conventional semiconductors such as GaAs [1] provides an attractive pathway for the creation of hybrid devices, coupling the exotic spin physics of TIs with the well-understood properties of spin coherence in semiconductors. We employ spatio-temporally resolved optoelectronic techniques to probe the carrier spin dynamics at the heterointerface between a TI and GaAs. Results are compared with interface band structure calculations.

This work is supported by ONR and NSF.

[1] A. Richardella, D. M. Zhang, J. S. Lee, A. Koser, D. W. Rench, A. L. Yeats, B. B. Buckley, D. D. Awschalom and N. Samarth, *Appl. Phys. Lett.* **97**, 262104 (2010).

11:27AM W14.00002 Optical Aharonov-Bohm Effect in Al_{0.08}Ga_{0.92}As/Al_{0.25}Ga_{0.75}As Quantum Wells¹, ANDREAS RUSS, LARS SCHWEIDENBACK, JOSEPH MURPHY, ALEXANDER CARTWRIGHT, ATHOS PETROU, SUNY at Buffalo, Buffalo, NY, GEORGE KIOSEOGLOU, University of Crete, Heraklion, Greece, ALEXANDER GOVOROV, Ohio University, Athens, OH, AUBREY HANBICKI, BEREND JONKER, Naval Research Laboratory, Washington DC — The photoluminescence (PL) from Al_{0.08}Ga_{0.92}As/Al_{0.25}Ga_{0.75}As quantum wells (QW) was studied as function of magnetic field applied along the normal to the QW planes. The PL intensity exhibits two maxima at 2.3 and 4.9 tesla. The time-resolved PL from the same sample has a decay time which is one order of magnitude longer than the PL from a GaAs/AlGaAs QW, indicating that the recombination in the AlGaAs QW is spatially indirect. The PL intensity oscillations are attributed to the optical Aharonov-Bohm effect associated with spatially quasi-indirect excitons, which are located in the vicinity of islands with lower Al composition. The holes are localized by the islands, while the electrons move around them in a ring-like geometry. This model is in agreement with the interpretation of earlier results from Al_xGa_{1-x}As/Al_yGa_{1-y}As Fe spin-LEDs.

¹Work at SUNY is supported by DOE-BES, ONR, AFOSR-DCT and NSF

11:39AM W14.00003 Optical response of relativistic electrons in the polar BiTeI semiconductor, J.S. LEE, Graduate program of Photonics and Applied Physics, Gwangju Institute of Science and Technology (GIST), Gwangju 500-712, Korea, G.A.H. SCHOBER, Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan, M.S. BAHRAMY, Correlated Electron Research Group (CERG) and Cross-Correlated Materials Research Group (CMRG), ASI, RIKEN, Wako 351-0198, Japan, H. MURAKAWA, Multiferroics Project, ERATO, Japan Science and Technology Agency (JST), Tokyo 113-8656, Japan, Y. ONOSE, R. ARITA, N. NAGAOSA, Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan, Y. TOKURA, Department of Applied Physics and Quantum Phase Electronics Center (QPEC), University of Tokyo, Tokyo 113-8656, Japan — The transitions between the spin-split bands by spin-orbit interaction are relevant to many novel phenomena such as the resonant dynamical magneto-electric effect and spin Hall effect. Here, we present a combined experimental and theoretical study of the dynamics of relativistic electrons in the recently discovered giant bulk Rashba spin splitting system BiTeI. Several novel features are observed in the optical spectra including sharp edge singularity due to the reduced-dimensionality of joint density of states and a systematic doping dependence of the intraband transitions between the Rashba-split branches. These confirm the bulk nature of the Rashba-type splitting in BiTeI and manifest relativistic nature of the electron dynamics in a solid.

11:51AM W14.00004 Room temperature ferromagnetism in transparent conducting Fe-doped In₂O₃ films, MICHAEL OSOFSKY, HEUNGSOO KIM, MICHAEL MILLER, SEYED QADRI, RAYMOND AUYEUNG, ALBERTO PIQUE, Naval Research Laboratory — Oxide semiconductors have been widely studied as a host compound for spintronic devices since they can be doped with transition metals to realize a higher Curie temperature and can produce high n-type carriers by either doping with Group IV elements or introducing oxygen vacancies. Among various oxide semiconductors, Fe-doped In₂O₃ is a promising ferromagnetic semiconductor due to the high solubility of Fe-ions into the In₂O₃ lattice. Recently, at NRL, In_{2-x}Fe_xO₃ thin films have been deposited on MgO, sapphire, and YSZ substrates by pulsed laser deposition. The lattice constant decreases linearly with increasing Fe-doping concentration suggesting the incorporation of Fe ions into the In₂O₃ lattice matrix. Magneto-transport characteristics including anomalous Hall effect along with structural analysis demonstrate that an intrinsic ferromagnetism is observed for some films grown under optimized conditions. In this presentation, we will discuss our work to date on the growth of In_{2-x}Fe_xO₃ thin films grown by pulsed laser deposition with various deposition conditions and present the structural, optical, magnetic, and transport properties along with spin-polarization measurements.

12:03PM W14.00005 Selective optical excitation of in-plane and out-of-plane spin polarizations with linearly polarized light in InGaAs¹, STEFAN GOEBBELS, FREDERIK KLEIN, PHILIPP SCHAEFERS, MARKUS HAGEDORN, KLAUS SCHMALBUCH, GERNOT GUENTHERODT, II. Physikalisches Institut, RWTH Aachen University, Germany, MIHAIL LEPSA, THOMAS SCHAEPEPERS, Peter Gruenberg Institut (PGI-9), Forschungszentrum Juelich GmbH, Germany, BERND BESCHOTEN, II. Physikalisches Institut, RWTH Aachen University, Germany — Excitation with circularly polarized light is a standard technique for optical spin orientation in semiconductors. This method is based on the transfer of angular momentum from the photons to the electrons and yields a polar spin polarization directed along the propagation direction of the exciting laser beam. Here we present linearly polarized all-optical pump-probe experiments to excite and detect coherent electron spins in InGaAs [1]. We find the magnitude and the orientation of the spin polarization strongly depend on the polarization axes of the exciting light. While in general the excited spin ensemble is composed of both polar and transverse spin components, the polarization axis of the exciting light can be chosen such that polar and transverse spin components can be excited separately. Thus, selective excitation of in-plane and out-of-plane spin polarizations is feasible with linearly polarized light.

[1] K. Schmalbuch *et al.*, *Phys. Rev. Lett.* **105**, 246603 (2010)

¹This work has been supported by DFG through FOR 912.

12:15PM W14.00006 Carrier Dynamics in Narrow Gap Ferromagnetic Semiconductors¹, D. SAHA, X. PAN, G.D. SANDERS, C.J. STANTON, University of Florida, M. BHOWMICK, T. MERRITT, G.A. KHODAPARAST, Virginia Tech, C. FEESER, B.W. WESSELS, Northwestern University, S. MCGILL, NHMFL — Narrow gap ferromagnetic semiconductors are promising materials for spin photonic and spin transport devices because of their small effective masses, small energy gap, and high carrier mobility. We use time resolved differential transmission (TRDT) experiments to study carrier dynamics in ferromagnetic InMnAs and InMnSb. Electronic structure for InMnAs and InMnSb is calculated using an 8-band Pidgeon-Brown model generalized to include the effects of an external magnetic field. Our model includes the effects of the ferromagnetic Mn ions and their coupling to electrons and holes with or without an external magnetic field. Optical transitions are calculated from Fermi's Golden rule and interband transitions at a given pump or probe laser energy are identified. This allows us to understand a sign change seen in the TRDT. Our results show that 1) Phase-Space Filling, 2) Band Gap Renormalization and 3) Free Carrier Absorption all contribute to the TRDT and that the relative importance of these effects depends on the laser probe energy.

¹Supported by NSF DMR-0846834, DMR-0800479 and DMR-1105437

12:27PM W14.00007 Ferromagnetism in cobalt-doped SrTiO₃ on Si grown by molecular beam epitaxy, AGHAM POSADAS, CHANDRIMA MITRA, ALEXANDER DEMKOV, University of Texas at Austin — We report the epitaxial growth of ferromagnetic cobalt-doped SrTiO₃ directly on silicon without the use of any buffer by molecular beam epitaxy (MBE). Magnetization as a function of magnetic field was performed for samples with varying doping concentration at room temperature and at 10 K. Room-temperature ferromagnetism is confirmed in single phase samples with composition 20-30% cobalt. We also performed x-ray photoelectron spectroscopy of the Co and Ti 2p levels to determine stoichiometry and cobalt oxidation state. In order to elucidate the origin of ferromagnetism, we also performed first-principles calculations of cobalt-doped SrTiO₃ with different doping concentrations and dopant configurations. The calculations show that intrinsic ferromagnetism can be stabilized beyond a critical concentration in SrTiO₃ under particular conditions. The ability to directly integrate a ferromagnet on silicon in epitaxial form may potentially overcome the problems of impedance mismatch and interface losses in applications involving spin injection in silicon.

12:39PM W14.00008 Two-dimensional MnGa_N Layer formed by Nitridation of Mn $\sqrt{3} \times \sqrt{3}$ -R30 structure on Wurtzite GaN (0001)¹, MENG SHI, ABHIJIT CHINCHORE, Department of Physics and Astronomy, Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, Ohio - 45701, YINHAO LIU, Los Alamos National Lab, Los Alamos, NM 87545, ARTHUR SMITH, Department of Physics and Astronomy, Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, Ohio - 45701 — There has been much interest in dilute Mn-doped GaN as a spintronic material. Recently, it has become of interest to consider the possible advantages of delta-doped magnetic layers, rather than a bulk alloy. Here we investigate experimentally the growth of single Mn-containing layers on top of wurtzite GaN as well as the overgrowth of GaN onto the Mn-containing layer, using a combination of N-plasma molecular beam epitaxy and reflection high energy electron diffraction. Sub-monolayer Mn deposition on GaN(0001) results in a novel $\sqrt{3} \times \sqrt{3}$ -R30 structure [1]. Upon nitrogen plasma exposure, this periodicity is removed; whereas, Mn is found remaining on the surface as measured by Auger electron spectroscopy. Unexpectedly, and in dramatic comparison to tiny lattice constant changes seen for bulk films, we find a huge -3.3 percent surface lattice contraction in both [1010] and [1120] azimuthal directions. This suggests the possible formation of a Mn_{0.25}Ga_{0.75}N 2-D alloy. Furthermore, subsequent overgrowth of GaN layers does not show significant lattice constant change compared to the nitridation process, up to a thickness of 20 ML or more.
[1] Chinchore et al., Applied Physics Letters **93**(18), 181908 (2008).

¹ Authors gratefully acknowledge DOE & NSF.

12:51PM W14.00009 Structural transition and giant spintronic response of two dimensional Manganese-Gallium $\sqrt{3} \times \sqrt{3}$ R30° surface structure¹, ABHIJIT CHINCHORE, MENG SHI, WENZHI LIN, KANGKANG WANG, Ohio University Nanoscale and Quantum Phenomena Institute, YIANGHAO LIU, Los Alamos National Laboratory, ARTHUR SMITH, Ohio University Nanoscale and Quantum Phenomena Institute, VALERIA FERRARI, ANDREA BARRAL, ANA MARIA LLOIS, Universidad de Buenos Aires and Comision Nacional de Energia Atomica — In recent experiments, we have found that gallium nitride surface when exposed to transition metal atoms, results in novel well-ordered two dimensional spintronic structure, with tunable spintronic properties. A 2000 Å N-polar *w*-gallium nitride (0001) layer is grown on a sapphire substrate, by molecular beam epitaxy. The growth is monitored using reflection high energy electron diffraction system. Post growth, the standard 1×1 gallium nitride surface, is exposed to sub monolayer doses of manganese. At low deposition temperature the diffraction patterns show manganese atoms forming a metastable 3×3 structure, on supplying little heat to the manganese 3×3 structure, it undergoes an irreversible transition to form a stable $\sqrt{3} \times \sqrt{3}$ R30° structure. Both the structures are studied using a scanning tunneling microscope. The $\sqrt{3} \times \sqrt{3}$ R30° structure shows a giant change in spectroscopic response on application of a very small out-of-plane magnetic field. The new findings suggest that the two dimensional magnetic nitride systems have excellent potential for both fundamental investigations and for use in future spintronic devices.

¹ Authors gratefully acknowledge the funding from NSF and DOE.

1:03PM W14.00010 Spinglass Dynamics of Amorphous Ferromagnetic Ge:Mn¹, SAMARESH GUCHAHAIT, SANJAY BANERJEE, RAYMOND ORBACH, The University of Texas at Austin — Ge_{0.84}Mn_{0.16} is an amorphous ferromagnetic semiconductor with a Curie temperature of about 160 K (measured at 1000 Oe). Magnetic field-cooled and zero-field-cooled experiments show existence of a spinglass phase well below the Curie temperature. The spinglass temperature is about 23 K at a 50 Oe field. The spinglass temperature scales monotonically with applied magnetic field. Magnetic hysteresis experiments show a non-zero coercive field below the spinglass temperature, and a very small coercive field or a superparamagnetic phase above it. Under a rapid quench, thermoremanent magnetization (TRM) decay experiments (at 14 K) exhibit a very large effective waiting time. This is associated with a slow rate of cooling, allowing communication between phase space states before the measuring temperature is reached, leading to an effective reduction in the attempt frequency. This is consistent with experiments on other more typical spin glass systems.

¹ This work was supported by SWAN-NRI, NSF DMR 0605828, and Welch Foundation F-1191.

1:15PM W14.00011 Magnetism in Iron-Titanium Oxide Nanostructures¹, PEGAH HOSSEINPOUR, Chemical Engineering Department, Northeastern University, EUGEN PANAITESCU, Physics Department, Northeastern University, LAURA H. LEWIS, Chemical Engineering Department, Northeastern University, LATIKA MENON, DON HEIMAN, Physics Department, Northeastern University — Modification of the titania nanotubes with magnetic transition metal additions is anticipated to provide the opportunity of creating a novel multifunctional nanostructured material with magnetic, semiconducting and catalytic properties. Incorporation of Fe into titania to produce ordered arrays of amorphous (Fe+Ti)₂O₃ nanotubes was achieved by electrochemical anodization. As-made nanotubes were subjected to a systematic thermal treatment in a variety of atmospheres for crystallization; their associated morphological, structural and magnetic character was examined. Preliminary results indicate that the Fe-modified nanotubes possess a unit cell volume that is slightly larger than that of titania (137 vs 136 Å³) confirming Fe incorporation into the lattice. The temperature-dependent magnetic susceptibility data obtained from the samples may be decomposed into a Curie-Weiss component that represents the localized magnetic character of titania nanotubes and a Pauli paramagnetic component that represents the semiconducting behavior of the nanotubes. It is noted that Fe incorporation causes an increase in both components of the magnetic signal, suggesting modification of the electronic structure of the crystalline titania phase with iron incorporation.

¹ Research supported by the National Science Foundation under Grant No. DMR-0906608.

1:27PM W14.00012 Magnetoluminescence Studies of Mn-doped PbS Quantum Dots¹, BIPLOB BARMAN, YUTSUNG TSAI, GEN LONG, SAVAS DELIKANLI, ATHOS PETROU, HAO ZENG, SUNY at Buffalo, Buffalo, NY — Diluted magnetic semiconductor quantum dots are interesting model systems for the investigation of carrier dopant exchange interactions. In this work, we report the carrier spin polarization studies in narrow band gap Mn-doped PbS quantum dots, a much less studied system compared to their II-VI counterparts. The PbMnS quantum dots were synthesized by hot colloidal solution technique. They are single crystalline with cubic structure. The doping concentration is 3-4% as measured by energy dispersive X-ray spectroscopy. The system is paramagnetic down to 2 K, as measured by VSM. We have recorded the PL spectra in the Faraday geometry for magnetic fields of up to 7 tesla in the 0-50 K temperature range. The PL was excited at 780 nm and the emission is centered at 940 meV with a FWHM of 100 meV. In the presence of a magnetic field the emission becomes strongly σ^+ polarized ($P = 35\%$ at 4 tesla), suggesting carrier spin polarization. The polarization is temperature sensitive and decreasing sharply with increasing temperature. The polarization vanishes at around $T = 40$ K. The degree of spin polarization can be tuned by quantum confinement.

¹This work is supported by NSF

1:39PM W14.00013 All-Optical observation of Nuclear Magnetic Resonance in a 2D electron system, YANG JI, XUAN QIAN, SKLSM, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, PR China, VLADIMIR UMANSKY, Braun Center for Submicron Research, Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel — Electron-nuclear spin interaction may be utilized to manipulate nuclear states coherently in quantum computation. Here we report on an all-optical observation of nuclear magnetic resonance (NMR) in a 2D electron system embedded in a GaAs/AlGaAs heterostructure. In analogy to radio-frequency fields used in traditional NMR, circularly polarized light creates electron spins in semiconductors whose hyperfine coupling with nuclei could tip nuclear moments. At a fixed time-delay ~ 12.5 ns, time-resolved Kerr-rotation (TRKR) signals were measured as a function of the modulation frequency (from 1 KHz to 100 kHz) of the pump laser. Spin-polarized carriers generated by the pump laser pulse train acts on the nuclear spins as an effective rf magnetic field synchronized at the pulse repetition frequency, which resonates nuclear spins at suitable frequencies in an external magnetic field in Voigt geometry. Several dips were observed in a TRKR trace at, which shift linearly with increasing magnetic field. They are ascribed to be NMR signals of elements As-75, Ga-69, Al-27 and Ga-71.

1:51PM W14.00014 Confinement and Diffusion Effects in Dynamical Nuclear Polarization in Low Dimensional Nanostructures, DAN HENRIKSEN, IONEL TIFREA, California State University, Fullerton — We investigate the dynamic nuclear polarization as it results from the hyperfine coupling between nonequilibrium electronic spins and nuclear spins in semiconductor nanostructures. The natural confinement provided by low dimensional nanostructures is responsible for an efficient nuclear spin - electron spin hyperfine coupling [1] and for a reduced value of the nuclear spin diffusion constant [2]. In the case of optical pumping, the induced nuclear spin polarization is position dependent even in the presence of nuclear spin diffusion. This effect should be measurable via optically induced nuclear magnetic resonance or time-resolved Faraday rotation experiments. We discuss the implications of our calculations for the case of GaAs quantum well structures.

[1] I. Tifrea and M. E. Flatté, Phys. Rev. B 84, 155319 (2011).

[2] A. Malinowski and R. T. Harley, Solid State Commun. 114, 419 (2000).

2:03PM W14.00015 ABSTRACT WITHDRAWN —

Thursday, March 1, 2012 11:15AM - 2:03PM —

Session W15 DMP FIAP GMAG: Focus Session: Spins in Metals - Domain Wall, Vortex, Magnonic Based Devices 213

11:15AM W15.00001 High speed domain wall motion in MgO-based magnetic tunnel junctions driven by perpendicular current injection¹, P.J. METAXAS, A. CHANTHBOUALA, R. MATSUMOTO, V. CROS, A. ANANE, J. GROLLIER, A. FERT, Unite Mixte de Physique CNRS/Thales, France, K.A. ZVEZDIN, Istituto P.M. s.r.l., Italy, A. FUKUSHIMA, S. YUASA, National Institute of Advanced Industrial Science and Technology (AIST), Japan — The ability to efficiently drive fast domain wall (DW) motion will pave the way for revolutionary new electronic devices ranging from DW-MRAMs to spintronic memristors. The majority of domain wall devices use a lateral, current-in-plane configuration in which critical current densities for domain wall motion remain quite high, typically being on the order of 100 MA/cm^2 with velocities generally limited to about 100 m/s . In this contribution we show that critical current densities can be decreased by up to two orders of magnitude using the current-perpendicular-to-plane geometry. Indeed, we demonstrate that a DW can be propagated back and forth along the free layer of a MgO-based magnetic tunnel junction (MTJ) in the absence of an external magnetic field using current densities that are on the order of 5 MA/cm^2 . More notably however, we obtain high domain wall velocities for these low current densities: the MTJ's large resistance variations allow us to carry out time-resolved measurements of the wall motion from which we evidence DW velocities exceeding 500 m/s .

¹The authors thank Canon ANELVA for magnetic film preparation. This work was supported by the European Research Council (ERC 2010 Stg 259068).

11:27AM W15.00002 Thermal activation energy for domain wall motion in out-of-plane magnetized submicron strips, SATORU EMORI, GEOFFREY BEACH, Massachusetts Institute of Technology — We have experimentally studied micrometer-scale domain wall (DW) motion driven by magnetic field and electric current in 500-nm wide out-of-plane magnetized Co/Pt multilayer strips with Co layer thicknesses $0.5\text{-}0.7 \text{ nm}$. The scaling of thermal activation energy for DW motion with driving field and current has been extracted directly from the temperature dependence of the DW velocity. For DWs driven by field, the activation energy follows creep and depinning dynamics below a critical field and collapses to zero above the critical field. DW motion assisted by current shows velocity enhancement independent of current polarity, but causes no measurable change in the activation energy barrier. Through this analysis, the observed current-induced DW velocity enhancement in these Co/Pt multilayer strips can be entirely and unambiguously attributed to Joule heating.

11:39AM W15.00003 Intrinsic domain wall flexing from current-induced spin torque , ELIZABETH

GOLOVATSKI, Dept. of Physics, Luther College, MICHAEL FLATTÉ, OSTC and Dept. of Physics and Astronomy, University of Iowa — Spin torque generated by coherent carrier transport in domain walls [1] is a major component in the development of spintronic devices [2]. We model spin torque in Néel walls [3] using a piecewise linear transfer-matrix method [4] to calculate spin torque on interior wall segments. For a π wall with a total positive torque (current left-to-right), we find the largest positive and negative spin torques left of the central region, 4-5 orders of magnitude larger than the center. The wall's rightward push comes from the back of the wall; all other significant regions pull to the left. Adding a second wall (both walls with positive total torque) changes the first wall little, but produces spin torques in the second wall with large canceling torques on the left, and the push rightward from a smaller torque on the right. The gradient of torque across the wall generates an intrinsic domain wall flexing (distinct from extrinsic wall flexing from pinning centers [5]). Work supported by an ARO MURI.

[1] M. Yamanouchi et al., Nature 428, 539 (2004).

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[4] E. Golovatski and M. Flatté, Phys. Rev. B, 84, 115210 (2011)

[5] A. Balk et al., Phys. Rev. Lett. 107, 077205 (2011).

11:51AM W15.00004 Spinmotive force due to domain wall motion in high field regime , JUN'ICHI

IEDA, Advanced Science Research Center, JAEA; CREST, JST, YUTA YAMANE, Institute for Materials Research, Tohoku University, SADAMICHI MAEKAWA, Advanced Science Research Center, JAEA; CREST, JST — Spinmotive force associated with a moving vortex domain wall is investigated numerically. Dynamics of magnetization textures such as a domain wall exerts a non-conservative spin-force on conduction electrons [1], offering a new concept of magnetic devices [2]. This spinmotive force in permalloy nanowires has been detected by voltage measurement [3] where magnitude of the signal is limited less than 500 nV. Theoretically it is suggested that the spinmotive force signal increases as a function of external magnetic fields. At higher magnetic fields, however, the wall propagation mode becomes rather chaotic involving transformations of the wall structure and it remains to be seen how the spinmotive force appears. Numerical simulations show that the spinmotive force scales with the field even in a field range where the wall motion is no longer associated coherent precession. This feature has been tested in a recent experiment [4]. Further enhancement of the spinmotive force is explored by designing ferromagnetic nanostructures [5] and materials. [1] S. Barnes and S. Maekawa, PRL (2007). [2] S. Barnes, J. Ieda, and S. Maekawa, APL (2006). [3] S. A. Yang et al., PRL (2009). [4] M. Hayashi, J. Ieda et al., submitted. [5] Y. Yamane, J. Ieda et al., APEX (2011).

12:03PM W15.00005 All-magnonic spin-transfer torque and domain wall propagation¹ , X.R. WANG,

P. YAN, X.S. WANG, The Hong Kong University of Science and Technology — In this talk, we will discuss the spin-transfer torque (STT) between magnons and magnetic domain wall (DW). It is found that a spin wave passes through a transverse magnetic DW in a magnetic nanowire without reflection. A magnon, the quantum of the spin wave, carries opposite spins on the two sides of the DW. As a result, there is a spin angular momentum transfer from the propagating magnons to the DW. This magnonic STT can efficiently drive a DW to propagate in the opposite direction to that of the spin wave. In comparison with the electronic STT, the energy consumption is much lower when the magnonic STT is used to drive a DW propagating at a useful velocity. Since this STT does not require any itinerant electrons, it opens a door of using magnetic insulators like YIG in spintronics devices. One extra benefit of using magnetic insulators is the low damping coefficient so that it should further lower the energy consumption and increase operation efficiency.

¹This work is supported by Hong Kong RGC Grants (604109, RPC11SC05, and HKUST17/CRF/08).

12:15PM W15.00006 Disentangling the physical contributions to the anomalous Hall effect and domain wall resistance in isoelectronic L1₀-FePd and L1₀-FePt alloys , KLAUS SEEMANN, FELIPE GARCIA-SANCHEZ, ATTILA KAKAY, CLAUS SCHNEIDER, Peter Gruenberg Institut, Research Centre Juelich, Germany, FRANK FREIMUTH, YURIY MOKROUSOV, STEFAN BLUEGEL, Institute for Advanced Simulation, Research Centre Juelich, Germany, RICCARDO HERTEL, Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg, CNRS UMR 7504, Strasbourg, France — We analyze the origin of the electrical resistance arising in domain walls of perpendicularly magnetized materials by considering a superposition of anisotropic magnetoresistance and the resistance implied by the magnetization chirality. The domain wall profiles of L1₀-FePd and L1₀-FePt are determined by micromagnetic simulations based on which we perform first principles calculations to quantify electron transport through the core and closure region of the walls. The wall resistance, being twice as high in L1₀-FePd than in L1₀-FePt, is found to be clearly dominated in both cases by a high gradient of magnetization rotation, and not by the spin-orbit interaction driven anisotropic magnetoresistance effect. Concerning the anomalous Hall effect on the other hand, we show that difference in spin-orbit interaction strength of Pt and Pd atoms leads to a pronounced cross-over from an extrinsic side jump mechanism in L1₀-FePd to an intrinsic Berry-phase anomalous Hall effect in L1₀-FePt.

12:27PM W15.00007 Stochastic dynamics of vortex cores in a pinning potential observed via torsional magnetometry¹ , ALASTAIR FRASER, JACOB BURGESS, JOSEPH LOSBY, FATEMEH FANISANI, University of Alberta, DOUG VICK, WAYNE HIEBERT, National Institute for Nanotechnology, JOHN DAVIS, University of Alberta, MARK FREEMAN, National Institute for Nanotechnology — Measurements of a single 1 micrometer diameter permalloy disk fabricated on a silicon nitride torsional resonator are presented. Sensitivity of this device is sufficiently high to allow study of the vortex core interaction with very weak pinning sites. Low speed stochastic dynamics are revealed and attributed to the vortex core hopping between bistable states around pinning sites. The temperature and field dependence of this noise around the pinning site was investigated. Analysis employing an analytical description of the vortex in a thin disk and an Arrhenius model allows determination of the pinning potential.

¹Research supported by NSERC, NINT, CIFAR, and CRC

12:39PM W15.00008 Dimensionality crossover in magnetic vortex dynamics¹ , TE-YU CHEN, MICHAEL ERICKSON, ANDREW GALKIEWICZ, CHRIS LEIGHTON, PAUL CROWELL, University of Minnesota — The ground state of a micron diameter ferromagnetic disk is often a single magnetic vortex, in which the gyrotropic mode of the vortex core is the lowest frequency excitation. In thin disks (thickness $L \ll$ diameter D), the vortex can be treated two-dimensionally (2D), and the gyrotropic frequency f_G is determined by L/D . We have observed a crossover from 2D to 3D dynamics as the thickness increases. Using time-resolved Kerr microscopy, we have investigated the gyrotropic mode in 1 μm diameter Ni₈₀Fe₂₀ disks as a function of L , which was varied from 20 nm to 200 nm. In thin disks ($L < 80$ nm), f_G is approximately proportional to L . For $L > 100$ nm, f_G increases less rapidly than predicted by the 2D model, and an additional gyrotropic mode appears at higher frequencies. We have explored the thickness dependences of both modes. In the ordinary gyrotropic mode, which is magnetostatic in character, the core oscillates uniformly through the thickness of the disk. The second gyrotropic mode is exchange-dominated, and the core oscillates with larger amplitude at the surfaces and a node in the equatorial plane of the disk. In the thickest disks, the exchange-dominated mode is the lowest in frequency.

¹This work supported primarily by the NSF MRSEC program.

12:51PM W15.00009 Magnonic band gaps in films with periodically modified surfaces¹, RODRIGO ARIAS, CLAUDIO JARUFE, Universidad de Chile — It is of current interest to understand the electromagnetic response of different nano-structures. In this study we focus on the role of geometry in ferromagnetic modes and response. Specifically we consider a ferromagnetic thin film with periodically perturbed surfaces, in the magnetostatic limit. We focus on the changing behavior of surface modes of the unperturbed film. Our film shows a behavior of interest since magnons propagate in it with band gaps associated to the geometry, i.e. they may be controlled by design. A reduced Brillouin zone scheme is introduced to describe the modes, which are of the Bloch type. Different bands are identified, and they are calculated numerically. For small geometric perturbations we develop a perturbation theory that agrees with our numerical results, and we obtain analytic expressions for the band gaps at the edges of the Brillouin zone. The underlying theory used to calculate the modes was previously developed, and relies on solving integral equations along the edges of the sample for the magnetostatic potential. We also calculate the response to magnetic field waves of a given wavevector that travel along the modulation direction, finding effective line width increments at the edge of the Brillouin zone, where the bands strongly couple.

¹Acknowledgment to Fondecyt (Chile) project 1100213, and Proyecto Basal FB0807-CEDENNA (Chile)

1:03PM W15.00010 Manipulation of propagating spin waves in straight and curved magnetic microstrips¹, ARABINDA HALDAR, HAU-JIAN LIU, Colorado State University, HELMUT SCHULTHEISS, Argonne National Laboratory, KATRIN VOGT, Technische Universität Kaiserslautern, AXEL HOFFMANN, Argonne National Laboratory, KRISTEN BUCHANAN, Colorado State University — The main challenges in realizing magnonics devices are the generation, manipulation and detection of spin waves, especially in metallic magnetic materials where the length scales are of interest for applications. We have studied the propagation of spin waves in transversely magnetized Permalloy (Py) microstrips of different shapes using micro-Brillouin light scattering. The Py stripe was 30-nm thick, several micrometers wide and $>50\text{ }\mu\text{m}$ long. Spin waves were excited in the Py strip using a $2\text{-}\mu\text{m}$ wide antenna. We compare the spin wave propagation along a straight wire to the propagation along a magnetic microstrip with a smooth bend. We will also discuss the use of a current through a gold wire under the Permalloy to provide a local magnetic field to maintain a transverse magnetization around the bend.

¹This work was supported by NIST and NSF.

1:15PM W15.00011 Dynamics of wavepacket of magnetostatic spin wave in magnet, RYO MATSUMOTO, SHUICHI MURAKAMI, Tokyo Institute of Technology — A semiclassical equation of motion of a wave packet of the magnetostatic spin wave is theoretically constructed. There appears the Berry curvature as an anomalous velocity term in the equation of motion, which causes characteristic orbital motions of the wave packet such as a self-rotational motion and a motion along the edge of the system. Due to the symmetry, the Berry curvature in the case of a thin film of an insulating ferromagnet appears when the magnetization is perpendicular to the film. We show a numerical calculation of the Berry curvature for this mode, i.e., the magnetostatic forward volume wave mode. Around the degeneracy point, the Berry curvature from the highest energy band enhances and that from other bands decreases. We also propose experimental settings to observe this effect.

1:27PM W15.00012 Nonlinear Behavior for the Uniform Mode and Horizontal Standing Spin Wave Modes in Metallic Ferromagnetic Microstrips: Experiment and Theory¹, B.W. SOUTHERN, M.P. WISMAYER, X.L. FAN, Y.S. GUI, C.-M. HU, University of Manitoba, R.E. CAMLEY, University of Colorado at Colorado Springs — Micron sized rectangular ferromagnetic bars have a variety of spin excitations, including a quasi-uniform mode, horizontal and vertical standing spin wave modes, and edge and corner modes. When driven by a strong microwave field, these modes differ from those found in the linear regime. For example, the resonance field or frequency becomes amplitude dependent. We study the nonlinear spin dynamics in such microstrips both experimentally and theoretically for a geometry where the static magnetic field is perpendicular to the plane of the sample. Experimentally it is found that, at a fixed microwave frequency, the resonance field for the uniform mode is significantly reduced as the microwave power is increased. In contrast, the resonance fields for the standing horizontal spin wave modes are only slightly reduced. This behavior is confirmed theoretically using micromagnetic calculations, and an intuitive explanation for this behavior is developed.

¹Supported by NSERC and NSF

1:39PM W15.00013 Efficient computation of Magnon dispersions within Time Dependent Density Functional Theory Using Maximally Localized Wannier Functions, BRUNO ROUSSEAU, CSIC - Centro de Física de Materiales, ASIER EIGUREN, AITOR BERGARA, Condensed Matter Physics Department, University of the Basque Country — An efficient scheme is presented to compute the transverse magnetic susceptibility within time dependent density functional theory from which magnon dispersions can be extracted. The scheme makes use of maximally localized Wannier functions in order to interpolate the band structure onto a fine k-mesh in order to converge sums on the first Brillouin zone. An optimal real space basis set containing few basis functions is shown to be sufficient to extract the magnon dispersion, making computations very efficient. The gap error in the magnon dispersion at Γ , numerically violating Goldstone's theorem, is analysed and a correction scheme is devised which can be generalized to systems where Goldstone's theorem does not apply. The method is applied to the computation of the magnon dispersion of bulk bcc iron and fcc nickel.

1:51PM W15.00014 Electron Paramagnetic Resonance of Transition Metal Ions: New Relativistic Effects at High Magnetic Fields, AYODEJI AWOBODE, University of Ibadan, Ibadan, Nigeria — We calculate the shift in the Electron Spin Resonance (ESR) frequency due to an inhomogeneous term in the equation of motion describing the precession of the angular momenta of relativistic electrons coupled to a static magnetic field. It is proposed that the calculated frequency shift may be observed in transition metal complexes in which the contributions from the ligand field are completely and precisely known. Furthermore, it is shown that a measurable transient oscillation of the dipole moment occurs after the external magnetic field is suddenly switched off.

Thursday, March 1, 2012 11:15AM - 2:15PM –
Session W16 DCMP: Quantum Criticality 251

11:15AM W16.00001 Pairing of critical Fermi-surface states, MAX METLITSKI, KITP, DAVID MROSS, MIT, SUBIR SACHDEV, Harvard University, TODADRI SENTHIL, MIT — States of matter with a sharp Fermi-surface but no well-defined Landau quasiparticles are expected to arise in a number of physical systems. Examples include i) quantum critical points associated with the onset of order in metals, ii) the spinon Fermi-surface (U(1) spin-liquid) state of a Mott insulator and iii) the Halperin-Lee-Read composite fermion charge liquid state of a half-filled Landau level. In this work, we use renormalization group techniques to investigate possible instabilities of such non-Fermi-liquids to pairing. We show that for a large class of phase transitions in metals, the attractive interaction mediated by order parameter fluctuations always leads to a superconducting instability, which preempts the non-Fermi-liquid effects. On the other hand, the spinon Fermi-surface and the Halperin-Lee-Read states are stable against pairing for a sufficiently weak attractive short-range interaction. However, once the strength of attraction exceeds a critical value, pairing sets in. We describe the ensuing quantum phase transition between i) the U(1) and the Z_2 spin-liquid states, and ii) the Halperin-Lee-Read and Moore-Read states.

11:27AM W16.00002 Fractionalized Fermi liquids as ground states of single band tJ models, MATTHIAS PUNK, SUBIR SACHDEV, Harvard University — Recently it has been argued that the normal state of underdoped cuprates might realize a fractionalized Fermi liquid (FL*), where electron-like quasiparticles couple to fractionalized excitations of a fluctuating antiferromagnetic background. The corresponding Fermi surface consists of pockets, the area of which is determined by the density of doped charge carriers alone as opposed to the total density of electrons, thereby violating Luttinger's theorem. Most previous studies of the FL* phase were based either on two-band models such as the Kondo lattice model, or on phenomenological models where Fermions are coupled to a fluctuating unit vector field representing the local Neel order. In this talk I will show that the FL* phase can indeed arise as the ground-state of a single band tJ model and discuss its implications.

11:39AM W16.00003 Doping the Kane-Mele-Hubbard model: A Slave-Boson Approach¹, JUN WEN, MEHDI KARGARIAN, University of Texas at Austin, ABOLHASSAN VAEZI, Institute for Research in Fundamental Sciences, IPM, 19395-5531, Iran; Department of Physics, Sharif University of Technology, Tehran 11155-9161, Iran, GREGORY FIETE, University of Texas at Austin — We study the Kane-Mele-Hubbard model both at half-filling and away from half-filling using a slave-boson mean-field approach at zero temperature. We obtain a phase diagram at half-filling and discuss its connection to recent results from quantum Monte Carlo, cellular dynamical mean field, slave-rotor, and Z_2 mean-field studies. In particular, we find a small window in parameter space where a spin liquid phase with gapped spin and charge excitations reside. Upon doping, we show the spin liquid state becomes a superconducting state by explicitly calculating the singlet pairing order parameters. Interestingly, we find an "optimal" doping for such superconductivity. Our work reveals some of the phenomenology associated with doping an interacting system with strong spin-orbit coupling and intermediate strength electron-electron interactions.

¹We gratefully acknowledge financial support from ARO Grant W911NF-09-1-0527 and NSF Grant DMR-0955778

11:51AM W16.00004 Stripe melting and quantum criticality in correlated metals, DAVID MROSS, SENTHIL TODADRI, Massachusetts Institute of Technology — In the last several years evidence for the occurrence of stripe and related orders has accumulated in many underdoped cuprates. With increasing doping the stripe ordering tendency disappears. This has given rise to the idea that a stripe melting quantum phase transition in the "underlying normal state" may play a role in some of the physics of the optimally doped strange metal. However there is currently no controlled understanding of a stripe-disordering phase transition in the presence of a Fermi-surface of electrons. We obtain a controlled critical theory of a continuous melting transition of charge stripes in a metal by proliferating pairs of dislocations in the stripe-order parameter, without proliferating single dislocations. At such a (deconfined) quantum critical point (QCP) the fluctuations of the stripe order parameter are strongly coupled, yet tractable. They also decouple dynamically from the Fermi-surface. We find that the full Fermi-surface and the associated Landau quasiparticles remain sharply defined at the QCP. On the stripe ordered side the reconstruction of the Fermi surface occurs at an energy scale that is parametrically different from that associated with the onset of stripe order.

12:03PM W16.00005 Quantum Criticality for Extended Nodes on the Bethe Lattice¹, JAMES MURRAY, Johns Hopkins University, ADRIAN DEL MAESTRO, University of Vermont, ZLATKO TESANOVIC, Johns Hopkins University — Theoretical description of anisotropic systems, such as layered superconductors and coupled spin chains, is often a challenge due to the different natures of interactions along different directions. As a model of such a system, we present an analytical study (1) of d -dimensional "nodes" arranged as the vertices of a Bethe lattice, where each node has nonzero spatial dimension and is described by an $O(N)$ quantum rotor model, and there is hopping between neighboring nodes. In the limit of large connectivity on the Bethe lattice, the hopping can be treated by constructing a self-consistent effective action for a single node. This procedure is akin to dynamical mean field theory, but generalized so that spatial as well as quantum fluctuations are taken into account on each node. The quantum phase transition is studied using this effective action for both infinite and finite N . The importance of the Perron-Frobenius uniform mode on the Bethe lattice is discussed, and its elimination via an "infinite range hopping" term shifts the transition, leading to nontrivial critical behavior. We calculate critical exponents and find that the internode hopping reduces the upper and lower critical dimensions each by one.
(1) arXiv:1111.2011

¹Supported by the Johns Hopkins-Princeton Institute for Quantum Matter, under No. DE-FG02-08ER46544 by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.

12:15PM W16.00006 Quantum Criticality on Graphs¹, ADRIAN DEL MAESTRO, University of Vermont, JAMES MURRAY, ZLATKO TESANOVIC, Johns Hopkins University — One of the tenets of our understanding of strongly correlated systems is that their macroscopic critical behavior is often universal and independent of any microscopic details. Continuous phase transitions driven by either thermal or quantum fluctuations can be placed in universality classes defined by the spatial dimension and the symmetry of a Landau-like order parameter. In an attempt to further understand the role of the spatial dimension in universality, we imagine a system whose symmetries and connectivities are controlled by the low-lying spectrum of degrees of freedom on a graph. As an elucidating example, we study a quantum phase transition on large random regular graphs, with coupled vertices described by d -dimensional $O(N)$ quantum rotor models.

¹This work was supported by the Johns Hopkins-Princeton Institute for Quantum Matter, under No. DE-FG02-08ER46544 by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.

12:27PM W16.00007 Entropic Signatures of Quantum Criticality in Itinerant Ferromagnets and Metamagnetic Systems, JIANDA WU, Rice University, LIJUN ZHU, LANL, QIMIAO SI, Rice University, ANDREAS ROST, ANDY MACKENZIE, University of St. Andrews — We investigate the thermodynamic properties of itinerant ferromagnets near quantum critical points described by a quantum Landau-Ginzburg ϕ^4 theory. We show that the quartic coupling in this theory, which is dangerously irrelevant, has a singular contribution to the renormalized Gaussian free energy. We trace this singularity to some ultraviolet contributions, thereby demonstrating its unphysical nature. We introduce a procedure to regularize this singularity, and apply the prescription to calculate thermodynamic quantities across ferromagnetic quantum critical points in both two and three dimensions. Our calculation illustrates various thermodynamic signatures of quantum criticality, including the entropy accumulation at the quantum critical point which was first proposed on scaling grounds [1]. We systematically compare our theoretical results with the experimental data on entropy and specific heat as a function of magnetic field in Sr3Ru2O7 [2]. We demonstrate that the thermodynamic data are compatible with a quantum critical scenario, but the critical behavior does not agree well with the conventional itinerant ferromagnetic quantum criticality picture. [1] L. Zhu et al PRL 91, 066404 (2003). [2] A.W. Rost et al, Science 325, 1360 (2009).

12:39PM W16.00008 Quantum criticality in a dissipative (2+1)-dimensional XY model of circulating currents in high- T_c cuprates¹, IVER B. SPERSTAD, EINAR B. STIANSEN, ASLE SUDBO, Norwegian University of Science and Technology — We present large-scale Monte Carlo results for the dynamical critical exponent z and the spatio-temporal two-point correlation function of a (2+1)-dimensional quantum XY model with bond dissipation, proposed to describe a quantum critical point in high- T_c cuprates near optimal doping. The phase variables of the model, originating with a parametrization of circulating currents within the CuO₂ unit cells in cuprates, are compact, $\{\theta_{vv\tau,\tau}\} \in [-\pi, \pi)$. The dynamical critical exponent is found to be $z \approx 1$, and the spatio-temporal correlation functions are explicitly demonstrated to be isotropic in space-imaginary time. The model thus has a fluctuation spectrum where momentum and frequency enter on equal footing, rather than having the essentially momentum-independent marginal Fermi liquid-like fluctuation spectrum previously reported for the same model.

¹Supported by the NRC under Grant No. 167498/V30 (STORFORSK).

12:51PM W16.00009 Strong Electron Correlation by Virtual Phonon Exchange in Jahn-Teller Crystals, MICHAEL KAPLAN, Simmons College, GEORGE ZIMMERMAN, Boston University, KAPLAN/ZIMMERMAN COLLABORATION — In Jahn-Teller crystals - crystals with at least one sublattice of ions with orbitally degenerate electronic states - virtual phonon exchange is a major source of strong electron correlation. This type of electron correlation leads to different structural and magnetic transitions the interplay of which is especially interesting in case of the triple degeneracy of the electronic ground states. The interest to these systems lately has increased as it is related to some unusual situations in perovskite and spinel structure compounds that are of big practical interest (multiferroicity, piezomagnetism, and others). Mutual influence of the antiferrodistortive XY-type and ferroelastic ZZ-type orderings mediated by magnetic external or internal interactions in such a type of crystals is under discussion. It is found that even in case of stronger interactions leading to the ferroelastic ordering the presence of magnetic interaction causes new type of structural phase transition from the ZZ- type of ordering to the XY-type. These structural transformations are accompanied by specific anomalies in the temperature and external magnetic field dependences. The thermodynamics of the systems with strong electron correlation leading to such a phase transitions is analyzed.

1:03PM W16.00010 Features of Fermi Systems near $\ell=0$ Pomeranchuk Instabilities: A Crossing Symmetric Approach, KELLY REIDY, KHANDKER QUADER, Kent State University, KEVIN BEDELL, Boston College — In Fermi systems, interactions can cause symmetry-breaking deformations of the Fermi surface, called Pomeranchuk instabilities. In Fermi liquid (FL) language, this occurs when one of the Landau harmonics $F_{\ell}^{a,s} \rightarrow -(2\ell + 1)$; e.g. $F_0^{a,s} = -1$ are related to ferromagnetic (a), and density instabilities (s) respectively. The corresponding point in parameter space may be viewed as a quantum critical point (QCP). Using graphical and numerical methods to solve coupled non-linear integral equations of a crossing symmetric equation (TSCE) scheme, we study the behavior of spin/density excitations; effective mass; ferromagnetic, spin density wave, phase separation, and pairing transitions near $\ell=0$ Pomeranchuk instabilities in a 3D Fermi system. Considering momentum dependence of the renormalized FL interactions, we find a number of results for repulsive and attractive couplings of arbitrary strengths; viz. attraction in both singlet and triplet pairing amplitudes (though singlet pairing is primarily favored); possibility of a second ferromagnetic transition due to spin waves, and possibility of phase separation with and without ferromagnetic transition. Some of our results may apply to ferromagnetic superconductors, such as UGe₂ and UIr.

1:15PM W16.00011 Phase reconstruction near to the two-dimensional ferromagnetic quantum critical point, CHRIS PEDDER, London Centre for Nanotechnology & UCL, UNA KARAHASANOVIC, FRANK KRUGER, University of St. Andrews, ANDREW GREEN, London Centre for Nanotechnology & UCL — We study the formation of new phases in two dimensions near to the putative quantum critical point of the itinerant ferromagnet to paramagnet phase transition. In addition to the first order and helimagnetic behaviour found in non-analytic extensions to Hertz-Millis theory [1] and in the quantum order-by-disorder approach [2], we find a small region of spin nematic order. Our approach also admits a concurrent formation of superconducting order. We further study the effect of small deformations from quadratic electron dispersion – as previously found in three dimensions, these enlarge the region of spin nematic order at the expense of spiral order.

[1] D. Belitz, T.R. Kirkpatrick and T. Vojta, Rev. Mod. Phys. **77**, 579 (2005). V. Efremov, J.J. Betouras, A.V. Chubukov Phys. Rev. B **77**, 220401(R), (2008)

[2] G. J. Conduit Phys. Rev. A **82**, 043604 (2010)

1:27PM W16.00012 Divergence of the effective mass in a strongly-interacting 2D electron system¹, SHIQI LI, City College of New York, New York, NY 10031; Graduate Center of CUNY, New York, NY 10016, ANISH MOKASHI, Northeastern University, Boston, MA 02115, BO WEN, City College of New York, New York, NY 10031, S.V. KRAVCHENKO, Northeastern University, Boston, MA 02115, A.A. SHASHKIN, V.T. DOLGOPOLOV, Institute of Solid State Physics, Chernogolovka, Moscow District 142432, M.P. SARACHIK, City College of New York, New York, NY 10031 — The diffusion thermopower in a low-disorder, strongly-interacting 2D electron system in silicon increases with decreasing electron density and tends to infinity at a finite density n_t . Comparison with earlier data for a high-disorder silicon system indicates that the critical density n_t does not depend on the degree of disorder. The increase of the thermopower is associated with a diverging electron mass in the close vicinity of an interaction-induced phase transition.

¹Work supported by DOE Grant DE-FG02-84ER45153, BSF grant #2006375, RFBR, RAS, and the Russian Ministry of Sciences.

1:39PM W16.00013 A New View of the Mott-Hubbard Transition: Renormalization of the Fermi-Surface Topology, LUCA FAUSTO TOCCHIO, Goethe University Frankfurt, FEDERICO BECCA, SISSA Trieste, CLAUDIUS GROS, Goethe University Frankfurt — We present the renormalization of the (underlying) Fermi-surface topology in the Hubbard model on a square lattice with frustrating hopping, that is relevant for the physics of high-temperature superconductors. With the help of novel high precision variational tools, including Jastrow factors and backflow correlations, we show that the Fermi surface renormalizes to perfect nesting at the interaction-driven Mott-Hubbard transition and in the large interaction limit. Moreover, we present new results for the density-driven Mott-Hubbard transition, investigating the Fermi-surface renormalization flow as a function of doping, where the renormalization occurs only when the half-filled case is insulating. We associate the flow to the appearance of a van Hove singularity at the Fermi level at small doping, that is interpreted as an instability to magnetic order. Finally, we show also that Fermi surface renormalization is associated to a strong crossover at finite doping for the critical U corresponding to the Mott-Hubbard transition.

1:51PM W16.00014 Detecting Quantum Phase Transitions using Classical Noises, YAN CHEN, YINCHEN HE, Fudan University — We theoretically propose that the classical noise spectra provide an efficient and straightforward way to detect the quantum phase transition points in low-dimensional quantum spin systems. By using Ornstein-Uhlenbeck noise, we employ both a quadratic response theory and time-dependent density matrix renormalization group method to study the quantum system. In the non-Markovian region, the time evolutions of physical observables exhibit distinct behaviors for different quantum phases. In addition, we have the freedom to choose various noises to detect peculiar quantum phases. This method can be used to measure the three body correlation function directly. We demonstrate that the method can determine faithfully the quantum transition points of the transverse Ising model as well as spin-1 bilinear-biquadratic Heisenberg model. The possible experimental realizations of noise detection are discussed.

2:03PM W16.00015 Topological non-Fermi liquids and continuous transitions to Fermi liquids in fractional Chern states, JOHN MCGREEVY, MIT, MAISSAM BARKESHLI, Stanford University — We develop a slave-particle formulation of the Halperin-Lee-Read (HLR) non-Fermi liquid state and extend it to situations without an external magnetic field. We use this formulation to develop a theory of a continuous transition to a Fermi liquid, producing an example in which we can understand how a Fermi surface is continuously destroyed to obtain a fractionalized Fermi liquid. We discuss senses in which the HLR state should be viewed as a topological non-Fermi liquid, and finally we discuss experimental possibilities for inducing such transitions by tuning the bandwidth of a topologically non-trivial bandstructure.

Thursday, March 1, 2012 11:15AM - 2:15PM –
Session W17 FIAP: Optics of Semiconductor Nanowires 252A

11:15AM W17.00001 Scalable Synthesis of Vertically Aligned, Catalyst-Free Gallium Arsenide Nanowire Arrays – Towards Optimized Optical Absorption and Reflection.¹, MAOQING YAO, ANUJ MADARIA, CHUNYUNG CHI, CHENXI LIN, NINGFENG HUANG, University of Southern California, RUIJUAN LI, None, MICHELLE POVINELLI, DANIEL DAPKUS, CHONGWU ZHOU, University of Southern California, USC NANOLAB TEAM, USC COMPOUND SEMICONDUCTOR LABORATORY TEAM, USC NANOPHOTONICS LABORATORY TEAM — Vertically aligned, catalyst-free nanowires hold great potential for photovoltaic applications, where scalable synthesis and optimized optical absorption are critical. Here, we report using nanosphere lithography, scalable synthesis of vertical gallium arsenide nanowires grown by selected area MOCVD. A comparative study was done between regular nanowires arrays using electron beam lithography and slightly more defective nanowire arrays using nanosphere lithography. Reflection of light by the nanowire array has been used as a measure to study the effects of defects in the patterned structures using NSL both experimentally and by simulation. Both studies show similar reflection behavior between nanowire prepared by EBL and NSL. GaAs nanowires as short as 130 nm show reflection of <10% over the visible range of solar spectrum. Optimized nanowire configuration to maximize the absorption has also been discussed.

¹This material is based upon work supported as part of the Center for Energy Nanoscience, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science and Office of Basic Energy Sciences

11:27AM W17.00002 Theory of photoluminescence polarization reversal in GaAs nanowires, W.R.L. LAMBRECHT, T. CHEIWCHANHAMNANGIJ, T. BIRKEL, CWRU, AL. L. EFROS, NRL — The polarization of photoluminescence (PL) in wurtzite (WZ) GaAs nanowires (NW) of diameter 100 nm has been observed to reverse as a function of temperature from perpendicular to parallel to the NW axis. We use the weak confinement limit for excitons and the envelope function approximation to study this phenomenon. The WZ GaAs crystal field and spin-orbit splittings were determined using GW calculations and agree well with resonant Raman spectra on WZ NWs. In contrast to zincblende (ZB) NWs, the crystal field splitting in WZ NWs leads to a perpendicularly polarized exciton ground state. The first excited state, however, has a parallel component and can be mixed in at slightly elevated temperature, leading to a polarization reversal. We find that a reversal can only take place for much smaller crystal field splittings than the one obtained in pure WZ. Strain induced reduction of the crystal field splitting would require an unrealistically large strain. On the other hand, multiple twinning, can lead to a substantially lower crystal field splitting as obtained from our GW calculations for lower hexagonality polytypes, such as 4H GaAs, and can thus explain the observed polarization reversals.

11:39AM W17.00003 Phonon Spectrum and Thermal Properties of free standing <100> and <111> InGaAs alloy nanowires, MEHDI SALMANI JELODAR, ABHIJEET PAUL, Purdue University, TIMOTHY BOYKIN, University of Alabama in Huntsville, GERHARD KLIMECK, Purdue University — The phonon spectra in zinc blende InAs, GaAs and their ternary alloy nanowires (NWs) are computed using an enhanced valence force field (EVFF) model. The physical and thermal properties of these nanowires such as sound velocity, elastic constant, specific heat (Cv), phonon density of states, phonon modes, and the ballistic thermal conductance are explored. The calculated transverse and longitudinal sound velocities along <100> direction in these NWs are ~25% and 20% smaller compared to the bulk velocities, respectively. These velocities along <111> direction are about twice smaller than bulk values. The Cv for NWs are about twice as large as the bulk values due to higher surface to volume ratio (SVR) and strong phonon confinement in the nanostructures. The temperature dependent Cv for InAs and GaAs nanowires show a cross-over at 180K and 155K along <100> and <111> directions respectively. It happens due to higher phonon density in InAs nanowires at lower temperatures. With the phonon spectra and Landauer's model the ballistic thermal conductance is reported for these III-V NWs. The results in this work demonstrate the potential to engineer the thermal behavior of III-V NWs.

11:51AM W17.00004 How and why a magnetized quantum wire can act as an optical amplifier, MANVIR KUSHWAHA, Rice University — The fundamental issues associated with the magnetoplasmon excitations are investigated in a quantum wire characterized by a confining harmonic potential and subjected to a perpendicular magnetic field. Essentially, we embark on the device aspects of the intersubband collective (magnetoroton) excitations which observe a negative group velocity between the maxon and the roton. The computation of the gain coefficient suggests an interesting and important application: the electronic device based on such magnetoroton modes can act as an optical amplifier.¹

¹M.S. Kushwaha, J. Appl. Phys. **109**, 106102 (2011).

12:03PM W17.00005 Electronic band structure calculations of bismuth-antimony nanowires, ANDREI LEVIN, Harvard University, MILDRED DRESSELHAUS, Massachusetts Institute of Technology — Alloys of bismuth and antimony received initial interest due to their unmatched low-temperature thermoelectric performance, and have drawn more recent attention as the first 3D topological insulators. One-dimensional bismuth-antimony (BiSb) nanowires display interesting quantum confinement effects, and are expected to exhibit even better thermoelectric properties than bulk BiSb. Due to the small, anisotropic carrier effective masses, the electronic properties of BiSb nanowires show great sensitivity to nanowire diameter, crystalline orientation, and alloy composition. We develop a theoretical model for calculating the band structure of BiSb nanowires. For a given crystalline orientation, BiSb nanowires can be in the semimetallic, direct semiconducting, or indirect semiconducting phase, depending on nanowire diameter and alloy composition. These “phase diagrams” turn out to be remarkably similar among the different orientations, which is surprising in light of the anisotropy of the bulk BiSb Fermi surface. We predict a novel direct semiconducting phase for nanowires with diameter less than ~15 nm, over a narrow composition range. We also find that, in contrast to the bulk and thin film BiSb cases, a gapless state with Dirac dispersion cannot be realized in BiSb nanowires.

12:15PM W17.00006 Gas phase interactions with bare and gold nanoparticle decorated gallium nitride nanowires by ultraviolet photoelectron spectroscopy¹, ISHWAR NIRLAULA, BLAISE-ALEXIS KENGNE, DAVID MCILROY, University of Idaho — Ultraviolet photoelectron spectroscopy (UPS) has been used to characterize the interaction of CO and H₂O with the surface of bare and gold nanoparticle (Au NP) decorated gallium nitride nanowires at 298 K, 77 K and 20 K. The average diameter of the Au NPs is 4.5 ± 0.5 nm and the average nanowire diameter is 105 ± 75 nm. CO and H₂O do not bond to the surface of the bare GaN nanowires at 298K, 77K, or 20K. Temperature dependent UPS analysis reveals that CO and H₂O weakly physisorbed to the Au NP decorated GaN nanowires with heats of adsorption of 4.37 ± 0.03 meV and 1.25 ± 0.04 meV, respectively. The adsorption at 298K of 50 Langmuir of CO followed by 50 Langmuir of H₂O showed that CO adsorption promotes H₂O adsorption, while 50 Langmuir of H₂O followed by 50 Langmuir of CO showed that H₂O inhibits CO adsorption. The findings of this study that the adsorption of H₂O inhibits CO adsorption onto the Au NP-GaN nanowires explains previous studies of the gas sensing properties of mats of Au NP- GaN nanowires.

¹The University of Idaho BANTech (Biological Applications of Nanotechnology) Initiative and the Office of Naval Research (Grant # N00014-10-1-0282).

12:27PM W17.00007 Genomic design of strong direct-gap optical transition in Si/Ge core/multishell nanowires¹, LIJUN ZHANG, MAYEUL D'AVEZAC, JUN-WEI LUO, National Renewable Energy Laboratory, ALEX ZUNGER, University of Colorado — Converting the electronically superior but optically impractical indirect-gap Si and Ge semiconductors into a strongly light-absorbing system has been a long-standing challenge, given that the phonon-assisted optical transition of the indirect gap has weak intensity, requiring thick absorbers. One of main strategies has been the use of two-dimensional (2D) layer-by-layer growth of Si/Ge superlattices (SLs). However, the maximum thickness of SLs that can be grown coherently on a substrate is limited by the lattice-mismatch-induced strain. This limitation can be greatly relaxed by changing from 2D SLs to one-dimensional quantum nanowire (NW), where much higher strain can be accommodated. With developed Vapor-Liquid-Solid based technique, experimental growth of Si/Ge core-multishell NWs has recently demonstrated a significant level of synthetic control. However, the number of possible core/multishell sequences and thicknesses might easily reach an astronomical value. We will present here a genomic search for targeted core/multishell NW geometries that give both a direct gap and a significantly enhanced dipole-allowed optical transition in the Si/Ge system, by using a combination of genetic algorithm with atomistic pseudopotential electronic-structure calculations.

¹Funded by DOE through Energy Frontier Research Center, Center for Inverse Design

12:39PM W17.00008 Axially-Resolved Luminescence of Individual ZnSe Nanowires¹, S.K. HARK, JUNPING ZHUANG, The Chinese University of Hong Kong, WAI-NING MEI, University of Nebraska at Omaha — Axially resolved distributions of luminescence intensity and lifetimes along individual ZnSe nanowires were studied using two-photon excited luminescence imaging and time-correlated single photon counting techniques. The nanowires were grown on GaAs substrates via the self-catalyzed VLS mode. An intense tip, to which a gallium particle is attached, is found for the deep level (DL) emissions via luminescence imaging, while the intensity for the near band edge (NBE) emissions is more uniform. The luminescence decays at all locations of the nanowires are dominated by a fast process at early times, followed by a slow one. In addition, the shape of distribution of the lifetimes along the length of nanowire resembles a flattened letter "U" for the NBE emissions, but it resembles a long tailed letter "L" for the DL emissions. Possible explanations of these results will be discussed.

¹Partially supported by a grant from the Research Grants Council of the HKSAR (Project No 417507).

12:51PM W17.00009 ABSTRACT WITHDRAWN —

1:03PM W17.00010 Studies of electronic excitations of rectangular ZnO nanorods by electron energy-loss spectroscopy, CHIEN-TING WU, National Nano Device Laboratories, National Applied Research Laboratories, Taiwan, MING-WEN CHU, Center for Condensed Matter Sciences, National Taiwan University, Taiwan, CHUAN-PU LIU, Dept. of Materials Science and Engineering, National Cheng Kung University, Taiwan, KUEI-HSIEN CHEN, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan, LI-CHYONG CHEN, Center for Condensed Matter Sciences, NTU, Taiwan, CHUN-WEI CHEN, Dept. of Materials Science and Engineering, NTU, Taiwan, CHENG-HSUAN CHEN, Center for Condensed Matter Sciences, NTU, Taiwan — Electronic excitations of single ZnO rectangular nanorod have been investigated by electron energy-loss spectroscopy in conjunction with scanning transmission electron microscopy (STEM-EELS). We focus primarily on the surface excitations greatly enhanced at the grazing incidence parallel to the surfaces of ZnO nanorods. An uncommon kind of surface excitation known as surface exciton polaritons occurring near interband transitions is found to dominate in the spectral range between the band gap at 3.4 eV and the surface plasmon peak at 15.8 eV. In addition, the dielectric function of ZnO up to 25 eV has also been derived from the bulk excitation spectra using the Kramers-Kronig analysis on a single nanorod. Theoretical EELS simulations are also compared with the experimental results and good agreements are obtained.

1:15PM W17.00011 Precise investigation of optical/electronic fine structures of nanostructures via cathodoluminescence spectroscopy, DAPENG YU, XINLI ZHU, JIASSEN ZHANG, ZHIMIN LIAO, XIAOBING HAN, QIANG FU, State Key Laboratory for Mesoscopic Physics, and Electron Microscopy Laboratory, Department of Physics, Peking University, Beijing 100871, P.R.China, WANLIN GUO, Institute of Nano Science, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, P.R.China, XUEWEN FU, JUN XU, State Key Laboratory for Mesoscopic Physics, and Electron Microscopy Laboratory, Department of Physics, Peking University, Beijing 100871, P.R.China, PEKING UNIVERSITY COLLABORATION, NANJING UNIVERSITY OF AERONAUTICS AND ASTRONAUTICS COLLABORATION — High special/energy resolution cathodoluminescence (CL) spectroscopy enables us to make precise investigation on the optical/electronic fine structures in nanostructures. The linear distribution of strain gradient from tensile to compression in bent ZnO nano/microwires provides ideal conditions to address the modification of the electronic structures by strain in semiconductor materials. Radial line scan of the CL spectroscopy along bent ZnO wires at liquid helium temperature shows very fine excitonic emission structures, which demonstrates systematic red shift towards the increase of tensile strain, and blue shift as well as excitonic peak splitting towards the increase of compressive strain. First-principle simulations reveal an electronic band structure evolution under continuously tuned strain.

1:27PM W17.00012 Raman scattering study of mixed metal oxide Ir_xRu_{1-x}O₂ nanowires grown by chemical vapor deposition, HAE-YOUNG SHIN, Department of Physics, Ewha Womans University, Seoul, 120-750, Korea, YUMIN LEE, SUNG HEE CHUN, JAEYEON LEE, MYUNG HWA KIM, Department of Chemistry and Nano Sciences, Ewha Womans University, Seoul, 120-750, Korea, SEOKHYUN YOON, Department of Physics and Department of Chemistry and Nano Sciences, Ewha Womans University, Seoul, 120-750, Korea — We present Raman scattering results of mixed metal oxide Ir_xRu_{1-x}O₂ nanowires that have been studied for their stability and for activity as electrocatalysts. For our study, 1-dimensional metallic mixed oxide single crystalline Ir_xRu_{1-x}O₂ nanowires were synthesized, for the first time, via a simple physical vapor transport process by controlling relative ratios of two precursors, RuO₂ and IrO₂, respectively. We measured Raman spectra of Ir_xRu_{1-x}O₂ nanowires using excitation laser sources with wavelengths of 488 nm and 632.8 nm. We observed that an E_g phonon mode of an Ir_xRu_{1-x}O₂ nanowire is being blue-shifted linearly with respect to the Ir contents. We could use our observation of frequency shift of the E_g phonon to determine stoichiometry information of nanowires which we also measured and confirmed by using EDS. From the shape of the phonon modes we measured, we could get information regarding crystalline quality that was also measured by HRTEM. We show that Raman scattering spectroscopy can provide a simple, prompt, and effective mean to measure the stoichiometry and crystalline quality of mixed metal oxide nanowires.

1:39PM W17.00013 Strain effects in polytypical wurtzite/zinc-blend nanowhiskers¹, GUILHERME SIPAHI, PAULO FARIA, Instituto de Física de Sao Carlos - Universidade de Sao Paulo — The recent interest on III-V nanowhiskers has led to the growth of high quality samples of systems with two different crystalline structures [1]. The crystals grown in [111]-direction for the zinc-blend (ZB) phase and [0001]-direction for the wurtzite (WZ) phase are very similar and can both be described as stacked hexagonal layers. The effect of two different structural phases coexisting in the same nanostructure is known as polytypism and creates confinement profiles similar to a heterostructure. One can notice band offsets at the interface and the formation of electronic minibands that can be explored to design systems for device applications. Although some of the III-V compounds do not present WZ structure in bulk form, recent calculations [2] presented a theoretical prediction of their band structure. However, as they considered that ZB and WZ to have the same lattice parameters no strain effects should appear on a first approach. Our theoretical approach introduces strain effects in our previous model [3] by using group theory arguments. It allows the analysis of the biaxial strain effects for both structures in a single matrix. [1] P. Caroff et al. Nature Nanotech. 4, 50, 2009. [2] A. De and C. E. Pryor, Phys. Rev. B 81, 155210, 2010 [3] <http://arxiv.org/abs/1012.022>

¹The users would like to acknowledge the support from Capes, CNPq and FAPESP (brazilian funding agencies)

1:51PM W17.00014 Quantum Zigzag Phase Transition in Quantum Wires¹, ABHIJIT C. MEHTA, Duke University, CYRUS J. UMRIGAR, Cornell University, HAROLD U. BARANGER, Duke University — We use Quantum Monte Carlo (QMC) techniques to study the quantum phase transition of interacting electrons in quantum wires to a quasi-one dimensional zigzag phase. The phase diagram of particles with Coulomb interaction that undergo a linear to zigzag transition is relevant to electrons in quantum wires [Meyer et al, PRL 2007] and ions in linear traps [Simshoni et al., PRL 2011]. Interacting electrons confined to a wire by a transverse harmonic potential form a Wigner crystal at low densities; as density increases, symmetry about the axis of the wire is broken and the electrons undergo a transition to a quasi-one-dimensional zigzag phase. Using QMC, we characterize this phase transition by measuring the power spectrum and addition energies.

¹Supported by the U.S. Department of Energy (Materials Sciences and Engineering, DE-SC0005237) and U.S. NSF (DMR-0908653).

2:03PM W17.00015 Raman Spectroscopy and Strain Mapping in Individual Ge- Si_xGe_{1-x} Core-Shell Nanowires¹, DAVID DILLEN, KAMRAN VARAHRAMYAN, EMANUEL TUTUC, University of Texas at Austin — Core-shell Ge-Si_xGe_{1-x} nanowires (NWs) are expected to contain large strain fields due to the lattice-mismatch at the core/shell interface. Here we report measurement of the core strain in such NW heterostructures by Raman Spectroscopy. We measure the diameter dependence of Raman spectra in individual Ge NWs, as well as Ge-Si_xGe_{1-x} core-shell NW heterostructures. We find that the bare Ge NWs show no diameter-dependence of the Ge-Ge peak at 300.5 cm^{-1} . On the other hand, the Ge-Ge peak of the Ge-Si_xGe_{1-x} core-shell NW shows a blue shift by comparison to the bare Ge NWs. This blue shift increases with reducing the NW diameter as a result of larger compressive strain in the Ge core. While the elastic strain is expected to split the triply degenerate Ge-Ge mode into separate singlet and doublet peaks, only the singlet mode was observed in experiment, a finding explained by the NW absorption and emission anisotropy. Using lattice dynamical theory and the Raman spectroscopy results we determine the strain in Ge-Si_xGe_{1-x} core-shell NWs as a function of the NW diameter. We compare the experimental results with the strain values calculated using a continuum elasticity model.

¹We thank the NSF for support.

Thursday, March 1, 2012 11:15AM - 2:15PM –

Session W18 DMP: Focus Session: Interfaces in Complex Oxides - Devices and Nanostructures

252B

11:15AM W18.00001 Mesoscopic transport properties of LaAlO₃/SrTiO₃ devices, DANIELA STORNAIUOLO, STEFANO GARIGLIO, ALEXANDRE FETE, NUNO COUTO GUIMARÃES, DANFENG LI, ANDREA CAVIGLIA, CLAUDIA CANCELLIERI, ALBERTO MORPURGO, JEAN-MARC TRISCONE, DPMC - University of Geneva — The conducting interface between the two band insulators LaAlO₃ and SrTiO₃ [1], with its unique electronic properties, stands as a prominent example of an oxide heterostructure for the realization of multifunctional devices. Using the electric field effect the ground state of this system can be tuned from insulating to superconducting [2]. Recently we demonstrated also the possibility to tune the carriers mobility by changing the deposition conditions of the LaAlO₃ film [3] and measured Shubnikov-de Haas oscillations, whose analyses demonstrate the 2D nature of the electronic states at the interface [3,4]. We are currently focusing on the realization of devices where the 2D quantum nature of the electronic states can be fully exploited. We show the feasibility of structures with lateral dimensions down to few hundreds nanometers, using an electron beam lithography based process. The lateral confinement of the electron gas in these devices is demonstrated by a phase coherent transport regime, which can be tuned by electric field.

[1] A.Ohtomo et al., Nature 427, 423 (2004)

[2] A.D.Caviglia et al., Nature 456, 624 (2008); C.Bell et al., PRL 103, 226802 (2009)

[3] A.D.Caviglia et al., PRL 105, 236802 (2010)

[4] M.Ben Shalom et al., PRL 105,206401 (2010)

11:27AM W18.00002 Sketched Oxide Single-Electron Transistor¹, JEREMY LEVY, GUANGLEI CHENG, JOSH VEAZEY, PATRICK IRVIN, MENGCHEN HUANG, Department of Physics and Astronomy, University of Pittsburgh, CHUNG-WUNG BARK, SANGWOO RYU, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison — Devices that confine and process single electrons represent an important scaling limit of electronics. Such devices have been realized in a variety of materials and exhibit remarkable electronic, optical and spintronic properties. Here, we use an atomic force microscope tip to reversibly “sketch” single-electron transistors by controlling a metal-insulator transition at the interface of two oxides.² In these devices, single electrons tunnel resonantly between source and drain electrodes through a conducting oxide island with a diameter of ~ 1.5 nm. We demonstrate control over the number of electrons on the island using bottom- and side-gate electrodes, and observe hysteresis in electron occupation that is attributed to ferroelectricity within the oxide heterostructure. These single-electron devices may find use as ultradense non-volatile memories, nanoscale hybrid piezoelectric and charge sensors, as well as building blocks in quantum information processing and simulation platforms.

¹This work is supported by NSF, ARO and AFSOR.

²Cheng *et al.*, Nature Nanotechnology 6, 343 (2011).

11:39AM W18.00003 Unexpected magnetic Exchange Interaction between Epitaxial $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$ film and a two Dimensional Electron Gas at an $\text{LaAlO}_3/\text{SrTiO}_3$ Interface¹, W.M. LU, X. WANG, Z.Q. LIU, K. GOPINADHAN, A. ANNADI, S.W. ZENG, Z. HUANG, S. DHAR, - ARIANDO, T. VENKATESAN, NUSNNI-Nanocore, University of Singapore, Singapore — We have examined the electrical and magnetic properties of LSMO films epitaxially grown on STO, LAO and LAO/STO substrates. Compared to LAO and STO the LSMO films on LAO/STO shows a higher metal-insulator transition temperature and also an order of magnitude larger magnetization. The magnetic hysteresis loops measured in pinning fields show a large exchange coupling for the case of the LAO/STO substrate and the sign of the coupling supports a ferromagnet to a ferromagnet exchange. The magnetization measured arises from a combination of substrate magnetism and that of the film and the enhanced conductivity, metal-insulator transition temperature and magnetization can be accounted for by the exchange coupling between the magnetic phase observed in the LAO/STO interfaces and the LSMO layer. The decay length of this interaction in LSMO is 90 nm which is surprisingly much longer than has been observed in ferromagnetic metals. Furthermore, the discovery of a long range oscillatory magnetic exchange coupling with LAO thickness suggests a role for the LAO layer beyond a simple insulator in this magnetic heterostructure.

¹We thank the National Research Foundation (NRF) Singapore under the Competitive Research Program (CRP) 'Tailoring Oxide Electronics by Atomic Control' NRF2008NRF-CRP002-024, National University of Singapore (NUS) cross-faculty grant and FRC for financial

11:51AM W18.00004 Quantum spin hall effect in $\text{LaAlO}_3/\text{SrTiO}_3$ nanostructures¹, GUANGLEI CHENG, University of Pittsburgh — $\text{LaAlO}_3/\text{SrTiO}_3$ heterostructures are known to exhibit strong spin-orbit coupling. We investigate local and non-local transport behavior of nanoscale Hall crosses created by conductive AFM lithography. The four-terminal resistance of these structures is consistently found to be $\sim h/e^2$, independent of the length of the channel. We also observe large (1-10 k Ω) non-local resistances and zero-field Hall resistance that are attributed to quantum spin Hall phase with a spin-orbit derived pseudo-magnetic fields $B_{\text{eff}} \sim 15$ T. The pure spin current is blocked by Cooper pairs that form below T_c 200 mK, leading to a collapse of the non-local and zero-field Hall resistances.

¹This work is supported by ARO and AFSOR.

12:27PM W18.00005 Nonvolatile Ferroelectric Manipulation of Electronic Structure at LAO/STO Heterointerface, JHIH-WEI CHEN, Department of Physics, National Cheng Kung University, Tainan, Taiwan, TRA-VU THANH, JIUNN-YUAN LIN, Institute of Physics, National Chiao-Tung University, Hsinchu, Taiwan, YING-HAO CHU, Department of Material Science and Engineering, National Chiao-Tung University, Hsinchu, Taiwan, YI-CHUN CHEN, CHUNG-LIN WU, Department of Physics, National Cheng Kung University, Tainan, Taiwan — Hetero-interfaces between different oxide insulators have attracted a lot of interests. One of the most important system is the 2D electron gas at LaAlO_3 (LAO) and SrTiO_3 (STO), which had been reported to possess metallic conduction and superconductivity. In this study, the top-patterned $\text{Pb}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{O}_3$ ferroelectric layer epitaxially grown on LAO/STO was proposed as a nonvolatile electronic modulation, and the interface band deformation was investigated using photoelectron spectroscopy (PES). Result showed different thickness and polarization state of top PZT significantly affected the band structure and its corresponding valence band offset at the LAO/STO hetero-interface. The transport data indicated that the as-grown PZT would deplete the conducting interface of LAO/STO, while switching the polarization of PZT would enhance the interface conduction.

12:39PM W18.00006 Non-local piezoresponse in 3 u.c. $\text{LaAlO}_3/\text{SrTiO}_3$, MENGCHEN HUANG, FENG BI, University of Pittsburgh, CHUNGWUNG BARK, SANGWOO RYU, CHANGBEOM EOM, University of Wisconsin, JEREMY LEVY, University of Pittsburgh — Nanoscale control of the metal-insulator transition in 3 unit cell (u.c.) $\text{LaAlO}_3/\text{SrTiO}_3$ heterostructures can be achieved by the conducting AFM lithography,¹ however the mechanism behind this transition is still not well understood. One proposed mechanism invokes ionic transport through the LaAlO_3 layer.² We have performed a variety of local and non-local piezoforce measurements on 3 u.c. $\text{LaAlO}_3/\text{SrTiO}_3$ heterostructures. The existence and nature of the non-local piezoelectric effect places strong constraints on the origin of the piezoelectric response. This work is supported by NSF DMR-1104191.

¹C. Cen, S. Thiel, G. Hammerl, C. W. Schneider, K. E. Andersen, C. S. Hellberg, J. Mannhart, and J. Levy, Nat. Mater. **7**, 2136 (2008)

²A. Kumar, S. Jesse, A. Gruverman, C. B. Eom, S.V.Kalinin, unpublished

12:51PM W18.00007 Piezoresponse Force Microscopy of Gated $\text{LaAlO}_3/\text{SrTiO}_3$ Heterostructures¹, FENG BI, MENGCHEN HUANG, Department of Physics and Astronomy, University of Pittsburgh, CHUNGWUNG BARK, SANGWOO RYU, CHANG-BEOM EOM, Department of Materials Science, University of Wisconsin, Madison, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — The quasi-two-dimensional (q-2DEG) electron liquid at the $\text{LaAlO}_3/\text{SrTiO}_3$ (LAO/STO) interface can be tuned through the metal-insulator transition using a metallic top gate. At low carrier densities, the capacitance between the top gate and q-2DEG is significantly enhanced beyond the geometric capacitance.² In order to understand the origins of this enhancement in capacitance, we have performed spatially resolved piezo-force microscopy (PFM) on a top-gated 5u.c. LAO/STO structure. A large enhancement in piezoresponse is observed as the interface is switched to the conducting phase. Within the transition region, spatial structures or domains are observed. We propose that such measurement can provide new insights into the metal-insulator transition of the interface, and the associated capacitance enhancement.

¹This work is supported by NSF DMR-1104191.

²Lu Li, C. Richter, S. Paetel, T. Kopp, J. Mannhart, R.C. Ashoori, Science **332**, 825 (2011)

1:03PM W18.00008 Ferroelectric control of two dimensional electron gas in oxide heterointerface¹, TRA VU THANH, Institute of Physics, National Chiao-Tung University, Hsinchu, Taiwan, JHIH-WEI CHEN, Department of Physics, National Cheng-Kung University, Tainan, Taiwan, CHAO-HUI YEH, Department of Electrical Engineering, National Tsing Hua University, Hsinchu, Taiwan, YI-CHUN CHEN, CHUNG-LIN WU, Department of Physics, National Cheng-Kung University, Tainan, Taiwan, JIUNN YUAN LIN, Institute of Physics, National Chiao-Tung University, Hsinchu, Taiwan, YING-HAO CHU, Department of Material Science and Engineering, National Chiao-Tung University, Hsinchu, Taiwan — Oxide heterointerfaces are emerging as one of the most exciting materials systems in condensed-matter science. One remarkable example is the $\text{LaAlO}_3/\text{SrTiO}_3$ (LAO/STO) interface, a model system in which a highly mobile electron gas forms between two band insulators. Our study to manipulate the conductivity at this interface by using ferroelectricity of $\text{Pb}(\text{Zr,Ti})\text{O}_3$. Our transport data strongly suggests that down polarization direction depletes the conducting interface of LAO/STO. After switching the polarization direction (up), it becomes accumulation. In addition, our experiments show there is obvious the band structure changed by cross-sectional scanning tunneling microscopy and combining with X-ray photoelectron spectroscopy (XPS) measurements. The transport properties are measured to build up the connection between macroscopic properties and local electronic structures that have been applied to study this structure. Controlling the conductivity of this oxide interface suggests that this technique may not only extend more generally to other oxide systems but also open much potential to ferroelectric field effect transistors.

¹This work was supported by National Science Council of Taiwan, ROC

1:15PM W18.00009 Anomalous High Mobility in $\text{LaAlO}_3/\text{SrTiO}_3$ Nanowires¹, PATRICK IRVIN, JOSHUA VEAZEY, GUANGLEI CHENG, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, C.W. BARK, S. RYU, C.B. EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, Madison, WI 53706 — Nanoscale control over the $\text{LaAlO}_3/\text{SrTiO}_3$ interface² provides a possible pathway for reconfigurable oxide-based nanoelectronics at densities that exceed conventional silicon electronics. One of the central challenges in replacing silicon relates to energy dissipation, which in turn depends on the carrier mobility. We have performed four-terminal transport measurements of $\text{LaAlO}_3/\text{SrTiO}_3$ nanowires at room temperature (300 K) and at low temperature (~ 500 mK). We find that the equivalent 2D mobility of nanowires greatly exceeds that of bulk SrTiO_3 ($\mu_{\text{STO}} = 6 \text{ cm}^2/\text{Vs}$), and approaches that of optimally doped Si at room temperature. Low-temperature mobilities can exceed $30,000 \text{ cm}^2/\text{Vs}$. We discuss possible physical mechanisms to explain the anomalously high mobility and the implications for future device technologies.

¹This work is supported by NSF NEB-1124131.

²C. Cen, S. Thiel, K. E. Andersen, C. S. Hellberg, J. Mannhart, and J. Levy, *Nature Materials* **7**, 2136 (2008).

1:27PM W18.00010 First-principles modeling of $\text{Pt}/\text{LaAlO}_3/\text{SrTiO}_3$ nanocapacitors under an external bias potential, CLAUDIO CAZORLA, MASSIMILIANO STENGEL, Institute of Materials Science of Barcelona — We study the electronic, structural and electrical properties of $\text{Pt}/\text{LaAlO}_3/\text{SrTiO}_3$ nanocapacitors under the action of an external applied bias, using first-principles calculations performed at fixed electric displacement D . In particular, we deduce a complete set of *ab initio* band diagrams and a simple analytical expression for the electric field within the LaAlO_3 (LAO) film as a function of thickness and applied potential. In addition, we investigate the capacitance of the metal-oxide heterostructure in a field-effect transistor setup. We find that the electric field within LAO is a non-intrinsic quantity that monotonically decreases with increasing LAO thickness. The occurrence of spontaneous Zener tunneling in this system, therefore, is ruled out. We discuss the implications of our results in the light of recent experimental observations involving biased LAO/STO junctions and metallic top electrodes.

1:39PM W18.00011 THz rectified optical response of $\text{LaAlO}_3/\text{SrTiO}_3$ nanojunctions, YANJUN MA, Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, USA, CHUNG WUNG BARK, SANGWOO RYU, CHANG-BEOM EOM, Department of Materials Science, University of Wisconsin, Madison, WI 53706, USA, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, USA — Conducting AFM lithography can be used to create a variety of nanoscale devices at the $\text{LaAlO}_3/\text{SrTiO}_3$ interface^{1,2}. Nanoscale junctions have been shown to exhibit strongly localized photoconductivity over a range of wavelengths spanning the visible and near-infrared regime³. Power-dependent and interferometric measurements of these nanostructures with ultrafast laser pulses reveal a nonlinear photoconductive response attributed to second-order nonlinear susceptibility of SrTiO_3 . The breaking of inversion symmetry comes from the strong local electric field that extends across the junction. The ultrafast response of these nanojunctions make them attractive candidates for generation and detection of THz radiation at molecular scales. This work is supported by NSF DMR-1104191.

¹C.Cen et al., *Nature Material*, **7**, 298 (2008)

²C.Cen et al., *Science*, **323**, 1026 (2009)

³P.Irvin et al., *Nature Photonics*, **4**, 849 (2010)

1:51PM W18.00012 Tuning the two-dimensional electron gas at the $\text{LaAlO}_3/\text{SrTiO}_3(001)$ interface by metallic contacts¹, ROSSITZA PENTCHEVA, REMI ARRAS, VICTOR G. RUIZ LOPEZ, Ludwig Maximilians University Munich, Germany, WARREN E. PICKETT, University of California, Davis — Density functional theory calculations reveal that adding a metallic overlayer on $\text{LaAlO}_3/\text{SrTiO}_3(001)$ reduces/eliminates the electric field within the polar LaAlO_3 film and thus suppresses the thickness-dependent insulator-to-metal transition observed in uncovered films. Independent of the LaAlO_3 thickness both the surface and the interface are metallic, with an enhanced interface carrier density relative to $\text{LaAlO}_3/\text{SrTiO}_3(001)$ after the metallization transition. Moreover, a monolayer thick metallic Ti-contact exhibits a finite magnetic moment and for a thin SrTiO_3 -substrate induces a spin-polarized 2D electron gas at the *n*-type interface due to confinement effects. The height of the Schottky barrier formed between the metal contact and LaAlO_3 depends strongly on the choice of the overlayer and allows to tune the carrier density at the interface [1].

[1] V. Ruiz López, R. Arras, W. E. Pickett, and R. Pentcheva, arXiv:1106.4205v1.

¹Funding by the DFT, SFB/TR80 is gratefully acknowledged.

2:03PM W18.00013 Spatial Analogue of Quantum Spin Dynamics via Spin-Orbit Interaction¹, VANITA SRINIVASA, JEREMY LEVY, University of Pittsburgh — We theoretically demonstrate the mapping of electron spin dynamics from time to space in quantum wires with built-in spatially uniform and oscillating Rashba spin-orbit coupling in orthogonal directions. The presence of the spin-orbit interaction introduces pseudo-Zeeman couplings of the electron spins to effective magnetic fields. By periodically modulating the spin-orbit coupling along the quantum wire axis, it is possible to create the spatial analogue of spin resonance, without the need for real magnetic fields. The mapping of time-dependent operations onto a spatial axis suggests a new mode for quantum information processing in which gate operations are encoded into the band structure of the material. We describe a potential realization of such a material within nanowires at the interface of $\text{LaAlO}_3/\text{SrTiO}_3$ heterostructures.

¹This work is supported by NDSEG, an Andrew Mellon Fellowship, NSF (DMR-0704022), and ARO MURI (W911NF-08-1-0317).

Thursday, March 1, 2012 11:15AM - 2:15PM —
Session W19 DCMP: Invited Session: Spin Coupling and Kondo Screening in Individual Magnetic Spins 253AB

11:15AM W19.00001 The Impact of the Local Environment on the Kondo Screening of a High-Spin Atom, CYRUS F. HIRJIBEHDIN, London Centre for Nanotechnology, Dept. of Physics & Astronomy, Dept. of Chemistry, UCL, London, UK — Spin 1/2 Kondo systems have been investigated extensively in theory and in a variety of experimental geometries. However the magnetic atoms that give rise to the Kondo effect in metals often have a larger spin, which makes the properties of the system more complex. Using low-temperature scanning tunneling microscopy and spectroscopy, we explore the Kondo effect of individual high-spin magnetic atoms on small islands of the thin insulator copper nitride (Cu_2N) in $\text{Cu}(100)$ surfaces. Using a combination of elastic spectroscopy to probe the local density of states features arising from the Kondo screening and inelastic tunneling spectroscopy to study the higher energy spin excitations, we determined the spin of the atom and explore its impact on the Kondo resonance [1]. We find that the local magnetic anisotropy plays a decisive role in the physics of Kondo screening. In addition, we find that the splitting of the Kondo peak matches the splitting of the underlying unscreened spin levels, and surprisingly does not show any evidence of a renormalization of energy scales even though large renormalizations have been predicted for lower spin system. In addition, we find remarkably large variations in the strength of both the Kondo screening and magnetic anisotropy for Co atoms on both small and large Cu_2N islands. In both cases, the anisotropy and Kondo screening are inversely related: the Kondo resonance weakens as the anisotropy increases. For small islands, the Kondo screening is strongest near the center of the island, while for large island this trend is reversed. We examine the possible origins of this phenomenon, including variations in the physical and electronic structure of the Cu_2N surface.

[1] AF Otte et al., Nature Physics 4, 847 (2008).

11:51AM W19.00002 Mechanical Control of Spin States in Spin-1 Molecules and the Under-screened Kondo Effect¹, DANIEL RALPH, Cornell University — The ability to make electrical contact to single molecules creates opportunities to examine fundamental processes governing electron flow on the smallest possible length scales. We report experiments in which we controllably stretched individual molecules with spin $S = 1/2$ and $S = 1$ while simultaneously measuring Kondo-assisted current flow through the molecule as a probe of its spin states. For molecules with $S = 1/2$, the temperature dependence of the Kondo signal is in excellent agreement with the predicted universal scaling curves for the $S = 1/2$ Kondo effect and the molecular spin states exhibit no energy splitting with stretching, consistent with Kramers' theorem. However, for cobalt complexes we observe temperature scaling curves that are very different from the $S = 1/2$ Kondo predictions, and instead are in quantitative agreement with the predictions of the underscreened Kondo model for $S = 1$, in which conduction electrons only partially compensate the molecular spin. This allows us to identify the spin state as $S = 1$. As a function of stretching, the $S = 1$ molecules exhibit energy splittings of the spin states in the absence of magnetic field due to magnetic anisotropy arising from modification of the molecular symmetry. These findings demonstrate a mechanism of spin control in single-molecule devices and establish that they can serve as model systems for making precision tests of correlated-electron theories.

¹This research was performed primarily by Joshua J. Parks, in collaboration with A. R. Champagne, T. A. Costi, W. W. Shum, A. N. Pasupathy, E. Neuscamman, S. Flores-Torres, P. S. Cornaglia, A. A. Aligia, C. A. Balseiro, G. K.-L. Chan, and H. D. Abruña.

12:27PM W19.00003 STEM in Kondo Lattices: a new window on correlated electron materials¹, PIERS COLEMAN, Physics and Astronomy, Rutgers University — The tremendous developments in scanning tunneling electron spectroscopy over the past decade, applied with tremendous success to the cuprate superconductors, are now beginning to be applied to other strongly correlated electron systems. One area where they offer tremendous potential, is in the context of heavy fermion materials. In the last few years, it has become possible to start probing the physics of the Kondo lattice using STEM methods. In this talk I will review this field, discussing the physics of tunneling into the Kondo lattice, showing how tunneling involves a co-operative process of electron transfer and spin-flip, called "cotunnelling" [1,2]. I will provide an overview of latest results in this field, especially URu_2Si_2 [3,4], YbRh_2Si_2 [5] and CeCoIn_5 [6], discussing how STEM can be used to probe various new theoretical proposals [7,8] for the exotic order and critical behavior.

[1] M. Maltseva, M. Dzero, and P. Coleman, Phys. Rev. Lett. 103, 206402 (2009).
 [2] J. Figgins and D. Morr, Phys. Rev. Lett. 104, 187202 (2010).
 [3] A. R. Schmidt et al, Nature 465, 570-576 (2010).
 [4] P. Aynajian et al., Proc. Natl. Acad. Sci. U.S.A. 107, 10383 (2010).
 [5] S. Ernst et al, Nature (2011).
 [6] S. Ernst et al, Physica Status Solidi 247, 624 (2010).
 [7] Y. Dubi and A.V. Balatsky, Phys. Rev. Lett. 106, 196407 (2011).
 [8] P. Chandra, P. Coleman and R. Flint, to be published (2012).

¹Research supported by NSF DMR 0907179.

1:03PM W19.00004 Pseudo-spin Resolved Transport Spectroscopy of the Double Dot Kondo Effect, SAMI AMASHA, Stanford University — The Kondo effect is a paradigmatic example of a highly correlated many-body state, describing how conduction electrons screen a localized spin via spin-flip scattering. Experimentally probing the spin physics of the Kondo effect is challenging, as spin-resolved measurements require either large magnetic fields that break the spin degeneracy of the localized site or ferromagnetic contacts that give the spin states different tunnel rates to the localized site. We demonstrate how the desired spin resolution can be achieved for arbitrary tunnel rates and fields in a double quantum dot system. A quantum dot consists of a confined droplet of electrons connected by tunnel barriers to conducting leads. We study two dots that are capacitively coupled with negligible inter-dot tunneling. In this system, one can have a degeneracy associated with an electron being in either dot 1 or dot 2, and this degeneracy acts as a pseudo-spin degree of freedom that gives rise to Kondo screening. We present transport spectroscopy measurements that show the zero-bias peak that is the hallmark of the Kondo effect. We use gate voltages to break the degeneracy between the pseudo-spin states, creating a pseudo-magnetic field. We show that spectroscopy measurements in this regime are analogous to measurements of the spin Kondo effect in a magnetic field. Finally, we demonstrate how measuring transport through each dot individually as a function of the bias voltage on the measured dot gives us the ability to perform pseudo-spin resolved measurements that are difficult to achieve in spin systems.

1:39PM W19.00005 Evolution of Kondo Resonance from a Single Impurity Molecule to the Two-Dimensional Kondo Lattice, NORIAKI TAKAGI, The University of Tokyo — We investigated the Kondo resonance formed by the adsorption of magnetic molecule, iron(II) phthalocyanine (denoted as FePc), on $\text{Au}(111)$ from a single impurity regime to the two-dimensional Kondo lattice by using scanning tunneling microscopy, the density functional theory (DFT) and numerical renormalization group (NRG). In the single molecule regime, FePc takes on-top and bridge configurations. These species show characteristic Kondo signatures in their one-particle energy spectra depending on the adsorption site. The on-top species shows a broad peak accompanied by a sharp dip, while the bridge species only a broad peak. The origin of these features comes from the difference in the local symmetry around the Fe ion. The two-stage Kondo screening occurs for two localized electrons in the different 3d orbitals characterized by low and high Kondo temperatures, reflecting the different coupling strength of these orbitals with $\text{Au}(111)$. For the on-top species, highly-symmetric $\text{SU}(4)$ Kondo effect is realized, leading to the sharp dip. The dip observed for the on-top species is also evolved from the single impurity regime to the two-dimensional lattice. The spectral evolution and the quantum phase of the lattice are discussed by the competition of the Kondo effect with antiferromagnetic RKKY coupling between the molecular spins.

11:15AM W20.00001 The Accident at TEPCO's Fukushima-Daiichi Nuclear Power Plant: Technical Description of What Happened and Lessons Learned for the Future, AKIRA OMOTO, The University of Tokyo — Tsunami that followed M9.0 earthquake on March 11th left the Fukushima-Daiichi Nuclear Power Plants without power and heat sink. While water makeup continued by AC-independent systems to keep the fuel core covered by coolant, operating team tried to depressurize and enable low pressure injection to the reactor to avoid overheating but was not successful enough primarily due to limited available resources. This resulted in core melt, hydrogen explosion and release of radioactivity to the environment. Key lessons learned are; 1) safety regulation and safety culture, 2) workable/executable severe accident management procedure, 3) crisis management and 4) design. Implications on security include revealed vulnerability and the nexus of safety and security. Given the scale of damage to the environmental, attention must be paid to defense against it and to societal safety goal of nuclear power by considering offsite remedial costs, compensation to damage, energy replacement cost etc. A sort of root cause analysis first by asking "Why nuclear community failed to prevent this accident?" was initiated by the University of Tokyo.

11:51AM W20.00002 The U.S. nuclear industry following the Fukushima event, STEPHEN KUCZYNSKI, Southern Nuclear Operating Co. — The nuclear industry is executing a coordinated, comprehensive and safety focused strategic plan in response to the accident in Japan. This beyond design basis external hazard driven event resulted in loss of core cooling due to a loss of offsite power as a result of the significant earthquake which was followed by a loss of on-site power due to the tsunami. Site response actions were impacted due to difficulty accessing the site. The current US fleet of operating reactors has over the last decades implemented numerous reviews assessing external hazards with post 911 actions being the most current. The industry took immediate actions following the March accident to verify existing capabilities to address events driven from external hazards and is now implementing a "Way Forward" plan that has as a priority the continued safe operation of the existing US fleet while examining both the technical and organizational root causes of the Fukushima Dai-ichi accident. Industry focus is to provide additional defense in depth through a "Flex" approach that adds the most significant safety benefit in the most efficient time frame. From a topical perspective, the industry is in agreement with the tier 1 recommendations from the NRC near term task force report. Southern Nuclear Operating Company operates 6 reactors and is building Vogtle 3&4 which is expected to be granted a COL in the near term. This generation III+ reactor design has passive safety features that would have mitigated an event similar to the Fukushima accident.

12:27PM W20.00003 Lessons from Fukushima for Improving the Safety of Nuclear Reactors, EDWIN LYMAN, Union of Concerned Scientists — The March 2011 accident at the Fukushima Daiichi nuclear power plant has revealed serious vulnerabilities in the design, operation and regulation of nuclear power plants. While some aspects of the accident were plant- and site-specific, others have implications that are broadly applicable to the current generation of nuclear plants in operation around the world. Although many of the details of the accident progression and public health consequences are still unclear, there are a number of lessons that can already be drawn. The accident demonstrated the need at nuclear plants for robust, highly reliable backup power sources capable of functioning for many days in the event of a complete loss of primary off-site and on-site electrical power. It highlighted the importance of detailed planning for severe accident management that realistically evaluates the capabilities of personnel to carry out mitigation operations under extremely hazardous conditions. It showed how emergency plans rooted in the assumption that only one reactor at a multi-unit site would be likely to experience a crisis fail miserably in the event of an accident affecting multiple reactor units simultaneously. It revealed that alternate water injection following a severe accident could be needed for weeks or months, generating large volumes of contaminated water that must be contained. And it reinforced the grim lesson of Chernobyl: that a nuclear reactor accident could lead to widespread radioactive contamination with profound implications for public health, the economy and the environment. While many nations have re-examined their policies regarding nuclear power safety in the months following the accident, it remains to be seen to what extent the world will take the lessons of Fukushima seriously and make meaningful changes in time to avert another, and potentially even worse, nuclear catastrophe.

1:03PM W20.00004 Nuclear Power in China, YUN ZHOU, Harvard University — In response to the Fukushima accident, China is strengthening its nuclear safety at reactors in operation, under construction and in preparation, including efforts to improve nuclear safety regulations and guidelines based on lessons learned from the accident. Although China is one of the major contributors in the global nuclear expansion, China's nuclear power industry is relatively young. Its nuclear safety regulators are less experienced compared to those in other major nuclear power countries. To realize China's resolute commitment to rapid growth of safe nuclear energy, detailed analyses of its nuclear safety regulatory system are required. This talk explains China's nuclear energy program and policy at first. It also explores China's governmental activities and future nuclear development after Fukushima accidents. At last, an overview of China's nuclear safety regulations and practices are provided. Issues and challenges are also identified for policy makers, regulators, and industry professionals.

1:39PM W20.00005 Nuclear Power in India, M.V. RAMANA, Program on Science and Global Security, Princeton University — India has ambitious plans for expanding nuclear power over the next few decades. A major accident in a densely populated country like India can be catastrophic and thus of concern. There are both technical and organizational requirements for safety of nuclear facilities. This talk will describe some of the organizational factors that safety theorists have identified and examine, from the publicly available information about incidents and failures at India's nuclear facilities to see if these requirements are met. It will also describe some of the reactions to the Fukushima accident from officials associated with nuclear energy in India.

Thursday, March 1, 2012 11:15AM - 2:15PM —
Session W21 DMP: Focus Session: Search for New Superconductors- Electron-Phonon Coupling 254A

11:15AM W21.00001 Correlation-enhanced electron-phonon coupling produces high-temperature superconductors, ZHIPING YIN, ANDREY KUTEPOV, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University — The microscopic origin of superconductivity has been established in numerous classes of materials. In elemental metals it results from the exchange of phonons whereas in copper oxides and iron pnictides it is intimately connected to magnetism. On the other hand, the cause of superconductivity in a large third class of isotropic high temperature superconductors is still mysterious and subject of debate. In this talk, we will demonstrate that dynamical correlations among electrons enhance their coupling to phonons in a large number of superconductors, raising significantly the previously underestimated theoretical superconducting critical temperature T_c of up to a few Kelvin to their experimental values of tens of Kelvin. The mechanism we propose is quite general, explains the magnitude and the doping dependence of superconductivity in many materials such as the celebrated $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ ($T_C=32$ K) compounds and the electron-doped $\beta\text{-HfNiCl}$ compounds ($T_c = 25.5$ K) and can be used to design other high temperature superconductors which have not yet been synthesized. We will also propose a few novel materials which are good superconductors in our theory and can be easily synthesized and tested by experiments.

11:27AM W21.00002 Spectral properties of correlated systems with electron-phonon coupling, ELIZABETH NOWADNICK, Stanford University and SLAC, STEVEN JOHNSTON, IFW Dresden, ANDREY MISHCHENKO, RIKEN and RRC Kurchatov Institute, BRIAN MORITZ, Stanford University and SLAC, NAOTO NAGAOSA, RIKEN and University of Tokyo, THOMAS DEVEREAUX, Stanford University and SLAC — Results from a variety of experiments, including single particle probes such as ARPES and STM, and multi-particle spectroscopies such as optical and Raman responses, have revealed the importance of the electron-phonon interaction in strongly correlated electron materials. We present a determinant quantum Monte Carlo study of the single-band Hubbard-Holstein model, which treats electron-electron and electron-phonon interactions on an equal footing. We focus on the behavior of the single- and multi-particle dynamical properties of the model, such as the spectral function and optical conductivity, as a function of electron-phonon coupling and Hubbard U.

11:39AM W21.00003 Vibrational spectrum and electron-phonon coupling of doped solid picene from first principles, LILIA BOERI, ALASKA SUBEDI, Max Planck Institute for Solid State Physics, Stuttgart — The search for new intercalated hydrocarbon superconductors was initiated by the report of a superconducting critical temperature (T_c) of 18 K in K- and Rb- doped picene ($C_{22}H_{14}$), followed by phenanthrene, coronene and di-benz-picene (27 K). These compounds, formed by just approx benzene rings, bear a strong resemblance both to fullerenes and intercalated graphites. Using first-principles linear response calculations have performed calculations of the phonon spectrum and electron-phonon (ep) interaction, we have shown that the coupling of the high-energy C bond-stretching phonons to the π molecular orbitals for a doping of 3 electrons per picene molecule is sufficiently strong to reproduce the experimental T_c of 18 K within Migdal-Eliashberg theory. For hole doping, we predicted a similar coupling leading to a maximum T_c of 6 K. However, we argue that, due to its molecular nature, picene may belong to the same class of strongly correlated *ep* superconductors as fullerides [1]. Our results are in agreement with estimates based on molecular orbital models; we also discuss possible reasons and implications of the discrepancy with linear response calculations that include explicitly the dopant.

11:51AM W21.00004 Strong Correlation Physics in Aromatic Hydrocarbon Superconductors¹, MASSIMO CAPONE, GIANLUCA GIOVANNETTI, CNR-IOM and International School for Advanced Studies (SISSA) — We show, by means of ab-initio calculations, that electron-electron correlations play an important role in doped aromatic hydrocarbon superconductors, including potassium doped picene with $T_c = 18K$ [1], coronene and phenanthrene [2]. For the case of picene the inclusion of exchange interactions by means of hybrid functionals reproduces the correct gap for the undoped compound and predicts an antiferromagnetic state for $x = 3$, where superconductivity has been observed [3]. The latter finding is compatible with a sizable value of the correlation strength. The differences between the different compounds are analyzed and results of Dynamical Mean-Field Theory including both correlation effects and electron-phonon interactions are presented. Finally we discuss the consequences of strong correlations in an organic superconductor in relation to the properties of Cs_3C_{60} , in which electron correlations drive an antiferromagnetic state [4] but also lead to an enhancement of superconductivity [5].

1. R. Mitsuhashi et al. Nature 464, 76 (2010)
2. X.F. Wang et al, Nat. Comm. 2, 507 (2011)
3. G. Giovannetti and M. Capone, Phys. Rev. B 83, 134508 (2011)
4. Y. Takabayashi et al., Science 323, 1585 (2009)
5. M. Capone et al. Rev. Mod. Phys. 81, 943 (2009)

¹This work is financed by European Research Council through ERC Starting Grant SUPERBAD

12:03PM W21.00005 Transport Anomalies and Possible High T_c Superconductivity in interconnected multiwall carbon nanotube sheets doped by ion implantation¹, ANVAR ZAKHIDOV, AUSTIN HOWARD, NICHOLAS CORNELL, ULAS GOSKUN, MYRON SALAMON, RAY BAUGHMAN, JULIA BYKOVA, NATHANAEAL MAYO, University of Texas at Dallas, XUEMEI WANG, EDUARD GALSTYAN, HERBERT FREYHARDT, WEI KAN CHU, University of Houston, UTD-UH TEAM COLLABORATION, UTD TEAM — Ion implantation offers an alternative doping method. In searching for superconductivity, we describe here the ion-implantation doping of MW-CNT interconnected networks by boron and other dopants (phosphorous, sulfur, arsenic) and report transport anomalies in oriented networks of ion implanted MWCNT sheets as compared to cross coated (non-oriented multilayer MWCNT sheets). The strong drop of resistance $R(T)$ with temperature decrease starting at $T_{c1} = 50-60$ K and even at higher T is reminiscent of inhomogeneous superconducting islands appearing in the non-SC matrix. An unusual anomaly of the 4-terminal resistance is observed in many samples, $R(T)$ becoming negative at lower $T < T_{c2} \sim 10-20$ K. This negative resistance is found to be associated with unusual I-V curves with s-shape at low $T < T_{c2}$ and $R(T)$ shows nonlinear dependence on excitation current and other features that are studied carefully in MWCNTs with different lengths and densities. This negative-resistance behavior gives a hint for the possible incorporation of superconducting areas and can be explained in terms of an imbalanced resistance bridge.

¹AFOSR grant FA 9550-09-10384

12:15PM W21.00006 Large Magnetoresistance and low temperature Transport anomalies in Ion implanted HOPG¹, NICHOLAS CORNELL, ANVAR ZAKHIDOV, MYRON SALAMON, YURI GARTSTEIN, University of Texas at Dallas, XUEMEI WANG, HERBERT FREYHARDT, WEI KAN CHU, University of Houston, UTD NANOTECH INST. TEAM, U. HOUSTON TEAM — Strong positive magnetoresistance (MR) was found in highly oriented pyrolytic graphite (HOPG) upon ion implantation by boron and phosphorous. Similar effects, but with smaller amplitude, are induced by carbon ion implantation, but due to structural disorder and defect formation without carrier concentration increase. The magnetic field dependence of the MR is linear at high fields with no sign of saturation, but different contact geometries result in a wide range of parameters. Two possible explanations of strong MR are suggested and analyzed. While the MR remains large at all temperatures, plots of $R(T)$ in constant field show a drop at lower T . Future experiments will clarify the origin of the $R(T)$ drop, in particular, whether this might be interpreted as the onset of inhomogeneous superconductivity, as proposed in some previous work, or could be explained in the context of strong linear MR effects seen in high-mobility, disordered materials.

¹NanoTech team supported by AFOSR grant FA 9550-09-10384

12:27PM W21.00007 Quantitative reliability of the Migdal-Eliashberg theory for strong coupling superconductors, JOHANNES BAUER, Max-Planck Institute for Solid State Research, Heisenbergstr.1, 70569 Stuttgart, Germany, JONG HAN, Department of Physics, SUNY at Buffalo, Buffalo, New York 14260, USA, OLLE GUNNARSSON, Max-Planck Institute for Solid State Research, Heisenbergstr.1, 70569 Stuttgart, Germany — The Migdal-Eliashberg (ME) theory for strong electron-phonon coupling and retardation effects of the Morel-Anderson type form the basis for the quantitative understanding of conventional superconductors. The validity of the ME theory for values of the electron-phonon coupling strength $\lambda > 1$ has been questioned by model studies. By distinguishing bare and effective parameters, and by comparing the ME theory with the dynamical mean field theory (DMFT), we clarify the range of applicability of the ME theory. Specifically, we show that ME theory is very accurate as long as the product of effective parameters, $\lambda\omega_{ph}/D$, where ω_{ph} is an appropriate phonon scale and D an electronic scale, is small enough [1]. The effectiveness of retardation effects is usually considered based on the lowest order diagram in the perturbation theory. We analyze these effects to higher order and find modifications to the usual result for the Coulomb pseudo-potential μ^* . Retardation effects are weakened due to a reduced effective bandwidth. Comparison with the non-perturbative DMFT corroborates our findings [2].

[1] J Bauer, J E Han, and O Gunnarsson, Phys. Rev. B. 84, 184531 (2011).

[2] J Bauer, J E Han, and O Gunnarsson, in preparation (2011).

12:39PM W21.00008 Influence of Surface Termination of Boron-Doped Diamond on Superconducting Property, KEISUKE NATSUI, TAKASHI YAMAMOTO, TAKESHI WATANABE, YASUAKI EINAGA, Keio University, JST-CREST TEAM — In 2004, a heavily boron-doped diamond was found to be a superconductor. Since then, a superconducting diamond has attracted considerable attention, mainly explored for fundamental properties and a theoretical basis. Meanwhile, it is known that the surface of diamond is easily modified by a chemical treatment, and the physical properties, such as surface conductivity, could be modulated through the surface modification. Here, we report modulation of superconducting properties of a heavily boron-doped diamond by tuning the surface electronic state. A heavily boron-doped diamond was prepared onto a silicon wafer substrate by a microwave plasma-assisted chemical vapor deposition method. The surface of a boron-doped diamond was changed between hydrogen- and oxygen-termination by thermal and electrochemical reactions, respectively. As a result, the critical current and the diamagnetic magnetization value could be modulated in a reversible manner between the hydrogen- and oxygen-terminated diamonds with maintenance of the superconducting transition temperature. It is assumed that the carrier density at grain boundaries would change due to the induced dipole moment via surface modification, resulting in modulation of the magnetic flux pinning effect at grain boundaries.

12:51PM W21.00009 Energy landscape of fullerene materials: A comparison of boron to boron nitride and carbon¹, SANDIP DE, University of Basel, Basel, Switzerland — After the discovery of the C₆₀ fullerene some 25 years ago, many more hollow and endohedrally doped structures made out of various elements have been proposed theoretically. However, since no other fullerenes have been synthesized up to date, the question arises whether experimentalists have just not yet found a way to synthesize these theoretically predicted fullerenes, or whether they do not exist at all in nature. Following the theoretical discovery of the B₈₀ fullerene by Szwacki et al, various other fullerene and stuffed fullerene structures were proposed but none of them could be synthesized in the laboratory yet. Using the minima hopping global geometry optimization method on the density functional potential energy surface we show that the energy landscape of boron clusters is glass like. Medium size boron clusters exhibit many structures which are lower in energy than the cages. This is in contrast to carbon and boron nitride systems which can be clearly identified as structure seekers. The differences in the potential energy landscape explain why carbon and boron nitride systems are found in nature whereas pure boron fullerenes have not been found. We thus present a methodology which can make predictions on the feasibility of the synthesis of new nano structures.

¹Indi-swiss research grant., Swiss national foundation, cscs swiss national super computer

1:03PM W21.00010 Light element ternary compounds – searching for new superconductors in the “upper left corner”¹, ANDREAS HERMANN, NEIL W. ASHCROFT, ROALD HOFFMANN, Cornell University — We propose here a new class of ternary compounds, composed entirely of light elements drawn from the upper left corner of the Periodic Table, as a new family of superconductors with the promise of high transition temperatures (T_c). In this explorative computational study, we have investigated stoichiometric 1:1:1 compounds of lithium, beryllium, and boron. We find layered metallic phases that are thermodynamically stable at P=1 atm, with still others stabilized at relatively low pressures and hence in principle accessible to synthesis and experimental characterization. At high pressures, close packed structures are again stabilized and a metal-to-insulator transition is predicted. Superconducting transition temperatures for the most structurally attractive metallic phases are estimated using BCS theory. An outlook on other stoichiometries, as well as the incorporation of different constituents, Mg instead of Be in particular, is given.

¹Research supported by U. S. DOE BES grant DE-SG0001057 and NSF grants CHE-0910623 and DMR-0907425. Computing resources provided by the TeraGrid initiative through grant TG-DMR060055N and the Cornell NanoScale Facility (supported by NSF grant ECS-0335765)

1:15PM W21.00011 Progress on Determining the alpha-beta Phase Boundary of Elemental Boron¹, TADASHI OGITSU, ERIC SCHWEGLER, LLNL — Recently, it was reported that the phase boundary between alpha-boron and beta-boron has been directly determined using high-pressure and temperature experiments down to P~4GPa and T~1400K [Scientific Reports 1, 96 (2011)]. Based on linear extrapolation of their results to lower pressure and temperature, these authors proposed that at P=0GPa alpha-boron is the stable form below about T~933(20)K, in conflict with the recent theoretical works based on DFT total energy calculations [JACS 129, 2458 (2007); PRB 77, 064113 (2008); JACS 131, 1903 (2009)], where it was concluded that beta-boron is the most stable at all temperature below melting temperature and down to zero Kelvin. At the talk, we show that the theoretical alpha-beta boundary obtained with a few approximations agrees well with the aforementioned experimental results within the error bars except for the lowest P, T point, and in this case, the ground state is still beta-boron [submitted]. We will also discuss on the recent experimental efforts in measuring the specific heat of boron allotropes that lead to a tentative conclusion supporting the aforementioned DFT results.

¹Prepared by LLNL under Contract DE-AC52-07NA27344.

1:27PM W21.00012 Calculation of electron-phonon coupling in Arsenic under pressure¹, KEVIN T. CHAN, MARVIN L. COHEN, Dept. of Physics, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — Elemental As undergoes a structural transformation from a rhombohedral A7 phase to a simple cubic (sc) phase at around 25 GPa as pressure is increased. At pressures near this phase transformation, As is superconducting, with a maximum superconducting transition temperature T_c of about 2.5 K. Experiments indicate that this maximum T_c occurs at the transition pressure for structural transformation, and the increase in T_c as the transition pressure is approached has been attributed to phonon softening. In this work, we calculate from first principles the electronic structure, phonon dispersions, and electron-phonon coupling constant λ for As in the A7 and sc phases at various pressures near the A7 to sc transition. Using these detailed quantitative calculations, we explain the trends in T_c as function of pressure in terms of phonon softening, electronic density of states, and electron-phonon matrix elements. We discuss the implications of these results for finding new superconducting materials.

¹This work was supported by NSF Grant No. DMR10-1006184 and DOE under Contract No. DE-AC02-05CH11231. Computational resources were provided by NSF through XSEDE and by DOE at NERSC.

1:39PM W21.00013 Physical properties of heavily boron doped silicon, AUDREY GROCKOWIAK, Institut Néel, CNRS and UJF, CHRISTOPHE MARCENAT, INAC, CEA, THIERRY KLEIN, Institut Néel, CNRS and UJF, GILLES PRUDON, CHRISTIANE DUBOIS, Institut des Nanotechnologies de Lyon, CNRS and INSA, France, THIERRY KOCINIEWSKI, DOMINIQUE DEBARRE, Institut d'Electronique Fondamentale, Université Paris Sud, Orsay, France — The discovery of superconductivity (SC) in heavily boron doped silicon in 2006 by [1] occurred shortly after diamond in 2004 by [2]. However, the SC in these 2 materials occurs differently. For diamond, the SC is obtained for a boron concentration close to the metal-insulator transition (MIT), while for silicon, the onset of superconductivity is obtained well above the MIT threshold. The aim of this study is to determine the influence of different parameters that impact the SC, such as the doping concentration nB, or the thickness of the layer. Interpolation between resistivity measurements of $T_c(nB)$ and ab initio calculations of the electron phonon coupling $\lambda(nB)$ showed a complete mismatch of the dependency of $\lambda(T_c)$ with the BSC MacMillan exponential law. The results obtained suggest rather a power law dependence such as $\lambda \propto T_c^2$. This dependency suggests a fractal dimension of the superconducting wave function as reported by Feigel'man et al. [3].

[1] E. Bustarret et al., Nature (London) 444, 465 (2006).

[2] E. Ekimov et al. (2004). Nature 428: 542

[3] Feigel'man et al., arXiv:1002.0859

1:51PM W21.00014 Eliashberg-McMillan Parameters of Polysulfur Nitride, (SN)_x, PAUL GRANT, W2AGZ Technologies, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA — Thirty-seven years following the discovery of superconductivity in polysulfur nitride, (SN)_x remains the lone conducting polymer exhibiting this phenomenon. The transition temperature is only 0.3 – 0.4 K, and details of its origin remain largely unknown, although it very likely arises from conventional phonon-mediated BCS pairing of normal state carriers. In pursuit of such a possible mechanism, we have performed density functional theory (DFT) investigations of the phonon and electron-phonon dispersion relationships in (SN)_x, and will present values for the coupling strength of the latter along with an estimate of T_c.

2:03PM W21.00015 Probing electronic order via coupling to phonons in Bi2Sr2CuO6 (Bi2201)¹, CRAIG BONNOIT, DILLON GARDNER, ROBIN CHISNELL, Massachusetts Institute of Technology, AYMAN SAID, Advanced Photon Source, Argonne National Laboratory, YOSHI OKADA, Nagoya University, TAKESHI KONDO, University of Tokyo, TSUNEHIRO TAKEUCHI, HIROSHI IKUTA, Nagoya University, DAVID MONCTON, YOUNG LEE, Massachusetts Institute of Technology — Recent work on several members of the cuprate family of high-temperature superconductors has revealed the occurrence of broken lattice translational, rotational, and time reversal symmetries in various materials at low temperatures. We report on measurements of acoustic phonons on Bi₂(La,Sr)₂CuO_{6+δ}, which reveal a coupling to an underlying electronic density-wave state. Longitudinal acoustic phonons are found to be anomalously broadened at a wavevector of q ≈ 1/4 rlu along the Cu-O direction. At low temperatures a disparity between the scattered intensity at positive and negative energy transfer is seen. These measurements indicates a breaking of time reversal and inversion symmetry in the bulk.

¹This work was supported by the US Department of Energy under Grant No. DE-FG02-07ER46134

Thursday, March 1, 2012 11:15AM - 2:15PM –
Session W22 DMP DCOMP: Focus Session: Fe-based Superconductivity - Magnetism in AxFe(1-y)Se2 254B

11:15AM W22.00001 NMR Study of Superconductivity and Spin Fluctuations in Intercalated Iron Selenides A_yFe_{2-x}Se₂¹, WEIQIANG YU, Department of Physics, Renmin University of China, Beijing 100872, China — The role of spin fluctuations in superconductivity is an essential topic in both cuprate and Fe-based superconductors. NMR works in several Fe-based superconductors proposed that the low-energy antiferromagnetic spin fluctuations (AFSF) is a possible pairing glue for superconductivity. However, studies on other systems such as KFe₂As₂ and Li_{1-x}FeAs does not support a strong correlation between low-energy spin fluctuations and superconductivity. In the newly discovered A_yFe_{2-x}Se₂ superconductors with T_c ~ 32 K, our NMR study identifies unambiguously a paramagnetic superconducting phase, which is phase separated from the block antiferromagnetic state. The low-energy AFSF is not seen at all, even though the T_c is high. The A_yFe_{2-x}Se₂ are singlet superconductors evidenced from the NMR Knight shift K; However, the absence of the coherence peak in the spin-lattice relaxation rate 1/T₁ suggests an unconventional behavior of superconductivity. In fact, we found that both the K and the 1/T₁T increase dramatically with temperature and follow a a + bT² form from T_c up to 300 K. Such behavior is strong evidence for spin fluctuations with a high-energy, local nature in 3D systems, and inconsistent with a band-gap effect. Furthermore, K and 1/T₁T saturate above 400 K, indicating an energy scale of 35 meV, which is distinct from the low-energy spin fluctuations. The above temperature enhanced spin fluctuations seem to be universal in Fe-based superconductors.

References: W. Yu et al., Phys. Rev. Lett. 106, 197001 (2011); Long Ma et al., Phys. Rev. B 83, 174510 (2011); L. Ma et al., arXiv:1103.4960.

¹Work support by the NSFC and the National Basic Research Program of China.

11:51AM W22.00002 Spin Waves and magnetic exchange interactions in insulating Rb_{0.89}Fe_{1.58}Se₂, MIAOYIN WANG, Dept. Phys., University of Tennessee, Knoxville, CHEN FANG, Dept. of Phys., Purdue University, DAOXIN YAO, State Key Laboratory of Optoelectronic Materials and Technologies, Sun Yat-sen University, GUOTAI TAN, College of Nuclear Science and Technology, Beijing Normal University, LELAND HARRIGER, YU SONG, TUCKER NETHERTON, CHENGLIN ZHANG, Dept. Phys., University of Tennessee, Knoxville, MENG WANG, IOP, Chinese Academy of Sciences, MATTHEW STONE, Neutron Scattering Science Division, ORNL, WEI TIAN, Ames Lab and Dept. Phys., Iowa State University, JIANGPING HU, Dept. of Phys., Purdue University, PENGCHENG DAI, Dept. Phys., University of Tennessee, Knoxville — Superconductivity in alkaline iron selenide AFe_{1.6+x}Se₂ (A = K, Rb, Cs) may have a different origin from the sign reversed s-wave electron pairing mechanism, because they are insulators near x = 0 and form a blocked AF structure that is completely different from the iron pnictides. We use neutron scattering to map out spin waves in the AF insulating Rb_{0.89}Fe_{1.58}Se₂. A comparison of the fitted effective exchange couplings using a local moment Heisenberg Hamiltonian in Rb_{0.89}Fe_{1.58}Se₂, (Ba,Ca,Sr)Fe₂As₂, and iron chalcogenide Fe_{1.05}Te reveals that their next nearest neighbor (NNN) exchange couplings are similar. Therefore, superconductivity in all Fe-based materials may have a common magnetic origin that is intimately associated with the NNN magnetic exchange interactions, even though they have metallic or insulating ground states, different AF orders and electronic band structures.

12:03PM W22.00003 77Se NMR Study of K_xFe_{2-y}Se_{2-z}S_z, DAVID TORCHETTI, MINGXUAN FU, TAKASHI IMAI, Department of Physics and Astronomy, McMaster University, H.C. LEI, C. PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory — We will present a ⁷⁷Se NMR study of the superconducting properties of the recently discovered K_xFe_{2-y}Se₂ (T_c ~ 33 K), in a temperature range of 4 to 250 K [1]. Our Knight shift data reflect the progressive decrease in uniform spin susceptibility with temperature, in analogy with FeSe and iron-arsenide systems. Nuclear spin-lattice relaxation rate data shows no Hebel-Slichter coherence peak, nor any enhancement of antiferromagnetic spin fluctuations (AFSF) toward T_c. We have also conducted ⁷⁷Se NMR measurements on K_xFe_{2-y}Se_{0.4}S_{1.6} (non-superconducting) and K_xFe_{2-y}Se_{1.2}S_{0.8} (T_c ~ 21 K) to study the effect of sulphur substitution in this superconductor [2]. Sulphur applies a chemical pressure on the lattice, because it has the same valence as Selenium but less than half the ionic radius. We again measure NMR Knight shift and nuclear spin-lattice relaxation rate 1/T₁, and find that both are suppressed with S substitution. We will discuss these results in comparison with K_xFe_{2-y}Se₂.

[1] D. Torchetti et. al., PRB 83, 104508 (2011)

[2] D. Torchetti et. al., arXiv:1111.2552 (2011)

12:15PM W22.00004 Magnetic state of $K_{0.8}Fe_{1.6}Se_2$ from a five-orbital Hubbard model in the Hartree-Fock approximation¹, QINLONG LUO, ANDREW NICHOLSON, ADRIANA MOREO, ELBIO DAGOTTO, Univ. of Tennessee/ORNL, JOSÉ RIERA, Universidad Nacional de Rosario, DAO-XIN YAO, Sun Yat-Sen Univ. — The five-orbital Hubbard model (without lattice distortions) is investigated to study theoretically the recently discovered Fe-based superconductors $K_{0.8}Fe_{1.6}Se_2$, by using the real-space Hartree-Fock approximation and employing a 10×10 Fe cluster with Fe vacancies in a $\sqrt{5} \times \sqrt{5}$ pattern[1]. The phase diagram contains an insulating state with the same spin pattern as observed experimentally, involving 2×2 ferromagnetic plaquettes coupled with one another antiferromagnetically. The magnetic moment $\sim 3\mu_B/Fe$ is in good agreement with experiments. Several other competing phases are also stabilized in the phase diagram, in agreement with recent calculations using phenomenological models. [1] Qinlong Luo *et al.*, Phys. Rev. B **84**, 140506(R) (2011), and references therein.

¹This work was supported in part by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

12:27PM W22.00005 Electronic structure and magnetic excitations in iron selenides, MARK VAN SCHILFGAARDE, King's College, London, UK, LIQIN KE, VLADIMIR ANTROPOV, Ames Laboratory — We calculate the electronic structure and magnetic excitations in the $K_4Fe_{4+x}Se_5$ alloy, with x between 0 and 1, within the local-density approximation. Analysis of the electronic structure with varying x leads to a prediction of the coexistence of two phases: one, strongly magnetic and another, weakly or nonmagnetic. Using linear response techniques we calculate spin wave spectra in $K_4Fe_{4+x}Se_5$, and find it is in excellent agreement with a recent experiment. The spectrum can be described rather well by an anisotropic J_1 - J_2 model. We confirm that exchange coupling between NN Fe magnetic moments is strongly anisotropic, and show directly that in the ideal system this anisotropy can be associated with higher order terms in spin Hamiltonian (biquadratic coupling). Structural relaxation provides an additional source of the exchange anisotropy of approximately the same strength. The dependence of spin wave spectra on filling of Fe vacancy sites is discussed.

12:39PM W22.00006 Novel Magnetism in $K_{0.8}Fe_{1.6}Se_2$ Explained in the Unified Picture, WEI-GUO YIN, CHIA-HUI LIN, WEI KU, Brookhaven National Laboratory — The novel block checkerboard antiferromagnetism in Fe-vacancy-ordered insulating $K_{0.8}Fe_{1.6}Se_2$ is investigated theoretically [1]. Neither of the Fermi surface nesting and the Mott insulator scenarios, which were widely employed to model previous Fe-vacancy-free iron-based superconductors, is supported by our first-principles analysis of its electronic structure including unfolded Fermi surface, band gap, and orbital polarization. Instead, the orbital-degenerate double-exchange model, previously proposed to unify the metallic collinear and bicollinear antiferromagnetism of iron-based superconductors, is found sufficient to explain this insulating spin order as well as associated quantum magnetic transition induced by tetramer lattice distortion. Our findings demonstrate that the iron-based superconductors be universally described in the framework of coexisting itinerant and localized electronic states, which are coupled by Hund's rule coupling on the Fe atoms. Work supported by DOE DE-AC02-98CH10886.

[1] W.-G. Yin, C.-H. Lin, and W. Ku, arXiv:1106.0881v1.

12:51PM W22.00007 Vacancy-driven orbital and magnetic order in $(K,Tl,Cs)_yFe_{2-x}Se_2$ ¹, WEI-CHENG LV, WEI-CHENG LEE, PHILIP PHILLIPS, Department of Physics, University of Illinois — We investigate the effects of the $\sqrt{5} \times \sqrt{5}$ Fe vacancy ordering on the orbital and magnetic order in $(K,Tl,Cs)_yFe_{2-x}Se_2$ using a three-orbital (t_{2g}) tight-binding Hamiltonian with generalized Hubbard interactions. We find that vacancy order enhances electron correlations, resulting in the onset of a block antiferromagnetic phase with large moments at smaller interaction strengths. In addition, vacancy ordering modulates the kinetic energy differently for the three t_{2g} orbitals. This results in a breaking of the degeneracy between the d_{xz} and d_{yz} orbitals on each Fe site, and the onset of orbital order. Consequently, we obtain a novel inverse relation between orbital polarization and the magnetic moment. We predict that a transition from high-spin to low-spin states accompanied by a crossover from orbitally-disordered to orbitally-ordered states will be driven by doping the parent compound with electrons, which can be verified by neutron scattering and soft X-ray measurements.

¹support by NSF DMR-0940992 and the Center for Emergent Superconductivity, a DOE Energy Frontier Research Center, Grant No. DE-AC0298CH1088

1:03PM W22.00008 Phase separation and magnetic order in K-doped iron selenide superconductor, XI CHEN, WEI LI, HAO DING, PENG DENG, KAI CHANG, CANLI SONG, Tsinghua University, KE HE, LILI WANG, XUCUN MA, Chinese Academy of Sciences, JIANG-PING HU, Purdue University, QI-KUN XUE, Tsinghua University — The newly discovered alkali-doped iron selenide superconductors exhibit unique characters that are absent in other iron-based superconductors, such as anti-ferromagnetically ordered insulating phases, extremely high Neel transition temperatures, and the presence of Fe vacancies and ordering. We have grown high-quality $K_xFe_{2-y}Se_2$ thin films on graphene by molecular beam epitaxy and measured their atomic and electronic structures by low-temperature scanning tunneling microscopy. We demonstrate that a typical $K_xFe_{2-y}Se_2$ sample contains two distinct phases: an insulating phase with well-defined $\sqrt{5} \times \sqrt{5}$ order of Fe vacancies, and a superconducting KFe_2Se_2 phase containing no Fe vacancies. An individual Fe vacancy can locally destroy superconductivity in a similar way as a magnetic impurity in conventional superconductors. The measurement of magnetic field dependence of the Fe-vacancy-induced bound states reveals a magnetically-related bipartite order in the tetragonal iron lattice. These findings elucidate the existing controversies on this new superconductor and provide atomistic information on the interplay between magnetism and superconductivity in iron-based superconductors.

1:15PM W22.00009 Magnetism and Superconductivity in $Rb_{1-x}Fe_{2-y}Se_2$, VLADIMIR TSURKAN, Academy of Sciences of Moldova, JOACHIM DEISENHOFER, AXEL GÜNTHER, JONAS FISCHER, ZHE WANG, MICHAEL SCHMIDT, HANS-ALBRECHT KRUG VON NIDDA, SEBASTIAN WIDMANN, ALOIS LOIDL, Augsburg University — We report on the structural, magnetic, and superconducting properties of $Rb_{1-x}Fe_{2-y}Se_2$ single crystals. The system exhibits a strongly anisotropic antiferromagnetic behavior below 400 K. For $1.53 < 2 - y < 1.6$ superconductivity is found, whereas for Fe concentrations $2 - y < 1.5$ and $2 - y > 1.6$ insulating and semiconducting behavior is observed, respectively. The sharpest transition to the superconducting state and the highest transition temperature T_c of 32.4 K is found for compositions close to $Rb_2Fe_4Se_5$. Comparison of the magnetic behavior of non-superconducting and superconducting samples provides evidence for the coexistence of superconductivity and static antiferromagnetic order [1]. THz time-domain transmission spectroscopy in superconducting samples evidences a metallic response and the superconducting transition of the system [2].

[1] V. Tsurkan et al., Phys. Rev. B **84**, 144520 (2011).

[2] A. Charnukha et al., arXiv:1108.5698.

1:27PM W22.00010 Defect formation, magnetic interaction and electron phonon coupling in iron selenides $M_{1-x}Fe_{2-y}Se_2$, XUHUI LUO, University of Illinois at Chicago & National Institute of Standard and Technology, SERDAR OGUT, University of Illinois at Chicago, TANER YILDIRIM, National Institute of Standard and Technology & University of Pennsylvania — We perform a systematic study to explore the electronic and magnetic structures in iron selenide superconductors $M_{1-x}Fe_{2-y}Se_2$ using first principles calculations. We show that there is an intimate relationship between Se-height and the underneath Fe-spin square in $M_{1-x}Fe_{2-y}Se_2$. A displacement of the Se atom by as small as $0.2\text{\AA}$ is enough to change the amount of charge in the Fe-plane as much as 0.7 e per Fe. The Se-height increases as the number of ferromagnetic Fe-Fe bonds increases, yielding an expansion of $2\text{\AA}$ expansion in the c-axis for fully ferromagnetic spin configuration, which indicates a giant magneto-elastic coupling in these systems. Our calculations also explain why the formation of Fe vacancies is favorable in iron selenides, but not in iron pnictides. Finally, we calculate the spin-resolved electron-phonon coupling in MFe_2Se_2 and $M_{1-x}Fe_{2-y}Se_2$ to shed light on the mechanism of superconductivity in these materials.

1:39PM W22.00011 Phononic, magnetic, and inter-band Raman scattering in $K_{0.75}Fe_{1.75}Se_2$ superconductor¹, ALEXANDER IGNATOV, PHIL LUBIK, Department of Physics & Astronomy, Rutgers University, Piscataway, NJ 08854, USA, R.H. YUAN, W.T. GUO, NAN-LIN WANG, Beijing Natl Lab for Condensed Matter Physics, CAS, Beijing 100190, China, GIRSH BLUMBERG, Department of Physics & Astronomy, Rutgers University, Piscataway, NJ 08854, USA — We have analyzed collective excitations in $K_{0.75}Fe_{1.75}Se_2$ single crystal ($T_c \sim 32$ K) by polarized Raman scattering in the energy shift range of 20-8000 cm^{-1} , the temperature range of 10-300 K, and laser excitation energies from 1.8 to 3.0 eV. Seven B_g and nine A_g phonon modes are observed at 300K. Below ~ 150 K an extra A_g mode appears at 165 cm^{-1} . The amplitudes of the A_g modes at ~ 67 , 112, and 124 cm^{-1} are reduced, while the amplitude of 183 cm^{-1} A_g mode is enhanced by factor of five as temperature decreases from 300 to 40 K. Magnetic scattering bands at 1000-2000 cm^{-1} consist of at least three distinct peaks each, implying different Fe-Fe AFM exchange coupling constants for underlying structure. Inter-band transitions are observed at ~ 3700 and 4600 cm^{-1} at 300 K in the A_g and B_g channels, respectively. Below 140 K these excitations are hardened to ~ 4040 and 4820 cm^{-1} .

¹Research at Rutgers was supported by the U.S. DOE, office of BES, Division of Materials Science and Engineering under award DE-SC0005463.

1:51PM W22.00012 Electronic structure and magnetism of doped $A_xFe_{2-y}Se_2$, YUAN-YEN TAI, Dept. of Physics, Univ. of Houston, Houston, Texas 77054, USA, JIAN-XIN ZHU, MATTHIAS J. GRAF, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, C.S. TING, Dept. of Physics, Univ. of Houston, Houston, Texas 77054, USA — We develop a new multiorbital t-J Hamiltonian with realistic tight-binding and Heisenberg parameters to study the electronic and magnetic structure of $A_xFe_{2-y}Se_2$ superconductors for $0 < y < 0.4$. The ARPES experiments are fitted by a tight-binding lattice model with random vacancy order. We find that the vacancy order greatly affects the electronic band structure. For intermediate doping levels $0 < y < 0.4$, the stable electronic structure is a compromise between the solution for $y=0$ and $y=0.4$. Based on this model, we study the paramagnetic and antiferromagnetic (AFM) phases of $A_{0.8}Fe_{1.6}Se_2$. In the AFM phase the calculated spin susceptibility for the bare band structure agrees with a block-spin structure. This theoretical result is in good agreement with neutron scattering experiments of the spin structure. Furthermore, we show the results on the evolution of low-energy quasiparticle states with electron filling factor in the vacancy-ordered magnetic state.

2:03PM W22.00013 Nodeless d-wave Superconductivity and spin resonance in iron-selenide superconductors, A.V. BALATSKY, TANMOY DAS, LANL — Iron-selenide based layered compounds have been realized to be high-transition temperature superconductor in December, 2010. The superconductivity is tuned by varying number of iron vacancies in the crystal. This unique tunability of the high-temperature superconducting properties has reinforced the debate of universal properties in Fe based superconductors. Experiments and band structure calculations have shown that the electronic and magnetic structures of these compounds are significantly different from other iron-based superconductors. This fact leads us to propose that the superconducting state is nodeless d-wave pairing which is still driven by magnetic interactions. Nodeless gap leads to the fully gapped quasiparticle spectrum. Sign-changing gap lends itself naturally to the sharp feature in neutron scattering spectrum, the so called spin resonance. We predict the upward “horseshoe” dispersion of the spin resonance, in a sharp contrast with the “hourglass” dispersion in high- T_c oxides where similar spin resonance is ubiquitously seen. In conclusion, despite iron-selenide systems exhibit very different observables, we show that the underlying pairing mechanism is driven by similar spin-fluctuation instabilities as in other high-temperature superconductors.

Thursday, March 1, 2012 11:15AM - 2:15PM —

Session W23 DMP DCOMP: Focus Session: Fe-based Superconductors - AFeAs and RFeAsO Families 255

11:15AM W23.00001 Quantum oscillations in LiFeAs, AMALIA COLDEA, MATTHEW WATSON, Oxford University, ANTONY CARRINGTON, CARSTEN PUTZKE, ISABEL I. GUILLAMON, University of Bristol, ALIX MCCOLLAM, HMFL, Nijmegen, DAVID VIGNOLLES, DAVID LEBOEUF, LNCMI, Toulouse, IGOR MAZIN, Naval Research Laboratory, USA, SHIGERU KASAHARA, T. TERASHIMA, T. SHIBAUCHI, Y. MATSUDA, Kyoto University — Quantum oscillations are a powerful technique to establish with accuracy the three-dimensional topology of the Fermi surface and it has been successfully used in the study of iron-based superconductors. Here we report quantum oscillations in the 111 pnictide superconductor, LiFeAs, with $T \sim 18$ K, by using highly sensitive torque magnetometry in high magnetic fields (up to 58T) and at very low temperatures (0.3-4.2K). We observe clearly three different orbits around 1.5kT, 2.4kT and 2.9kT. By comparing the angular dependence of the measured frequencies with the predictions given by the first principle band calculations we conclude that the observed orbits belong to the electronic bands. The values of the quasiparticle masses for these orbits are significantly enhanced as compared with the band masses (a factor 4-5) suggesting that either that electron-electron and/or electron-phonon correlations are significant. We will compare our data with available APRES data on the same material and discuss the effect of the spin-orbit coupling. The details of the Fermi surface of LiFeAs will be compared with other iron-based superconductors. This work was supported by EPSRC (UK), EuroMagNET II, KAKENHI from JSPS and National Science Foundation, State of Florida and the U.S. Department of Energy.

11:27AM W23.00002 Effects of correlations in LiFeAs and LiFeP, JOHANNES FERBER, KATERYNA FOYEVTSOVA, HARALD O. JESCHKE, ROSER VALENTI, Institut fuer Theoretische Physik, Goethe-Universitaet Frankfurt, 60438 Frankfurt, Germany — We will discuss the role of electronic correlations in the iron-based superconductors LiFeAs and LiFeP by considering the effects on band structure, mass enhancements, and Fermi surface in the framework of density functional theory combined with dynamical mean field theory calculations. We show that LiFeAs shows characteristics of a moderately correlated metal and that the strength of correlations is mainly controlled by the value of the Hund's rule coupling J . The hole pockets of the Fermi surface show a distinctive change in form and size with implications for the nesting properties. We discuss our results in view of recent angle-resolved photoemission spectroscopy and de Haas-van Alphen experiments.

11:39AM W23.00003 Anisotropic Energy-Gaps of Iron-based Superconductivity from Intra-band Quasiparticle Interference in LiFeAs, Part I, M.P. ALLAN, Brookhaven National Laboratory, University of St Andrews, Cornell University, A.W. ROST, Cornell University, University of St Andrews, A.P. MACKENZIE, University of St Andrews, YANG XIE, Cornell University, J.C. DAVIS, Brookhaven National Laboratory, Cornell University, University of St Andrews, Kavli Institute at Cornell for Nanoscale Science, K. KIHOU, C.-H. LEE, A. IYO, H. EISAKI, Institute of Advanced Industrial Science and Technology, Tsukuba, Japan, T.-M. CHUANG, Academia Sinica, Taipei, Taiwan — Cooper pairing in the iron-based high- T_c superconductors is thought to occur due to the projection of the antiferromagnetic interactions between neighboring iron atoms onto the complex momentum-space electronic structure. It is thus pivotal to have an exact measurement of the electronic structure in these materials. In this talk, I will introduce intra-band Bogoliubov quasiparticle scattering interference (QPI) to iron-based superconductor studies. We report a precise determination of the low energy band structure of LiFeAs using QPI. We observe three hole-like bands, in qualitative agreement with dHvA and ARPES studies (“ γ ”, α_2 & α_1). The quantitative determination of the bandstructure is the foundation that we later use to measure the superconducting gap structure with QPI.

11:51AM W23.00004 Non-magnetic impurity effects in LiFeAs studied by STM/STS, T. HANAGURI, RIKEN, SEUNG HYUN KHIM, BUMSUNG LEE, KEE HOON KIM, Seoul National Univ., K. KITAGAWA, K. MATSUBAYASHI, Y. MAZAKI, Y. UWATOKO, M. TAKIGAWA, ISSP, Univ. Tokyo, H. TAKAGI, RIKEN/Univ. Tokyo — Detecting the possible sign reversal of the superconducting gap in iron-based superconductors is highly non-trivial. Here we use non-magnetic impurity as a sign indicator. If the sign of the superconducting gap is positive everywhere in momentum space, in-gap bound state should not be observed near the impurity site unless it is magnetic. On the other hand, if there is a sign-reversal in the gap, even non-magnetic impurity may create in-gap bound state [1]. We performed STM/STS experiments on self-flux and Sn-flux grown LiFeAs crystals and examined the effects of Sn impurity. In STM images of Sn-flux grown samples, we found a ring-like object which may represent Sn. Tunneling spectrum taken at this defect site exhibits in-gap bound state. Together with flat-bottom superconducting gap observed far from the defects, sign-reversing *s*-wave gap is the most plausible gap structure in LiFeAs. [1] T. Kariyado and M. Ogata, JPSJ **79**, 083704 (2010).

12:03PM W23.00005 Bogoliubov Electronic Structure at Individual Impurity Atoms in LiFeAs, YANG XIE, Laboratory of Solid State Physics, Department of Physics, Cornell University, Ithaca, NY 14853, USA, MILAN ALLAN, CMPMS Department, Brookhaven National Laboratory, Upton, NY 11973, USA, ANDREAS ROST, Laboratory of Solid State Physics, Department of Physics, Cornell University, Ithaca, NY 14853, USA, ANDY MACKENZIE, SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews, Fife KY16 9SS, UK, KUNIHITO KIHOU, HIROSHI EISAKI, Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8568, Japan, TIEN-MING CHUANG, JAMES DAVIS, CMPMS Department, Brookhaven National Laboratory, Upton, NY 11973, USA — Individual impurity atoms in a superconductor can strongly perturb the surrounding electronic environment and can therefore be used to probe high-temperature superconductivity at the atomic scale. Spectroscopic imaging scanning tunneling microscopy (SI-STM) is an ideal technique for the study of such effects. This has provided the motivation for several theoretical studies predicting the spatial and energetic structure of Bogoliubov electronic states at single impurity atoms in Fe-based superconductors. Here we report on a type of impurity atom that forms a strong in-gap quasi-particles interference (QPI) pattern nearby in the Fe-based superconductor LiFeAs. Our result puts a number of restrictions on theoretical studies of Fe-based superconducting mechanism.

12:15PM W23.00006 Theory of quasiparticle vortex bound states in Fe-based superconductors: application to LiFeAs, YAN WANG, PETER HIRSCHFELD, Department of Physics, University of Florida, Gainesville, Florida 32611, USA, ILYA VEKHTER, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803-4001, USA — Spectroscopy of vortex bound states can provide valuable information on the structure of the superconducting order parameter. Quasiparticle wavefunctions are expected to leak out in the directions of gap minima or nodes, if they exist, and scanning tunneling spectroscopy (STS) on these low-energy states should probe the momentum dependence of the gap. Anisotropy can also arise from band structure effects, however. We perform a quasiclassical calculation of the density of states of a single vortex in an anisotropic superconductor, and show that if the gap itself is not highly anisotropic, the Fermi surface anisotropy dominates, preventing direct observation of superconducting gap features. This serves as a cautionary message for the analysis of STS data on the vortex state on Fe-based superconductors, in particular LiFeAs, which we treat explicitly. YW and PJH were supported by the DOE under DE-FG02-05ER46236, and I. V. under DE-FG02-08ER46492.

12:27PM W23.00007 Local electronic structure near a vortex in LiFeAs within self-consistent BdG, KYUNGMIN LEE, MARK FISCHER, EUN-AH KIM, Cornell University — A major question in Fe-based superconductors is whether the pairing is of an unconventional nature with a sign change. The electronic structure in the presence of vortices can serve as a platform for phase sensitive measurements to answer this question. However as Fe-based superconductors are in the intermediate regime of correlation strength, a delicate balance between band structure effects and interaction effects may challenge a simple guess. We perform a microscopic self-consistent BdG calculation for LiFeAs in the presence of a perpendicular magnetic field and calculate the energy-dependent local electronic structure near a vortex. We use a band structure in agreement with recent experiments and compare different gap-symmetry possibilities. We find the low-energy local density of states to be dominated by the geometry of the Fermi surface, with tails along the directions perpendicular to the flat portions of the Fermi surface. These are the directions of the gap *maxima* on the square-like hole pocket around the Γ point according to recent observations. We discuss how the gap symmetry affects high-energy local density of states.

12:39PM W23.00008 Elastic neutron scattering on Co-doped NaFeAs superconductors, CHENGLIN ZHANG, GUOTAI TAN, YU SONG, TUCKER NETHERTON, SCOTT CARR, Univ of Tennessee, Physics dept, WEI TIAN, Oak Ridge National Lab, PENGCHENG DAI, Univ of Tennessee, Physics dept, UTK TEAM, ORNL COLLABORATION — NaFeAs and LiFeAs are the only two members in the Pnictide superconductors 111 family. Without doping, NaFeAs shows filamentary superconductivity coexisting with static antiferromagnetic (AF) order. In addition to the superconducting transition at 9 K, structural and AF transitions appear at ~ 50 K and ~ 40 K, respectively. By gradually doping Co on Fe sites, the AF order is suppressed and bulk superconductivity occurs. Although the electronic phase diagram of Co-doped NaFeAs is similar to the phase diagram of Co-doped 122 family, the NaFeAs system is much simpler because it does not have strong *c*-axis magnetic coupling and therefore a detailed investigation of this system will shed new light to our understanding on the common features amongst different classes of Fe-based superconductors. We will report our elastic neutron scattering results about this system.

12:51PM W23.00009 Temperature-dependent resistivity in single crystals $\text{Na}_{1-\delta}\text{Fe}_{1-x}\text{Co}_x$, M. A. TANATAR, Ames Laboratory US DOE, Ames, Iowa, N. SPYRISON, K. CHO, Ames Laboratory US DOE, Ames Iowa, G.T. TAN, J.Q. YAN, P.C. DAI, C.L. ZHANG, Oak Ridge National Laboratory, Knoxville, TN, R. PROZOROV, Ames Laboratory US DOE, Ames Iowa — Stoichiometric NaFeAs superconductor is representative of the slightly underdoped part of the doping phase diagram, with a sequence of tetragonal-to-orthorhombic, $T_s \approx 60$ K, magnetic, $T_m = 45$ K, and superconducting, $T_c = 12$ K transitions. Doping level in the compound can be tuned with Co substitution of Fe, acting as electron donor. This doping suppresses structural and magnetic instabilities and induces superconductivity with T_c up to 25 K. Doping with Co allows for studying complete doping phase diagram. We performed systematic measurements of the temperature-dependent in-plane, $\rho_a(T)$, and inter-plane, $\rho_c(T)$, electrical resistivities in the compounds. At optimal doping, both $\rho_a(T)$ and $\rho_c(T)$ show close to T -linear temperature dependence above the superconducting T_c . With doping this dependence gradually evolves towards T^2 . At much higher temperatures a slope-change is observed in $\rho_a(T)$, which we relate with onset of carrier activation over a pseudogap.

¹The work at Ames was supported by the U.S. DOE, under contract No. DE-AC02-07CH11358. The single crystal growth is supported by U.S. DOE BES U.S. DOE BES under Grant No. DE-FG02-05ER46202.

1:03PM W23.00010 Oxidative deintercalation of single crystal $\text{Na}_{1-\delta}\text{FeAs}$ upon Interaction with the environment, NICHOLAS SPYRISON, M.A. TANATAR, K. CHO, E. BLOMBERG, The Ames Laboratory, Ames, IA, G. TAN, J. YAN, P. DAI, C. ZHANG, Oak Ridge National Laboratory, Knoxville, TN, R. PROZOROV, The Ames Laboratory, Ames, IA — Due to high mobility of Na ions, NaFeAs superconductor exhibits pronounced reaction with the environment, leading to a bulk change in stoichiometry. We study the doping evolution of the same single crystals as a function of time of the environmental exposure. In NaFeAs, a controlled reaction with air increases the superconducting transition temperature, T_c , from the initial value of 12 K to 27 K as probed by transport and magnetic measurements. Temperature dependent resistivity, $\rho_a(T)$, shows a dramatic change with the exposure time. In freshly prepared samples, $\rho_a(T)$ reveals clear features at the structural, $T_s \approx 60$ K, and magnetic, $T_m = 45$ K, transitions and superconductivity with onset $T_{c,ons} \approx 16$ K and offset $T_{c,off} \approx 12$ K. The exposed samples show T -linear variation of $\rho_a(T)$ above $T_{c,ons} \approx 30$ K ($T_{c,off} \approx 26$ K). This suggests bulk doping and implies the existence of a quantum critical point at the optimal doping. The resistivity for different doping levels is affected below ~ 200 K suggesting the existence of a characteristic energy scale that caps the T -linear regime, which could be identified with a pseudogap.

1:15PM W23.00011 Some magnetic and electronic properties of Vanadium (hole) doped NaFeAs, SCOTT CARR, University of Tennessee, Knoxville — We examine the magnetic properties of the hole doped system $V_x\text{Na}_{1-x}\text{FeAs}$. It's known that the Na111 system exhibits structural, magnetic, and superconducting phase transitions. As opposed to the better studied electron doped systems, we successfully grew homogeneous single crystals with holes doped into the iron sites. Preliminary results show a total suppression of the superconducting phase and partial suppression of the AF order with doping as low as 1%. I will present a range of susceptibility measurements to examine the effect of Vanadium doping on T_c and the Neel Temperature.

1:27PM W23.00012 Cerium-Iron Magnetic Coupling in Single Crystal CeFeAsO at Low Temperatures¹, QIANG ZHANG, WEI TIAN, H.-F. LI, J.-Q. YAN, T.A. LOGRASSO, Ames Laboratory, U.S. DOE, R.W. MCCALLUM, Ames Laboratory; Department of Materials Science and Engineering, Iowa State University, J.L. ZARESTKY, DAVID VAKNIN, Ames Laboratory; Department of Physics and Astronomy, Iowa State University, J.W. KIM, Argonne National Laboratory, H. CAO, Oak Ridge National Laboratory — Neutron and synchrotron resonant X-ray scattering techniques have been used to determine the intricate magnetic structure of single crystal CeFeAsO at low temperatures, way below the spin-density wave (SDW) transition around 130 K associated with Fe moments ordering. Our synchrotron X-ray scattering results at the Ce L_{II} -edge clearly show a magnetic transition that is specific to the Ce ordering at $T_{Ce} = 4$ K, whereas neutron diffraction data indicate a transition at $T^* = 12$ K with unusual order parameter. Detailed order parameter measurements on the (100) & (101) magnetic reflections by neutrons show an anomaly at $T = 4$ K which we associate with the Ce ordering. The successive transitions at T_{Ce} and T^* can also be clearly identified by two anomalies in heat capacity measurements. We argue that the higher transition temperature observed in neutron measurements reflects Fe-Ce combined rearrangement prior to the complete ordering of the Ce. The effect of the weak Ce-Fe coupling on the rearrangement of Fe ordering is yet another example of the vulnerability of the Fe-SDW as influenced by minute doping or by relatively low applied pressures.

¹Supported by U.S. DOE Office of Basic Energy Sciences, Cont. No. DE-AC02-07CH11358

1:39PM W23.00013 FT-IR evaluation of SmFeAsO_{1-x}F_x (x = 0, 0.069), HAJIME SHINOHARA, YOICHI KAMIHARA, Department of Applied Physics and Physico-Informatics, Keio University — Optical properties of superconducting SmFeAsO_{1-x}F_x (x=0, 0.069) were demonstrated by reflection measurement with FT-IR method. Polycrystalline SmFeAsO_{1-x}F_x samples were synthesized using two-step solid state reaction described elsewhere [New J. Phys. **12**, 033005 (2010)]. Purity of samples was checked by X-ray diffraction patterns using Cu K- α radiation. The reflection measurement was performed at the range from 9000 cm^{-1} to 18000 cm^{-1} that was corresponded to an energy region from 1.12 eV to 2.25 eV. A photoconductivity of SmFeAsO_{1-x}F_x was determined by Kramer-Kronig (KK) relation. Reflectivity and photoconductivity measurements, as well as by FT-IR, at various areas were performed to define an energy level of materials [EPL, **84** 67013 (2008), and J. Phys. Soc. Jpn. **80** 013707 (2011)]. Obtained photoconductivity and reflection spectra were similar to those of LaFeAsO_{1-x}F_x that was a basic compound of LnFeAsO_{1-x}F_x (Ln=La, Ce, Sm), reported by Z. G. Chen et al [Phys. Rev. B **81**, 100502 (2010)]. Our result suggests that the energy band structure of SmFeAsO was affected by F-doping even in visible area. Details and temperature dependence of the reflection and photoconductivity spectra will be presented at the conference.

1:51PM W23.00014 Superconducting and normal state properties of single crystalline RFeAsO-based materials¹, J.J. HAMLIN, C.A. MCELROY, B.D. WHITE, D.Y. TUTUN, N. KANCHANAVATEE, Y. HEO, A.N. ELLINGTON, M.B. MAPLE, Department of Physics, University of California, San Diego, La Jolla, CA 92093, USA — We report electrical resistivity, Hall effect, magnetoresistance, magnetization, and specific heat measurements on single crystals of several RFeAsO-based materials (R = rare-earth). We also discuss the effects of lattice compression on the magnetic and superconducting transition temperatures. These single crystal studies benefit from significantly sharper signatures of the transitions, compared to earlier studies on polycrystalline samples.

¹Synthesis and superconductivity screening supported by AFOSR-MURI, Grant FA9550-09-1-0603. Physical properties characterization supported DOE, Grant DE-FG02-04-ER46105. High pressure measurements supported by DOE grant DE-FG52-06NA26205.

2:03PM W23.00015 Growth conditions of oxypnictide compounds LaFePnO Pn={P,As,Sb}, JASON VIELMA, SEAN MUIR, M.A. SUBRAMANIAN, A.W. SLEIGHT, GUENTER SCHNEIDER, Oregon State University — The discovery of superconductivity in layered ferro-oxypnictides LaFePO ($T_c \sim 4$ K) and LaFeAsO_{1-x}F_x ($T_c \sim 26$ K) lead to an intense search for other iron based superconducting materials. For the hypothetical compound LaFeSbO, ab initio density functional theory (DFT) calculations predict an enhanced density of states at the Fermi level together with increased nesting between the electron and hole sheets in the tetragonal structure (isostructural to LaFeAsO) and an enhanced spin-density wave ground state in a closely related orthorhombic structure; indicating the potential for superconductivity with a higher transition temperature [1]. We report ab initio DFT calculations of the phase stability of the oxypnictides LaFePnO Pn={P,As,Sb} and find growth conditions where LaFePO and LaFeAsO are thermodynamically stable, but LaFeSbO is unstable with respect to the formation of La₂SbO₂. Indeed, our attempt to synthesize LaFeSbO led to the synthesis and characterization of La₂SbO₂. The phonon spectrum of hypothetical LaFeSbO shows no soft modes, indicating that LaFeSbO is potentially metastable and leaving open the possibility of a nonequilibrium synthesis route.

[1] C-Y. Moon, S. Y. Park, and H. J. Choi, Phys. Rev. B, **78**, 212507 (2008)

Thursday, March 1, 2012 11:15AM - 2:15PM – Session W24 FIAP: Integer Quantum Hall Effect 256

11:15AM W24.00001 A quantitative examination of the collapse of spin splitting in the quantum Hall regime¹, W. PAN, Sandia National Labs, K.W. BALDWIN, K.W. WEST, L.N. PFEIFFER, D.C. TSUI, Princeton University — There is a great deal of current interest in understanding electron spin physics in semiconductors for potential quantum computation applications. The quantum Hall effect in the two-dimensional electron system (2DES) has proved to be a unique system in this avenue due to a tunability in the difference of spin population and thus the strength of exchange interaction provided by the formation of Landau levels. In this talk, we want to present our experimental results to *quantitatively* examine the theoretical model of spin splitting collapse in the quantum Hall regime [by Fogler and Shklovskii, Phys. Rev. B **52**, 17366 (1995)] at fixed magnetic fields as a function of electron density in a high quality heterojunction insulated-gate field effect transistor. In the density range between $n = 2 \times 10^{10}$ and $2 \times 10^{11} \text{ cm}^{-2}$, the Landau level number N follows a power-law dependence on the critical electron density n_c , where the spin splitting collapses, and $N = 11.47 \times n_c^{0.64 \pm 0.01}$. This power law dependence is in good agreement with the theoretical prediction in the low density regime.

¹SNL is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

11:27AM W24.00002 Single electron wave packets probed by Hanbury-Brown and Twiss interferometry, GWENDAL FEVE, ERWANN BOCQUILLON, FRANCOIS PARMENTIER, Ecole Normale Supérieure, Paris, CHARLES GRENIER, Ecole Normale Supérieure, Lyon, JEAN-MARC BERROIR, Ecole Normale Supérieure, Paris, PASCAL DEGIOVANNI, Ecole Normale Supérieure, Lyon, CHRISTIAN GLATTLI, BERNARD PLACAIS, Ecole Normale Supérieure, Paris, ANTONELLA CAVANNA, YONG JIN, Laboratoire de Photonique et Nanostructures — The ballistic propagation of electronic waves in the quantum Hall edge channels of a 2DEG bears strong analogies with photon optics which inspired a whole set of experiments, including the realization of electronic Mach-Zehnder [1] and Hanbury-Brown and Twiss [2] interferometers. So far, these experiments have been performed with continuous sources, but the recent realization of on-demand single electron emitters [3] has risen the hope to reach, in these experiments, the single charge control. We report here on the first realization of a Hanbury-Brown and Twiss experiment on a single electron beam generated by the single electron emitter recently developed by our group [3]. Using the chiral edge channels of the quantum Hall effect, single electron emitted by the source are directed towards an electronic beam-splitter. From the low frequency current correlations at the output of the beam splitter, we are able to count and characterize the elementary excitations produced by the source. By analyzing their antibunching with thermal excitations, we show that we are able to shape single particle states in a tuneable way. [1] Ji et al., Nature 422, 415 (2003) [2] Henny et al., Science 284 296 (1999) [3] Fève et al., Science 316, 1169 (2007)

11:39AM W24.00003 Hall Viscosity I: Linear Response Theory for Viscosity, BARRY BRADLYN, MOSHE GOLDSTEIN, NICHOLAS READ, Yale University — In two dimensional systems with broken time-reversal symmetry, there can exist a non-dissipative viscosity coefficient [1,2,3]. This Hall viscosity is similar in nature to the non-dissipative Hall conductivity. In order to investigate this phenomenon further, we develop a linear response formalism for viscosity. We derive a Kubo formula for the frequency dependent viscosity tensor in the long wavelength limit. We compute the viscosity tensor for the free electron gas, integer quantum Hall systems, and two-dimensional paired superfluids. In the zero frequency limit, we show how the known results [3,4] for the Hall viscosity are recovered.

[1] J. Avron, R. Seiler, and P. Zograf, Phys. Rev. Lett. **75**, 697 (1995).

[2] P. Levay, J. Math. Phys. **36**, 2792 (1995).

[3] N. Read, Phys. Rev. B **79**, 045308 (2009).

[4] N. Read and E. Rezayi, Phys. Rev. B **84**, 085316 (2011).

11:51AM W24.00004 Hall Viscosity II: Extracting Viscosity from Conductivity, MOSHE GOLDSTEIN, BARRY BRADLYN, NICHOLAS READ, Yale University — When time reversal symmetry is broken, the viscosity tensor of a fluid can have non-dissipative components, similarly to the non-dissipative off-diagonal Hall conductivity. This "Hall viscosity" was recently shown to be half the particle density times the orbital angular momentum per particle. Its observation can thus help elucidate the nature of the more exotic quantum Hall states and related systems (e.g., p+ip superconductors). However, no concrete measurement scheme has hitherto been proposed. Motivated by this question we use linear response theory to derive a general relation between the viscosity tensor and the wave-vector dependent conductivity tensor for a Galilean-invariant quantum fluid. This relation enables one to extract the Hall viscosity, as well as other viscosity coefficients (shear and bulk) when relevant, from electromagnetic response measurements. We also discuss the connection between this result and a similar one recently derived by C. Hoyos and D. T. Son [arXiv:1109.2651].

12:03PM W24.00005 Four-point characterization using capacitive and ohmic contacts, WANG ZHOU, BRIAN KIM, YASH SHAH, CHUANLE ZHOU, MATTHEW GRAYSON, Dept. of Electrical Engineering and Computer Science, Northwestern University, NEBILE İŞIK, Walter Schottky Institut, Technische Universität München — A four-point characterization method is developed for semiconductor samples that have either capacitive or ohmic contacts. When capacitive contacts are used, capacitive current- and voltage-dividers result in a capacitive scaling factor which is not present in four-point measurements with only ohmic contacts. Both lock-in amplifier and pre-amplifier are used to measure low-noise response over a wide frequency range from 1 Hz – 100 kHz. From a circuit equivalent of the complete measurement system after carefully being modeled, both the measurement frequency band and capacitive scaling factor can be determined for various four-point characterization configurations. This technique is first demonstrated with a discrete element four-point test device and then with a capacitively and ohmically contacted Hall bar sample using lock-in measurement techniques. In all cases, data fit well to a circuit simulation of the entire measurement system over the whole frequency range of interest, and best results are achieved with large area capacitive contacts and a high input-impedance preamplifier stage. Results of samples (substrates grown by Max Bichler Dieter Schuh, and Frank Fischer of the WSI) measured in the QHE regime in magnetic fields up to 15 T at temperatures down to 1.5 K will also be shown.

12:15PM W24.00006 Growth and magnetotransport measurements of triple-valley high mobility, miscut (111) AlAs quantum wells, SUNANDA PRABHU-GAUNKAR, M. GRAYSON, Dept. of Electrical Engineering and Computer Science, Northwestern University, F. HERZOG, G. KOBLMUELLER, Walter Schottky Institut, Tech. Univ. Munchen — We optimize growth of AlAs on (111)B GaAs substrates and perform magnetotransport measurements on vicinal (111)AlAs quantum wells (QWs). Previous literature reports that MBE growth on exactly oriented GaAs (111)B substrates is difficult, and the grown epi-layers are obscured by pyramid-like surface faceting and twin defect formation; slight substrate miscut results in stable step-flow growth. We perform a combined structural analysis with AFM, TEM and XRD to correlate MBE growth conditions with defect density scaling. We find that a high growth temperature of 690° C and low As beam fluxes reduce micro-twin formation for exactly oriented substrates and eliminate them for miscut substrates. A slight miscut of 2°, at which slip-step growth is known to occur, lead to AlAs QWs with record electron mobility $\mu = 13000 \text{ cm}^2/\text{Vs}$ at a sheet density $n_{2D} = 2.17 \times 10^{11} \text{ cm}^{-2}$. Numerical calculations reveal that valley splitting is about 1 meV per degree of miscut, which compares to typical Fermi energies of 2DEGs in AlAs QWs. Signatures in the transport data indicate that not only miscut but also exchange splitting between valleys can play an important role. Magnetotransport data at 15 mK in magnetic fields up to 15 T will also be presented.

12:27PM W24.00007 Chiral heat transport in driven quantum Hall and spin Hall edge states, LILIANA ARRACHEA, Universidad de Buenos Aires, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — We consider a model for an edge state of electronic systems in the quantum Hall regime with filling $\nu = 1$ as well as in the quantum spin Hall regime. In both cases the system is in contact with two reservoirs by tunneling at point contacts. Both systems are locally driven by applying an ac voltage in one of the contacts. By weakly coupling them to a third reservoir, the transport of the generated heat is studied in two different ways: i) when the third reservoir acts as a thermometer the local temperature is sensed, and ii) when the third reservoir acts as a voltage probe the time-dependent local voltage is sensed. Our results indicate a chiral propagation of the heat along the edge in the quantum Hall case and in the quantum spin Hall case (if the injected electrons are spin polarized). The temperature profile shows that electrons along the edge thermalize with the closest upstream reservoir.

12:39PM W24.00008 Wigner path integral solution for the integer quantum Hall effect, DRIES SELS, FONS BROSENS, WIM MAGNUS, BART SÖREE, Universiteit Antwerpen — The real time propagator of the Wigner distribution function can be constructed from the Wigner-Liouville equation as a phase space path integral. By analogy with the Feynman path integral one can define a new effective Lagrangian of the system in the Wigner-Weyl representation. The effects of gauge transformations and geometric constraints on the action are discussed. In particular we discuss the dynamics of a non-interacting 2DEG on a Hall strip.

12:51PM W24.00009 Microwave reflection study of GaAs/AlGaAs devices in the regime of the radiation-induced magnetoresistance oscillations¹, TIANYU YE, A.N. RAMANAYAKA, R.G. MANI, Georgia State University, W. WEGSCHEIDER, ETH-Zurich, ETH-ZURICH COLLABORATION — The microwave-induced magnetoresistance oscillations are revealed in the GaAs/AlGaAs two dimensional electron system (2DES) under microwave and terahertz photo-excitation at liquid helium temperatures. Such oscillations are understood in terms of the displacement and inelastic models for photo-excited transport in this system. In order to identify the relative physical contributions, we have concurrently examined magnetotransport and microwave reflection from the 2DES. For the reflection measurements, a sensitive microwave detector was assimilated into the standard experimental setup. Here, we report on the observed magnetic field induced changes in the microwave reflection, and correlate the observations with concurrent transport response of the photo-excited 2DES.

¹Work has been supported by the ARO under W911NF-07-01-0158, and by the DOE under DE-SC0001762.

1:03PM W24.00010 Observation of linear-polarization-sensitivity in the microwave-radiation-induced magneto-resistance oscillations¹, RAMESH MANI, ARUNA RAMANAYAKA, Georgia State University, WERNER WEGSCHEIDER, ETH Zurich — In the quasi two-dimensional GaAs/AlGaAs system, we investigate the effect of rotating *in-situ* the electric field of linearly polarized microwaves relative to the current, on the microwave-radiation-induced magneto-resistance oscillations. We find that the frequency and the phase of the photo-excited magneto-resistance oscillations are insensitive to the polarization. On the other hand, the amplitude of the resistance oscillations are remarkably responsive to the relative orientation between the microwave antenna and the current-axis in the specimen. The results suggest a striking linear polarization sensitivity in the radiation-induced magnetoresistance oscillations.

¹DOE: DE-SC0001762, ARO: W911NF-07-01-015

1:15PM W24.00011 Non-equilibrium bosonization and its applications to quantum Hall systems, IVAN LEVKIVSKYI, EUGENE SUKHORUKOV, University of Geneva — Bosonization is a powerful theoretical method allowing one to treat interactions in 1D systems non-perturbatively. This technique in its original formulation applies to equilibrium states. In order to describe recent experiments on 1D systems far from equilibrium, we introduce a new bosonization method: A non-equilibrium state is described by imposing non-trivial boundary conditions for collective boson fields. This method allows to reduce the problem of finding correlation functions in an interacting 1D system to the calculation of full counting statistics of a process, which creates a non-equilibrium state. The full counting statistics has been extensively studied, and it is well known in several important situations. We apply the non-equilibrium bosonization technique to explain recent experiments on noise-induced dephasing in quantum Hall interferometers and to the energy equilibration at quantum Hall edge states.

1:27PM W24.00012 Single-electron quantum tomography in quantum Hall edge channels¹, PASCAL DEGIOVANNI, CNRS / ENS Lyon, CHARLES GRENIER, CPHT - Ecole Polytechnique Paris, RÉMY HERVÉ, INSA Lyon, ERWANN BOCQUILLON, Laboratoire Pierre Aigrain ENS Paris, FRANÇOIS D PARMENTIER, CNRS - Laboratoire de Photonique et Nanostructures, JEAN-MARC BERROIR, GWENDAL FÈVE, BERNARD PLAÇAIS, Laboratoire Pierre Aigrain ENS Paris — The recent demonstration of an on demand single electron source [1,2] has opened the way to a new generation of "electron quantum optics" experiments aimed at preparing, manipulating and measuring coherent single electron excitations propagating in ballistic conductors such as the edge channels of a 2DEG in the integer quantum Hall regime. In this talk, I will describe a proposal [3] for measuring single electron coherence using an Hanbury Brown and Twiss interferometer. This quantum tomography protocol could be used to characterize single electron sources and to perform quantitative studies of decoherence.

[1] Science 316, 1169 (2007)

[2] Phys. Rev. B 82, 201309 (2010)

[3] New Journal of Physics 13, 093007 (2011)

¹ANR GRant 1shot (ANR-2010-BLANC-0412)

1:39PM W24.00013 Linear polarization rotation study of the radiation-induced magnetoresistance oscillations¹, A.N. RAMANAYAKA, R.G. MANI, Georgia State University, Atlanta, GA, J. INARREA, Universidad Carlos III, Madrid, Spain, W. WEGSCHEIDER, ETH Zurich, Zurich, Switzerland — The polarization sensitivity of microwave-radiation-induced magneto-resistance oscillations is investigated by rotating, by an angle θ , the polarization of linearly polarized microwaves with respect to the long-axis of GaAs/AlGaAs Hall-bar electron devices. At low microwave power, P , experiments show a strong sinusoidal variation in the diagonal resistance R_{xx} vs. θ at the oscillatory extrema, indicating linear polarization sensitivity in the microwave radiation-induced magneto-resistance oscillations. Surprisingly, the phase shift θ_0 for maximal oscillatory R_{xx} response under photo-excitation appears dependent upon the radiation-frequency f , the extremum in question, and the magnetic field orientation or $\text{sgn}(B)$.

¹ARO: W911NF-07-01-0158, DOE: DE-SC0001762

1:51PM W24.00014 Wave function multifractality and dephasing at quantum Hall transitions: A numerical investigation, S. BERA, Institut Neel, CNRS, Grenoble., I.S. BURMISTROV, L. D. Landau Institute for Theoretical Physics, Moscow, Russia, F. EVERS, Karlsruhe Institut für Technologie, Germany, I. GORNYI, Karlsruhe Institut für Technologie, Germany and A. F. Ioffe Physico Technical Institute, St. Petersburg, Russia, A.D. MIRLIN, Karlsruhe Institut für Technologie, Germany and Petersburg Nuclear Physics Institute, St. Petersburg, Russia — To understand the effect of the Coulomb interaction is one of the most challenging problems in the context of Anderson localization and the quantum Hall effect. In our study we address this question by following a perturbation theory in the interaction near the non-interacting fixed point. In each order diagrams appear which contain correlation functions characterizing the fluctuation properties of wavefunctions at the (non-interacting) critical fixed point. It turns out that the correlators relevant for dephasing combine in a way such that the *leading* multifractal powerlaws cancel; the subleading terms govern the interaction corrections. We present a numerical study based on the Chalker-Coddington network, in which we determine quantitatively the subleading multifractal exponents of the salient wavefunction correlators.

2:03PM W24.00015 Corrections to scaling near the quantum Hall transition, FERDINAND EVERS, HIDEAKI OBUSE, SOUMYA BERA, Institute of Nanotechnology, Karlsruhe Institute of Technology, ILYA GRUZBERG, James Franck Institute, University of Chicago — Corrections to scaling near critical points are important to understand, because they superimpose and often obscure the true asymptotics of critical scaling laws. This is true, in particular, for studies near the quantum Hall transition where recent numerical work by Slevin and Ohtsuki (Phys. Rev. B **80**, 041304 (2009)) reports a very small value for the leading irrelevant scaling index $|y| \approx 0.17$. We here report a numerical study of two-point conductances and two-terminal conductances at the integer quantum Hall transition within the Chalker-Coddington network. The scaling of these observables will be analyzed in the two-dimensional and the quasi-one-dimensional geometries. We confirm the relation between the conductance exponents X_q and the anomalous dimensions Δ_q known from the multifractal wavefunction analysis: $X_q = 2\Delta_q$. For a consistent picture it is essential to carefully account for corrections to scaling due to subleading power laws and irrelevant scaling operators.

Thursday, March 1, 2012 11:15AM - 2:15PM –

Session W25 DCOMP: Focus Session: Modeling of Rare Events: Methods and Applications I

257A

11:15AM W25.00001 Pathways to forming glass¹, DAVID CHANDLER, University of California, Berkeley — Upon super-cooling at a finite rate, many liquids transform to glass. It is a non-equilibrium transition that depends upon both the material and the cooling protocols. We have used methods of transition path sampling to study this phenomenon in models of glass forming liquids. For the models considered, we establish the order of the transition and the nature of excitations that distinguish a melt from a glass.

¹This research has been supported in the past by grants from NSF and currently by BES-DOE.

11:51AM W25.00002 The kinetic activation-relaxation technique: an off-lattice, self-learning kinetic Monte Carlo algorithm with on-the-fly event search¹, NOMAND MOUSSEAU, Université de Montréal — While kinetic Monte Carlo algorithm has been proposed almost 40 years ago, its application in materials science has been mostly limited to lattice-based motion due to the difficulties associated with identifying new events and building usable catalogs when atoms moved into off-lattice position. Here, I present the kinetic activation-relaxation technique (kinetic ART) is an off-lattice, self-learning kinetic Monte Carlo algorithm with on-the-fly event search [1]. It combines ART nouveau [2], a very efficient unbiased open-ended activated method for finding transition states, with a topological classification [3] that allows a discrete cataloging of local environments in complex systems, including disordered materials. In kinetic ART, local topologies are first identified for all atoms in a system. ART nouveau event searches are then launched for new topologies, building an extensive catalog of barriers and events. Next, all low energy events are fully reconstructed and relaxed, allowing to take complete account of elastic effects in the system's kinetics. Using standard kinetic Monte Carlo, the clock is brought forward and an event is then selected and applied before a new search for topologies is launched. In addition to presenting the various elements of the algorithm, I will discuss three recent applications to ion-bombarded silicon, defect diffusion in Fe and structural relaxation in amorphous silicon.

This work was done in collaboration with Laurent Karim Béland, Peter Brommer, Fedwa El-Mellouhi, Jean-François Joly and Laurent Lewis.

[1] F. El-Mellouhi, N. Mousseau and L.J. Lewis, *Phys. Rev. B*, **78**, 153202 (2008); L.K. Béland *et al.*, *Phys. Rev. E* **84**, 046704 (2011).

[2] G.T. Barkema and N. Mousseau, *Phys. Rev. Lett.* **77**, 4358 (1996); E. Machado-Charry *et al.*, *J. Chem Phys.* **135**, 034102, (2011).

[3] B.D. McKay, *Congressus Numerantium* **30**, 45 (1981).

¹This work was supported by the FQRNT (Quebec), NSERC (Canada) and the Canada Research Chair Foundation.

12:27PM W25.00003 An improved Activation-Relaxation Technique method for finding transition pathways¹, FREDERIC LEGOLL, Ecole Nationale des Ponts et Chaussées — The Activation-Relaxation Technique nouveau (ARTn) is an eigenvector following method for systematic search of saddle points and transition pathways on a given potential energy surface. We propose a variation of this method aiming at improving the efficiency of the local convergence close to the saddle point. The efficiency of the method is demonstrated in the case of point defects in body centered cubic iron. We also prove the convergence and robustness of a simplified version of this new algorithm. Joint work with E. Cancès, M.-C. Marinica, K. Minoukadeh and F. Willaime.

¹This work was partially supported by the Agence Nationale de la Recherche (LN3M project, Contract No. ANR-05-CIGC-0003).

12:39PM W25.00004 ABSTRACT WITHDRAWN –

12:51PM W25.00005 Entropic stabilization of nanoscale voids in materials under tension, DANNY PEREZ, ARTHUR F. VOTER, TIMOTHY C. GERMAN, Theoretical Division T-1, Los Alamos National Laboratory, Los Alamos, NM — While preexisting defects are known to act as nucleation sites for plastic deformation in strained materials, the kinetics of the early stages of plastic yield are still poorly understood. We use a wide range of atomistic simulation techniques (molecular dynamics, accelerated molecular dynamics, umbrella sampling, etc) to investigate the kinetics of plastic yield around small nanoscale voids in copper under uniaxial tensile strain. We demonstrate that, at finite temperatures, these voids are stabilized by strong entropic effects and show that their lifetime is significant even when the static mechanical instability limit is exceeded. This stabilization phenomenon dramatically affects the yield kinetics: the lifetime of the voids is seen to increase with increasing temperature, in contrast with the usual thermally-activated behavior. Even accounting for thermal activation, very small voids prove to be extremely inefficient nucleation sites for plasticity.

1:03PM W25.00006 Estimate Exponential Large Mean Exit Time for Diffusion Process, XIANG ZHOU, HUI WANG, Brown University — We propose an efficient numerical method to estimate the mean exit time of a high dimensional diffusion process associated with an Ito SDE with a gradient drift and small ϵ diffusion coefficient, starting from a stable equilibrium of the drift. It is well-known that the mean exit time is exponential large in ϵ and thus the direct simulation of the SDE requires long time integration. Our method only requires the simulation time $O(1/\epsilon)$ and is based on the Ornstein-Uhlenbeck diffusion in each dimension.

1:15PM W25.00007 K-ART study of defect evolution on experimental time scales in bcc iron and Cu–Zr interfaces, PETER BROMMER, NORMAND MOUSSEAU, Département de physique, Université de Montréal, Québec, Canada — Defects in metals are challenging to study in linear simulation schemes like molecular dynamics (MD), as diffusive activation barriers are typically high compared to $k_B T$, and most resources are devoted to integrating out thermal vibration. Simultaneously, low-energy non-diffusive rearrangements (so-called basins) are serious obstacles for methods that use state-to-state trajectories like kinetic Monte Carlo (KMC). We combined the kinetic Activation-Relaxation technique (k-ART, [1]), an off-lattice, self-learning KMC method which correctly reproduces long-range interactions, with an autonomous basin identification scheme that averages over all in-basin transitions. This allows us to study defect evolution on much longer time scales than MD. In this talk, we present results on the vacancy cluster formation in bcc iron and interface diffusion in the Cu–Zr system.

[1] Béland, Brommer, *et al.*, *Phys. Rev. E*, **84**, 046704 (2011).

1:27PM W25.00008 Accelerated Molecular Dynamics of GaAs(001) Homoepitaxy: Effects of Long-Range Disorder¹, YANGZHENG LIN, KRISTEN FICHTHORN, Penn State University — GaAs homoepitaxy and heteroepitaxy are both fundamentally and technologically significant. From a fundamental perspective, recent experimental work has shown that the GaAs(001) $\beta 2(2\times 4)$ substrate can transform and play an active role in diffusion and the morphologies that form during thin-film growth. Structural transformations lead to a substrate with local (2×4) domains that exhibit long-range disorder characteristic of $c(2\times 8)$. At experimentally relevant temperatures, these transformations are mediated by rare events that occur over time scales ranging from ns to ms, which makes it difficult to probe the kinetics with conventional rare-event techniques. We develop an accelerated molecular dynamics (MD) protocol to deal with this challenge and we apply it to describe the temperature-dependent long-range structure of the surface. Our results are in agreement with experiment. Adatom diffusion occurs over longer time scales than those associated with transformations of the surface. Our accelerated MD studies indicate that adatom diffusion on this surface occurs via different mechanisms than those suggested by previous theoretical studies based on first-principles density-functional theory.

¹Supported by NSF DMR-1006452

1:39PM W25.00009 Ultimate self-learning metabasin escape algorithm for supercooled liquids and glasses, PENGHUI CAO, HAROLD S. PARK, XI LIN, Department of Mechanical Engineering, Boston University — A generic history-penalized metabasin escape algorithm is presented in this work without any predetermined parameters. The configuration space location and volume of imposed penalty functions are determined in self-learning processes as the complete 3N-dimensional potential energy surface is sampled. The computational efficiency is demonstrated using the binary Lennard-Jones liquid supercooled to the glass transition temperature, which shows an exponential enhancement over previous algorithm implementations.

1:51PM W25.00010 Modeling Correlation and Defect Effects on Mixed Polaronic and Ionic Transport in Rare-Earth Phosphates, NICOLE ADELSTEIN, University of California at Berkeley — Rare-earth phosphates are promising candidates for intermediate-temperature proton-conducting fuel cell membranes, with Sr-doped CePO_4 showing particularly high conductivity in oxidizing conditions. Since this high conductivity is likely due to hole-polarons rather than protons, the defect chemistry of incorporating charge carriers (protons versus holes versus oxygen vacancies) is currently being investigated with experiments and calculations. In this work, the dominant charge carrier and its transport in CePO_4 is calculated with density functional theory and compared to conductivity and photon beam experiments. In particular, we present ab-initio calculations on the thermodynamics of the dopants and defects and proton and hole-polaron mobilities. For the case of hole-polaron mobilities, the strength of the coupling with the lattice and the electronic coupling between sites will be investigated.

2:03PM W25.00011 ABSTRACT WITHDRAWN —

Thursday, March 1, 2012 11:15AM - 2:03PM —
Session W26 DCOMP: Focus Session: What is Computational Physics? New Technologies and Their Application 257B

11:15AM W26.00001 The Future of Scientific Computing, THOM DUNNING, National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign — Computing technologies are undergoing a dramatic transition. Multicore chips with up to eight cores are now available from many vendors. This trend will continue, with the number of cores on a chip continuing to increase. In fact, many-core chips, e.g., NVIDIA GPUs, are now being seriously explored in many areas of scientific computing. This technology shift presents a challenge for computational science and engineering—the only significant performance increases in the future will be through the increased exploitation of parallelism. At the same time, petascale computers based on these technologies are being deployed at sites across the world. The opportunities arising from petascale computing are enormous—predicting the behavior of complex biological systems, understanding the production of heavy elements in supernovae, designing catalysts at the atomic level, predicting changes in the earth's climate and ecosystems, and designing complex engineered systems. But, petascale computers are very complex systems, built from multi-core and many-core chips with 100,000s to millions of cores, 100s of terabytes to petabytes of memory, and 10,000s of disk drives. The architecture of petascale computers has significant implications for the design of the next generation of science and engineering applications. In this presentation, we will provide an overview of the directions in computing technologies as well as describe the petascale computing systems being deployed in the U.S. and elsewhere.

11:51AM W26.00002 GPU Acceleration of the Qbox First-Principles Molecular Dynamics Code¹, WILLIAM DAWSON, FRANCOIS GYGI, Department of Computer Science, University of California Davis, Davis CA 95616 — The availability of double precision graphics cards provides an opportunity to speed up electronic structure computations. We modify the Qbox [1] code to utilize Fermi GPUs on the Keeneland [2] platform. We use the CUFFT library to speed up Fourier transforms and perform asynchronous communication to cut down the cost of data transfers. The modified code is used in simulations of a 64-molecule water system with an 85 Ry plane wave energy cut off. Preliminary results show a 2-3 times speedup in the calculation of the charge density and in the application of the Hamiltonian operator to the wave function. We present these findings as well as further speedups measured in other parts of the code.

[1] <http://eslab.ucdavis.edu/software/qbox>

[2] <http://keeneland.gatech.edu>

¹Supported by NSF OCI 60000572 and DOE SciDAC DE-FC02-06ER25794

12:03PM W26.00003 Quantum Monte Carlo in the era of petascale computers, JEONGNIM KIM, University of Illinois at Urbana-Champaign and Oak Ridge National Laboratory, KENNETH ESLER, Stone Ridge Technology, JEREMY MCMINIS, University of Illinois at Urbana-Champaign, MIGUEL MORALES, Lawrence Livermore National Laboratory, BRYAN CLARK, Princeton University, LUKE SHULENBURGER, Sandia National Laboratories, DAVID CEPERLEY, University of Illinois at Urbana-Champaign — Continuum quantum Monte Carlo (QMC) methods are a leading contender for high accuracy calculations for the electronic structure of realistic systems, especially on massively parallel high-performance computers (HPC). The performance gain on recent HPC systems is largely driven by increasing parallelism: the number of compute cores of a SMP and the number of SMPs have been going up, as the Top500 list attests. However, the available memory as well as the communication and memory bandwidth per element has not kept pace with the increasing parallelism. This severely limits the applicability of QMC and the problem size it can handle. (OpenMP,CUDA)/MPI hybrid programming provides applications with simple but effective solutions to overcome efficiency and scalability bottlenecks on large-scale clusters based on multi/many-core SMPs. We discuss the design and implementation of hybrid methods in QMCPACK and analyze its performance on multi-petaflop platforms characterized by various memory and communication hierarchies. Also presented are QMC calculations of bulk systems, including defects in semiconductors.

12:15PM W26.00004 GPU accelerated replica-exchange simulations of polymers, JONATHAN GROSS, MICHAEL BACHMANN, Center for Simulational Physics, University of Georgia, Athens, Georgia 30602, USA — Precise estimation of physical quantities using Monte Carlo computer simulations strongly depends on the amount of statistical data gathered during the simulation. Being able to increase the performance of the sampling process will allow more accurate results in a shorter time period. To employ the parallel tempering replica-exchange algorithm on parallel hardware such as multicore CPUs and GPUs turns out to be very suitable for the task. We achieve rapid speedups in our investigation of an exemplified bead-spring polymer model. Identification and classification of phase-like transitions were done by analyzing the microcanonical entropy.

12:27PM W26.00005 Graphics Processing Unit Accelerated Hirsch-Fye Quantum Monte Carlo, CONRAD MOORE, SAMEER ABU ASAL, KAUSHIK RAJAGOPLAN, DAVID POLIAKOFF, JOSEPH CAPRINO, Louisiana State University, KAREN TOMKO, Ohio State University, BHUPENDER THAKUR, SHUXIANG YANG, JUANA MORENO, MARK JARRELL, Louisiana State University — In Dynamical Mean Field Theory and its cluster extensions, such as the Dynamic Cluster Algorithm, the bottleneck of the algorithm is solving the self-consistency equations with an impurity solver. Hirsch-Fye Quantum Monte Carlo is one of the most commonly used impurity and cluster solvers. This work implements optimizations of the algorithm, such as enabling large data re-use, suitable for the Graphics Processing Unit (GPU) architecture. The GPU's sheer number of concurrent parallel computations and large bandwidth to many shared memories takes advantage of the inherent parallelism in the Green function update and measurement routines, and can substantially improve the efficiency of the Hirsch-Fye impurity solver.

12:39PM W26.00006 ABSTRACT WITHDRAWN —

12:51PM W26.00007 ABSTRACT WITHDRAWN —

1:03PM W26.00008 A simple yet powerful open-source tool for scientific computing, LARRY ENGELHARDT, Francis Marion University — I will introduce new open-source software for easily carrying out common mathematical task (plotting, animating, differentiating, integrating, and solving systems of equations) and fitting experimental data. This software requires no special syntax or programming, and it is designed to allow you to communicate mathematical results to your colleagues or students in a manner that is interactive, productive, and efficient. The current version can be downloaded from <http://www.compadre.org/osp/items/detail.cfm?ID=11250>.

1:15PM W26.00009 Multicanonical Modeling of Commercial WDM Optical Communication Systems¹, DAVID YEVICK, GEORGE SOLIMAN, University of Waterloo — The multicanonical method has been extensively applied to optical and more recently wireless communication systems. Here we outline our recent work on the simulation of electronically compensated polarization multiplexed wavelength-division-multiplexed quadrature phase shift keyed optical communication systems influenced by polarization mode dispersion and fiber nonlinearities. This constitutes to our knowledge the first complete multicanonical analysis of a realistic commercial system.

¹Work supported by CIENA and NSERC

1:27PM W26.00010 Mantid, A high performance framework for reduction and analysis of neutron scattering data, JON TAYLOR, ISIS STFC, O. ARNOLD, Tessella PLC, J. BILHEAUX, ORNL, A. BUTS, ISIS STFC, S. CAMPBELL, M. DOUCET, ORNL, N. DRAPER, Tessella PLC, R. FOWLER, STFC, M. GIGG, Tessella PLC, V. LYNCH, ORNL, A. MARKVARDSEN, K. PALMEN, P. PARKER, ISIS STFC, P. PETERSON, S. REN, M. REUTER, A. SAVICI, ORNL, R. TAYLOR, R. TOLCHENOV, Tessella PLC, R. WHITLEY, ISIS STFC, W. ZHOU, J. ZIKOVSKY, ORNL — The use of large scale facilities by researchers in the field of condensed matter, soft matter and the life sciences is becoming ever more prevalent in the modern research landscape. Facilities such as SNS and HiFNR at ORNL and ISIS at RAL have ever increasing user demand and produce ever increasing volumes of data. One of the single most important barriers between experiment and publication is the complex and time consuming effort that individual researchers apply to data reduction and analysis. The objective of the Manipulation and Analysis Toolkit for Instrument Data or MANTID [1] framework is to bridge this gap with a common interface for data reduction and analysis that is seamless between the user experience at the time of the experiment and at their home institute when performing the final analysis and fitting of the data.

[1] <http://www.mantidproject.org/>

1:39PM W26.00011 SU(N) Clebsch-Gordan coefficients and non-Abelian symmetries, ARNE ALEX, LUKAS EVERDING, Arnold Sommerfeld Center, LMU Munich, PETER LITTELMANN, University of Cologne, JAN VON DELFT, Arnold Sommerfeld Center, LMU Munich — The numerical treatment of models with SU(N) benefits greatly from the Wigner-Eckart theorem. Its application requires the explicit knowledge of the Clebsch-Gordan coefficients (CGCs) of the group SU(N). We present an algorithm for the explicit numerical calculation of SU(N) CGCs based on the *Gelfand-Tsetlin pattern* calculus. Further exploitation of the Weyl symmetry of SU(N) irreducible representations (irreps) leads to a significant speed-up compared to our previous algorithm (J. Math. Phys. 52, 023507, 2011). Our algorithm works for arbitrary N and tensor products of two arbitrary SU(N) irreps. It is well-suited for numerical implementation; we provide a well-tested computer code for download and online use. Possible applications of our code include numerical treatments of quantum many-body systems using the numerical renormalization group (NRG), the density matrix renormalization group (DMRG), and general tensor network methods.

1:51PM W26.00012 Efficient interacting many body simulations using GPUs, TOBIAS KRAMER, Universität Regensburg — Graphics Processing Units (GPUs) provide an ideal tool to study interacting systems using classical mechanics with huge speedups for example in molecular dynamics. The quantum-mechanical calculations of many-body systems require additional work, but are feasible using additional degrees of freedom to incorporate quantum-mechanical effects [1]. As an example of the method I show the self-consistent solution to the current transport in a magnetic field can be obtained from a microscopic model with thousands of Coulomb interacting electrons. This yields a microscopic model of the Hall effect [2]. For few electron systems I compare the electronic density evolution based on the GPU classical-quantum model to TD-DFT calculations and discuss prospects of GPUs for solving the Schrodinger equation for many-particles.

[1] Time dependent approach to transport and scattering in atomic and mesoscopic systems, T. Kramer AIP Conf. Proc., 1334, 142 (2011)

[2] Self-consistent calculation of electric potentials in Hall devices, T. Kramer, V. Krueckl, E. Heller, and R. Parrott Phys. Rev. B, 81, 205306 (2010)

Thursday, March 1, 2012 11:15AM - 2:15PM —

Session W27 DCMP: Invited Session: Electrons, Spins, and Collective Modes in Nanofilms

11:15AM W27.00001 Plasmons under extreme dimensional confinement, HANNO WEITERING, Department of Physics and Astronomy, The University of Tennessee — In our studies, we explore how surface and bulk plasmons emerge under extreme dimensional confinement, i.e., dimensions that are orders of magnitude smaller than those employed in ‘nanoplasmonics’. Atomically-smooth ultrathin Mg films were epitaxially grown on Si(111), allowing for atomically-precise tuning of the plasmon response.¹ While the single-particle states in these 3-12 monolayer (ML) thick films consist of a series of two-dimensional subbands, the bulk-plasmon response is like that of a thin slice carved from bulk Mg subject to quantum-mechanical boundary conditions. Remarkably, this bulk-like behavior persists all the way down to 3 ML. In the 3-12 ML thickness range, bulk loss spectra are dominated by the $n=1$ and $n=2$ normal modes, consistent with the excitation of plasmons involving quantized electronic subbands. The collective response of the thinnest films is furthermore characterized by a thickness-dependent spectral weight transfer from the high-energy collective modes to the low-energy single-particle excitations, until the bulk plasmon ceases to exist below 3 ML. Surface- and multipole plasmon modes even persist down to 2 ML. These results are striking manifestations of the role of quantum confinement on plasmon resonances in precisely controlled nanostructures. They furthermore suggest the intriguing possibility of tuning resonant plasmon frequencies via precise dimensional control.

¹M.M. Özer, E.J. Moon, A.G. Eguluz, and H.H. Weitering, Phys. Rev. Lett. **106**, 197601 (2011).

11:51AM W27.00002 Radial band structure of a ultrathin liquid metal film¹, HAN WOONG YEOM, Department of Physics, POSTECH — Understanding the properties of strongly disordered materials has been one of the long standing and most challenging problems in condensed matter physics. One major difficulty lies in the failure of the band structure concept to describe electronic properties due to the lack of the periodicity, as notorious for electrons in liquid metals without any well-established and well-tested alternative until now. In this work, we experimentally, using angle-resolved photoelectron spectroscopy, establish the formation of an intriguing “double radial band structure” in a strongly disordered electronic system of a liquid metal Pb. A monolayer Pb film was formed on Si(111) with an unusually low melting temperature and its detailed band dispersions and Fermi contours were mapped throughout the melting process. Furthermore, we introduce the way to understand this characteristic band structure based on an old theoretical idea proposed in 1962 invoking the coherent radial scattering of electrons, which can be widely encountered in wave scatterings within disordered media. In conclusion, liquid metals, or possibly other strongly disordered electronic systems, have well defined radial bandstructures through the coherent radial scattering of electrons and the radial correlation of atoms.

¹This work was supported by National Research Foundation of Korea through the CRi program.

12:27PM W27.00003 Ultrafast mass transport during decay of gigantic Pb mesas on Ni(111), BENE POELSEMA, Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente — We have studied the initial growth of Pb films on Ni(111) at elevated temperatures of 424 K and 474 K. Quantum Well States (QWS's) have been found to be responsible for the morphology of these Pb films on Ni(111). The delicate balance between surface energies, elastic energies and QWS's is initially tilted towards QWS's, as discrete layer heights are observed. First, a strong preference for 5 and 7 layers high, flat topped Pb islands is observed, showing several striking similarities with Pb films on Si(111) and on Cu(111). Key examples of these will be discussed. When the character of the rough film gradually changes from 2D to 3D, the balance between these forces becomes more and more dominated by interfacial energies. A tipping point is reached by very slowly heating the surface to about 520 K. As the energetic balance is tipped for good in favor of the interface free energy, the electronically stabilized, extended, about 40 layers high mesas suddenly decay towards compact hemispheric structures. The spectacular speed at which the transition takes place (billions of atoms move over several microns during a few milliseconds!) is many orders of magnitude larger than what is expected, based on arguments involving thermally activated behavior on atomic scales. I will discuss peculiarities of the wetting layer and its changes, which appear to coincide with the ultrafast transition of the film morphology. With a widespread interest in nanostructures in general, our results illustrate the generic need to characterize all aspects of nanostructures, both structural and electronic, since small excursions away from equilibrium can have dramatic consequences. T.R.J. Bollmann, R. van Gastel, H.J.W. Zandvliet and B. Poelsema; Phys. Rev. Lett. **107**, 116101 (2011); T.R.J. Bollmann, R. van Gastel, H.J.W. Zandvliet and B. Poelsema; New J. Phys. **13**, 103025 (2011).

1:03PM W27.00004 Regulating spin and Fermi surface topology of a quantum metal film by the surface (interface) monatomic layer, IWAO MATSUDA, the Institute for Solid State Physics, the University of Tokyo — Spin and current controls in solids have been one of the central issues in researches of electron and spin transport. Nowadays, electronics/spintronics deals with nanometer- or atomic-scale structures and miniaturization of these systems implies emergence of various quantum phenomena, intimately linked to the formation of electronic states different from those of the corresponding bulk materials. For example, valence electrons of films with the thickness comparable to the electron wavelength form discrete quantum-well states (QWSs) under opportune conditions of confinement (quantum size effect). Furthermore, the size reduction also increases the surface/volume ratio and a film possibly changes its electronic (spin) properties by the surface effect. Concerning metal films, the quantum size effect requires the thickness in a range of nanometers and the length corresponds to several tens of atoms, indicating the very large ratio of a surface (interface) monatomic layer to film atomic layers. Thus, we have been interested in combining the quantum size effects and the surface effect on the metal films to induce new physical phenomena. In the present talk, two research cases are shown. 1) Instead of isotropic two-dimensional in-plane states expected for an isolated metal film, quasi-one-dimensional quantized states were measured by photoemission spectroscopy in an epitaxial Ag(111) ultra thin film, prepared on an array of atomic chains [1]. 2) High-resolution spin-resolved photoemission and magneto-transport experiments of ultrathin Ag(111) films, covered with a $\sqrt{3}\times\sqrt{3}$ -Bi/Ag surface ordered alloy, were performed. The surface state (SS) bands, spin-split by the Rashba interaction, selectively couple to the originally spin-degenerate QWS bands in the metal film, making the spin-dependent hybridization [2,3]. Magnetoconductance of the films, measured in situ by the micro-four-point probe method as a function of the applied magnetic field [4], has shown that the formation of the Rashba-type surface alloy reduces the spin-relaxation time in the ultrathin film significantly [5]. These results demonstrate that spin and Fermi surface topology of a quantum metal film can be regulated by the surface (interface) monatomic layer.

[1] T. Okuda, Y. Takeichi, K. He, A. Harasawa, A. Kakizaki, and I. Matsuda, Phys. Rev. B **80**, 113409 (2009).

[2] K. He, T. Hirahara, T. Okuda, S. Hasegawa, A. Kakizaki, and I. Matsuda, Phys. Rev. Lett. **101**, 107604 (2008).

[3] K. He, Y. Takeichi, M. Ogawa, T. Okuda, P. Moras, D. Topwal, A. Harasawa, T. Hirahara, C. Carbone, A. Kakizaki, and I. Matsuda, Phys. Rev. Lett. **104**, 156805 (2010).

[4] N. Miyata, R. Hobara, H. Narita, T. Hirahara, S. Hasegawa, and I. Matsuda, Japanese Journal of Applied Physics **50**, 036602 (2011).

[5] N. Miyata, H. Narita, M. Ogawa, A. Harasawa, R. Hobara, T. Hirahara, P. Moras, D. Topwal, C. Carbone, S. Hasegawa, and I. Matsuda, Phys. Rev. B, **83**, 195305 (2011).

1:39PM W27.00005 Quantum Oscillations of Surface Electronic Structure: Inter-relation Between Quantum Well States, Work Functions and Surface Energies, CHIH-KANG SHIH, The University of Texas at Austin — Quantum size effects (QSE) in ultra-thin metallic film has been a topic of intense investigations. Of particular interests are the inter-relationship between the quantum well states (QWS), work function (W) and surface energy (E_s). In ultrathin Pb films on semiconductors, quantum oscillations of E_s as a function of layer thickness (L) have been investigated by various experimental methods which have all yielded identical results. Experimental studies of work function, however, took a longer journey. Photoemission can probe the work function for a uniform film but in this case uniform film only exists for certain thicknesses. Scanning tunneling microscopy, can probe “local” properties for all thicknesses, but the very existence of QWS in these films profoundly affects the measured tunneling decay constant κ . Consequently, L-dependence of κ also depends on the bias voltage. It was then discovered that at a very low sample bias ($|V_s| < 0.03$ V) the measured κ vs. L accurately reflects the quantum size effect on the work function [1]. With this last obstacle removed, we are able to simultaneously measure the W vs. L, E_s vs. L and to correlate these quantities with the measured QWS locations, yielding the quantitative phase relationship between the quantum oscillations of work function and surface energy. To our surprise, instead of a predicted $1/4$ wavelength phase shift, we find that the quantum oscillations of these two quantities are exactly in-phase. A new model is proposed.

Thursday, March 1, 2012 11:15AM - 1:51PM —

Session W29 GQI: Focus Session: Superconducting Qubits: Resonators and Loss Mechanisms

259A

11:15AM W29.00001 Microwave Loss in Josephson Junction Embedded Superconducting Resonators¹, STEVEN WEBER, KATER MURCH, I. SIDDIQI, UC Berkeley, QNL — We report on progress to identify and mitigate sources of microwave frequency loss in Josephson junction resonant circuits at low temperature and power—the operating regime of superconducting qubits. Large critical current junctions (>500nA) were embedded in lumped element 4–8 GHz superconducting resonators based on single crystal silicon dielectric overlap capacitors. Small critical current junctions (25-100nA) were characterized by measuring the T_1 relaxation time of transmon qubits. For both sets of measurements, the critical current density was varied from 20-800 A/cm². We present the dependence of junction loss on junction area and environmental factors such as shielding and filtering.

¹This research was supported by the IARPA CSQ program.

11:27AM W29.00002 Superconducting Microwave Resonators, CHARLES NEILL, ANTHONY MEGRANT, MIKE LENANDER, RAMI BARENDs, JIM WENNER, TED WHITE, DANIEL SANK, YU CHEN, YI YIN, BEN CHIARO, JULIAN KELLY, PETER O'MALLEY, PEDRAM ROUSHAN, ERIK LUCERO, AMIT VAINSENER, JOERG BOCHMANN, MATTEO MARIANTONI, CHRIS AXLINE, JOHN MARTINIS, ANDREW CLELAND, UCSB — High quality factor superconducting microwave resonators play a key role in applications to quantum computation and single photon detection schemes. We have optimized our aluminum quarter wavelength coplanar waveguide resonators in an effort to improve energy decay times. As the characteristic decay times in our samples begin to approach the requirements set out by fault tolerant error correction algorithms, reproducibility becomes a growing focus. Consistent reproduction of high quality factor resonators requires reliable determination of device parameters independent of experimental imperfections and environmental influences. These measurements permit an improved understanding of the variations between nominally identical resonators as well as variations in an individual sample over time. Recent experimental results will be discussed.

11:39AM W29.00003 Improving the Quality Factor of Superconducting Resonators¹, ANTHONY MEGRANT, CHARLES NEILL, RAMI BARENDs, BEN CHIARO, MIKE LENANDER, CHRIS PALMSTROM, JOHN MARTINIS, ANDREW CLELAND, UC Santa Barbara, UCSB SUPERCONDUCTING QUANTUM INFORMATION GROUP TEAM — Superconducting resonators hold great promise for quantum information storage in quantum computing. Improving the coherence lifetimes is therefore of central interest. We have focused on improving the interface between the resonator's underlying dielectric and superconducting metallization, as simulations have shown this interface to be a major source of loss, possibly associated with two-level states. After mitigating for stray light and magnetic fields, we have achieved low power intrinsic quality factors in excess of one million at single photon energies, with high power Q's in excess of ten million. Attaining such high quality factors is dependent on substrate preparation before depositing the superconductor, as well as the deposition method. We will describe the fabrication method and characterization of resonators that consistently achieve quality factors above one million.

¹IARPA\ARO Grant : W911NF-09-1-0375

11:51AM W29.00004 Investigation of superconducting resonator designs for measuring the microwave response of vortices, I. NSANZINEZA, H. CHEN, C. SONG, B.L.T PLOURDE, Syracuse University — The microwave response of superconductors can be influenced by the presence of vortices and the dynamics they exhibit at high frequencies. We present measurements of vortices trapped in superconducting resonators fabricated from thin aluminum films, a common material for superconducting qubit circuits. In particular, we are studying the dependence of the threshold magnetic field for trapping vortices on the resonator geometry. We perform field-cooled measurements of various configurations of coplanar waveguide resonators to study the magnetic field, frequency, and temperature dependence of the microwave vortex response. The addition of vortices results in a downward shift in resonant frequency and a reduction in the resonator quality factor. We discuss the optimization of the resonator layout for detecting the response from only a few vortices trapped in the superconducting film.

12:03PM W29.00005 Anomalous magnetic field effects in high Q superconducting resonators, M. LENANDER, R. BARENDs, YU CHEN, J. KELLY, ERIK LUCERO, MATTEO MARIANTONI, A. MEGRANT, P.J.J. O'MALLEY, C. NEILL, D. SANK, A. VAINSENER, H. WANG, J. WENNER, T.C. WHITE, Y. YIN, J. ZHAO, C. PALMSTROM, A.N. CLELAND, JOHN M. MARTINIS, UCSB — Superconducting coplanar wave guide resonators are an important tool in quantum computing for use as memory elements. Recent process improvements have allowed for quality factors in excess of 1.5 million at single photon excitations. While allowing for more sensitive experiments, the most recent group of resonators exhibit very high sensitivity to magnetic fields. Ordinarily Abrikosov vortex physics is expected to govern the magnetic response of the resonators. During field cooling, vortices begin to form at a threshold field, B_{th} , that depends quadratically on the width of the resonator. However these resonators show an observed B_{th} two orders of magnitude lower than predicted by theory and without any scaling with resonator width. We explore increased sensitivity to frequency fluctuations at nonzero field as a possible explanation for reduced quality factor long before vortices are expected to form.

12:15PM W29.00006 Quality Factor Measurements with Improved Superconducting Stripline Resonators¹, ERIC HOLLAND, LUYAN SUN, MATTHEW REAGOR, KEVIN CHOU, LUIGI FRUNZIO, ROBERT SCHOELKOPF, Yale University — Superconducting microwave resonators can be coupled to a superconducting qubit to manipulate, read out and protect the qubit from the environment. Improvements in resonator quality factors, Q, offer a variety of benefits. One benefit of higher Qs is the possibility for longer coherence times. Alternatively, higher Q resonators could be implemented as a quantum memory. We fabricated and tested superconducting stripline resonators which are designed to minimize sensitivity to surface dielectric losses. These devices allow the possibility of sensitive testing of superconducting film quality and/or losses in the bulk substrate dielectric. By measuring these losses we can better understand possible mechanisms of decoherence in superconducting qubits. Preliminary quality factor results, taken at milliKelvin temperatures, will be given.

¹Funded by IARPA

12:27PM W29.00007 Dielectric loss analysis using linear resonators with different impedances, BAHMAN SARABI, M.S. KHALIL, M.A. KHASAWNEH, M.J.A. STOUTIMORE, SERGIY GLADCHENKO, University of Maryland and Laboratory for Physical Sciences, F.C. WELLSTOOD, C.J. LOBB, University of Maryland, K.D. OSBORN, Laboratory for Physical Sciences — It is known that amorphous dielectrics are a major source of decoherence in superconducting qubits due to energy absorption by two-level systems coupled to the electric fields. Linear resonators have been applied extensively to study loss in different dielectrics used in qubit circuits due to their versatility and relative simplicity in design, fabrication and measurement. We have designed linear resonators with multi-turn inductors and parallel-plate capacitors with resonance frequencies of 4.8-6.4 GHz. We achieve substantially different L/C values and capacitor volumes by varying the number of inductance turns and the area of the capacitors. We will present results of continuous wave measurements with SiN_x capacitors and show how loss tangent and phase noise are related to impedance and capacitor volume.

12:39PM W29.00008 ABSTRACT WITHDRAWN —

12:51PM W29.00009 Reduction of Microwave Loss in Titanium Nitride CPW Resonators, MICHAEL VISSERS, National Institute of Standards and Technology, Boulder, CO, DAVID WISBEY, St Louis University, St Louis, MO, JIANGSONG GAO, JEFFREY KLINE, MARTIN SANDBERG, MARTIN WEIDES, DAVID PAPPAS, National Institute of Standards and Technology, Boulder, CO — Titanium Nitride (TiN) thin films, when optimally grown and processed, exhibit very low microwave loss at high and low power. We investigate reducing the loss by systematically removing Si substrate material from the gap region in TiN coplanar waveguides (CPWs) fabricated on intrinsic Si substrates. By exploiting the radial dependence of the etch rate in a parallel plate reactive ion etcher, otherwise identical CPWs with only the gaps etched to varying depth, i.e. trenched, were created in a single TiN film within a single processing step. The high power loss is similar for all resonators, $< 2 \times 10^{-7}$. However, when comparing the loss from all trench depths in the single photon regime at 50 mK we find that loss was reduced for the deeper trenches with the deepest reduced by a factor of 2. Predictions from finite-element analysis, with a reduced participation of lossy surface oxides in the deeper trenched CPW gaps, fit well to the measured reduction.

1:03PM W29.00010 Cooper Pair Transistor Embedded in a dc-Biased High-Q Microwave Cavity¹, JULIANG LI, FEI CHEN, JOEL STETTENHEIM, Dartmouth College, A.J. SIROIS, University of Colorado, Boulder, R.W. SIMMONDS, National Institute of Standards and Technology, Boulder, M.P. BLENCOWE, A.J. RIMBERG, Dartmouth College — A high-Q microwave cavity design based on the circuit quantum electrodynamics architecture has been developed to introduce a dc bias to the center conductor of the cavity without significantly degrading the Q at high frequencies [1]. Here we directly couple Cooper pair transistors (CPTs) to such a cavity. In the subgap region of the CPT, the dc bias generates a tunable oscillating current through the CPT via the ac Josephson effect. Evidence of such self-oscillations has been observed as current peaks in our dc measurements, which are in good agreement with calculated cavity modes, and indicate the strong coupling between the CPT and the cavity. Recent experimental results will be discussed.

[1] F. Chen, A. J. Sirois, R. W. Simmonds and A. J. Rimberg, Appl. Phys. Lett., 98, 132509 (2011).

¹This work is supported by the NSF, AFOSR and DARPA

1:15PM W29.00011 Photon Emission from a Self-oscillating Cavity-Embedded-Cooper Pair Transistor¹, FEI CHEN, JOEL STETTENHEIM, JULIANG LI, Dartmouth College, A.J. SIROIS, University of Colorado, Boulder, R.W. SIMMONDS, National Institute of Standards and Technology, Boulder, M.P. BLENCOWE, A.J. RIMBERG, Dartmouth College — A strongly non-linear superconducting device consisting of a Cooper pair transistor embedded in a dc voltage biased microwave cavity is investigated. The cavity-embedded-Cooper pair transistor (CECPT) is driven via the ac Josephson effect by an applied dc bias and exhibits self-oscillation without an external ac drive. Tunneling Cooper pairs can both emit photons into and absorb photons from microwave cavity modes. Photons emitted into the cavity are directly probed and are in good agreement with dc measurements. Photon emission arising from both sequential tunneling and cotunnelling processes has been observed. The CECPT offers an interesting system for studying nonlinear quantum dynamics and the quantum-to-classical transition. Recent experimental results will be discussed.

¹This work is supported by the NSF, AFOSR and DARPA.

1:27PM W29.00012 Superconducting microstrip resonators for circuit QED experiments¹, M. HAEBERLEIN, M. KRAWCZYK, A. BAUST, J. GOETZ, E. HOFFMANN, E. P. MENZEL, M. SCHWARZ, F. WULSCHNER, L. ZHONG, F. DEPPE, A. MARX, R. GROSS, Walther-Meissner-Institut — Superconducting microstrip resonators have several advantages when designing scalable circuit QED systems. Their simple geometry facilitates the implementation of additional circuit elements and control lines, and, most importantly, their spectrum tends to exhibit nearly no parasitic modes up to 20 GHz even for more complicated geometries. However, due to their specific field configuration they are not expected to yield high Q-factors at very low temperatures. We analyzed such resonators at Millikelvin temperatures and find experimentally useful quality factors of approximately 1500 even in the low temperature low power limit. Our analysis indicates that even ten times higher quality factors can be achieved straightforwardly by choosing substrates with better dielectric properties. Supported by the DFG via SFB 631 and by the German Excellence Initiative via NIM

¹Supported by the DFG via SFB 631 and by the German Excellence Initiative via NIM.

1:39PM W29.00013 Superconducting Resonators with Parasitic Electromagnetic Environments, JOHN HORNIBROOK, School of Physics, University of Sydney, 2006, Australia, EMMA MITCHELL, CSIRO Materials Science and Engineering, Lindfield 2070 Australia, DAVID REILLY, School of Physics, University of Sydney, 2006, Australia — Microwave losses in niobium superconducting resonators are investigated at milli-Kelvin temperatures and with low drive power. In addition to the well-known suppression of Q-factor that arises from coupling between the resonator and two-level defects in the dielectric substrate [1-4], we report strong dependence of the loaded Q-factor and resonance line-shape on the electromagnetic environment. Methods to suppress parasitic coupling between the resonator and its environment are demonstrated.

[1] Day, P.K. et al., Nature 425, 817-821 (2003).

[2] Wallraff, A. et. al., Nature 451, 162-167 (2004).

[3] Macha, P. et. al., Appl. Phys. Lett., 96, 062503 (2010).

[4] O'Connell, A.D. et. al., Appl. Phys. Lett., 92, 112903 (2008).

Thursday, March 1, 2012 11:15AM - 2:15PM – Session W30 GQI: Quantum Entanglement 259B

11:15AM W30.00001 Entanglement, Fluctuations, and Quantum Critical Points, STEPHAN RACHEL, Department of Physics, Yale University, New Haven, CT 06520, USA, NICOLAS LAFLORENCIÉ, Laboratoire de Physique Theorique, Universite de Toulouse, UPS, (IRSAMC), F-31062 Toulouse, France, H. FRANCIS SONG, Department of Physics, Yale University, New Haven, CT 06520, USA, KARYN LE HUR, Center for Theoretical Physics, Ecole Polytechnique, 91128 Palaiseau Cedex, France and Department of Physics, Yale University, New Haven, CT 06520 — We show that bipartite fluctuations F can be considered an entanglement measure. We further demonstrate that the concept of bipartite fluctuations F provides a very efficient tool to detect quantum phase transitions in strongly correlated systems. We investigate paradigmatic examples for both quantum spins and bosons in one and two dimensions. As compared to the von Neumann entanglement entropy, we observe that F allows to find quantum critical points with a much better accuracy in one dimension. We further demonstrate that F can be successfully applied to the detection of quantum criticality in higher dimensions with no prior knowledge of the universality class of the transition. Promising approaches to experimentally access fluctuations are discussed for quantum antiferromagnets and cold gases.

11:27AM W30.00002 A statistical portrait of the entanglement decay of two-qubit memories¹, KAREN FONSECA-ROMERO, JULIAN MARTINEZ-RINCON², Universidad Nacional de Colombia — We present a novel approach to the study of entanglement decay, which focuses on collective properties. As an example, we investigate the entanglement decay of a two-qubit memory, produced by local identical reservoirs acting on the qubits, for three experimentally and theoretically relevant cases: depolarizing, dephasing and amplitude-damping channels. We study the probability distributions of disentanglement times, a quantity independent of the measure used to quantify entanglement, and the time-dependent probability distribution of concurrence. Uniformly distributed pure states are assumed for the two-qubit system. The calculation of these probability distributions gives a clearer insight on how different decoherence channels affect the entanglement initially contained in the set of two-qubit pure states. The entanglement evolution of mixed states, under the Hilbert-Schmidt metric, is also considered.

¹Fundación para la Promoción de la Investigación y la Tecnología (Colombia)

²Now at University of Rochester

11:39AM W30.00003 Quantum Mutual Information Capacity for High Dimensional Entangled States¹, P. BENJAMIN DIXON, Research Laboratory of Electronics, MIT, GREGORY A. HOWLAND, JAMES SCHNEELOCH, JOHN C. HOWELL, University of Rochester — High dimensional Hilbert spaces used for quantum communication channels offer the possibility of large data transmission capabilities and improved security. We propose a method of characterizing the channel capacity of an entangled photonic state in high dimensional position and momentum bases. We use this method to measure the channel capacity of a parametric downconversion state, achieving a channel capacity over 7 bits/photon in either the position or momentum basis, by measuring in up to 576 dimensions per detector. The channel strongly violated an entropic separability bound, indicating the performance cannot be replicated classically.

¹DARPA DSO InPho grant W911NF-10-1-0404 and USARO MURI grant W911NF-05-1-0197

11:51AM W30.00004 Entangling Qubits in a One-Dimensional Harmonic Oscillator, EDMUND OWEN, MATTHEW DEAN, CRISPIN BARNES, University of Cambridge — We present a method for generating entanglement between qubits associated with a pair of particles interacting in a one-dimensional harmonic potential. By considering the effect of the interaction on the energy spectrum of the system, we show that, under certain approximations, a “power-of-SWAP” operation is performed on the initial two-qubit quantum state without requiring any time-dependent control. Initialization errors and deviations from our approximation are shown to have a negligible effect on the final state. Using a GPU-accelerated iteration scheme to find numerical solutions to the two-particle time-dependent Schrödinger equation, we demonstrate that it is possible to generate maximally entangled Bell states between the two qubits with high fidelity for a range of possible interaction potentials.

12:03PM W30.00005 Entanglement entropy for arbitrary quantum lattice models from quantum Monte Carlo, TOMMASO ROSCILDE, Ecole Normale Supérieure de Lyon (France), STEPHAN HUMENIUK, Ecole Normale Supérieure de Lyon (France) and Ludwig-Maximilians-Universität, Munich (Germany) — We present a general scheme to numerically calculate the Renyi entropy for the reduced density matrix of a subsystem in a quantum lattice model at finite and (physically) zero temperature. This scheme is based on an extended-ensemble formulation of quantum Monte Carlo, which can be applied in principle to any quantum Monte Carlo algorithm. It improves on the existing approach of R. G. Melko et al., Phys. Rev. B 82, 100409(R) (2010) and of M. B. Hastings et al., Phys. Rev. Lett. 104, 157201 (2010) in that it allows to probe the ground-state properties of lattice models regardless of their symmetry – as long as they admit an efficient quantum Monte Carlo algorithm. We test the entanglement entropy scaling of fundamental quantum spin models, showing e.g. that the two-dimensional XX model, describing lattice hardcore bosons, exhibits an area law despite lacking an intrinsic length scale for the decay of correlations.

12:15PM W30.00006 Different Measures of Entanglement in Spin Chains, VLADIMIR KOREPIN, Yang Institute for Theoretical Physics in Stony Brook — Different measures of entanglement in spin chains are considered. Main example is VBS state, it is important because of measurement based quantum computation. Entanglement spectrum and negativity are considered in the lecture. These measures are calculated analytically in one dimension. In 2D we have only estimates. Lecture follows the papers: <http://arxiv.org/abs/1109.4971> and <http://arxiv.org/abs/1110.3300>

[1] Heng Fan, Vladimir Korepin, Vwani Roychowdhury, PRL, vol 93, (2004), 227203

12:27PM W30.00007 Rényi entropy of d -wave Bose metal phases on multi-leg ladders, JAMES R. GARRISON, RYAN V. MISHMASH, MATTHEW P.A. FISHER, University of California, Santa Barbara — In recent years, much progress has been made toward understanding 2D Bose metal-type phases by accessing them through a series of controlled quasi-1D ladder studies [1]. Crucially, such quasi-1D descendants of these exotic phases are expected to have a number of gapless Luttinger modes, c , that grows with the width of the ladder. Therefore, characterizing scaling of the entanglement entropy has become an essential tool for establishing the existence of these phases, as it provides a direct measure of c . With density-matrix renormalization group (DMRG) methods, it is easy to calculate the entanglement entropy but the results converge prohibitively slowly as the ladder becomes wider. Here, we present results where we have calculated, using Variational Monte Carlo (VMC), the Rényi entropy S_2 for Gutzwiller-projected d -wave Bose metal (DBM) [2] trial wave functions on ladders, following the method employed in [3]. We compare with DMRG results (where they are available), and comment on what our findings mean for the ability of our trial wave functions to faithfully represent the DBM phase.

[1] D. N. Sheng et. al., PRB **78**, 054520 (2008).

[2] O. I. Motrunich and M. P. A. Fisher, PRB **75**, 235116 (2007).

[3] Y. Zhang et. al., PRL **107**, 067202 (2011).

12:39PM W30.00008 Rényi Entanglement Entropies and the Entanglement Spectrum, FRANCIS SONG, STEPHAN RACHEL, KARYN LE HUR, Yale University — We describe a simple method for computing the full entanglement spectrum of any finite density matrix from the Rényi entropies of integer order. This has important implications for non-interacting fermionic systems where the Rényi entropies are directly related to the cumulants of charge number fluctuations, and for quantum Monte Carlo simulations where it is now becoming possible to compute the Rényi entropies but not the von Neumann entropy or the full entanglement spectrum.

12:51PM W30.00009 Entanglement Entropy of Fermi Liquids via Multi-dimensional Bosonization¹, WENXIN DING, National High Magnetic Field Laboratory & Florida State University, ALEXANDER SEIDEL, Washington University in St. Louis, KUN YANG, National High Magnetic Field Laboratory & Florida State University — The logarithmic violations of the area law, i.e. an “area law” with logarithmic correction of the form $S \sim L^{d-1} \log L$, for entanglement entropy are found in both 1D gapless system and for high dimensional free fermions. The purpose of this work is to show that both violations are of the same origin, and in the presence of Fermi liquid interactions such behavior persists for 2D fermion systems. In this paper we first consider the entanglement entropy of a toy model, namely a set of decoupled 1D chains of free spinless fermions, to relate both violations in an intuitive way. We then use multi-dimensional bosonization to re-derive the formula by Gioev and Klich [Phys. Rev. Lett. **96**, 100503 (2006)] for free fermions through a low-energy effective Hamiltonian, and explicitly show the logarithmic corrections to the area law in both cases share the same origin: the discontinuity at the Fermi surface (points). In the presence of Fermi liquid (forward scattering) interactions, the bosonized theory remains quadratic in terms of the original local degrees of freedom, and after regularizing the theory with a mass term we are able to calculate the entanglement entropy perturbatively up to second order in powers of the coupling parameter for a special geometry via the replica trick.

¹This work is supported support by National Science Foundation under NSF Grant No. DMR-1004545 (W.X.D. and K.Y.). AS is supported by the National Science Foundation under NSF Grant No. DMR-0907793.

1:03PM W30.00010 Multipartite Entanglement classes via Negativity Fonts¹, SANTOSH SHELLEY SHARMA, Depto. de Física, Universidade Estadual de Londrina, Londrina PR, Brazil, NARESH KUMAR SHARMA, Depto. de Matemática, Universidade Estadual de Londrina, Londrina — The number and types of K-way negativity fonts in canonical form of an N-qubit state depends on the nature and amount of quantum coherences in the state. Non zero determinants of negativity fonts, characterizing a given state, are easily written down and reflect the entanglement microstructure of the superposition. A classification criterion for multipartite entangled states, based on negativity fonts in canonical state and decomposition of global partial transpose in terms of K-way partially transposed operators, is proposed. Inequivalent sub-classes are labelled by N-qubit local unitary invariants. A complete classification of four qubit states is obtained. The number of major families for $N > 3$ is found to be $2^N - 2N$. Classification of four qubit states indicates that a small number of relevant polynomial invariants is enough to classify N-qubit states.

¹This work is supported by Faep Uel, Fundação Araucária and CNPq, Brazil.

1:15PM W30.00011 Entanglement Spectrum Classification of Disordered Class AII Symplectic Systems¹, MATTHEW GILBERT, TAYLOR HUGHES, University of Illinois at Urbana-Champaign, ANDREI BERNEVIG, Princeton University — Of the available classes of random matrices which have been shown to contain topologically non-trivial properties², one of the most intriguing is class AII, which characterizes a system that possesses time-reversal symmetry. This class of random matrices has been the subject of significant attention as it encompasses Z_2 topological systems of which the quantum spin Hall (QSH) state is a member³. We calculate the entanglement spectrum for disordered class AII symplectic systems in two-dimensions as a function of disorder strength, chemical potential, and bulk inversion asymmetry. We show that there is a one to one correspondence between the full system Hamiltonian and that of the entanglement spectrum not only in terms of level statistics but also in terms of the scaling of the inverse participation ratios. We also use the properties of the entanglement spectrum to illustrate the nature of the symplectic metal phase which appears when inversion symmetry is broken.

¹MJG is supported by the AFOSR under grant FA9550-10-1-0459

²A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, *Phys. Rev. B* **55**, 195125 (2008).

³C. L. Kane and E. J. Mele, *Phys. Rev. Lett.* **95**, 146802 (2005).

1:27PM W30.00012 Experimental entanglement estimation for a general unknown input state of a multiqubit system, ELIZABETH BEHRMAN, Department of Mathematics and Physics, Wichita State University, JAMES STECK, Department of Aerospace Engineering, Wichita State University — Measurement of entanglement remains an important problem for quantum information. We present the design and simulation of an experimental method for entanglement estimation for a general, unknown, state of a multiqubit system. The state can be in pure or mixed, and it need not be “close” to any particular state. Our method, based on dynamic learning, does not require prior state reconstruction or lengthy optimization. Results for three-qubit systems compare favorably with known entanglement measures. The method is then extended to four- and five-qubit systems, with relative ease. As the size of the system grows the amount of training necessary diminishes, raising hopes for applicability to large computational systems.

1:39PM W30.00013 Entanglement Spectrum of the Kugel-Khomskii Model, REX LUNDGREN, VICTOR CHUA, GREGORY A. FIETE, Department of Physics, University of Texas at Austin — We study the entanglement spectrum of the Kugel-Khomskii model in one dimension. The Kugel-Khomskii Hamiltonian describes transition metal oxides with orbital degeneracy, and is rich with both gapless and gapped phases with interesting symmetries. The entanglement spectrum reveals much more information than the commonly studied entanglement entropy. In this work, we investigate the entanglement spectrum for different phases and different partitions. We also make comparisons with previous field theoretic and numerical studies.

1:51PM W30.00014 Entanglement Spectrum In Topological Phases¹, B. ANDREI BERNEVIG, Princeton University — I will review the information that entanglement spectra give for a wide range of systems in condensed matter physics, such as fractional quantum hall effect, quantum spin chains, topological insulators, and disordered systems. I will also show how the entanglement spectrum is a unique tool to examine previously unknown many-body wavefunctions such as the ground-states of Fractional Chern Insulators (the results are based on a series of works performed in collaboration with N. Regnault, M. Hermanns, B. Estienne, Yangle Wu, Aris Alexandradinata, R. Thomale, A. Sterdyniak, Z. Papić, T.L. Hughes, E. Prodan, D.P. Arovas, P. Bonderson)

¹NSF CAREER, ONR, DARPA, Packard

2:03PM W30.00015 Topological Order in Three Dimensions and Entanglement Entropy of Gapped Phases, TARUN GROVER, UC Berkeley, ARI TURNER, University of Amsterdam, ASHVIN VISHWANATH, UC Berkeley — In this talk, I will present two very general, yet easy to understand results in the entanglement entropy of the ground states corresponding to the gapped phases of matter. In particular, I will focus on the following two results: 1) In contrast to the familiar result in two dimensions, a size independent constant contribution to the entanglement entropy can appear for non-topological phases in any odd spatial dimension. 2) The “topological entanglement entropy” corresponding to discrete gauge theories in any given spatial dimension D (and in particular, $D = 3$) has an interesting dependence on the Betti numbers of the boundary manifold defined by the entanglement cut.

Thursday, March 1, 2012 11:15AM - 2:15PM –
Session W31 DMP: Focus Session: Topological Insulators: Synthesis & Characterization - Quantum Transport & Nanostructures 260

11:15AM W31.00001 Evidence for a Dirac Spectrum in the Topological Insulator $\text{Bi}_2\text{Te}_2\text{Se}$ from High-Field Shubnikov-de Haas Oscillations, JUN XIONG, Princeton University, YONGKANG LUO, Zhejiang University, YUEHAW KHOO, SHUANG JIA, ROBERT CAVA, NAI PHUAN ONG, Princeton University — The transport properties of surface states in the 3D topological insulators based on bismuth have been observed in a number of experiments. However, there is still no direct evidence for the Dirac dispersion predicted for these states. We have measured the Shubnikov-de Haas (SdH) oscillations in $\text{Bi}_2\text{Te}_2\text{Se}$ in intense dc fields. At $B > 40$ T, we can reach the $n=1$ surface Landau Level. In the index plot (of $1/B$ versus n), the relatively large oscillation amplitudes in our crystals (as large as 17% of the total conductance) enables us to resolve, in the high-field limit, the $\frac{1}{2}$ -shift predicted from the Berry phase in the Dirac spectrum. In addition, the linearity of the index plot shows that the surface Lande g-factor is quite small (less than 5) in $\text{Bi}_2\text{Te}_2\text{Se}$, in contrast with recent inferences based on low-B SdH experiments. Supported by NSF DMR 0819860

11:27AM W31.00002 Thin films of topological insulators in a parallel or tilted magnetic field, SERGEY PERSHOGUBA, VICTOR YAKOVENKO, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park, Maryland 20742-4111 — In thin films of topological insulators, the surface states on the opposite edges are coupled by a tunneling coupling t . We discuss the energy spectrum and the transport properties of the system in a magnetic field. When an electron tunnels between the edges, the Lorentz force due to the in-plane magnetic field $\mathbf{B} = (0, B_y, 0)$ changes the in-plane electron momentum by $\Delta p_x \propto B_y$. As a result, the Fermi circles on the opposite edges shift by Δp_x in the momentum space. We propose that this effect can be detected by measuring the tunneling conductance $\sigma_{zz}(B_y)$ between the edges of the system. We show that $\sigma_{zz}(B_y)$ has special signatures due to the helical spin configuration of the surface Dirac cones. In case of a tilted field $\mathbf{B} = (0, B_y, B_z)$, the perpendicular component B_z quantizes the in-plane motion to the Landau levels, while the in-plane component B_y spatially shifts the wave functions on the different edges. As the overlap between the wave functions changes, the tunneling amplitude t is renormalized and acquires dependence on both B_y and B_z . This effect can be observed as the dependence of the interlayer conductance and in-plane conductivity on the tilt angle θ of the magnetic field $\tan\theta = B_y/B_z$.

11:39AM W31.00003 Clear Revelation of Topological Surface States in Bi_2Se_3 Thin Films by *in situ* Al Passivation, MURONG LANG, LIANG HE, XINXIN YU, JIANSHI TANG, XUFENG KOU, KANG L. WANG, UCLA Electrical Engineering, ALEXEI V. FEDOROV, Lawrence Berkeley National Laboratory — We report that *in situ* aluminum (Al) passivation of Bi_2Se_3 can inhibit the degradation process and clearly reveal the massless, Dirac-like topological surface states. In this work, an 8 quintuple layers Bi_2Se_3 film was passivated with 2 nm Al, immediately after the MBE growth, which prevents native oxide (BiO_x) formation, isolates the film from ambient n -type doping or contaminations in the subsequent fabrication process. Dual evidences from both Shubnikov-de Haas (SdH) oscillations and weak antilocalization (WAL) effect, originated from the π Berry phase of the nontrivial surface states, were clearly revealed in the sample with *in situ* Al passivation. In contrast, we show that the two dimensional carrier density was increased 39.2% for the un-passivated control samples. Also, the SdH oscillations were completely absent and a large deviation from the WAL was observed

11:51AM W31.00004 High Field Magnetoresistance in ultra pure Bi_2Se_3 , PAUL SYERS, University of Maryland, NICHOLAS BUTCH, Lawrence Livermore National Laboratory, CYRIL PROUST, BAPTISTE VIGNOLLE, LNCMI-Toulouse, JOHNPIERRE PAGLIONE, University of Maryland — The longitudinal and transverse components of magnetoresistance were measured in bulk crystals of undoped, high purity Bismuth Selenide in pulsed magnetic fields of up to 60 Tesla. Data is presented from samples with a range of carrier concentrations extending into the quantum limit. Measurements were also performed at multiple angles along the plane containing the current direction to investigate the angular dependence of the linear behavior of the magnetoresistance in this material.

12:03PM W31.00005 Surface-dominated conduction in a 6nm-thick Bi_2Se_3 thin, LIANG HE, XINXIN YU, XUFENG KOU, MURONG LANG, KANG L. WANG, UCLA Electrical Engineering, FAXIAN XIU, Iowa State University, Department of Electrical and Computer Engineering, MARCUS TEAGUE, NAI-CHANG YEH, CalTech, department of Physics — We report a direct observation of surface dominated conduction in an intrinsic Bi_2Se_3 thin film with a thickness of 6 quintuple layers (QLs) grown on lattice-matched CdS (0001) substrates by molecular beam epitaxy (MBE). Shubnikov-de Haas (SdH) oscillations from the topological surface states suggest that the Fermi level falls inside the bulk band gap and is 53 $\pm$ 5 meV above the Dirac point, in agreement with 70 $\pm$ 20 meV obtained from scanning tunneling spectroscopies (STS). Our results demonstrate a great potential of producing genuine topological insulator devices using Dirac Fermions of the surface states.

12:15PM W31.00006 Magnetoconductance in high-mobility topological insulator Bi_2Se_3 devices, HADAR STEINBERG, VALLA FATEMI, JAVIER SANCHEZ-YAMAGISHI, LUCAS ORONA, PABLO JARILLO-HERRERO, MIT — We report the fabrication and measurement of gate-tunable high mobility exfoliated ($<100\text{nm}$ thick) Bi_2Se_3 devices. We measure electronic transport of these devices in magnetic fields up to 35T, and find a complex pattern of quantum oscillations consistent with both the surface and the bulk channels. We study the dependence of the oscillations on the magnetic field angle and gate voltage and discuss models for coexistence of surface and bulk oscillations.

12:27PM W31.00007 Magnetic Field Signatures of Topological States in 3D Time-Reversal Invariant Insulators, BRIAN DELLABETTA, Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, TAYLOR HUGHES, Department of Physics, University of Illinois at Urbana-Champaign, BENJAMIN LEV, Department of Applied Physics, Stanford University, MATTHEW GILBERT, Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign — While the topological behavior of Bi_2Se_3 has been identified experimentally^{1, 2}, characterization by electron transport has been difficult due to high bulk transport caused by inadvertent doping of the crystal.³ We perform self-consistent quantum transport calculations to show that patterned surfaces offer a unique environment in which the system may be characterized by resultant magnetic field distributions. We compare doped and undoped Bi_2Se_3 samples with normal metals to show a qualitative difference in current flow around the patterned surface. We find that the surface to bulk conductance ratio can be inferred from the magnetic field in patterned systems due to the spatial separation of bulk and surface currents created by the corrugation, which applies even in heavily doped systems. The magnetic field is sufficiently large so as to be observed using ultracold atom microscopy.

¹Y.L. Chen et al., *Science* **325**, 178 (2009).

²P. Roushan et al., *Nature* **460**, 7259 (2010).

³N. P. Butch et al., *Phys. Rev. B*, **81**, 24 (2010).

12:39PM W31.00008 Quantum Hall effect from Dirac fermions of the 3D topological insulator HgTe , A.V. STIER, R. VALDÉS AGUILAR, S. HUANG, T. MCQUEEN, N.P. ARMITAGE, Department of Physics & Astronomy, Johns Hopkins University, Baltimore, MD 21218, B. UELAND, F. RONNING, Los Alamos National Laboratory, Los Alamos NM 87545 — Three dimensional (3D) topological insulators (TI) exhibit two dimensional (2D) topologically protected conducting surface states created by strong spin-orbit coupling. Time reversal invariance (TRI) of those states manifest itself in spin-momentum locking and a dispersion relation of massless Dirac fermions. We present our results of magneto-transport of the 3D TI HgTe [1]. Our samples are 70 nm HgTe films strained on slightly Zn doped CdTe substrates. Tensile strain due to the lattice mismatch between the HgTe film and the substrate lifts the heavy hole - light hole degeneracy, which results in TI states at the Brillouin zone center. We observe evidence for a quantized Hall (QH) resistance developing at temperatures below $T=50\text{K}$. The observed effect is confirmed to derive from Dirac fermions of the two TI surfaces as shown through a non-zero Berry's phase by an extrapolation of the filling factors of the QH plateaus to the large magnetic field limit. We have also confirmed the 2D character of the probed states through tilted magnetic field measurements. If time allows, we will discuss our results for very high magnetic fields and dilution refrigeration temperatures experiments. Work supported by the Gordon and Betty Moore Foundation. [1] C. Brüne et.al., PRL 106, 126803 (2011)

12:51PM W31.00009 Topological insulator Bi_2Te_3 nanowire field effect devices, LUIS A. JAUREGUI, GENQIANG ZHANG, YUE WU, YONG P. CHEN, Purdue University — Bismuth telluride (Bi_2Te_3) has been studied extensively as one of the best thermoelectric materials and recently shown to be a prototype topological insulator with nontrivial conducting surface states. We have grown Bi_2Te_3 nanowires by a two-step solution phase reaction and characterized their material and structural properties by XRD, TEM, XPS and EDS. We fabricate both backgated (on SiO_2/Si) and top-gated (with ALD high-k gate dielectric such as Al_2O_3 or HfO_2) field effect devices on such nanowires with diameters $\sim 50\text{nm}$. Ambipolar field effect and a resistance modulation of up to 600% at low temperatures have been observed. The 4-terminal resistance shows insulating behavior (increasing with decreasing temperature) from 300 K to 50K, then saturates in a plateau for temperatures below 50K, consistent with the presence of metallic surface state. Aharonov-Bohm (AB) oscillations are observed in the magneto-resistance with a magnetic field parallel to the nanowire, providing further evidence of the presence of surface state conduction. Finally, a prominent weak anti-localization (WAL) feature that weakens with increasing magnetic field and/or temperature is observed in the magneto-resistance with a magnetic field perpendicular to the nanowire.

1:03PM W31.00010 Analysis of quantum interference in mesoscopic channels of epitaxial Bi_2Se_3 , ABHINAV KANDALA, DUMING ZHANG, ANTHONY RICHARDELLA, NITIN SAMARTH, Penn State University, University Park PA 16802 — Predictions of topologically protected surface states lead to expectations of longer scattering lengths from the surface channel in candidate topological insulators such as Bi_2Se_3 . In this context, we probe coherent transport in mesoscopic channels of MBE-grown Bi_2Se_3 at temperatures down to 0.5K and magnetic fields up to 6T. The magnetoresistance reveals two types of quantum corrections superimposed upon a classical background: low-field weak antilocalization and an aperiodic, reproducible fingerprint. Analysis and comparison of the quantum corrections data are used to extract important length scales and provide insights into the origin of these corrections. The channel length and temperature dependence of the magnetofingerprint is consistent with the theory of universal conductance fluctuations for diffusive systems that are two dimensional in phase coherent phenomena. Periodic oscillations in the autocorrelation of the fingerprint, persistent to high fields and high temperatures, point towards the presence of dominant scattering centers. Work supported by NSF-MRSEC and ONR.

1:15PM W31.00011 Synthesis and Transport Measurements of Catalyst-Free Topological Insulator Bi_2Se_3 Nanostructures, JEROME T. MLACK, ATIKUR RAHMAN, GARY L. JOHNS, NINA MARKOVIC, Johns Hopkins University — The semiconductor bismuth selenide (Bi_2Se_3) was predicted to be a topological insulator (TI) with a single Dirac cone, which was observed using Angle-Resolved-Photo-Emission-Spectroscopy in 2008. TI's are materials which exhibit electrically insulating properties in the bulk, but they have metallic surface states. The surface states are topologically protected from perturbations, defects, and impurities. Nano-sized structures might be well suited for the study of surface states because the surface effects are likely to dominate over bulk properties due to the high surface-to-volume ratio. So far, nanowires and nanoribbons of TI's have been synthesized using metal catalysts, such as gold, iron, or nickel. However, it has been found that these catalysts dope the nanostructures, which has the potential to modify their properties. We show catalyst-free growth of nanowires and nanoribbons of Bi_2Se_3 using the Vapor-Liquid-Solid method. Analysis by EDAX and TEM imaging suggest high purity samples. We have fabricated devices from these nanostructures and present electron transport measurements.

1:27PM W31.00012 Topological Insulator Nanoribbon Synthesis by Metal-Organic Chemical Vapor Deposition¹, LOREN ALEGRIA, MICHAEL SCHROER, GERALD POIRIER, MICHAEL PRETKO, ANASUA CHATTERJEE, Princeton University, SHIVANG PATEL, None, JASON PETTA, Princeton University — We report a method for metal-organic chemical vapor deposition (MOCVD) synthesis of Bi_2Se_3 topological insulator nanoribbons. We use gold nanoparticles to catalyze nanoribbon growth on silicon substrates. Trimethyl Bismuth and Diethyl Selenium are used as the metal-organic precursors. The growth parameters can be varied to control the morphology from narrow nanoribbons to wide platelets. Resulting nanostructures are characterized by electron diffraction, energy dispersive X-ray spectroscopy, and low-temperature transport measurements. We also investigate the synthesis of ternary compounds using this growth method.

¹Funded by the Sloan and Packard Foundations, and the NSF supported Princeton Center for Complex Materials.

1:39PM W31.00013 Electrical, Thermal, and Thermoelectric Characterizations of Vapor Solid Bi₂Te₃ Nanoplates, MICHAEL PETTES, LI SHI, The University of Texas at Austin — Single-crystal nanoplates of Bi₂Te₃ synthesized by the vapor solid method are characterized by electrical, thermal, and thermoelectrical measurements. The Bi₂Te₃ domains investigated are less than 12 nm thick and are suspended to remove substrate doping effects. A room temperature thermal conductivity of 1.5 Wm⁻¹K⁻¹ was measured, lower than the 1.8–3.3 Wm⁻¹K⁻¹ range reported for bulk crystals with different carrier types and concentrations. The room temperature electrical conductivity was measured at 1.5×10⁵ Sm⁻¹. Applying the Wiedemann-Franz Law, the electron contribution to the total thermal conductivity is nearly 40 % at room temperature. The electrical conductivity is similar to that reported for bulk single crystals at an electron concentration of 3.5×10¹⁹ cm⁻³. However, the room-temperature Seebeck coefficient of -66 μVK⁻¹ indicates *n*-type doping and is lower than that reported for *n*-type Bi₂Te₃ single crystals at an electron concentration as high as 14.6×10¹⁹ cm⁻³. Consequently, the figure of merit is only 0.11 at room temperature, a factor of 7.9 lower than the highest ZT reported for *n*-type single crystals at the optimized doping level.

1:51PM W31.00014 Hybrid Bismuth Selenide Nanostructures Synthesized by Chemical Vapor Deposition, EUGEN PANAITESCU, FANGZE LIU, SWASTIK KAR, LATIKA MENON, Physics Department, Northeastern University — The recent demonstration of theoretically predicted topologically ordered states in real bismuth based chemical compounds such as bismuth antimony, bismuth selenide, bismuth telluride etc opened the field of topological insulators (materials exhibiting insulator properties in bulk, but metallic behavior on the surface) for a plethora of possible applications. Topological insulator nanostructures in particular are of great interest due to their large surface to volume ratio. We will report on the CVD synthesis of various hybrid 1D and 2D nanostructures of the bismuth-selenium complex, and their morphological and structural properties (investigated by SEM and TEM imaging coupled with EDAX and XRD spectroscopy). Optical and transport properties will be also presented and related to possible spintronics and no dissipation electronics applications.

2:03PM W31.00015 Electronic transport of Sb-doped Bi₂Se₃ topological insulator nanoribbons, SEUNG SAE HONG, JUDY CHA, DESHENG KONG, YI CUI, Stanford University — Vapor-liquid-solid (VLS) grown nanoribbons, having large surface / volume ratio and high crystal quality, provide a unique opportunity to study topological insulator materials by electronic transport. However, clear observation of the surface states is often hindered due to materials' imperfections. Bulk impurities and environmental doping effects are known to contribute to dominant background transport signal, so that appropriate doping and surface protection are necessary to reduce the excess carriers. We report that Antimony (Sb), known to be an effective compensational dopant for bulk crystals, can be incorporated into Bi₂Se₃ nanoribbons and it reduces the bulk electron contribution significantly. With a Zinc Oxide protective layer, the carrier density of thin ribbons reaches below 10¹²cm⁻². This talk will include magnetotransport studies and temperature dependant transport of nanoribbons as well.

Thursday, March 1, 2012 11:15AM - 2:15PM –

Session W32 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides - Bandgaps, Surfaces, Oxides on Semiconductors 261

11:15AM W32.00001 Band Gap and Edge Engineering of SrTiO₃ and Related Compounds via Ferroic Distortion and Anisotropic Strain, ROBERT BERGER, The Molecular Foundry, Lawrence Berkeley National Laboratory — Due to its electronic band edge energies and its stability in water, the perovskite strontium titanate (SrTiO₃) is a promising water splitting photocatalyst. However, its ability to use solar photons to split water into hydrogen and oxygen would be more efficient if its wide optical band gap (3.2 eV) better matched the solar spectrum. Therefore, there is interest in modifying the crystal structure of SrTiO₃ (e.g., via chemical doping or epitaxial strain) to tune its electronic and optical properties. We use density functional theory (DFT) and many-body perturbation theory within the GW approximation to calculate the effects of structural and chemical modifications of SrTiO₃ on its band gap and edges. Much of our work (Berger, Fennie, and Neaton, Phys. Rev. Lett. 107, 146804 [2011]) focuses on the effects of epitaxial strain and the associated ferroic distortions. Anisotropic strains are shown to reduce the SrTiO₃ gap by breaking degeneracies at the band edges. Ferroic distortions are shown to widen the gap by allowing new band edge orbital mixings. To reduce the SrTiO₃ gap, one must lower the symmetry from cubic while suppressing ferroic distortions. Our calculations indicate that for engineered orientation of the growth direction along [111], the SrTiO₃ gap can be controllably and considerably reduced at room temperature. Chemical doping and substitution can, in combination with strain and distortion, further tune the band gap and edges. Our results and their favorable qualitative agreement with experiment suggest achievable paths toward engineering efficient solar water splitting catalysts, and more generally provide fundamental insight into the relationships between crystal and electronic structure in the property-rich perovskite family.

11:51AM W32.00002 Epitaxial strain tuning of polarization and band gap in perovskite SnTiO₃¹, WILLIAM PARKER, SERGE NAKHMANSON, Argonne National Laboratory, JAMES RONDINELLI, Drexel University — Lead toxicity has motivated theoretical studies of a tin-based perovskite ferroelectric material. Density-functional calculations predict a polar perovskite ground state for SnTiO₃. Simulated epitaxial strain up to ±2% tunes both the magnitude of the polar distortion, its direction, and the electronic band gap — compressive bi-axial strain creates the largest polar distortions, which occur entirely in the growth direction, while tensile strain reorients the polar displacements, enlarging the band gap. Projected densities of states indicate that the broken four-fold symmetry of the non-growth-oriented distortion allows Ti *d_{xy}* bands to mix with O *p_x* bands, further separating the valence band maximum and conduction band minimum. Comparing Sn and Pb in the perovskite titanate phases shows similar trends and suggests that SnTiO₃ ferroelectrics may be viable thin-film alternatives to Pb-based oxides.

¹The U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences and American Recovery and Reinvestment Act through the Office of Advanced Scientific Computing Research under contract no. DE-AC02-06CH11357 funded this work.

12:03PM W32.00003 Ferroelectric Properties of TiO₂ Rutile Bulk and Surfaces Investigated by Ab Initio Calculations¹, ANNA GRÜNEBOHM, PETER ENTEL, Department of Physics, University Duisburg-Essen and CeNIDE, CLAUDE EDERER, School of Physics, Trinity College, Dublin — TiO₂ rutile is an incipient ferroelectric material [Lee et al., Phys. Rev. B **50**, 13379 (1994)] and theoretical studies have shown that a ferroelectric transition can be enforced [Montanari et al., J. Phys. Condens. Matter **16**, 273 (2004)]. The experimental realization of ferroelectric TiO₂ (110) surfaces would have great technical impact and already the tuning of the electric permittivity would be of interest, e.g., for optical coating. In order to get an insight into the ferroelectric trends, we have studied the atomic and electronic structure, as well as phonon spectra, dipolar interactions and the polarization, using density functional theory (VASP and PWscf). Accordingly, ferroelectric states polarized along (110) and (001) can be stabilized within bulk. We demonstrate the different strain dependencies of the corresponding polar modes, which opens up the possibility of strain engineering the polarization direction, and the resulting dielectric response [Grünebohm et al., Phys. Rev. B **84**, 132105 (2011) and Grünebohm et al. arxiv:1111.2575]. Although the dipolar interaction and the short range repulsion are both modified at the (110) surface, stable local dipoles are obtained within the surface planes, which increase with increasing strain.

¹Computational time was granted by the Jülich Supercomputing Center (JSC) and the Center for Computational Sciences and Simulation (CCSS) of the University of Duisburg-Essen

12:15PM W32.00004 XPS measurements of interface dipole switching at the a-Al₂O₃/Si interface, STEPHANIE FERNANDEZ-PENA, Geneva University, D.P. KUMAR, Yale University, Z. ZHANG, Argonne National Laboratory, A.M. KOLPAK, MIT, S. ISMAIL-BEIGI, C.H. AHN, F.J. WALKER, Yale University — In this work, we describe work on polarization switching at a high-*k* oxide-silicon interface. The procedure involves inserting a monolayer (ML) of ZrO₂ in-between an amorphous-Al₂O₃ and Si. Theoretical calculations using density functional theory (DFT) predict that the ZrO₂ should display two stable configurations of the polarization. Deposition of the ZrO₂ in UHV is used to avoid SiO₂ formation. The device is transferred in vacuum and the interface chemistry analyzed using x-ray photoelectron spectroscopy (XPS) to determine the oxidation state of the Si. When the ZrO₂ is in direct contact with the Si, chemical shifts as large as 0.58 [eV] are observed, implying a polar interface. In addition, XPS measurements on devices under applied voltage, along with electron transport measurements, show a switching of the interface dipole of 0.25 [eV]. These voltage dependent XPS results are consistent with the magnitude and direction of hysteresis loops observed in Capacitance-Voltage measurements. Finally, the microscopic structure has been investigated using extended x-ray absorption fine structure (EXAFS) at the Zr K-edge. The results are compared to DFT-calculated atomic positions.

12:27PM W32.00005 Macroscopic electrostatics at the nanoscale: From ferroelectric capacitors to confined electron gases, MASSIMILIANO STENGEL, ICREA - Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona — Complex oxides are characterized by a multitude of coupled electronic and lattice degrees of freedom, and therefore constitute an unusually rich playground for experimentalists and theoreticians alike. These microscopic variables manifest themselves in macroscopically measurable quantities such as polarization, magnetization and strain, whose mutual coupling is sought after for applications in multifunctional electronic devices. To understand the interplay of these many factors, density functional theory (DFT) has proven an invaluable tool. However, the treatment of the macroscopic electrical variables (electric fields and polarization), which are a crucial ingredient in describing the experimentally observed response properties, has traditionally been difficult within first-principles calculations. In this talk I will first review a number of recent methodological developments that removed this limitation, thus extending the scopes of first-principles theory to the simulation of realistic devices within arbitrary electrical boundary conditions. Next, I will discuss the evolution of the band offset at a metal/ferroelectric interface as a function of polarization, and its implications for the electrical properties of nanocapacitors. Finally, I will show that, depending on the polarization of the film, a problematic regime might occur where the metallic carriers populate the energy bands of the insulator, making it metallic. As the most common approximations of density functional theory are affected by a systematic underestimation of the fundamental band gap of insulators, this scenario is likely to be an artifact of the simulation. I will discuss a number of criteria to systematically identify this situation in simulations, and effective modeling strategies to describe this peculiar charge compensation mechanism.

1:03PM W32.00006 Band Alignment of Plasma-Enhanced ALD High-*k* Dielectrics on Gallium Nitride, JIALING YANG, BRIANNA ELLER, CHIYU ZHU, ROBERT NEMANICH, Arizona State University — GaN-based transistors have shown immense promise because of their high saturation velocity and breakdown field, but their performance is limited by the high gate leakage. This limitation is mitigated with the use of metal/high-*k* oxide/III-N structures. This experiment investigates three promising high-*k* dielectrics deposited by plasma enhanced ALD: Al₂O₃, HfO₂, and La₂O₃. The band gaps of these materials are 6.5eV, 5.8eV, and 4.3eV, while the dielectric constants are 9, 20, and 27, respectively. The large band gap associated with Al₂O₃ reduces the leakage current; however, the lower dielectric constant increases the equivalent oxide thickness. The band alignment of the high-*k* oxide/GaN interface plays a critical role in determining the confinement properties of semiconductor carriers and ultimately device performance. In situ photoemission gave valence band offsets for Al₂O₃, HfO₂, and La₂O₃ with GaN as 1.8eV, 1.3eV, and 0.9eV. The results are described by the charge neutrality level and interface dipole models. We also investigated the use of Al₂O₃ as an interfacial passivation layer between HfO₂ and GaN. This research is supported by the Office of Naval Research.

1:15PM W32.00007 High-*k* dielectrics on n-Al_{0.25}Ga_{0.75}N via atomic layer deposition, N. NEPAL, N.Y. GARCES, D. MEYER, T.J. ANDERSON, J.K. HITE, M.A. MASTRO, C.R. EDDY, JR., U.S. Naval Research Laboratory, Washington, DC 20375, USA — AlGaIn/GaN and AlInN/GaN high-electron-mobility transistors (HEMTs) are promising devices for high-temperature and high-power electronics applications. A key issue with these devices is the high gate leakage current, particularly for enhancement-mode HEMTs. There has been an increased interest in developing high quality gate insulators to reduce gate leakage current. Al₂O₃ and HfO₂ layers (21nm thick) were deposited via atomic layer deposition on n-Al_{0.25}Ga_{0.75}N pretreated with one of two different surface preparations, H₂O₂:H₂SO₄ (1:5) (piranha) or HF:H₂O (1:3). Dielectrics were characterized using spectroscopic ellipsometry, X-ray photoelectron spectroscopy, atomic force microscopy (AFM), and capacitance-voltage (C-V) measurements. AFM shows that Al₂O₃ and HfO₂ layers are continuous and uniform in thickness on both HF and piranha pretreated surfaces. However, C-V measurement shows smaller (15%) hysteresis for HF pretreated samples. The estimated dielectric constants (ϵ) are 9 and 18 for Al₂O₃ and HfO₂ on HF pretreated surfaces, respectively, in general agreement with theoretical values of 9 and 25. Al₂O₃ layers on Al_{0.25}Ga_{0.75}N exhibited a lower leakage (7×10^{-8} A/cm² at 5 V) current and higher forward breakdown voltage of 7.5 MV/cm compared to that of HfO₂ layer. The higher breakdown voltage and lower leakage current for Al₂O₃ is due to larger conduction band offset with Al_{0.25}Ga_{0.75}N.

1:27PM W32.00008 The growth of c-axis oriented BaTiO₃ films on Si and Ge for a non-volatile field-effect transistor¹, J.H. NGAI, D. KUMAR, M. MARSHALL, Y. SEGAL, C.H. AHN, F.J. WALKER, Dept. of Applied Physics, Yale University — The reorientable polarization of a ferroelectric material can be utilized in a variety of applications, including the development of novel memory devices. Of particular interest is the use of a ferroelectric's spontaneous polarization to maintain "on" and "off" conductivity states in a field effect transistor. BaTiO₃ has been proposed as a Pb-free ferroelectric for such an application. Direct coupling of the ferroelectric polarization with the channel of a field effect transistor requires c-axis oriented BaTiO₃ films to be grown on Si or Ge. However, due to the small thermal expansion coefficients of Si and Ge, BaTiO₃ films tend to be a-axis oriented, having the polarization lying in the plane of the film. In order to achieve c-axis oriented BaTiO₃ films, we have developed a graded buffer layer that imparts in-plane compressive strain to overcome the incompatibility in thermal expansion. Ferroelectric, c-axis oriented, BaTiO₃ films with thicknesses exceeding 120 nm have been achieved. We will discuss the growth and characterization of these films in the development of a non-volatile, ferroelectric transistor.

¹This work was supported by the National Science Foundation under Contract No. MRSEC DMR 0520495

1:39PM W32.00009 First principles analysis of the capacitance density of high-k nanocapacitors utilizing the orbital separation approach, SHUSUKE KASAMATSU, Department of Materials Engineering, the University of Tokyo, SEUNGWU HAN, Department of Materials Science and Engineering, Seoul National University, SATOSHI WATANABE, Department of Materials Engineering, the University of Tokyo — In order to realize further scaling of electronic devices, capacitors and transistors with higher capacitance density are necessary. To this end, higher-k films of nanometer thickness are being considered for next-generation devices. However, high-k/metal interfaces often suffer from degraded dielectric properties due to, e.g., contamination, defects, and the intrinsic dead layer effect [1]. In this work, we developed a new first principles approach based on the Kohn-Sham formalism that we call orbital separation approach [2] to calculate the capacitance of nano-sized capacitors and examine the limit in capacitance density. In this method, the Kohn-Sham orbitals around the Fermi level of a metal/insulator/metal slab are separated into left and right electrode. The separated orbitals are occupied according to different Fermi levels to simulate the effect of bias voltage. We applied this approach to Au/MgO/Au and SrRuO₃/SrTiO₃/SrRuO₃ systems to examine the effect of the interface on the dielectric response. We confirmed that this method gives reasonable results. The impact of the intrinsic dead layer and that of defects on the capacitance are also examined.

[1] M. Stengel and N. Spaldin, *Nature* 443, 679 (2006).

[2] S. Kasamatsu et al., *Phys. Rev. B* 84, 085120 (2011).

1:51PM W32.00010 Properties of Ultrathin Al₂O₃-TiO₂ Nanolaminate Films for Gate Dielectric Applications Deposited by Plasma-Assisted Atomic Layer Deposition, NELSON GARCES, DAVID MEYER, NEERAJ NEPAL, VIRGINIA WHEELER, CHARLES EDDY, U.S. Naval Research Laboratory — High permittivity dielectrics such as Al₂O₃, HfO₂, Ta₂O₅, TiO₂, etc., are an essential component of aggressively-scaled III-V and graphene field effect transistors (FETs) where insulators are necessary to reduce gate leakage current while maintaining high gate capacitance and charge control of the channel. Atomic layer deposition (ALD) has the capability to deposit hybrid films, or nanolaminates, of two or more dielectrics that have unique properties. Thin [Al₂O₃+TiO₂] nanolaminates with varying TiO₂ and Al₂O₃ content were deposited on *n*-Si substrates at ~225-300 °C using ALD. A nanolaminate is composed of bilayers, defined as the sum of (x)Al₂O₃ and (y)TiO₂, where x, and y indicate the number of times a component monolayer is repeated. While the overall thickness of the dielectric was held at ~ 17-20 nm, the relative ratio of Al₂O₃ to TiO₂ in the bilayer stack was varied to evaluate changes in the material properties and electrical performance of the oxides. C-V and I-V measurements on various [(x)TiO₂+(y)Al₂O₃] MOS capacitors were taken. The high-TiO₂-content films show limited evidence of oxide charge trapping and relatively large dielectric constants ($\kappa \sim 15$), whereas the high-Al₂O₃-content films offer a larger optical bandgap and improved suppression of leakage current. We will discuss the properties of very thin nanolaminates and their possible use as gate oxides. Morphological, electrical, and XPS composition assessments will be presented.

2:03PM W32.00011 Ferroelectric Surface Chemistry: First-principle study of NO_x Decomposition¹, ARVIN KAKEKHANI, SOHRAB ISMAIL-BEIGI, Yale University, SOHRAB ISMAIL-BEIGI'S TEAM — NO_x molecules are critical and regulated air pollutants produced during automotive combustion. As part of a long-term effort to design viable catalysts for NO_x decomposition that operate at higher temperatures and thus would allow for greater fuel efficiency, we are studying NO_x chemistry on ferroelectric perovskite surfaces. Changing the direction of the ferroelectric polarization can modify surface properties and thus can lead to switchable surface chemistry. We will discuss our results for NO and NO₂ on the polar (001) surfaces of PbTiO₃ as function of ferroelectric polarization, surface stoichiometry, and various molecular or dissociated binding modes.

¹Primary support from Toyota Motor Engineering and Manufacturing, North America, Inc.

Thursday, March 1, 2012 11:15AM - 2:15PM –
Session W33 GERA: Physics of Hydrogen Production, Storage, Delivery 106

11:15AM W33.00001 Boron Doping Carbon Structures Using Decaborane? A Theoretical Study¹, CARLOS WEXLER, MATTHEW CONNOLLY, MATTHEW BECKNER, PETER PFEIFER, University of Missouri Physics Department, ALLIANCE FOR COLLABORATIVE RESEARCH IN ALTERNATIVE FUEL TECHNOLOGY COLLABORATION — Boron-doped carbon materials have been shown to improve hydrogen storage. Boron-doped activated carbons have been produced using a novel process involving the pyrolysis of a boron containing compound and subsequent high-temperature annealing. A model for the boron doping process based on a Langmuir isotherm is presented. A theoretical study of the interaction of the boron containing compound with the undoped carbon precursor will be presented. Ab-initio calculations of the potential energy surface and the Langmuir isotherm parameters derived from them are also presented. The theoretical study outlines the unique capabilities and limits of this doping procedure.

¹This material is based on work supported by the US Department of Defense under Awards No. N00164-07-P-1306 and N00164-08-C-GS37 and the US Department of Energy under Awards No. DE-FG02-07ER46411 and DE-FG36-08GO18142.

11:27AM W33.00002 Mass Transport in the Dehydrogenation Reaction of B₂₀H₁₆, KYLE MICHEL, CHRISTOPHER WOLVERTON, Northwestern University — The compound B₂₀H₁₆ has been predicted to decompose directly into 20B and 8H₂ with favorable hydrogen release (6.9 wt. %) and equilibrium temperature ($T = 20$ °C at a pressure of 1 bar H₂) [W.Q. Sun, et. al. *Phys. Rev. B*, **83**, 064112, 2011]. The segregation of B and H during this reaction is investigated using density functional theory assuming that this process is mediated by the diffusion of native point defects in solid B₂₀H₁₆. Using the calculated formation energies under relevant chemical conditions, those defects that form in the largest concentrations, and thus those that facilitate mass segregation, are identified. These results are used to gain insight into the possible kinetic limitations of this hydrogen storage reaction.

11:39AM W33.00003 Theoretical prediction of intermediates in the decomposition of Mg(BH₄)₂, ERIC MAJZOUB, Center for Nanoscience, and Department of Physics and Astronomy, University of Missouri, YONGSHENG ZHANG, Materials Science and Engineering, Northwestern University, VIDVUDS OZOLINS, Materials Science and Engineering, University of California, Los Angeles, CHRISTOPHER WOLVERTON, Materials Science and Engineering, Northwestern University — We have studied the decomposition pathway of Mg-borohydride using density-functional theory (DFT) calculations of the free energy (including vibrational contributions) in conjunction with a Monte Carlo-based crystal structure prediction method, the prototype electrostatic ground state (PEGS) method. We find that a recently proposed Mg(B₃H₈)₂ intermediate [Chong, et al., *Chem. Commun.* **47**, 1330, (2011)] is energetically highly unfavorable with respect to decomposition into MgB₁₂H₁₂. We systematically search for low-energy structures of Mg-triboranes [Mg(B₃H₈)₂, MgB₃H₇, and Mg₃(B₃H₆)₂], closo-borane MgB_nH_n (n=6,7,8,9,10,11), and Mg(B₁₁H₁₄)₂ compounds using PEGS+DFT simulations. We find that only the reaction enthalpy to Mg₃(B₃H₆)₂ is close to the stable MgB₁₂H₁₂ pathway, and falls within the thermodynamic conditions for reversibility [e.g., $\Delta H = 20 \sim 50$ kJ/(mol H₂)]. Careful control over experimental conditions might allow for Mg₃(B₃H₆)₂ as a possible intermediate in the decomposition of Mg(BH₄)₂, and might allow Mg₃(B₃H₆)₂ to be rehydrided back to Mg(BH₄)₂ under modest H₂(*T, p*) conditions.

11:51AM W33.00004 Industrial Scale Measurements of Hydrogen Uptake and Delivery in KOH Activated Carbons¹, TYLER RASH, DAVE STALLA, MATT BECKNER, JIMMY ROMANOS, G. SUPPES, A TEKEEI, University of Missouri, P. BUCKLEY, P. DOYNOV, MRIGlobal, PETER PFEIFER, University of Missouri, ALL-CRAFT TEAM — The Alliance for Collaborative Research in Alternative Fuel Technologies (ALL-CRAFT) has been producing high surface area activated carbons. Here we will investigate the hydrogen adsorption characteristics of these activated carbons using a custom built 10 liter hydrogen adsorption apparatus filled with 4 kg of activated carbon. We will discuss problems and solutions specific to filling and delivering hydrogen from industrial scale systems. Results show that activated carbons can produce a significant but surmountable, amount of impedance to hydrogen flow. The 10 liter hydrogen storage system measures adsorption at temperatures between -78 Celsius and 100 Celsius and at pressures between zero and 100 bar. The 10 liter hydrogen adsorption uptakes are compared against results obtained with the Hiden Isochema HTP1 volumetric gas analyzer.

¹This material is based on work supported by the US Department of Energy under Award Number DE-FG36-08GO18142 and the US NAVY under Awards Number N00164-07-P-1306 and N00164-08-C-GS37.

12:03PM W33.00005 Reversible Storage of Hydrogen and Natural Gas in Nanospace-Engineered Activated Carbons¹, JIMMY ROMANOS, MATT BECKNER, TYLER RASH, PING YU, GALEN SUPPES, PETER PFEIFER, Department of Physics, University of Missouri — An overview is given of the development of advanced nanoporous carbons as storage materials for natural gas (methane) and molecular hydrogen in on-board fuel tanks for next-generation clean automobiles. High specific surface areas, porosities, and sub-nm/supra-nm pore volumes are quantitatively selected by controlling the degree of carbon consumption and metallic potassium intercalation into the carbon lattice during the activation process. Tunable bimodal pore-size distributions of sub-nm and supra-nm pores are established by subcritical nitrogen adsorption. Optimal pore structures for gravimetric and volumetric gas storage, respectively, are presented. Methane and hydrogen adsorption isotherms up to 250 bar on monolithic and powdered activated carbons are reported and validated, using several gravimetric and volumetric instruments. Current best gravimetric and volumetric storage capacities are: 256 g CH₄/kg carbon and 132 g CH₄/liter carbon at 293 K and 35 bar; 26, 44, and 107 g H₂/kg carbon at 303, 194, and 77 K respectively and 100 bar. Adsorbed film density, specific surface area, and binding energy are analyzed separately using the Clausius-Clapeyron equation, Langmuir model, and lattice gas models.

¹ This material is based upon work supported by the U.S. Department of Energy under Award No. DE-FG36-08GO18142 and the California Energy Commission under Contract No. 500-08-022.

12:15PM W33.00006 The Stationary States of Adsorbed Hydrogen, RAINA OLSEN, EERE Postdoctoral Fellow, Oak Ridge National Laboratory, HASKELL TAUB, CARLOS WEXLER, University of Missouri Columbia — In order to investigate the impact of quantum effects on hydrogen adsorption, it is important to understand the stationary states occupied by adsorbed hydrogen molecules. We present experimental inelastic neutron scattering spectra which provide evidence for significant mixing of degrees of freedom which are normally decoupled in free space. Results suggest that simultaneous treatment of translational and rotational degrees of freedom and consideration of the potential corrugation are necessary for improved theoretical understanding of the problem. Numerical calculations of the full five dimensional single body potential are used to understand the origins of the experimentally observed stationary states. In addition, we briefly discuss how our results may be used to understand the shape of hydrogen adsorption isotherms.

12:27PM W33.00007 Measured Enthalpies of Adsorption of Boron-Doped Activated Carbons¹, M. BECKNER, J. ROMANOS, E. DOHNKE, A. SINGH, J. SCHAEFERKOETTER, D. STALLA, J. BURRESS, S. JALISATGI, G. SUPPES, M.F. HAWTHORNE, P. YU, C. WEXLER, P. PFEIFER, University of Missouri — There is significant interest in the properties of boron-doped activated carbons for their potential to improve hydrogen storage.² Boron-doped activated carbons have been produced using a process involving the pyrolysis of decaborane (B₁₀H₁₄) and subsequent high-temperature annealing. In this talk, we will present a systematic study of the effect of different boron doping processes on the samples' structure, hydrogen sorption, and surface chemistry. Initial room temperature experiments show a 20% increase in the hydrogen excess adsorption per surface area compared to the undoped material. Experimental enthalpies of adsorption will be presented for comparison to theoretical predictions for boron-doped carbon materials. Additionally, results from a modified version of the doping process will be presented.

¹This material is based on work supported by the US Department of Energy under Award No. DE-FG36-08GO18142.

²Multiply Surface-Functionalized Nanoporous Carbon for Vehicular Hydrogen Storage, P. Pfeifer et al. DOE Hydrogen Program 2011 Annual Progress Report, IV.C.3, 444-449 (2011).

12:39PM W33.00008 Performance of Carbon Hydrogen Storage Materials as a Function of Post-Production Thermal Treatment¹, E. DOHNKE, J. ROMANOS, M. BECKNER, J.W. BURRESS, P. YU, P. PFEIFER, University of Missouri — High-surface-area activated carbons for hydrogen storage were investigated as a function of post-synthesis surface treatment. Thermal treatment of the initial carbon in high vacuum at temperatures 200-1000 °C leads to materials with significantly different surface chemistries and hydrogen storage capacities. Results from nitrogen pore-structure analyses, FT-IR spectroscopy before and after the treatment, and thermogravimetric analysis and mass spectroscopy of volatile reaction products during treatment, are reported. For treatment at 600 °C, excess hydrogen adsorption at 80 K and 303 K is found to be 20-30% higher than for the untreated sample. At temperatures below 450 °C, volatiles are mostly water and air; volatiles above 450 °C are mostly carbon dioxide and carbon monoxide. The results are interpreted as that high-temperature treatment produces materials with a large fraction of high-binding-energy sites.

¹This material is based on work supported by the US Department of Energy under Award No. DE-FG36-08GO18142.

12:51PM W33.00009 Size-scaling behavior of hydriding phase transformations in nanocrystals, LESTER HEDGES, RIZIA BARDHAN, Lawrence Berkeley National Laboratory, CARY PINT, ALI JAVEY, University of California, Berkeley, STEPHEN WHITELAM, JEFFREY URBAN, Lawrence Berkeley National Laboratory — By partnering data obtained from a novel in-situ luminescence-based probe with a statistical mechanical model we derive size-scaling laws for hydriding phase transformations relevant for hydrogen storage. We conclude that the observed experimental trends are consistent with thermally-driven nucleation, and derive scaling relations that reveal the fundamental size-dependence of nucleation barriers in nanocrystals for first-order phase transformations: near the critical point, the barrier to nucleation is controlled directly by the size of the nanocrystal. Consequently, phase transformation can occur in a nanocrystal even at the critical point, in stark contrast to the classical bulk scenario. Our results provide a detailed framework for understanding how nanoscale interfaces impact broad classes of thermally-driven solid-state phase transformations of relevance for hydrogen storage, catalysis, batteries, and fuel cells.

1:03PM W33.00010 Hydrogen affinity and structural stability of Mg-films on substrates¹, MINA YOON, Oak Ridge National Laboratory, Oak Ridge, MURAT OZER, HANNO WEITERING, University of Tennessee, Knoxville — Using first-principles density functional theory we investigated the binding mechanism of hydrogen to thin Mg films and alloyed films. In ultrathin Mg films the stability of hydrides is much lower than in the corresponding bulk systems and it can be modified by metal alloying. We calculated the chemical potential of hydrogen in Mg films for different dopant species and film thicknesses while including all vibrational degrees of freedom. By comparing the chemical potential with that of free hydrogen gas at finite temperature and pressure, we construct a hydrogenation phase diagram and identify the conditions for hydrogen absorption/desorption. Experimentally those films were synthesized on the Si substrate using MBE technique, where we observed the formation of both Mg and Mg silicides. We studied the competing mechanism of Mg/Mg₂Si formation and their structural stabilities on the substrate.

¹Supported by the US DOE, Office of Basic Energy Sciences, Materials Sciences and Engineering Division

1:15PM W33.00011 Hydrogen storage through spillover at sub-2nm Pt nanoparticle - support interfaces, SOMIK MUKHERJEE, BALAVINAYAGAM RAMALINGAM, SHUBHRA GANGOPADHYAY, University of Missouri — Hydrogen generation and storage are essential components in the increasingly important field of energy storage. Electrochemical generation of Hydrogen atoms at the surface of Pt like metals at select potentials is a widely studied phenomenon. However, moving these adsorbed Hydrogen atoms to high surface area support systems (primarily Carbon) for storage is an issue. We show spillover of these adsorbed Hydrogen atoms to the conducting transition-metal oxide support for sub-2 nm Pt nanoparticles sputtered on fluorine doped tin oxide (FTO) using cyclic voltammetry. The sub-2 nm Pt nanoparticles are deposited on oxide and carbon support systems using a unique tilted target sputtering (TTS) system developed by our lab. The resultant Pt nanoparticles are highly homogeneous, have high number density and are crystalline in nature. We propose integrating this sub-2 nm Pt nanoparticle-FTO system with different carbon structures to see if the spilled over hydrogen can be stored reversibly on adjacent carbon support systems and study the involved hydrogen spillover and storage mechanisms.

1:27PM W33.00012 Activated carbon monoliths for methane storage, NAGARAJU CHADA, JIMMY ROMANOS, RAMSEY HILTON, GALEN SUPPES, JACOB BURRESS, PETER PFEIFER, University of Missouri — The use of adsorbent storage media for natural gas (methane) vehicles allows for the use of non-cylindrical tanks due to the decreased pressure at which the natural gas is stored. The use of carbon powder as a storage material allows for a high mass of methane stored for mass of sample, but at the cost of the tank volume. Densified carbon monoliths, however, allow for the mass of methane for volume of tank to be optimized. In this work, different activated carbon monoliths have been produced using a polymeric binder, with various synthesis parameters. The methane storage was studied using a home-built, dosing-type instrument. A monolith with optimal parameters has been fabricated. The gravimetric excess adsorption for the optimized monolith was found to be 161 g methane for kg carbon.

1:39PM W33.00013 A DFT Study of Atomic Hydrogen and Oxygen Chemisorption on the γ -U Surface¹, DAYLA MORRISON, ASOK RAY, Physics Department, University of Texas at Arlington — Generalized gradient approximation to density functional theory has been used to compute O and H atomic adsorption properties on the (100) surface of γ -U. The computational method used is the all-electron full-potential linearized augmented plane wave plus local orbitals basis method as implemented in the WIEN2k code. The adatom was allowed to approach the five-layer slab surface at the top, center and bridge sites. The bridge site was found to be most stable with chemisorption energies of 8.43 and 3.76 eV for O and H, respectively, spin-orbit coupling (SOC) included. The optimized distances to the surface for the O atom was 1.98 Å at the top, 0.75 Å at center and 1.32 Å and at the bridge sites. For H, these distances were found to be 2.07, 0.57, and 1.40 Å at the corresponding sites, respectively. Inclusion of SOC has significant effects on the energies, changing the chemisorption energy by as much as 0.63 eV for O and 0.43 eV for H. Possible changes in work function, magnetic moment, and charge density distributions have been investigated and will be presented. We will also present results on interstitial sites, by incorporation of O and H atoms inside the slab. Different properties were observed for the O adatom as compared to the H atom.

¹This work is partially supported by a GAANN fellowship and a grant from the Welch foundation.

1:51PM W33.00014 Effect of Nitrogen Doping on the Electronic and Optical Properties of TaON, NABIL AL-AQTASH, FLORIN APOSTOL, RENAT SABIRIANOV, University of Nebraska at Omaha — TaON is considered as a potential candidate as a visible-light responsive photocatalyst. We report the results of ab initio studies of electronic structure of TaON in monoclinic and hypothetical cubic phases using VASP code. Specifically, we show that the position of conduction and valence band can be modified by varying the nitrogen (N) concentration in TaO_{1+x}N_{1-x}. The bandgap decreases monotonically with the increase of N concentration from near 2.7eV to just over 1.1eV (i.e. by 230%) when N concentration is reduced from x=0.5 to 1.5. The bandgap reduction is mostly associated with the change in the position of the valence band, while the conduction band is not sensitive to nitrogen content. We calculated the optical absorption spectra and discuss the effect of nitrogen doping on the photocatalytic activity of oxinitrides.

2:03PM W33.00015 Determination of crystal structure and the study of electronic properties of AgBiW₂O₈ by density functional theory¹, PRANAB SARKER, MUHAMMAD N. HUDA, Physics Department, University of Texas at Arlington, Texas 76019 — AgBiW₂O₈ shows promising features in solar energy to hydrogen conversion through photoelectrochemical (PEC) approach because of moderate band gap, stability in the liquid solution, suitable band edge positions and low production cost. However, there is not much study available to determine its crystal structure. Using mineral database of relevant oxides and density functional theory (DFT) total energy calculation, we have determined the crystal structures of AgBiW₂O₈ to be a wolframite structure, which contradicts a previous report. Our theoretical electronic structure and optical properties calculation agrees well with the recent experimental result.

¹This work is supported by NREL and NSF.

Thursday, March 1, 2012 11:15AM - 2:03PM —

Session W34 DCP: Focus Session: Nano V: Nanoscale Materials and Properties II 107A

11:15AM W34.00001 In Quest of a Systematic Framework for Unifying and Defining Nanoscience¹, DONALD TOMALIA, NanoSynthons LLC — A *central paradigm driven, Mendeleev-like nano-periodic system* has been cited as a critical missing link in the transformation of nanotechnology from an empirical to a highly predictive science. A systematic framework is proposed based on the same first principles underpinning “central paradigms” for chemistry/physics.² As such, a **Nanomaterials Classification Roadmap** considers *structure controlled* nanoparticles defined by **Critical Nanoscale Design Parameters (CNDPs)**; namely, **size, shape, surface chemistry, flexibility, architecture and elemental composition**. Classified as either **hard (H)** (inorganic) or **soft (S)** (organic) **nano-element categories**, these nanoparticles (e.g., nano-clusters) generally manifest pervasive **atom mimicry** features.³ Many literature examples demonstrate chemical bonding/assembly of these nano-element categories to produce extensive libraries of **hard-hard [H_n:H_n], soft-soft [S_n-S_n] or hard-soft [H_n-S_n]** nano-element combinations, referred to as **nano-compounds**. Due to their quantized CNDP features, these nano-element/compounds exhibit many well-defined **nano-periodic property patterns**. These property patterns are observed in their intrinsic physico-chemical properties (i.e., melting points, reactivity/self-assembly, sterics), as well as important functional/ performance properties (i.e., magnetic, photonic, and electronic behavior). The importance of these CNDP directed property patterns was recently demonstrated by publication of **first Mendeleev-like nano-periodic tables** by Percec, et al.⁴ Similarly, Mirkin, et al.⁵ recently reported six CNDP dependent nano-periodic rules for predicting hard-soft nano-element assemblies. These two independent reports appear to fulfill/validate this proposed nano-periodic concept. This lecture will overview this unifying **nano-periodic system** suitable for tuning optimal nanostructure/application properties, as well as predicting important risk/benefit/performance boundaries in the nanoscience field.

¹NSF

²D.A. Tomalia, *J. Nanopart. Res.* (2009), 11, 1251.

³S.N. Khanna, A.W. Castleman, et al., *PNAS* (2006), 103 (49), 18405.

⁴V. Percec, et al., *J. Am. Chem. Soc.* (2009), 131, 17500.

⁵C.A. Mirkin, et al., *Science* (2011), 334, 204.

11:51AM W34.00002 DFT-based Modeling of Field-Dependent Control and Response of Nano-magnetic Molecules¹, MARK PEDERSON, Chemical Sciences, Biosciences, and Geosciences Division, Office of Basic Energy Sciences, Department of Energy — Regardless of whether one is interested in characterizing, utilizing or controlling molecular-scale systems [1], one requisite to their understanding, design, and improvement is the ability to realistically model their response to electromagnetic fields. Since such responses are often collective their description requires an understanding of the interplay between bonding, spin, spin-orbit, vibrations, and electromagnetic fields. Inclusion of spin and magnetism influences the behaviors significantly. I provide an overview of a density-functional-based method (NRLMOL) for determining resonant tunneling of magnetization and Berry's phase oscillations in molecular magnets (primarily Mn₁₂-Acetate and derivatives) [2] and spin-electric effects in frustrated spin systems [Na₁₂Cu₃(AsW₉O₃₃)₂·3H₂O] [3]. The complexities related to spin- and magnetically dependent transport are compared to those of a nonmagnetic case [4]. Direct comparisons to experiments will be made. Challenges and recent progress associated with incorporating these effects into a realistic description of the frequency and amplitude dependent field driven response of many-electron/spin nanosystems will be discussed.

[1] MRP and SN Khanna, *PRB* **60** 9566 (1999).

[2] AV Postnikov, J. Kortus & MRP, *PSSB* **243** 2533 (2006).

[3] MF Islam, JF Nossa, CM Canali, & MRP, *PRB* **82** 15546 (2010).

[4] N.A. Zimbovskaya, MRP, AS Blum, BR Ratna and R. Allen, *JCP* **130** 094702 (2009).

¹Early parts of this work were supported in part by NRL, ONR, DOE and NSF. Views expressed in this work do not necessarily represent the priorities of any government agency.

12:27PM W34.00003 On the mechanism of enhanced photocatalytic activity of composite TiO₂/carbon nanofilms¹, DINKO CHAKAROV, RAJA SELLAPPAN, Department of Applied Physics, Chalmers University of Technology — We fabricated and analyzed well-defined model samples consisting of anatase and graphitic carbon films with and without modifying the interface between them by a thin SiO₂ space layer. The study was performed in the search for the origin of the enhanced photocatalytic activity of composite TiO₂-carbon systems observed previously by us, but also reported in number of publications. We found that the films with a TiO₂/C interface show noticeably lower photoluminescence intensity and shorter carrier life times compared to single TiO₂ films with the same thickness and composition. The stronger non-radiative recombination was mainly assigned to charge carrier leakage (transfer) at the interface between TiO₂ nanocrystallites and the carbon film.

¹The study is performed with financial support from N-INNER, project Solar Hydrogen (P30938-1).

12:39PM W34.00004 Light-sensitive gold nanoparticles designed for solar energy use, SUNGSOOK AHN, SUNG YONG JUNG, SEUNGGOON KIM, SANG JOON LEE, POSTECH, POSTECH TEAM — Light-sensitive organic ligands are incorporated with gold nanoparticles (AuNPs) to utilize solar energy. The physical properties of the ligand-AuNP systems are mainly modulated by the ligand/AuNP ratio. Hydrodynamic size measurement, laser Doppler electrophoresis and transmission electron microscopy are used for physical characterization. The interconnectivity of the AuNPs by dual-functional ligands also has a great impact on the physical properties. In addition, fs-THz spectroscopy is applied to evaluate electron activation of the designed AuNPs. Electron beams of different energy levels are applied to change the surface energy of AuNPs, which strongly affects the absorption energy band. This study contributes to the basic understanding on the nanoparticle technology for solar energy use.

12:51PM W34.00005 Factors controlling thermodynamic properties at the nanoscale: Ab initio study of Pt nanoparticles¹, GHAZAL SHAFI, MARISOL ALCANTARA ORTIGOZA, TALAT S. RAHMAN, University of Central Florida — We analyze via density-functional-theory calculations how factors such as size, shape, and hydrogen passivation influence the bond lengths, vibrational density of states (VDOS), and thermodynamic quantities of 0.8-1.7 nm diameter Pt nanoparticles (NPs), whose shape was previously characterized via extended X-ray absorption fine structure spectroscopy (EXAFS) [1]. For a given shape, unsupported NPs display increasingly broader bond-length distributions with decreasing size. Since the VDOS is remarkably non-Debye-like (even for the largest NPs), the VDOS and the thermal properties are not correlated as they are in the bulk. Generally, the fundamental vibrational frequency of a NP is associated with the shape and decreases with increasing size, as in macroscopic systems. Not surprisingly, we find that the frequency of this fundamental mode largely characterizes the thermal properties. We demonstrate that the qualitative difference between the atomic mean-square-displacement and the corresponding mean bond-projected bond-length fluctuations should be taken into account when interpreting the Debye-Waller factor of NPs measured by X-ray (or neutron) scattering or EXAFS. We find that in H-passivated Pt NPs, H desorption with increasing temperature explains the appearance of negative thermal expansion.

[1] B. Roldan Cuenya, et al. (2011), preprint available

¹Work supported in part by DOE-BES grant DE-FG02-07ER46354

1:03PM W34.00006 Nucleation in the Anatase-to-Rutile Transformation of Nanocrystalline Anatase¹, YA ZHOU, KRISTEN FICHTHORN, Penn State University — We use molecular dynamics (MD) simulations to investigate the anatase-to-rutile transformation of titania nanocrystals in vacuum. By comparing energies of various Wulff-shaped nanocrystals, we find that rutile becomes favored over anatase past a critical size that is significantly smaller than that predicted by thermodynamic models based on surface energies, indicating that edges play a profound role in the energetics of nanocrystals. We develop a local order parameter to distinguish anatase from rutile and intermediate anatase (112) twins at the resolution of a single TiO₂ unit and we apply it in direct MD simulations of spherical and Wulff-shaped anatase nanocrystals, as well as nanocrystal aggregates. To further characterize the transformation, we simulate X-ray diffraction of the nanoparticles. The anatase-to-rutile transformation originates at surfaces and interfaces, where alternating anatase (112) twin planes form. Rutile nuclei form via transformation of anatase (112) twins and they grow rapidly when they reach a critical size that can be as small as 10 TiO₂ units. Rutile nuclei tend to have planar structures bounded by (101) surfaces and the ease with which they form is dependent on the structure of the nanocrystal.

¹Supported by DOE DE-FG0207ER46414

1:15PM W34.00007 Local Ionic Environment around Polyvalent Nucleic-Acid Functionalized Gold Nanoparticles¹, MONICA OLVERA DE LA CRUZ, JOS ZWANIKKEN, Department of Materials Science and Engineering, Northwestern University, CHAD MIRKIN, Department of Chemistry, Northwestern University — Polyvalent oligonucleotide-functionalized gold nanoparticles (DNA-AuNPs) are remarkably stable in a cellular environment against degradation by nucleases, a property that was recently attributed to the local high concentration of mono- and divalent ions (Ref 1). In order to evaluate this hypothesis, we investigated the composition of the ion cloud around spherical nanoparticles that are functionalized by stiff, highly charged polyelectrolyte chains by means of classical density functional theory and molecular dynamics simulations. We developed a cell model that includes ligands explicitly and both applies over the entire relevant parameter space and is in excellent quantitative agreement with simulations (Ref 2). The ion distribution around the DNA-AuNPs as a function of DNA grafting densities and bulk ionic concentrations, as well as different sizes of nanoparticles and chains, is studied. For small particles with high DNA surface densities, we find strongly enhanced local salt concentrations, a pronounced localization of divalent ions near the surface of the nanoparticle, and a large radial component of the electric field between the ligands. Therefore, we conclude that enzyme activity in general may be heavily influenced by the local environment around DNA-AuNPs.

¹Funding: U.S. AFOSR award FA9550-10-1-0167 / FA9550-11-1-0275; Ref 1: A. E. Prigodich, et al., ACS Nano 3, 2147 (2009); Ref 2: J. W. Zwanikken, et al. J. Phys. Chem. C 115 (33), 16368 (2011)

1:27PM W34.00008 Mechanical properties of Ge nanowire, ALEX LEE, MINJUNG KIM, JAMES CHELIKOWSKY, The University of Texas at Austin — Nanowires possess unique properties owing to their low dimensionality and high surface-to-volume ratio. Although numerous calculations exist for the electronic properties of nanowires, the mechanical properties have not been addressed to the same extent. Here, we present real-space pseudopotential calculations for the mechanical properties of Ge nanowires. In particular, we examine three different orientations of Ge nanowires, with the axis along the [111], [110], and [100] directions. We present calculations for the elastic properties as a function of wire diameter. We find that Young's modulus is decreased as the surface-to-volume ratio increases, except for the [110] orientation, which shows the opposite trend. In addition, we will discuss the band structure under strain for each nanowire system.

1:39PM W34.00009 Chemisorption on Palladium and Silver Clusters, AJIT HIRA, CHRISTELLA LOVATO, Northern New Mexico College — We continue our interest on the chemisorption of different atomic and molecular species on small clusters of metallic elements, by examining the interactions of H, O and F atoms with Pd_n and Ag_n clusters (n = 6 thru 12). The hybrid ab initio methods of quantum chemistry (particularly the DFT-B3LYP model) are used to derive optimal geometries for the clusters of interest. We compare calculated binding energies, bond-lengths, ionization potentials, electron affinities and HOMO-LUMO gaps for the clusters of the two different metals. Of particular interest are the comparisons of binding strengths at the three important types of sites: edge (E) sites, hollow sites (H) site and on-top (T) sites. Effects of crystal symmetries corresponding to the bulk structures for the two metals will also be investigated. Our theoretical results will be compared with the experimental studies where they are available. Implications for the molecular dissociation of the H₂ and O₂ species will be considered.

1:51PM W34.00010 Blinking in nanoscale systems: a universal theoretical framework, SANDOR VOLKAN-KACSO, California Institute of Technology, PAVEL FRANTSUZOV, BOLDIZSAR JANKO, University of Notre Dame — Fluctuations of fluorescence intensity (blinking) is observed in many different kinds of optically active nanoscale objects. These fluctuations with extremely long-term correlations manifest on timescales longer than seconds and were observed in the emission of colloidal and self-assembled quantum dots, nanorods, nanowires, and some organic dyes. We suggest the idea of a universal physical mechanism underlying the blinking phenomenon. Here we show that the features of this universal mechanism can be captured phenomenologically by the multiple recombination center model (MRC) we proposed in a recent work to explaining single colloidal QD intermittency. Within the framework of the MRC model we qualitatively explain all the important features of fluorescence intensity fluctuations for a broad spectrum of nanoscale emitters.

Thursday, March 1, 2012 11:15AM - 2:15PM –

Session W35 DCP: Focus Session: DFT VIII: Time-Dependent Processes II: Excitations 107B

11:15AM W35.00001 Watching excitons move: the time-dependent transition density matrix¹, CARSTEN ULLRICH, University of Missouri — Time-dependent density-functional theory allows one to calculate excitation energies and the associated transition densities in principle exactly. The transition density matrix (TDM) provides additional information on electron-hole localization and coherence of specific excitations of the many-body system. We have extended the TDM concept into the real-time domain in order to visualize the excited-state dynamics in conjugated molecules. The time-dependent TDM is defined as an implicit density functional, and can be approximately obtained from the time-dependent Kohn-Sham orbitals. The quality of this approximation is assessed in simple model systems. A computational scheme for real molecular systems is presented: the time-dependent Kohn-Sham equations are solved with the OCTOPUS code and the time-dependent Kohn-Sham TDM is calculated using a spatial partitioning scheme. The method is applied to show in real time how locally created electron-hole pairs spread out over neighboring conjugated molecular chains. The coupling mechanism, electron-hole coherence, and the possibility of charge separation are discussed.

¹This work is supported by NSF Grant DMR-1005651.

11:51AM W35.00002 A minimal TDDFT model for excitons¹, YONGHUI LI, ZENGHUI YANG, CARSTEN ULLRICH, University of Missouri — Optical processes in insulators and semiconductors, including excitonic effects, can be accurately described with linear-response TDDFT, provided one uses suitable exchange-correlation kernels. We have developed a conceptually and computationally simple formalism for calculating exciton binding energies with TDDFT, based on a two-band approximation. This formalism is implemented in a one-dimensional Kronig-Penney model, and we discuss the requirements for excitonic binding in this model. The performance of different types of exchange-correlation kernels (long- versus short-ranged, adiabatic versus nonadiabatic) is analyzed, with a particular emphasis on the excitonic Rydberg series.

¹This work is supported by NSF Grant DMR-1005651.

12:03PM W35.00003 Nonlinear ultrafast optical response in organic molecular crystals¹, TALAT S. RAHMAN, VOLODYMYR TURKOWSKI, MICHAEL N. LEUENBERGER, Physics Department and NSTC, University of Central Florida — We analyze possible nonlinear excitonic effects in the organic molecule crystals by using a combined time-dependent DFT and many-body approach. In particular, we analyze possible effects of the time-dependent (retarded) interaction between different types of excitations, Frenkel excitons, charge transfer excitons and excimers, on the electric and the optical response of the system. We pay special attention to the case of constant electric field and ultrafast pulses, including that of four-wave mixing experiments. As a specific application we examine the optical excitations of pentacene nanocrystals and compare the results with available experimental data.[1] Our results demonstrate that the nonlinear effects can play an important role in the optical response of these systems. [1] A. Kabakchiev, "Scanning Tunneling Luminescence of Pentacene Nanocrystals", PhD Thesis (EPFL, Lausanne, 2010).

¹Work supported in part by DOE Grants No. DOE-DE-FG02-07ER15842 and No. DOE-DE-FG02-07ER46354.

12:15PM W35.00004 Electronic and dielectric properties of organic photovoltaic compounds from first principles, ISMAILA DABO, CERMICS, Université Paris-Est, ANDREA FERRETTI, Istituto Nanoscienze, CNR, CHEOL-HWAN PARK, Department of Materials, Oxford University, NICOLAS POILVERT, Rowland Institute, Harvard University, MATTEO COCCIONI, CEMS, University of Minnesota, NICOLA MARZARI, Department of Materials, Oxford University — The initial step towards the design of organic photovoltaic (OPV) devices from first principles is to predict the electronic spectra and dielectric responses of molecular and polymer OPV compounds to quantitative accuracy [*Phys. Rev. B* **71**, 041306 (2005)]. To date, determining the frontier levels and dielectric properties of materials within conventional density-functional theory approximations has been elusive. To address current limitations, orbital-dependent density-functional methods, namely, hybrid density-functional theory (hybrid-DFT) and self-interaction-corrected density-functional theory (SIC-DFT) approximations, represent promising alternatives. In this presentation, we provide a critical comparison of hybrid-DFT and SIC-DFT functionals in determining electronic energies for families of OPV materials. We demonstrate that SIC-DFT based upon Koopmans' condition [*Phys. Rev. B* **82**, 115121 (2010)] is apt at describing donor and acceptor levels within 0.1-0.4 eV and 0.2-0.6 eV relative to experiment. Furthermore, SIC-DFT dielectric responses for semiconducting polymers are predicted in close agreement with more expensive wave-function methods, thereby allowing the accurate and computationally tractable description of donor-acceptor molecular complexes.

12:27PM W35.00005 Discontinuities of the exchange-correlation kernel and charge-transfer excitations in time-dependent density functional theory, MARIA HELLGREN, Max-Planck-Institute, Weinberg 2, Halle(Saale), Germany, E.K.U. GROSS, Max-Planck-Institute, Weinberg 2, Halle (Saale), Germany — We identify the key property that the exchange-correlation (XC) kernel of time-dependent density functional theory (TDDFT) must have in order to describe long-range charge-transfer excitations. We show that the discontinuity of the XC potential as a function of particle number induces a frequency-dependent discontinuity of the XC kernel which diverges in the dissociation limit. This divergency compensates for the exponentially small overlap between the acceptor and donor orbitals, thereby yielding a finite correction to the Kohn-Sham eigenvalue differences. This mechanism is illustrated to first order in the Coulomb interaction.

12:39PM W35.00006 Density Functional Resonance Theory: The Complex Density Function, Orbital Energies and Lifetimes, and Results for Simple Systems¹, DANIEL WHITENACK, Purdue University Department of Physics, ADAM WASSERMAN, Purdue University Department of Chemistry and Department of Physics — Density Functional Resonance Theory (DFRT) is a recently developed complex-scaled version of ground-state Density Functional Theory (DFT) for metastable systems. This work is a detailed study of the formalism itself, its consequences and its application. The meaning of the complex "density" function, which is used as the primary variable, is discussed along with its possible application to study the reactivity of metastable systems. In addition, orbital energies and lifetimes are defined and related to physical quantities. Finally, results for energies and lifetimes are presented for simple systems.

¹Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund for support of this research under grant No. PRF # 49599-DN16.

12:51PM W35.00007 Meta-GGA-based adiabatic time-dependent density-functional theory¹, VLADIMIR NAZAROV, Research Center for Applied Sciences, Academia Sinica, GIOVANNI VIGNALE, University of Missouri-Columbia — The local-density approximation (LDA) to the ground-state density functional theory (DFT) is well known to allow for a generalization to the time-dependent case [1]. The assumption of the adiabaticity of the process greatly simplifies the theory. The further extension of the time-dependent DFT (TDDFT) to the generalized gradient approximation (GGA) is trivial. Here we address lifting the adiabatic TDDFT to the third rung of the "Jacobs ladder" [2]: We work out the kinetic energy density dependent (meta-GGA) TDDFT formalism. The new theory possesses remarkable properties not present in LDA and GGA: (i) It is non-local with respect to the particle density; (ii) In the case of bulk semiconductors, it supports the $1/q^2$ singularity of the exchange-correlation kernel, where q is the wave-vector, the latter being important to reproduce the excitonic effect. We also present illustrative calculations of the optical absorption in semiconductors [3].

[1] A. Zangwill and P. Soven, *Phys. Rev. A*, **21**, 1561 (1980).

[2] J. Tao, J. P. Perdew, V. N. Staroverov, and G. E. Scuseria, *Phys. Rev. Lett.* **91**, 146401 (2003).

[3] V. U. Nazarov and G. Vignale, *Phys. Rev. Lett.* **107**, 216402(2011).

¹VN acknowledges partial support from National Science Council, Taiwan, Grant No. 100-2112-M-001-025-MY3; GV acknowledges support from DOE Grant No. DEFG02-05ER46203

1:03PM W35.00008 Describing electronic excitations using electron-hole density functional theory (eh-DFT), ARINDAM CHAKRABORTY, Syracuse University — The electron-hole interaction play a crucial role in calculating optical properties of atoms, molecules, clusters and solids. In this talk, the density functional treatment of electron-hole quasiparticle interaction will be presented in the framework of electron-hole density functional theory (eh-DFT). The electron-hole correlation functional plays a central role in accuracy of any eh-DFT calculations. In the present work, the development of eh-correlation functional using the eh-reduced density matrix will be presented. Benchmark calculation using the developed functional will be compared with HF, full CI, R12-full CI, and explicitly correlated Hartree-Fock calculations. Exciton binding energies in CdSe quantum dots have been calculated and the eh-DFT results will be compared with experimental and pseudopotential+CI results. Discussion on construction of electron-hole adiabatic connection curve (ACC) using density-constrained minimization will be presented and the results from the ACC will be compared with eh-DFT calculations. Finally, similarity and difference between the GW+Bethe-Salpeter method and eh-DFT approach for treating electron-hole interaction will be presented.

1:15PM W35.00009 Applying state-of-the-art signal processing to time-dependent density functional theory, JACOB SANDERS, XAVIER ANDRADE, ALAN ASPURU-GUZI, Harvard University Department of Chemistry and Chemical Biology — Real-time time-dependent density functional theory (TDDFT) is a computationally efficient method that can be used to calculate optical absorption spectra, circular dichroism spectra, and other properties including non-linear ones. These properties are often obtained via time-propagation methods, and a discrete Fourier transform is used to convert from the time domain to the frequency domain. However, a Fourier transform requires long time propagations to resolve spectra, especially if they contain closely-spaced frequencies. Instead, we apply a state-of-the-art signal processing technique known as compressed sensing to the spectral analysis of electron dynamics. Compared to a Fourier transform, compressed sensing provides higher-resolution absorption spectra with shorter propagation times. In the systems we study, the method requires about 80% less time series data to obtain comparable frequency resolution, thus reducing total computational cost by approximately a factor of five. By combining the computational efficiency and parallelizability of real-time TDDFT for large systems with the dramatic reduction in simulation time enabled by compressed sensing, we increase the feasibility of studying electron dynamics in large biological molecules and organic photovoltaics.

1:27PM W35.00010 Density Functional Theory Investigation of Tunable Surface Composition of CdS Quantum Dots¹, OLEG PREZHDO, AMANDA NEUKIRCH, JEREMY YOUNG, HELEN WEI, CHRISTOPHER EVENS, TODD KRAUSS, University of Rochester — It has recently been observed that surface composition of CdS QDs greatly affects photoluminescence. Band edge emission is quenched in sulfur terminated CdS QDs and recovered when QDs were cadmium terminated. However, in all cases the absorption spectra remained relatively unchanged. To understand the origin of this phenomenon, the density of states in a stoichiometric, Cd rich, and S rich dots was investigated using density functional theory (DFT). It was found that in the S rich system states within the band gap were introduced, providing a channel for non-radiative electronic relaxation. Gap states were also introduced in the Cd rich system compared to the stoichiometric system, but a significant band gap remained in even the most Cd rich systems. Finally, time dependent (TD)DFT was used to calculate the spectra of the various systems. It was found that created gap states were largely optically inactive. Therefore the new states would not participate in optical absorption or emission, but could participate in electron phonon relaxation. This study clarifies the role of surface defects in QD optical properties and provides a route for tuning those optical properties by controlling surface composition.

¹This work was supported by NSF grant numbers CHE-1050405 and CHE-1012681

1:39PM W35.00011 First-Principles Approach to Chemical Raman Enhancement of Organic Adsorbates on Metal Surfaces¹, ALEXEY ZAYAK, Molecular Foundry, LBNL, HYUCK CHOO, California Institute of Technology, YING S. HU, Rice University, DANIEL GARGAS, STEFANO CABRINI, JEFFREY BOKOR, P. JAMES SCHUCK, JEFFREY B. NEATON, Molecular Foundry, LBNL — A first-principles density functional theory (DFT)-based approach is developed [1] to determine chemical contributions to surface-enhanced Raman spectroscopy (SERS) for molecular adsorbates on metal surfaces. While SERS applications are often directed at sensing trace amounts of chemical species, quantitative calculations of how Raman spectra of molecules are altered on chemisorption [1], coupled to experiments, can contribute significantly to our understanding of the electronic structure of the metal-adsorbate interface. For two adsorbates on Au – benzene thiol and trans-1,2-bis(4-pyridyl) ethylene (BPE) – DFT calculations of the static Raman tensor demonstrate a strong mode-dependent modification of Raman spectra by Au substrates. Raman active modes with the largest enhancements result from stronger contributions from Au to their electron-vibron coupling, as quantified through a deformation potential. Based on our calculations, we introduce a straightforward analysis to extract “chemical enhancement” from measurements, and demonstrate how SERS spectra of BPE change as a function of the relative fraction of BPE molecules chemisorbed to the substrate.

[1] Zayak et al, Phys. Rev. Lett. 106, 083003 (2011)

¹We acknowledge DOE for support, and NERSC for computational resources.

1:51PM W35.00012 Electron-Hole Pairs during Adsorption Dynamics of O₂ on Pd(100) – Exciting or not?, JOERG MEYER, KARSTEN REUTER, TU Muenchen — *Ab initio* modeling can provide important atomistic insights into the dynamics of elementary reaction steps in heterogeneous catalysis. But already an apparently simple example like the adsorption of O₂ on a frozen Pd(100) surface brings up several fundamental challenges: The corresponding six-dimensional potential energy surface (PES) is required, and excitations of electron-hole (eh) pairs as well as the transition from the ³Σ_g⁻ spin-triplet in the gas phase to a singlet-like state of adsorbed oxygen might require to go beyond the Born-Oppenheimer approximation. We tackle the PES by neural network interpolation, based on a coordinate transformation that correctly includes and exploits the underlying symmetry. Classical molecular dynamics thereon yields the initial sticking coefficient in good agreement with experimental data. Scrutinizing this result, we calculate spin-resolved eh pair spectra for several trajectories of different statistical relevance using a computationally appealing perturbative approach building on time-dependent DFT.¹ Although non-adiabatic energy losses do not exceed 5% of the chemisorption energy, their importance for the spin transition is finally discussed.

¹J. Meyer and K. Reuter, New J. Phys. 13, 085010 (2011)

2:03PM W35.00013 Self-consistent GW calculations with basis of dominant products, PETER KOVAL, Centro de Fisica de Materiales, DIETRICH FOERSTER, University of Bordeaux 1, DANIEL SANCHEZ PORTAL, Centro de Fisica de Materiales — Hedin's GW approximation (GWA) is a well known method to study charged excitations in electronic systems with a moderate computational cost [1]. Already one-shot GWA delivers a considerable improvement if compared with Green's functions from density-functional theory (DFT). However, the one-shot results are dependent on the used starting point. This unphysical dependence can be eliminated by iterating a GW calculation to self-consistency. We implemented self-consistent GWA for molecules [2], within our original framework of dominant products basis. We use the DFT calculation by SIESTA code as starting point. The framework allowed to calculate Green's functions on a fine frequency mesh for such small molecules as benzene. We demonstrate the level of independence on starting point achievable within pseudo-potential framework, validating the implementation. Effects of the self-consistency on the interacting Green's function will be discussed along with different levels of self-consistency and mixing schemes. Finally, we compare the self-consistency with so-called quasi-particle self-consistent GW [3].

[1] F.Aryasetiawan, O.Gunnarsson, Rep. Prog. Phys. 61, 237 (1998).

[2] D.Foerster, P.Koval, D.Sanchez Portal, J. Chem. Phys. 135, 074105 (2011).

[3] T.Kotani, M.van Schilfgaarde, S.V.Falleev, Phys. Rev. B 76, 165106 (2007).

Thursday, March 1, 2012 11:15AM - 2:15PM – Session W37 DMP: Topological Insulators: Fractionalization 108

11:15AM W37.00001 Zoology of Fractional Chern Insulators, YANG-LE WU, B. ANDREI BERNEVIG, Princeton University, N. REGNAULT, Ecole Normale Supérieure, CNRS — We study four different models of Chern insulators in the presence of strong electronic repulsion at partial fillings. We observe that all cases exhibit a Laughlin-like phase at filling fraction $1/3$. We provide evidence of such a strongly correlated topological phase by studying both the energy and the entanglement spectra. In order to identify the key ingredients of the emergence of Laughlin physics in these systems, we show how they are affected when tuning the band structure. We also address the question of the relevance of the Berry curvature flatness in this problem. Using three-body interactions, we show that some models can also host a topological phase reminiscent of the $\nu = 1/2$ Pfaffian Moore-Read state. Additionally, we identify the structures indicating cluster correlations in the entanglement spectra.

11:27AM W37.00002 Time-reversal symmetric hierarchy of fractional incompressible liquids, LUIZ SANTOS, Harvard University, TITUS NEUPERT, Paul Scherrer Institute, SHINSEI RYU, University of Illinois at Urbana-Champaign, CLAUDIO CHAMON, Boston University, CHRISTOPHER MUDRY, Paul Scherrer Institute — In this talk I shall establish a hierarchical construction for a class of BF theories and present it as a candidate topological field theory to describe fractional topological insulators in 2D. The structure of the K matrix and the universal properties that it describes will be discussed, and the properties of the time-reversal symmetric edge theory will be derived via the bulk-edge correspondence.

11:39AM W37.00003 Fractional Chern Insulator, NICOLAS REGNAULT, Ecole Normale Supérieure Paris, CNRS, BOGDAN ANDREI BERNEVIG, Princeton University — Chern insulators are band insulators exhibiting a nonzero Hall conductance but preserving the lattice translation symmetry. We conclusively show that a partially filled Chern insulator at $1/3$ filling exhibits a fractional quantum Hall effect and rule out charge-density wave states that have not been ruled out by previous studies. By diagonalizing the Hubbard interaction in the flat-band limit of these insulators, we show the following: the system is incompressible and has a 3-fold degenerate groundstate whose momenta can be computed by postulating an generalized Pauli principle with no more than 1 particle in 3 consecutive orbitals. The groundstate density is constant, and equal to $1/3$ in momentum space. Excitations of the system are fractional statistics particles whose total counting matches that of quasiholes in the Laughlin state based on the same generalized Pauli principle. The entanglement spectrum of the state has a clear entanglement gap which seems to remain finite in the thermodynamic limit. The levels below the gap exhibit the identical counting of Laughlin $1/3$ quasiholes. The 3 groundstates and excited states exhibit spectral flow upon flux insertion. All the properties above disappear in the trivial state of the insulator.

11:51AM W37.00004 Fractional Chern Insulators from the n th Root of Bandstructure¹, BRIAN SWINGLE, Harvard University, KY-ANH TRAN, JOHN MCGREEVY, MIT — I will describe some recent theoretical results pertaining to fractional Chern insulators. These are interacting lattice models of partially filled Chern bands which have been numerically shown to realize some universal aspects of fractional quantum Hall physics. We use parton/slave-particle techniques to provide model wavefunctions for these phases. We also provide a strong coupling expansion that gives new insights into the foundations of the parton approach. I will conclude by describing some of the practical uses of our results, including suggesting candidate models to realize non-Abelian fractional Chern insulators.

¹This work partially supported by a Simons Fellowship.

12:03PM W37.00005 Wannier states and pseudopotential Hamiltonians for fractional Chern insulators, CHING HUA LEE, Department of Physics, Stanford University, DONG-NING SHENG, Department of Physics and Astronomy, California State University, RONNY THOMALE, XIAO-LIANG QI, Department of Physics, Stanford University — Fractional Chern insulators are fractional quantum Hall states realized in lattice models with full lattice translational symmetry in the absence of an external magnetic field. In fractional quantum Hall systems, pseudopotential Hamiltonians have been constructed for which the ideal ground states such as Laughlin states are exact ground states. In this work, we constructed pseudopotential Hamiltonians for the fractional Chern insulators by making use of the Wannier function representation. The physical interaction Hamiltonians can be expanded in pseudopotentials, from which one can analyze the preferred fractional quantum Hall states in the corresponding systems. The results of this analysis are compared with exact diagonalization. Our approach may be generalized to studying nonabelian fractional Chern insulator states and time-reversal invariant fractional topological insulators.

12:15PM W37.00006 Topological insulators and fractional quantum Hall effect on the ruby lattice¹, XIANG HU, MEHDI KARGARIAN, GREGORY A. FIETE, The University of Texas at Austin — We study a tight-binding model on the two-dimensional ruby lattice. This lattice supports several types of first and second neighbor spin-dependent hopping parameters in an s -band model that preserves time-reversal symmetry. We discuss the phase diagram of this model for various values of the hopping parameters and filling fractions, and note an interesting competition between spin-orbit terms that individually would drive the system to a $\mathbb{Z}_2$ topological insulating phase. We also discuss a closely related spin-polarized model with only first and second neighbor hoppings and show that extremely flat bands with finite Chern numbers result, with a ratio of the band gap to the band width approximately 70. Such flat bands are an ideal platform to realize a fractional quantum Hall effect at appropriate filling fractions. The ruby lattice can be possibly engineered in optical lattices, and may open the door to studies of transitions between quantum spin liquids, topological insulators, and integer and fractional quantum Hall states.

¹We acknowledge support from ARO Grant W911NF-09-1-0527 and NSF Grant DMR-0955778, and the Texas Advanced Computing Center (TACC) for providing computing resources.

12:27PM W37.00007 Charge and spin fractionalization in strongly correlated topological insulators¹, PREDRAG NIKOLIC, George Mason University, TANJA DURIC, Max Planck Institute, Dresden — The recently discovered two-dimensional topological insulators (TI) with time-reversal symmetry are closely related to integer quantum Hall states in which electron spin plays the role of charge. The appearance of protected edge states in these systems can be understood by describing the spin-orbit coupling as the source of an SU(2) (spin-dependent) magnetic flux. However, the absence of spin conservation cripples the quantum spin-Hall effect. In this talk we will explore the possibility of obtaining strongly correlated TIs with fractional quasiparticles. Such states are the SU(2) analogues of fractional quantum Hall states, but with modified topological orders due to the spin non-conservation. We will discuss two heterostructure designs featuring a “conventional” TI quantum well that could host a fractional TI state of Cooper pairs or excitons. These devices exploit a quantum critical point for electron localization to provide a fragile spectrum that can be dramatically reshaped by the strong spin-orbit coupling. Then, we will present a topological spinor-field theory of fractional TIs and explain how the spin-orbit coupling can produce a combined charge and spin fractionalization despite the spin non-conservation.

¹Supported by ONR, NIST and DOE (IQM at Johns Hopkins University)

12:39PM W37.00008 Symmetry protected fractional Chern insulators and fractional topological insulators, YUAN-MING LU, Department of Physics, University of California at Berkeley, Berkeley, CA 94720, USA, YING RAN, Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467, USA — We construct fully symmetric wavefunctions for the spin-polarized fractional Chern insulators (FCI) and time-reversal-invariant fractional topological insulators (FTI) using the parton approach. We show that the lattice symmetry gives rise to many different FCI and FTI phases even with the same filling fraction ν (and the same quantized Hall conductance σ_{xy} in FCI case). They have different symmetry-protected topological orders, which are characterized by different projective symmetry groups. We mainly focus on FCI phases with which are realized in a partially filled band with Chern number one and filling fraction $\nu = 1/m$. Examples of FCI/FTI wavefunctions on honeycomb lattice and checkerboard lattice are explicitly given. Possible non-Abelian FCI phases which may be realized in a partially filled band with Chern number two are discussed. Generic FTI wavefunctions preserving all lattice symmetries in the absence of spin conservation are also presented for filling fraction $\nu = 2/m$.

12:51PM W37.00009 High-temperature fractional quantum Hall states, EVELYN TANG, XIAO-GANG WEN, Massachusetts Institute of Technology — Using a suitable combination of geometric frustration, ferromagnetism, and spin-orbit coupling in a hopping model on the kagome lattice, we obtain a flat band with nonzero Chern number. Partial filling of this band could give rise to the fractional quantum Hall effect in this system which, when considering realistic parameters, would persist at room temperature. Possible material realizations that indicate new directions for exploration and synthesis are discussed.

1:03PM W37.00010 Fractional Quantum Hall states in strongly correlated multi-orbital systems¹, MARIA DAGHOFER, JÖRN W.F. VENDERBOS, STEFANOS KOURTIS, JEROEN VAN DEN BRINK, IFW Dresden — For topologically nontrivial and very narrow bands, Coulomb repulsion between electrons has been predicted to give rise to a spontaneous fractional quantum-Hall (FQH) state in absence of magnetic fields. We will discuss how orbital degrees of freedom in frustrated lattice systems lead to a narrowing of topologically nontrivial bands [1]. This robust effect does not rely on fine-tuned long-range hopping parameters and is directly relevant to a wide class of transition metal compounds. In addition, we will show that strongly correlated electrons in a t_{2g} -orbital system on a triangular lattice self-organize into a spin-chiral magnetic ordering pattern that induces precisely the required topologically nontrivial and flat bands [2]. On top of a self-consistent mean-field approach, we use exact diagonalization to study an effective one-band model for the emerging flat band in the presence of longer-range interactions and establish the signatures of a spontaneous $\nu = \frac{1}{3}$ FQH state.

[1] J. W.F. Venderbos, M. Daghofer, J. van den Brink, PRL **107**, 076405 (2011)

[2] J. W.F. Venderbos, S. Kourtis, J. van den Brink, M. Daghofer, arXiv:1109.5955

¹Supported by DFG (Emmy-Noether program) and the Interphase Program of the Dutch Science Foundation NWO/FOM.

1:15PM W37.00011 Hall Crystal States in Fractionally Filled Chern Bands, GANPATHY MURTHY¹, University of Kentucky, RAMAMURTI SHANKAR², Yale University — Two-dimensional time-reversal-invariant topological insulators can be thought of as a time-reversed pair of Chern bands. Numerical evidence shows the existence of states at fractional filling which are analogous to FQH states[1]. In [2] it was noted that at small momenta, the algebra of the density operators projected to the Chern band resembles the magnetic translation algebra. The authors have constructed a mapping[3] between Chern bands and a Landau level in a periodic potential which works at all momenta. This mapping is dynamically faithful, and reproduces the commutators of the projected density operator. There turn out to be Hall Crystal states, characterized by a Hall conductance, and another integer which described the charged dragged when the potential is adiabatically moved by a lattice unit. Using the Hamiltonian formalism developed by the authors some time ago for the FQHE[4], we calculate gaps and collective mode dispersions for such states. 1. D. N. Sheng et al, arxiv:1102.2568, N. Regnault and B. A. Bernevig, arxiv:1105.4867. 2. S. Parameswaran, R. Roy, and S. L. Sondhi, arxiv:1106.4025. 3. G. Murthy and R. Shankar, arxiv:1108.5501 4. G. Murthy and R. Shankar, Rev. Mod. Phys. **75**, 1101 (2003)

¹NSF-DMR0703992, NSF-PHY0970069

²NSF-DMR0901903

1:27PM W37.00012 Chiral Topological Phases and Fractional Domain Wall Excitations in One-Dimensional Chains and Wires¹, JUKKA VAYRYNEN, Yale University, TEEMU OJANEN, Harvard University — According to the general classification of topological insulators, there exist one-dimensional chirally (sublattice) symmetric systems that can support any number of topological phases. We introduce a zigzag fermion chain with spin-orbit coupling in magnetic field and identify three distinct topological phases. Zero-mode excitations, localized at the phase boundaries, are fractionalized: two of the phase boundaries support $\pm e/2$ charge states while one of the boundaries support $\pm e$ and neutral excitations. In addition, a finite chain exhibits $\pm e/2$ edge states for two of the three phases. We explain how the studied system generalizes the Peierls-distorted polyacetylene model and discuss possible realizations in atomic chains and quantum spin Hall wires.

¹Academy of Finland (T.O), KAUTE, Emil Aaltonen Foundation, ERC Grant No. 240362-Heattronics (J. I. V)

1:39PM W37.00013 Quantum Hall Effect and Bound Fractional Charge in Topological Insulator Magnetic Tunnel Junctions, TAYLOR HUGHES, QINGLEI MENG, SMITHA VISHVESHWARA, University of Illinois at Urbana Champaign — Proximity coupling 2D and 3D time-reversal invariant topological insulators to ferromagnetic domain walls is known to lead to bound fractional charge and an integer quantum Hall effect respectively. Here we show that by correctly engineering the sample geometry these effects can appear in the presence of only a single magnet with no domain walls, thus reducing the experimental complexity. We will prove that a magnetic layer sandwiched between 3D topological insulator films will exhibit the quantum Hall effect, possibly leading to a room-temperature realization of the quantum Hall effect.

1:51PM W37.00014 Phase Diagram of a Simple Model for Fractional Topological Insulator, HUA CHEN, Zhejiang Institute of Modern Physics and Department of Physics, Zhejiang University, Hangzhou 310027, China, KUN YANG, National High Magnetic Field Laboratory and Department of Physics, Florida State University, Tallahassee, FL 32306, USA — We study a simple model of two species of (or spin-1/2) fermions with short-range intra-species repulsion in the presence of opposite (effective) magnetic field, each at filling factor 1/3. In the absence of inter-species interaction, the ground state is simply two copies of the 1/3 Laughlin state, with opposite chirality. Due to the overall time-reversal symmetry, this is a fractional topological insulator. We show this phase is stable against moderate inter-species interactions. However strong enough inter-species repulsion leads to phase separation, while strong enough inter-species attraction drives the system into a superfluid phase. We obtain the phase diagram through exact diagonalization calculations. Nature of the fractional topological insulator-superfluid phase transition is discussed using an appropriate Chern-Simons-Ginsburg-Landau effective field theory.

2:03PM W37.00015 Fractional Chern Insulators and the W_∞ Algebra, RAHUL ROY, Rudolf Peierls Centre for Theoretical Physics, Oxford University, SIDDHARTH PARAMESWARAN, University of California, Berkeley, SHIVAJI SONDHI, Princeton University — A set of recent results indicates that fractionally filled bands of Chern insulators in two dimensions support fractional quantum Hall states analogous to those found in fractionally filled Landau levels. We provide an understanding of these results by examining the algebra of Chern band projected density operators. We find that this algebra closes at long wavelengths and for constant Berry curvature, whereupon it is isomorphic to the W_∞ algebra of lowest Landau level projected densities first identified by Girvin, MacDonald and Platzman [Phys. Rev. B 33, 2481 (1986).] For Hamiltonians projected to the Chern band this provides a route to replicating lowest Landau level physics on the lattice.

Thursday, March 1, 2012 11:15AM - 2:15PM –
Session W39 DMP DBIO DPOLY: Focus Session: Materials and Functional Structures for Biological Interfaces: Cells 109B

11:15AM W39.00001 Controlling Cell Function with Geometry, MILAN MRKSICH, Northwestern University — This presentation will describe the use of patterned substrates to control cell shape with examples that illustrate the ways in which cell shape can regulate cell function. Most cells are adherent and must attach to and spread on a surface in order to survive, proliferate and function. In tissue, this surface is the extracellular matrix (ECM), an insoluble scaffold formed by the assembly of several large proteins—including fibronectin, the laminins and collagens and others—but in the laboratory, the surface is prepared by adsorbing protein to glass slides. To pattern cells, gold-coated slides are patterned with microcontact printing to create geometric features that promote cell attachment and that are surrounded by inert regions. Cells attach to these substrates and spread to adopt the shape defined by the underlying pattern and remain stable in culture for several days. Examples will be described that used a series of shapes to reveal the relationship between the shape of the cell and the structure of its cytoskeleton. These geometric cues were used to control cell polarity and the tension, or contractility, present in the cytoskeleton. These rules were further used to control the shapes of mesenchymal stem cells and in turn to control the differentiation of these cells into specialized cell types. For example, stem cells that were patterned into a “star” shape preferentially differentiated into bone cells whereas those that were patterned into a “flower” shape preferred a fat cell fate. These influences of shape on differentiation depend on the mechanical properties of the cytoskeleton. These examples, and others, reveal that shape is an important cue that informs cell function and that can be combined with the more common soluble cues to direct and study cell function.

11:51AM W39.00002 Role of fiber functionality and angle on cell migration.¹, SISI QIN, RICHARD CLARK, MIRIAM RAFILOVICH, Stony Brook University, DEPARTMENT OF MATERIALS SCIENCES AND ENGINEERING, STONY BROOK UNIVERSITY TEAM, DEPARTMENT OF BIOMEDICAL ENGINEERING, STONY BROOK UNIVERSITY TEAM — In order to determine the role of surface interactions on cell migration we compared the cell velocity on electrospun PMMA fibers which were either etched with UV/ozone plasma, had pre-adsorbed Fibronectin or both. It shows that dermal fibroblasts (CF-29, ATCC) did not adhere to the fibers without treatment, and the migration of cells was fastest on with both etching and pre-coat FN fibers. Vinculin was used to stain for the focal adhesion points and the largest number per cell were found on the FN pre-incubated samples, and nearly none on the plasma etched surface, despite good proliferation and migration. The results indicate that the migration velocity need not directly correlate to the cell adhesion. Using FN coated fibers we also studied the effect of angle on crossed fibers. We found that there was a clear preference by the cells for crossing a matrix where the fibers were oriented at 30 degrees. At this angle the migration velocity was slowest. Movies of the migrating cells indicate that the residence time of the cells at junctions with this angle is the longest cut to the interactions of the motion between fibers. The largest speed was observed for fibers placed at 90 degree.

¹NSF-DMR-MRSEC Program

12:03PM W39.00003 Anomalous cell migration properties on electrospun fibers¹, RICHARD CLARK, SISI QIN, MIRIAM RAFILOVICH, Stony Brook University, DEPARTMENT OF MATERIALS SCIENCES AND ENGINEERING, STONY BROOK UNIVERSITY TEAM, DEPARTMENT OF BIOMEDICAL ENGINEERING, STONY BROOK UNIVERSITY TEAM — We have studied the influence of substrate morphology on the en-mass cell migration from an agarose droplet. On flat surfaces, the cell velocity decreases asymptotically towards the single cell value as the radial distance increases, and remains constant thereafter. On fibers, the velocity remains constant at the single cell limit for the first 24 hours and then begins to increase continuously for the next four days. On flat surfaces we have shown that migration was triggered by nuclear deformation [Pan Z. et al, 2009], whereas on fibers the nucleus is constantly deformed as the cell assumes the shape of the fiber and hence does not seem to play as major a role. Vinculin and paxillin immunofluorescent staining were performed to determine the role of traction forces. We found that whereas polarization remains constant on flat surfaces with time, it increases on the fiber surfaces after the first 24 hours, and may explain the increased migration speed.

¹NSF-DMR-MRSEC Program

12:15PM W39.00004 Control cell adhesion with dynamic bilayer films, ANDREAS KOUROUKLIS, Department of Chemical Engineering, Umass Amherst, RONALD LERUM, Department of Polymer Science & Engineering, Umass Amherst, HARRY BERMUDEZ, Department of Polymer Science & Engineering and Department of Chemical Engineering, Umass Amherst — Interfacially-directed assembly of amphiphilic block copolymers was employed to create ultrathin films having the potential to correlate the dynamics of ECM cues with cell adhesion and cytoskeletally-generated forces. The mobility of the polymeric bilayer films were tuned by the incorporation of hydrophobic homopolymer chains, which are thought to reduce interlayer friction. Labeling of the block copolymer chains with an adhesive peptide ligand (RGD) provided a specific means to study integrin-mediated cellular processes and the corresponding mechanotransduction. By seeding anchorage-dependent cells on “dynamic” (laterally mobile) and “static” films that display the same amount of RGD, we have found that cells recognize the difference in RGD diffusivity and develop distinct responses over time. We intend to examine changes in cell response by controlling the extent of cytoskeletally-generated forces and the assembly dynamics of focal adhesion complexes. Such films provide a unique platform to unveil the biomechanical signals related with ECM dynamics, and may ultimately facilitate a deeper understanding of cellular processes.

12:27PM W39.00005 Diblock Copolymer Foams with Adhesive Nano-domains Promote Stem Cell Differentiation¹, ADAM ENGLER, UC San Diego — Adhesions play an important role in cell behavior, including differentiation. Substrates are typically modified with homogeneous protein coatings; extracellular matrices *in vivo* provide heterogeneous adhesive sites. To mimic adhesive heterogeneity, internal phase emulsion foams were polymerized with polystyrene-polyacrylic acid (PAA) and polystyrene-polyethylene oxide (PEO) to determine if interface de-mixing would form patch-like surfaces. PEO/PAA mole ratios were confirmed by XPS and water contact angle while spatial distribution was measured by chemical force spectroscopy. This method confirmed the presence of patch-like PAA domains. Protein differentially adsorbs on PEO and PAA, so adsorption on foam mixtures was copolymer ratio dependent. Bone marrow-derived mesenchymal stem cell (BMSC) adhesion was ratio dependent, but the highest density and vinculin expression was observed for 75PEO/25PAA. BMSCs appeared to change lineage expression the most on this composition, suggesting that this foam, which exhibits small adhesive PAA domains, may be more biomimetic than uniformly adhesive scaffolds, e.g. 0PEO/100PAA.

¹Funding from HFSP grant RGY0064/2010 and NIH New Innovator Award.

1:03PM W39.00006 Dental Pulp Stem Cell Differentiation on Poly-4-vinyl-pyridine surfaces¹, GIULIA SUARATO, Department of Materials Science and Engineering, SUNY at Stony Brook, ANEEL BHERWANI, Oral Biology and Pathology, SUNY at Stony Brook, CHUNG-CHUEH CHANG, MIRIAM RAFAILOVICH, Department of Materials Science and Engineering, SUNY at Stony Brook, MARCIA SIMON, Oral Biology and Pathology, SUNY at Stony Brook — In the regeneration of a natural tissue, the mechanics and the chemical properties of the artificial substrate play a critical role. In this study, the influence of poly-4-vinyl-pyridine scaffold morphology on dental pulp stem cell differentiation was analyzed. Cells were plated on spun cast films and electrospun fibers with diameters ranging from nano to micrometers. Confocal microscopy showed the presence of various cell morphologies: on microfibers cells conform precisely to the main axis of elongation, while on nanometric scaffolds they result spread and in contact with several fibers. Even if the surface chemistry was identical, a great variation in the curvature was present. From day 9 of incubation, spontaneous biomineralization in the absence of induction agents occurred only on the fibrous structures. The SEM revealed template deposits directly on the microfibers, while on the nanofibers large spherical islands were also present. EDAX determined hydroxyl apatite nature of the deposits. RT-PCR indicated upregulation of osteogenic markers, confirming differentiation. SEM also revealed the presence of ECM fibers covering the polymer structure, which may enhance the expression of focal adhesion sites on the cell membrane.

¹NSF-DMR-MREC program and the DMR-CBET program

1:15PM W39.00007 Spontaneous Differentiation of Dental Pulp stem cells on Dental polymers, ANEEL BHERWANI, Oral Biology and Pathology, Stony Brook University, GIULIA SUARATO, SISI QIN, CHUNG-CHUEH CHANG, Materials Science, Stony Brook University, AARON AKHAVAN, Ramban Mesizta High School, JOSEPH SPIEGEL, VLADIMIR JURUKOVSKI, MIRIAM RAFAILOVICH, Materials Science, Stony Brook University, MARCIA SIMON, Oral Biology and Pathology, Stony Brook University — Dental pulp stem cells were plated on two dentally relevant materials i.e. PMMA commonly used for denture and Titanium used for implants. In both cases, we probed for the role of surface interaction and substrate morphology. Different films of PMMA were spun cast directly onto Si wafers; PMMA fibers of different diameters were electro spun onto some of these substrates. Titanium metal was evaporated onto Si surfaces using an electron beam evaporator. In addition, on some surfaces, P4VP nanofibers were spun cast. DPSC were grown in alpha-MEM supplemented with 10% fetal bovine serum, 0.2mM L-ascorbic acid 2-phosphate, 2mM glutamine and 10mM beta-glycerol phosphate either with or without 10nM dexamethasone. After 21 days samples were examined using confocal microscopy of cells and by scanning electron microscopy (SEM) and Energy dispersive X-ray Analysis (EDAX). In the case of Titanium biomineralization was observed independent of dexamethasone, where the deposits were templated along the fibers. Minimal biomineralization was observed on flat Titanium and PMMA samples. Markers of osteogenesis and specific signaling pathways are being evaluated by RT-PCR, which are up regulated on each surface, to understand the fundamental manner in which surfaces interact with cell differentiation.

1:27PM W39.00008 Interaction of Substrate Mechanics with Dental Pulp Stem Cells (DPSCs) differentiation to generate a scaffold for Bone regeneration, MIRIAM RAFAILOVICH, DIVYA BHATNAGAR, Department of Materials Science and Engineering, SUNY Stony Brook, ANEEL BHERWANI, MARCIA SIMON, School of Dental Medicine, SUNY Stony Brook — This work investigates the interaction of the substrate mechanics with the differentiation in the absence of chemical induction and only resulting from the stimuli of the substrate mechanics and chemistry. We chose enzymatically cross-linked gelatin hydrogels substrates of different stiffness varying from 8KPa to 100Pa. DPSCs were cultured and differentiated on the substrates for 7, 14 and 21 days with and without dexamethasone induction media. SEM and EDX analysis after 21 days indicate that cells produced a sheet of biomineralized deposits, several tenths of mm thick on the hard substrate irrespective of chemical induction. Moduli of the cells was independent of the induction and stiffness of the hydrogels. RT-PCR assays indicated that cells expressed more osteocalcin when cultured in non-induction media and harder substrate. The shape of the deposits was more uniform and in close packing on the harder substrate with a higher Ca:P ratio. On soft substrate the deposits were more flat with less Ca:P ratio. Further experiments indicated that conformational change due to the crosslinking of gelatin could be the reason for biomineralization.

1:39PM W39.00009 Neuron Growth on Carbon Nanotube Thread Bio-Scaffolds for Repair of Central Nervous System Damage, DAVID MAST, SARAH PIXLEY, MARK SCHULZ, VESSILIN SHANOV, University of Cincinnati — Approximately 11,000 new spinal cord injuries occur each year. Repairing such central nervous system (CNS) damage has proven to be very difficult. We report on *in vitro* experiments using carbon nanotube (CNT) threads as a bio-scaffold for promoting CNS repair via directed neuron regrowth along the CNT material. Mouse brain neurospheres, containing neuronal stem cells, neurons and support glia, were observed to attach to and grow along laminin-coated CNT threads *in vitro*. However, due to their limited mobility, only neurospheres close to the threads attach. To increase cellular attachment to the threads, we exploit the fact that these cells can exhibit enhanced, directed migration along an externally applied electric field. Recent *in vitro* cell growth was carried out in chambers containing several parallel CNT threads with electrical connections extending out of the incubator so that a voltage applied across adjacent threads established an appropriate electric field. Electrochemical Impedance Spectroscopy, Cyclic Voltammetry and dc and ac IV measurements were used to monitor cell growth and attachment as a function of applied electric field and time. Cell migration and attachment were also investigated using time lapse photography in a separate growth chamber mounted on the stage of an optical microscope.

1:51PM W39.00010 Stiffness nanotomography of human epithelial cancer cells, JACK R. STAUNTON, BRYANT L. DOSS, C. MICHAEL GILBERT, Arizona State University, SANDOR KASAS, EPFL, ROBERT ROS, Arizona State University — The mechanical stiffness of individual cells is important in both cancer initiation and metastasis. We present atomic force microscopy (AFM) based nanoindentation experiments on various human mammary and esophagus cell lines covering the spectrum from normal immortalized cells to highly metastatic ones. The combination of an AFM with a confocal fluorescence lifetime imaging microscope (FLIM) in conjunction with the ability to move the sample and objective independently allow for precise alignment of AFM probe and laser focus with an accuracy down to a few nanometers. This enables us to correlate the mechanical properties with the point of indentation in the FLIM image. We are using force-volume measurements as well as force indentation curves on distinct points on the cells to compare the elastic moduli of the nuclei, nucleoli, and the cytoplasm, and how they vary within and between individual cells and cell lines. Further, a detailed analysis of the force-indentation curves allows study of the cells' mechanical properties at different indentation depths and to generate 3D elasticity maps.

2:03PM W39.00011 Snakeskin tribology: How snakes generate large frictional anisotropy , HAMIDREZA MARVI, JEFFREY STREATOR, DAVID HU, Georgia Institute of Technology — The limbless locomotion of snakes relies fundamentally upon friction. Snakes can adjust their spatial and temporal frictional properties in order to get friction anisotropies of around 2. Ventral scales play a major role in friction adjustment. In this combined experimental and theoretical study we measure the mechanical and frictional properties of snakeskin. We report the effect of substrate roughness and compliance on snake frictional anisotropy. We numerically model a snake scale interacting with an elastic rough substrate using contact mechanics. The scale is modeled as an isotropic rigid material attached to the body using a torsional spring. We find that the combined effect of the scales geometry and angle of attack leads to the scale high frictional anisotropy. Our results suggest that fabricating engineering surfaces such as artificial snakeskin with optimized geometry and orientation of scales will improve the efficiency of snake-like robots.

Thursday, March 1, 2012 11:15AM - 2:15PM –
Session W40 DBIO DPOLY DCOMP: Focus Session: Single Molecule Biological Physics - Nucleic acids and Proteins 156A

11:15AM W40.00001 Single-molecule Imaging Reveals Molecular Mechanisms of A DNA Strippase , ERIC GREENE, Columbia University and HHMI — No abstract available.

11:51AM W40.00002 ABSTRACT WITHDRAWN –

12:03PM W40.00003 Sequence-dependent sliding kinetics of p53 , JASON LEITH, ANAHITA TAFVIZI, Harvard University, Massachusetts Institute of Technology, FANG HUANG, Cambridge University, WILLIAM USPAL, PATRICK DOYLE, Massachusetts Institute of Technology, ALAN FERSHT, Cambridge University, LEONID MIRNY, Massachusetts Institute of Technology, ANTOINE VAN OIJEN, Rijksuniversiteit Groningen — Theoretical work has long proposed that one-dimensional sliding along DNA while simultaneously reading its sequence can accelerate transcription factors' (TFs) search for their target sites. More recently, functional sliding has been shown to require TFs to possess at least two DNA-binding modes. The tumor suppressor p53 has been directly observed to slide on DNA, and structural and single-molecule studies have provided evidence for a two-mode model for the protein. If the model is in fact applicable to p53, then the requirement that TFs read while they slide implies that p53's mobility on DNA should be affected by non-cognate sites and thus that its diffusivity should be generally sequence-dependent. Here we confirm this prediction with single-molecule microscopy measurements of p53's local diffusivity on non-cognate DNA. We show how a two-mode model accurately predicts the variation in local diffusivity while a single-mode model does not. Our work provides evidence that p53's sliding is indeed functional and suggests that the timing and efficiency of its activating and repressing transcription can depend on its non-cognate binding properties and its ability to change between multiple modes of binding, in addition to the much better-studied effects of cognate-site binding.

12:15PM W40.00004 Single-molecule study of protein-DNA target search mechanisms for dimer-active protein complexes¹ , MARKITA LANDRY, Dept of Chemistry, University of Illinois at Urbana-Champaign, WAI MUN HUANG, Dept of Pathology, University of Utah Health Sciences Center, YANN CHEMLA, Dept of Physics, University of Illinois at Urbana-Champaign — Protein-DNA interactions are essential to cellular processes, many of which require proteins to recognize a specific DNA target-site. This search process is well-documented for monomeric proteins, but not as well understood for systems that require dimerization at the target site for activity. We present a single-molecule study of the target-search mechanism of Protelomerase TelK, a recombinase-like protein that is only active as a dimer. We observe that TelK undergoes 1D diffusion on non-target DNA as a monomer, as expected, but becomes immobile on DNA as a dimer or oligomer despite the absence of its target site. We further show that TelK condenses non-target DNA upon dimerization, forming a tightly bound nucleo-protein complex. Together with simulations, our results suggest a search model whereby monomers diffuse along DNA, and subsequently dimerize to form an active complex on target DNA. These results show that target-finding occurs faster than nonspecific dimerization at biologically relevant protein concentrations. This model may provide insights into the search mechanisms of proteins that are active as multimeric complexes for a more accurate and comprehensive model for the target-search process by sequence specific proteins.

¹NSF (grant 082265, Physics Frontier Center: Center for the Physics of Living Cells). M.P.L. acknowledges a NSF Graduate Research Fellowship (Grant No. 0913128) and an EAPSI fellowship (Award ID OISE-0913128)

12:27PM W40.00005 Single-Molecule Encoders for Tracking Motor Proteins on DNA , EVERETT A. LIPMAN, Department of Physics, University of California, Santa Barbara — Devices such as inkjet printers and disk drives track position and velocity using optical encoders, which produce periodic signals precisely synchronized with linear or rotational motion. We have implemented this technique at the nanometer scale by labeling DNA with regularly spaced fluorescent dyes. The resulting molecular encoders can be used in several ways for high-resolution continuous tracking of individual motor proteins. These measurements do not require mechanical coupling to macroscopic instrumentation, are automatically calibrated by the underlying structure of DNA, and depend on signal periodicity rather than absolute level. I will describe the synthesis of single-molecule encoders, data from and modeling of experiments on a helicase and a DNA polymerase, and some ideas for future work.

1:03PM W40.00006 Tuning Cargo Travel via Single Motor Velocity , JING XU, University of California, Merced, ZHANYONG SHU, University of California, Irvine, STEPHEN KING, University of Central Florida, STEVEN GROSS, University of California, Irvine — Active intracellular transport is crucial for cell function, and defects are linked to diseases including neurodegeneration. Single molecule biophysical studies have revealed a great deal about the function of individual motors in vitro. However, it remains challenging to use single molecule properties of molecular motors to explain the complex range of cargo motions observed in vivo, in particular how motors work together in small ensembles. Recent reports have highlighted the sensitivity of ensemble transport to the single motor properties of processivity and force production. Here we investigate the previously unexplored role of motor velocity, and report a combined experimental and theoretical demonstration that single motor velocity crucially controls the ensemble function of two-motor transport.

1:15PM W40.00007 Study of Large Multimeric Biomolecules by Single-Molecule Manipulation and Imaging , KAI LOU, SITARA S. WIJERATNE, Department of Physics and Astronomy, Rice University, JERAHME MARTINEZ, Department of Biochemistry and Cell biology, Rice University, HUI-CHUN YEH, Puget Sound Blood Center and Division of Hematology, Department of Medicine, University of Washington, JOEL MOAKE, Department of Bioengineering, Rice University, JING-FEI DONG, Puget Sound Blood Center and Division of Hematology, Department of Medicine, University of Washington, MARY C. FARACH-CARSON, Department of Biochemistry and Cell biology, Rice University, CHING-HWA KIANG, Department of Physics and Astronomy, Rice University — Single-molecule manipulation enables us to study the properties of long chain, multimeric biomolecules. Perlecan, a giant secreted heparin sulfate proteoglycan, is a major component of basement membrane, bone stroma and blood vessels. It is involved in processes such as cell adhesion, migration and modulation of apoptosis. The changes in its synthesis and function are closely associated with many diseases, including cancer. Von Willebrand factor is a large multimeric protein circulating in blood, and is crucial for initiation of blood coagulation. We use atomic force microscope to obtain force curves and images of these proteins. We characterized the mechanical property of perlecan as well as the domain conformational changes of von Willebrand factor. The results demonstrate that single-molecule manipulation can probe directly the dynamics of large biomolecules that are usually not accessible with other methods.

1:27PM W40.00008 Uncovering the microscopic mechanism of strand exchange during RecA mediated homologous recombination using all-atom molecular dynamics simulations¹, MANISH SHANKLA, JEJOONG YOO, ALEKSEI AKSIMENTIEV, University of Illinois at Urbana-Champaign — Homologous recombination (HR) is a key step during the repair process of double-stranded DNA (dsDNA) breakage. RecA is a protein that mediates HR in bacteria. RecA monomers polymerize on a single-stranded DNA (ssDNA) separated from the broken dsDNA to form a helical filament, thus allowing strand exchange to occur. Recent crystal structures depict each RecA monomer in contact with three contiguous nucleotides called DNA triplets. Surprisingly, the conformation of each triplet is similar to that of a triplet in B-form DNA. However, in the filament the neighboring triplets are separated by loops of the RecA proteins. Single molecule experiments demonstrated that strand exchange propagation occurs in 3 base-pair increments. However, the temporal resolution of the experiments was insufficient to determine the exact molecular mechanism of the triplet propagation. Using all-atom molecular dynamics simulations, we investigated the effect of both the RecA protein and the conformation of the bound ssDNA fragment on the stability of the duplex DNA intermediate formed during the strand-exchange process. Specifically, we report simulations of force-induced unzipping of duplex DNA in the presence and absence of the RecA filament that explored the effect of the triplet ladder conformation.

¹This work was supported by the Center for the Physics of Living Cells through a grant from the National Science Foundation (PHY0822613).

1:39PM W40.00009 Transduction of Glycan-Lectin Binding using Near Infrared Fluorescent Single Walled Carbon Nanotubes for Glycan Profiling, NIGEL REUEL, JIN-HO AHN, MIT - Chemical Engineering, JONG-HO KIM, Hanyang University, Ansan, Republic of Korea, JINGQING ZHANG, ARDEMIS BOGHOSSIAN, MIT - Chemical Engineering, LARA MAHAL, NYU - Chemistry, MICHAEL STRANO¹, MIT - Chemical Engineering — In this work, we demonstrate a sensor array employing recombinant lectins as glycan recognition sites tethered via Histidine tags to Ni²⁺ complexes that act as fluorescent quenchers for semi-conducting single walled carbon nanotubes embedded in a chitosan to measure binding kinetics of model glycans. Two higher-affined glycan-lectin pairs are explored: fucose (Fuc) to PA-IIL and N-acetylglucosamine (GlcNAc) to GafD. The dissociation constants (KD) for these pairs as free glycans (106 and 19 μ M respectively) and streptavidin-tethered (142 and 50 μ M respectively) were found. The absolute detection limit for the current platform was found to be 2 μ g of glycosylated protein or 100 ng of free glycan to 20 μ g of lectin. Glycan detection is demonstrated at the single nanotube level (GlcNAc to GafD). Over a population of 1000 nanotubes, 289 of the SWNT sensors had signals strong enough to yield kinetic information (KD of $250 \pm 10 \mu$ M). We are also able to identify the locations of "strong-transducers" on the basis of dissociation constant (4 sensors with KD < 10 μ M) or overall signal modulation (8 sensors with > 5% quench response). The ability to pinpoint strong-binding, single sensors is promising to build a nanoarray of glycan-lectin transducers as a method to profile glycans without protein labeling or glycan liberation pretreatment steps.

¹Corresponding Author

1:51PM W40.00010 Comprehensive single molecule dynamics and functions of lysozyme upon linear and cross-linked substrate using a carbon nanotube circuit, YONGKI CHOI, PATRICK C. SIMS, BRAD L. CORSO, Department of Physics and Astronomy, University of California, Irvine, ISSA S. MOODY, Department of Molecular Biology, University of California, Irvine, DAVID SEITZ, LARRY BLASZCAZK, Muroplex Therapeutics, Inc., GREGORY A. WEISS, Department of Molecular Biology, University of California, Irvine, PHILIP G. COLLINS, Department of Physics and Astronomy, University of California, Irvine — The dynamic processivity of individual lysozyme molecules was monitored in the presence of either linear or cross-linked peptidoglycan substrates using a single-walled carbon nanotube transistor. The substrate-driven, hinge bending motions of lysozyme induce dynamic electronic signals in the underlying transistor to allow long-term monitoring of the same molecule, all without the limitations of fluorophore quenching or bleaching. For both types of substrates, lysozyme exhibits slow, processive turnover at 20 Hz and also rapid, nonproductive motions at 300 Hz. However, the latter type of motion nearly vanishes with the linear substrate, which lacks cross-links. Specifically, the nonproductive binding fills 43% of the enzyme's total activity when the substrate has cross-links, but only 7% with the cross-links are absent. The continuous, uninterrupted processing indicates that lysozyme can catalytically hydrolyze glycosidic bonds all the way to the end of a linear substrate, and that the motion attributed to nonproductive binding may be the lysozyme sidestepping the peptide cross-links.

2:03PM W40.00011 A hierarchical coarse-grained (all-atom to all residue) approach to peptides (P1, P2) binding with a graphene sheet¹, RAS PANDEY, University of Southern Mississippi, ZHIFENG KUANG, BARRY FARMER, SANG KIM, RAJESH NAIK, Air Force Research Laboratory — Recently, Kim et al. [1] have found that peptides P1: HSSYWAFNNKT and P2: EPLQLKM bind selectively to graphene surfaces and edges respectively which are critical in modulating both the mechanical as well as electronic transport properties of graphene. Such distinctions in binding sites (edge versus surface) observed in electron micrographs were verified by computer simulation by an all-atomic model that captures the pi-pi bonding. We propose a hierarchical approach that involves input from the all-atom Molecular Dynamics (MD) study (with atomistic detail) into a coarse-grained Monte Carlo simulation to extend this study further to a larger scale. The binding energy of a free amino acid with the graphene sheet from all-atom simulation is used in the interaction parameter for the coarse-grained approach. Peptide chain executes its stochastic motion with the Metropolis algorithm. We investigate a number of local and global physical quantities and find that peptide P1 is likely to bind more strongly to graphene sheet than P2 and that it is anchored by three residues ⁴Y⁵W⁶Y. [1] S.N. Kim et al J. Am. Chem. Soc. 133, 14480 (2011).

¹This work is supported by the Air Force Research Laboratory.

Thursday, March 1, 2012 11:15AM - 2:03PM –
Session W41 DBIO: Focus Session: Quantum Coherence in Biological Systems 156B

11:15AM W41.00001 Quantum Coherence in Biology, BIRGITTA WHALEY, University of California, Berkeley — Discussion of quantum mechanical effects in biology is generally restricted to molecular energetics, stability, and kinetics as determined by potential energy barriers. In recent years however, an increasing number of experiments have shown evidence for the existence of dynamical phenomena in biological systems that involve coherent quantum motion. One prominent instance is electronic quantum coherence in photosynthesis. I shall present theoretical studies that analyze the nature of this coherence, its relation to the non-local quantum correlations characteristic of entanglement, implications for relevance of quantum information processing in natural systems and address the question of whether and how such quantum coherence might result in a biological advantage.

11:51AM W41.00002 Absence of quantum oscillations in electronic excitation transfer in the Fenna-Matthews-Olson complex¹, ALEXANDER EISFELD, Harvard University, GERHARD RITSCH, JAN RODEN, Max-Planck-Institute for the Physics of Complex Systems, WALTER STRUNZ, TU Dresden, ALAN ASPURU-GUZIK, Harvard University — Energy transfer in the photosynthetic Fenna-Matthews-Olson (FMO) complex of the Green Sulfur Bacteria is studied theoretically taking all three subunits (monomers) of the FMO trimer and the recently found eighth bacteriochlorophyll (BChl) molecule into account. For the calculations we use the efficient Non-Markovian Quantum State diffusion approach. Since it is believed that the eighth BChl is located near the main light harvesting antenna we look at the differences in transfer between the situation when BChl 8 is initially excited and the usually considered case when BChl 1 or 6 is initially excited. We find strong differences in the transfer dynamics, both qualitatively and quantitatively. When the excited state dynamics is initialized at site eight of the FMO complex, we see a slow exponential-like decay of the excitation. This is in contrast to the oscillations and a relatively fast transfer that occurs when only seven sites or initialization at sites 1 and 6 is considered. Additionally we show that differences in the values of the electronic transition energies found in the literature lead to a large difference in the transfer dynamics.

¹AE acknowledges financial support from the DFG under Contract No. Ei 872/1-1

12:03PM W41.00003 Progress Towards Room-Temperature Electron Spin Detection in Biological Systems, NICHOLAS CHISHOLM, IGOR LOVCHINSKY, ALEX SUSHKOV, Harvard University, DAVID HUNGER, Ludwig-Maximilians-Universität (LMU) Munich, ALEXEY AKIMOV, Lebedev Physics Institute, PEGGY LO, AMY SUTTON, JACOB ROBINSON, NORMAN YAO, STEVEN BENNETT, HONGKUN PARK, MIKHAIL LUKIN, Harvard University — We report on recent progress of room-temperature electron spin sensing for biological applications using nitrogen-vacancy (NV) centers in diamond. Our approach involves room-temperature detection of a small number of electron spins, situated outside the measurement substrate. Potential applications will be discussed, including detection of magnetic resonance signals from individual electron or nuclear spins of complex biological molecules, measurement of concentrations of radicals in living cells, and monitoring the ion channel function across cell membranes (important for exploring drug delivery mechanisms).

12:15PM W41.00004 Coherent transfer in biological systems: a study of the role of environmental noise, NAYELI ZUNIGA-HANSEN, MARK S. BYRD, Southern Illinois University Carbondale — We study the effects of environmental noise on quantum mechanical systems, we focus mainly on biological systems in which noise is believed to assist coherent transport of energy. We use error correction methods aimed at avoiding decoherence and dissipation due to coupling to a reservoir, with the purpose of investigating if modifying the coupling to a noisy bath can provide further insight on its effects on transport mechanisms, and propose that this work is carried out experimentally.

12:27PM W41.00005 Noise induced quantum effects in photosynthetic complexes, KONSTANTIN DORFMAN, DMITRI VORONINE, Texas A&M University, College Station, Texas 77843, SHAUL MUKAMEL, University of California, Irvine, California 92697, MARLAN SCULLY, Texas A&M University, College Station, Texas 77843 — Recent progress in coherent multidimensional optical spectroscopy revealed effects of quantum coherence coupled to population leading to population oscillations as evidence of quantum transport. Their description requires reevaluation of the currently used methods and approximations. We identify couplings between coherences and populations as the noise-induced cross-terms in the master equation generated via Agarwal-Fano interference that have been shown earlier to enhance the quantum yield in a photocell. We investigated a broad range of typical parameter regimes, which may be applied to a variety of photosynthetic complexes. We demonstrate that quantum coherence may be induced in photosynthetic complexes under natural conditions of incoherent light from the sun. This demonstrates that a photosynthetic reaction center may be viewed as a biological quantum heat engine that transforms high-energy thermal photon radiation into low entropy electron flux.

12:39PM W41.00006 FMO complex: exciton transfer and interaction with vibronic modes, LEV MOUROKH, Physics Department, Queens College of CUNY, ANATOLY SMIRNOV, FRANCO NORI, Frontier Research System, RIKEN, Japan and Physics Department, The University of Michigan — We examine transport of excitons through Fenna-Matthews-Olson (FMO) complex from a receiving antenna to a reaction center, using methods of condensed matter and statistical physics. Writing equation of motion for creation/annihilation operators, we are able to describe the exciton dynamics in the regime when the reorganization energy is of the order of the intra-system couplings. Well-known quantum oscillations of the site populations are obtained, in particular. We determine the exciton transfer efficiency and its dependencies of the system parameters. While the majority of vibronic modes are treated as a heat bath, we address the situation when specific modes are strongly coupled to excitons and examine the effects of these modes on the quantum oscillations and the energy transfer efficiency.

12:51PM W41.00007 Non-Markovian harmonic bath model for molecular systems: Influence of the bath spectral density, JAN RODEN, Department of Chemistry, University of California, Berkeley, California 94720, USA, ALEXANDER EISFELD, Department of Chemistry and Chemical Biology, Harvard University, 12 Oxford Street, Cambridge, MA 02138, K. BIRGITTA WHALEY, Department of Chemistry, University of California, Berkeley, California 94720, USA — In quantum mechanical simulations of the electronic excitation dynamics in molecular complexes, like natural or artificial light-harvesting complexes, often open quantum system descriptions are applied, to treat a large number of degrees of freedom involved. A popular approach is then, to include only the electronic degrees of freedom into the system part and to couple them to a non-Markovian bath of harmonic vibrational modes. The coupling to the bath, representing intra-molecular as well as external vibrations, is usually described via the bath spectral density, which therefore is an important ingredient in this approach. Here, we discuss different aspects of the influence of the bath spectral density on dynamics and optical spectra. In particular, we consider structured spectral densities, consisting of multiple broadened peaks. It is often assumed that the strong coupling to an intra-molecular vibrational mode, which is damped by coupling to other vibrational modes, is described reasonably by such a broadened peak in the spectral density. Here we demonstrate that this interpretation should be used with caution, because the damping of the mode differs from the model for an intra-molecular mode that one would usually apply when including the mode directly in the system part.

1:03PM W41.00008 Curvature, torsion and temperature in energy transfer, YASSER OMAR, ISEG, Technical University of Lisbon & Instituto de Telecomunicações — Curvature and torsion can play a role in energy transfer in alpha-helical proteins [New J. Phys. 12, 055003 (2010)]. The phenomenon is specific to alpha-helices and not to beta-sheets in proteins due to the three strands of hydrogen bonds constituting the alpha-helical backbone. In this work we analyse and discuss how temperature can affect the role of geometry in the energy transfer.

1:15PM W41.00009 Quantum Process Tomography for Energy Transfer Systems via Ultrafast Spectroscopy, JOEL YUEN-ZHOU, Harvard University, Chemistry and Chemical Biology — The description of excited state dynamics in energy transfer systems constitutes a theoretical and experimental challenge in modern chemical physics. A spectroscopic protocol that systematically characterizes both coherent and dissipative processes of the probed chromophores is desired [1,2]. In this talk, I show that a set of two-color photon-echo experiments performs quantum state tomography (QST) of the one-exciton manifold of a dimer by reconstructing its density matrix in real time. This possibility in turn allows for a complete description of excited state dynamics via quantum process tomography (QPT). Simulations of a noisy QPT experiment for an inhomogeneously broadened ensemble of model excitonic dimers show that the protocol distills rich information about dissipative excitonic dynamics, which appears nontrivially hidden in the signal monitored in single realizations of four-wave mixing experiments. Progress on the experimental side will be discussed, as well as new insights that QPT has offered on the understanding of 2D electronic and vibrational spectroscopy. [1] J. Yuen-Zhou, J. J. Krich, A. Aspuru-Guzik, Quantum state and process tomography of energy transfer systems via ultrafast spectroscopy Joel Yuen-Zhou, Jacob J. Krich, Masoud Mohseni and Alán Aspuru-Guzik Proc. Nat. Acad. Sci. USA, Early Edition (2011). [2] J. Yuen-Zhou, A. Aspuru-Guzik, Quantum process tomography of molecular dimers from two-dimensional electronic spectroscopy I: General theory and application to homodimers Joel Yuen-Zhou and Alán Aspuru-Guzik. Chem. Phys. 134, 134505 (2011).

1:27PM W41.00010 Coherent vs. dissipative nonequilibrium dynamics in spectroscopy of molecular aggregates¹, DARIUS ABRAMAVICIUS, ANDRIUS GELZINIS, VYTAUTAS BUTKUS, LEONAS VALKUNAS, Physics Faculty, Vilnius University, Sauletekio al. 9, 10222 Vilnius, Lithuania — Molecular aggregates embedded in a protein environment are the core elements in photosynthetic antennae units. Photoexcitations in these systems experience multistep relaxation, which could be traced using various time-resolved spectroscopy techniques. Initiated coherent processes turn into dissipative. Understanding of these processes is still a major theoretical task. We study theoretically spectroscopic properties of simple molecular aggregates coupled to a bath, which contains main ingredients of protein environment: high-energy vibrations, long-range correlations, and smooth spectrum of frequencies. At short times after the optical excitation high-energy coherent vibrational resonances can be observed in two-dimensional repumping spectroscopy. Their beats overlap with electronic quantum coherences, responsible for the quantum transport. We show the way to discriminate between them. At the long times we find that the conventional excitonic picture of eigenstates is valid only in the Markovian regime. In the non-Markovian regime the exciton concept breaks down and renormalized system parameters must be introduced: effective intermolecular coupling, widely used in polaron theories, can be used to account for the effects of the bath.

¹Support of Research Council of Lithuania Grant No. VP1-3.1-SMM-07-K-01-020 is greatly acknowledged

1:39PM W41.00011 New quantum state of protons and electrons in nano-confined water¹, GEORGE REITER, University of Houston, ALEXANDER KOLESNIKOV, ORNL, STEPHEN PADDISON, University of Tennessee, Knoxville, JERRY MAYERS, ISIS, PHIL PLATZMAN, University of Houston — Neutron Compton Scattering provides a means of directly and accurately measuring the momentum distribution of protons in water, which is determined primarily by the protons ground state wavefunction. We find that in water confined on scales of $\sim 20\text{\AA}$, this wave function responds to the details of the confinement, corresponds to a strongly anharmonic local potential, shows evidence in some cases of coherent delocalization in double wells, and involves differences in zero point kinetic energy of the protons from that of bulk water at room temperature of -40 to $+120$ meV. This behavior is a generic feature of nanoscale confinement, and in particular, this state should be that which is present in water confined in biological cells. It is exhibited here in $16\text{\AA}$ inner diameter carbon nanotubes, two different hydrated proton exchange membranes (PEMs), Nafion 1120 and Dow 858, and has been seen earlier in xerogel and $14\text{\AA}$ diameter carbon nanotubes. The existence of this state is confirmed by x-ray Compton scattering measurements of the electron momentum distribution.

¹G. Reiter's work was supported by the DOE, Office of Basic Energy Sciences, Contract No.DE-FG02-08ER46486. Work at ORNL was managed by UT-Battelle, under DOE contract DE-AC05-00OR22725.

1:51PM W41.00012 Spectroscopic Characterization of the Water Oxidation Intermediates in the Blue Dimer Ru-Based Catalyst for Artificial Photosynthesis¹, DOOSHAYE MOONSHIRAM, YULIA PUSHKAR, Purdue University, JONAH JURSS, JAVIER CONCEPCION, THOMAS MEYER, University of North Carolina at Chapel Hill, TAI SIYA ZAKHAROVA, IGOR ALPEROVICH, Purdue University — Utilization of sunlight requires solar capture, light-to-energy conversion and storage. One effective way to store energy is to convert it into chemical energy by fuel-forming reactions, such as water splitting into hydrogen and oxygen. Ruthenium complexes are among few molecular-defined catalysts capable of water splitting. Mechanistic insights about such catalysts can be acquired by spectroscopic analysis of short-lived intermediates of catalytic water oxidation. Use of techniques such as EPR and X-ray absorption spectroscopy (XAS) are used to determine electronic requirements of catalytic water oxidation. About 30 years ago Meyer and coworkers reported first ruthenium-based catalyst for water oxidation, the "blue dimer". We performed EPR studies and characterized structures and electronic configurations of intermediates of water oxidation by the "blue dimer". Intermediates were prepared chemically by oxidation of Ru-complexes with defined number of Ce (IV) equivalents and freeze-quenched at controlled times. Changes in oxidation state of Ru atom were detected by XANES at Ru K-edges. K-edges are sensitive to changes in Ru oxidation state for Blue Dimer $[3,3]^{4+}$, $[3,4]^{4+}$, $[3,4]^{4+}$ and $[4,5]^{3+}$ allowing a clear assignment of Ru oxidation state in intermediates. EXAFS demonstrated structural changes.

¹DOE

Thursday, March 1, 2012 11:15AM - 2:15PM —
Session W42 DBIO DPOLY: Focus Session: The Physics of Genome Folding I: Fractal Globules and Condensed Polymer States 156C

11:15AM W42.00001 How the genome folds¹, EREZ LIEBERMAN AIDEN, Harvard Society of Fellows — I describe Hi-C, a novel technology for probing the three-dimensional architecture of whole genomes by coupling proximity-based ligation with massively parallel sequencing. Working with collaborators at the Broad Institute and UMass Medical School, we used Hi-C to construct spatial proximity maps of the human genome at a resolution of 1Mb. These maps confirm the presence of chromosome territories and the spatial proximity of small, gene-rich chromosomes. We identified an additional level of genome organization that is characterized by the spatial segregation of open and closed chromatin to form two genome-wide compartments. At the megabase scale, the chromatin conformation is consistent with a fractal globule, a knot-free conformation that enables maximally dense packing while preserving the ability to easily fold and unfold any genomic locus. The fractal globule is distinct from the more commonly used globular equilibrium model. Our results demonstrate the power of Hi-C to map the dynamic conformations of whole genomes.

¹E.L.A. is supported by NIH Grants 1P50HG006193-01 (Center for Cell Circuits) and 1DP2OD008540-01 (NIH New Innovator Award).

11:51AM W42.00002 Contact probability scaling of the Hilbert curve¹ , ADRIAN SANBORN, JIAN LI, Harvard College, EREZ L. AIDEN, Harvard Society of Fellows — Using Hi-C experiments, it has become possible to measure contact probability scalings for genomic polymers. However, the theoretical analysis of such scalings remains in its infancy. Here, we prove that contact probability scales with linear distance for lattice approximations of the Hilbert curve. These results point to the potential for new theoretical approaches to the study of contact probability, and shed light on the analysis behind the fractal globule, a recent model for the three-dimensional structure of the human genome.

¹This work is supported by NIH Grants 1P50HG006193-01 (Center for Cell Circuits) and 1DP2OD008540-01 (NIH New Innovator Award).

12:03PM W42.00003 Territorial Polymers and Large Scale Genome Organization , ALEXANDER GROSBERG, New York University, Center for Soft Matter Research and Department of Physics — Chromatin fiber in interphase nucleus represents effectively a very long polymer packed in a restricted volume. Although polymer models of chromatin organization were considered, most of them disregard the fact that DNA has to stay not too entangled in order to function properly. One polymer model with no entanglements is the melt of unknotted unconcatenated rings. Extensive simulations indicate that rings in the melt at large length (monomer numbers) N approach the compact state, with gyration radius scaling as $N^{1/3}$, suggesting every ring being compact and segregated from the surrounding rings. The segregation is consistent with the known phenomenon of chromosome territories. Surface exponent β (describing the number of contacts between neighboring rings scaling as N^β) appears only slightly below unity, $\beta \approx 0.95$. This suggests that the loop factor (probability to meet for two monomers linear distance s apart) should decay as $s^{-\gamma}$, where $\gamma = 2 - \beta$ is slightly above one. The later result is consistent with HiC data on real human interphase chromosomes, and does not contradict to the older FISH data. The dynamics of rings in the melt indicates that the motion of one ring remains subdiffusive on the time scale well above the stress relaxation time.

12:39PM W42.00004 Diffusion of Particles in the Melt of Polymeric Rings and Diffusion of Proteins in the Cell Nucleus¹ , KURT KREMER, Max Planck Institute for Polymer Research, Mainz, Germany, JONATHAN HALVERSON, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY, GARY GREEST, Center for Integrated Nanotechnologies, Sandia National Laboratories, Albuquerque, NM, ALEXANDER GROSBERG, Department of Physics, New York University, New York, NY — Ring polymers in the melt are partially collapsed and partially segregated as revealed by both simulation and experiment. This behavior is qualitatively consistent with the arrangement of chromosomes in the cell nucleus which are found in distinct territories. Working under the hypothesis that a melt of nonconcatenated rings serves as a simple model for the packing of chromatin fibers in the nucleus of higher eukaryotes, we have investigated the dynamic behavior of a non-sticky spherical particle in polymer melts composed of rings using molecular dynamics simulation. Linear chains are also studied for comparison. In the case of rings such systems are thought to represent protein diffusion in the cell nucleus. The sub-diffusive motion of the particle is found to be independent of the polymer architecture and chain length but depends strongly on particle size. The long-time behavior suggests that these particles diffuse faster in the rings. We compare our results to existing models of protein diffusion.

¹Research carried out in part at the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

12:51PM W42.00005 Spatial autocorrelation in fractal and knotted globules , MIRIAM HUNTLEY, EREZ LIEBERMAN AIDEN, Harvard University — The unknotted fractal globule is a model for the state of nuclear chromatin, and has properties that are distinct from those of knotted globules. One crucial property is a stronger correspondence between one-dimensional position along the polymer contour and three-dimensional position in the bulk. Here we introduce measures of spatial autocorrelation, such as Moran's I and Geary's C, and investigate spatial autocorrelation in both fractal and knotted globules. We show that fractal globules exhibit higher levels of spatial autocorrelation at both small and intermediate length scales. This autocorrelation may be relevant to the study of how proteins find their DNA targets inside the nucleus.

1:03PM W42.00006 Simulation of Interphase DNA , RALF EVERAERS, Ecole Normale Supérieure de Lyon — No abstract available.

1:39PM W42.00007 In silico simulations of polymer condensation: the fractal globule as a metastable state¹ , LEON FURCHTGOTT*, ASHOK CUTKOSKY*, NAJEEB TARAZI, Harvard University, EREZ LIEBERMAN AIDEN, Harvard Society of Fellows — The fractal globule is a model for the metastable conformation of a long polymer after initial immersion in a poor solvent. Recent experimental findings describing the conformation of the human genome at the megabase scale are consistent with a fractal globule conformation. Here, we simulate the collapse of a polymer in a poor solvent using both molecular dynamics and Monte-Carlo simulations. We show that the statistics of the resulting configuration, such as radius of gyration, end-to-end distance, and contact probability, are independent of the approach used to simulate the condensation process. (* contributed equally).

¹This work is supported by NIH Grants 1P50HG006193-01 (Center for Cell Circuits) and 1DP2OD008540-01 (NIH New Innovator Award).

1:51PM W42.00008 Fractal Globule as a model of DNA folding in eukaryotes , MAKSIM IMAKAEV, LEONID MIRNY, Massachusetts Institute of Technology — A recent study (Lieberman-Aiden et al., Science, 2009) observed that the structure of the genome, on the scale of a few megabases, is consistent with a fractal globule. The fractal globule is a quasi-equilibrium state of a polymer after a rapid collapse. First proposed theoretically in 1988, this structure had never been simulated. Fractal globule was seen as a state, in which each subchain is compact, and doesn't mix with other subchains due to their mutual unentanglement (topological constraints). We use GPU-assisted dynamics to create fractal globules of different sizes and observe their dynamics. Our simulations confirm that a polymer after rapid collapse has compact subchains. We measure the scaling of looping probability of a subchain with its length, and observe the remarkably robust inverse proportionality. Dynamic simulation of the equilibration of this state show that it exhibits Rose type subdiffusion. Due to diffusion, fractal globule quickly degrades to a quasi-equilibrium state, in which subchains of a polymer are mixed, but topologically unentangled. We propose that separation of spatial and topological equilibration of a polymer chain might have implications in different fields of physics.

2:03PM W42.00009 High-order chromatin architecture shapes the landscape of chromosomal alterations in cancer¹ , GEOFFREY FUDENBERG, Harvard, GAD GETZ, MATTHEW MEYERSON, Broad Institute, LEONID MIRNY, MIT — The rapid growth of cancer genome structural information provides an opportunity for a better understanding of the mutational mechanisms of genomic alterations in cancer and the forces of selection that act upon them. Here we test the evidence for two major forces, spatial chromosome structure and purifying (or negative) selection, that shape the landscape of somatic copy-number alterations (SCNAs) in cancer (Beroukhi et al, 2010). Using a maximum likelihood framework we compare SCNA maps and three-dimensional genome architecture as determined by genome-wide chromosome conformation capture (HiC) and described by the proposed fractal-globule (FG) model (Lieberman-Aiden and Van Berkum et al, 2009). This analysis provides evidence that the distribution of chromosomal alterations in cancer is spatially related to three-dimensional genomic architecture and additionally suggests that purifying selection as well as positive selection shapes the landscape of SCNAs during somatic evolution of cancer cells.

¹Physical Sciences Oncology Center at MIT (U54CA143874)

Thursday, March 1, 2012 11:15AM - 2:15PM –

Session W43 DBIO DPOLY: Invited Session: Physical Mechanisms of Collective Microbial Dynamics 157AB

11:15AM W43.00001 Chiral patterning in *Paenibacillus* colonies under stress, HERBERT LEVINE, University of California, San Diego — One of the most striking examples of bacterial colony patterning occurs in the C-morphotype of *Paenibacillus* strains. Here, macroscopic chirality results from the interaction of local liquid-crystal ordering of the long bacterial cells with the self-propelled motility driven by the non-reflection-symmetric flagella. This talk will review some of the original experimental data from the Ben-Jacob lab as well as recent insight obtained via genomics. I will then discuss attempts to model and simulate the chiral patterns via solving reaction-diffusion equations on random lattices. At the end, I will introduce the challenges still to be faced in understanding transitions between these patterns and more common branching structures

11:51AM W43.00002 The effects of self-induced noise on the onset of collective behavior in suspensions of swimming bacteria¹, IGOR ARONSON, Argonne National Laboratory, 9700 South Cass Av, Argonne, IL60439 — Collective dynamics of self-locomoting micro-organisms, such as bacteria and algae have attracted enormous attention, with a large number of experimental and theoretical works published in the last few years. A plethora of nontrivial properties have been predicted and consequently studied, including dynamic instabilities, anomalous density fluctuations, nontrivial stress-strain relations, rectification of chaotic motion, and viscosity reduction. Here we investigate the viscosity of a suspension of swimming bacteria analytically and numerically. We propose a simple model that takes into account excluded volume constraints and allows for efficient computation for a large number of bacteria. Our calculations show that long-range hydrodynamic interactions, intrinsic to self-locomoting objects in a viscous fluid, result in a dramatic reduction of the effective viscosity. In agreement with experiments on suspensions of *Bacillus subtilis*, we show that the viscosity reduction is related to the onset of large-scale collective motion due to interactions between the swimmers. The simulations reveal that the viscosity reduction occurs only for relatively low concentrations of swimmers: further increases of the concentration yield an increase of the viscosity. We derive an explicit asymptotic formula for the effective viscosity in terms of known physical parameters and show that hydrodynamic interactions are manifested as self-induced noise in the absence of any explicit stochasticity in the system. We also explain the increase in the viscosity for pullers by analysis of the deviations from the mean field approximation

¹The work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering, under Contract DE-AC02-06CH11357.

12:27PM W43.00003 Synchronization of flagella, THOMAS R. POWERS, Brown University — Motivated by the observed coordination of nearby beating flagella, we use highly controlled simple model experiments with rotating paddles to study how hydrodynamic interactions can lead to phase-locking. The agreement between our numerical models and experimental results confirms that hydrodynamic interactions can lead to synchronization or phase-locking if the system has sufficient flexibility. We also present a simple theory, valid for weakly interacting paddles, for both viscous and viscoelastic fluids.

1:03PM W43.00004 Formation and propagation of high density waves during swarming of *P. aeruginosa*¹, MARK ALBER, Department of Applied and Computational Mathematics and Statistics, University of Notre Dame — We will describe in this talk how the bacterium *P. aeruginosa* alters its local physical environment by propagating high density waves of cells into branched tendrils during surface motility described as swarming. Biologically justified model simulations will be used to suggest a mechanism of wave propagation and branched tendril formation that depend upon competition between the changing viscosity of the bacterial liquid suspension and the liquid film boundary expansion caused by Marangoni forces. Thus, *P. aeruginosa* controls physical forces responsible for liquid film expansion to efficiently colonize surfaces.

¹This research was partially supported by NIH grant 1R01GM100470-01

1:39PM W43.00005 Alignment vs noise in self-propelled particles: minimal models for collective motion and their continuous descriptions, HUGUES CHATE, CEA - Saclay — Two important 1995 papers have marked the birth of collective motion studies in physics: Vicsek et al introduced what could now be described as the "Ising model" of this new subfield. This prompted Toner and Tu to propose a continuum theory of flocks which they showed to give rise to long-range orientational order even in two space dimensions. In this setting, the complexity of most natural instances of collective motion is reduced to the competition between local alignment and noise in interacting self-propelled particles. As I will show, this nevertheless gives rise to important and new physics. In this talk, I will give an update of our current knowledge about the Vicsek model, the Toner-Tu theory, and their relationship. I will also present the emerging picture of universality classes brought about by recent progress in the study of Vicsek-like models together with their continuous descriptions.

Thursday, March 1, 2012 11:15AM - 2:15PM –

Session W44 DPOLY: Focus Session: Interparticle Interactions in Polymer Nanocomposites - Mechanical, Electrical, and Optical Properties 157C

11:15AM W44.00001 Bio-inspired Fillers for Mechanical Enhancement, LASHANDA KORLEY, Case Western Reserve University — An examination of natural materials has offered a new perspective on the development of multi-functional materials with enhanced mechanical properties. One important lesson from nature is the utilization of composite structures to impart improved mechanical behavior and enhanced functionality using nanofillers. A relatively unexplored expansion of this bio-inspired, nanoscale filler approach to high performance materials is the incorporation of responsive, multi-functional reinforcing elements in polymeric composites with the goal of combining superior mechanical behavior that can be tuned with additional functionality, such as sensing and bioactivity. One approach is the use of self-assembling small molecules that form uniform, one-dimensional nanostructures as an emerging class of filler components. Another pathway toward mechanical enhancement is the incorporation of stimuli-responsive and high-modulus electrospun nanofibers. We have probed the utilization of high-aspect ratio, self-assembled small molecules and responsive electrospun nanofibers as all-organic nanofillers to achieve significant modulus changes within elastomeric matrices. The influence of matrix-filler interactions and the role of hierarchical organization in these nature-inspired composites will be discussed. Potential applications in barrier technology and drug delivery have also been explored.

11:51AM W44.00002 Temperature sensitive mechanical properties of Graphene-epoxy nanocomposites¹, ARDAVAN ZANDIATASHBAR, CATALIN PICU, NIKHIL KORATKAR, Rensselaer Polytechnic Institute — Carbon-based polymeric nanocomposites have potential applications including structural parts in aerospace vehicles and civil infrastructure. In this work various aspects of mechanical properties of Graphene-epoxy nanocomposites are studied at different scales. The quasi-static tensile yield stress and stiffness of the nanocomposite are larger than those of neat epoxy. While the creep response of the nanocomposite is similar to that of neat epoxy at lower stress and room temperature, a significant discrepancy is observed at high temperature and/or large stress, the nanocomposite creeping less. The fracture toughness for the nanocomposite with the optimum filler fraction is larger than the toughness of unfilled epoxy at room temperature. This difference decreases at higher temperatures. Local mechanical properties were investigated using nanoindentation and similar trends are observed.

¹We gratefully acknowledge support from the NSF under grant CMMI 0900188 and from the ONR under grant N00014-09-1-0928.

12:03PM W44.00003 Mechanical Properties of Polymer Nanocomposites under Large Amplitude Deformation, ERKAN SENSES, PINAR AKCORA, Stevens Institute of Technology — Bare silica nanoparticle dispersion in polystyrene and poly(methyl methacrylate) homopolymers are found to be controlled upon changing the evaporation condition. In this study, we deformed the polymer nanocomposites at different states of particle dispersion under large amplitude oscillatory shearing (LAOS). As the structure evolved during LAOS, the TEM images and small-angle X-ray scattering results obtained for different states of deformation together with the measured moduli allowed us to relate the mechanical reinforcement and nonlinearities such as strain stiffening/softening or shear thinning/thickening to the particle-polymer and particle-particle interactions effective at nanometer dimensions. Our results show that well-dispersed system with attractive interactions between particle and polymer becomes more elastic under large shear and behaves as attractive gels.

12:15PM W44.00004 Polymer Nanocomposite Mechanical Properties as a Function of Nanoparticle Dispersion¹, JOSEPH MOLL, Columbia University, SHUSHAN GONG, RALPH COLBY, Pennsylvania State University, DIMITRIS VLASSOPOULOS, IESL-FORTH, SANAT KUMAR, Columbia University — Nanoparticle (NP) dispersion critically affects the properties of polymer nanocomposites (PNCs), especially mechanical properties. Previous work by our group and others has shown optimal material properties occur when particles form a percolated network. Particle dispersion is a function of the interaction between the polymer and nanoparticle surface, and as such is difficult to control as an independent variable. In our previous work, dispersion was controlled via polymer grafts. Thus in order to vary the particle dispersion states the length and density of the grafted chains were necessarily simultaneously varied. Here we consider bare silica nanoparticles, 14nm in diameter, in 97kg/mol poly(2-vinyl pyridine). Although the particles are bare, the dispersion can still be controlled by proper solvent casting of the material; we use varying amounts of pyridine to charge stabilize the particles in solution and thus vary the dispersion state. We use TEM to probe PNP structure and NP dispersion state, and rheology is used to quantify mechanical properties. We look at the recovery of the storage modulus after large amplitude oscillatory shear and use this to probe the mechanism of particle reinforcement. Because the dispersion is an independently controlled variable, we are able to more accurately quantify its effect on nanocomposites.

¹Funding from: NSF DMR-1006659

12:27PM W44.00005 Elastic Moduli of Polymeric Thin Films of Nanocomposites and Blends via Buckling on Elastomeric Substrates, HONGYI YUAN, JOLANTA MARSZALEK-KEMPKE, Department of Polymer Engineering, The University of Akron, Akron, OH 44325, PRATEEK VERMA, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332, ALAMGIR KARIM, Department of Polymer Engineering, The University of Akron, Akron, OH 44325, THE UNIVERSITY OF AKRON TEAM, GEORGIA INSTITUTE OF TECHNOLOGY TEAM — Mechanical properties are important for the long term durability of polymeric thin films. Unfortunately, there are very few methods for mechanical characterization of sub-micron thin films with high accuracy and repeatability. The technique of Strain-Induced Elastic Buckling Instability for Mechanical Measurements (SIEBIMM) was employed to determine the elastic moduli of nanocomposite and blend films, which were calculated from the buckling patterns generated by applying compressive stresses. In this study, polylactic acid (PLA) / Cloisite 30B nanocomposite thin films and polycaprolactone (PCL) / PLA blend thin films were prepared via spin-coating and then transferred to crosslinked polydimethylsiloxane (PDMS) flexible substrates. Results showed the strengthening effect of Cloisite 30B on PLA systems. The effect of nanoparticle concentrations and the influences of crystallinity and phase separation of blends will be presented.

12:39PM W44.00006 Electrical Conductivity in Transparent Silver Nanowire Networks: Simulations and Experiments, MICHELLE SHERROTT, ROSE MUTISO, University of Pennsylvania, AARON RATHMELL, BENJAMIN WILEY, Duke University, KAREN WINEY, University of Pennsylvania — We model and experimentally measure the electrical conductivity of two-dimensional networks containing finite, conductive cylinders with aspect ratio ranging from 33 to 333. We have previously used our simulations to explore the effects of cylinder orientation and aspect ratio in three-dimensional composites, and now extend the simulation to consider two-dimensional silver nanowire networks. Preliminary results suggest that increasing the aspect ratio and area fraction of these rods significantly decreases the sheet resistance of the film. For all simulated aspect ratios, this sheet resistance approaches a constant value for high area fractions of rods. This implies that regardless of aspect ratio, there is a limiting minimum sheet resistance that is characteristic of the properties of the nanowires. Experimental data from silver nanowire networks will be incorporated into the simulations to define the contact resistance and corroborate experimentally measured sheet resistances of transparent thin films.

12:51PM W44.00007 Effect of Nanowire Size Dispersity and Orientation on Electrical Conductivity in Polymer Nanocomposites, ROSE MUTISO, MICHELLE SHERROTT, University of Pennsylvania, JU LI, Massachusetts Institute of Technology, KAREN WINEY, University of Pennsylvania — We model the percolation threshold (ϕ_c) and electrical conductivity of isotropic and oriented three-dimensional networks containing finite, conductive cylinders with experimentally typical (Gaussian) and engineered (bidisperse) distributions in their length and/or diameter. Our results show that narrow Gaussian distributions do not affect the threshold concentration or electrical conductivity significantly in either isotropic or oriented networks. In contrast, the addition of a small fraction of longer rods in a bidisperse system can improve the electrical properties considerably. We have also successfully extended the excluded volume percolation theory to predict ϕ_c of polydisperse networks of soft-core rods with finite-L/D by generalizing the monodisperse case and applying an empirical calibration factor from our simulations. Our analytical expression finds the critical concentration in nanocomposites with arbitrary distributions in L and/or D.

1:03PM W44.00008 Finite-size effects in nanocomposites: experimental and computational studies, L.I. CLARKE, M.P. ROMAN, E.W. SKAU, D.R. STEVENS, L.N. DOWNEN, T.J. HOFFMAN, J.R. BOCHINSKI, Department of Physics, NC State University — Many proposed applications for electrically-conducting composite materials (smart textiles, e-m shielding coatings, tissue scaffolds) are nanostructured - that is, characteristic sample length scales may be similar to at least one dimension of the embedded particle. This is particularly true for long aspect-ratio particles such as nanotubes where the length of the particle can approach or exceed the thickness of a thin nanocomposite film or a nanofiber diameter. In these cases, the formation of a particle network and thus the electrical conductivity enhancement is affected by finite size effects, that is, percolation thresholds and the width of the transition to percolation differ with sample size [Stevens et al., *Phys. Rev. E* **84**, 021126 (2011)]. We present experimental electrical conductivity and 3-D continuum Monte-Carlo simulation results on such finite-sized percolation effects for particles with aspect ratios of 1 to 1000 and discuss proposed scaling laws and techniques to improve conductance in the finite-size regime.

1:15PM W44.00009 Spectral and polarization modulation of quantum dot emission in a one-dimensional liquid crystal photonic cavity¹, ANDREA RODARTE, C. GRAY, L.S. HIRST, S. GHOSH, University of California, Merced — We demonstrate spectral and polarization modulation of chemically synthesized core shell CdSe/ZnS quantum dots (QDs) embedded in a one-dimensional photonic cavity formed by a cholesteric liquid crystal (CLC) matrix. A Cano-wedge cell varies the pitch of the CLC leading to the formation of Grandjean steps. This spatially tunes the photonic stop band, changing the resonance condition and continuously altering both the emission wavelength and polarization state of the QD ensemble. Using high resolution spatially- and spectrally-resolved photoluminescence measurements we find that the emission is elliptically polarized and that the tilt of the ellipse, while dependent on the emission wavelength, additionally varies with distance across the Grandjean steps. This work opens up the possibility of designing new QD based optical devices, such as tunable single photon sources, where spatial control of wavelength and polarization of the embedded QDs would allow great flexibility and added functionalities.

¹This work is funded by NSF, UC MEXUS and UC MERI

1:27PM W44.00010 Self-assembly of silicon quantum dot clusters in polymer nanocomposites, AUSTIN R. VAN SICKLE, JOSEPH B. MILLER, North Dakota State University, REBECCA R. ANTHONY, UWE R. KORTSHAGEN, University of Minnesota, DANIEL M. KROLL, ERIK K. HOBBIE, North Dakota State University — We measure the influence of polymer-driven silicon nanocrystal (SiNC) self-assembly on the photoluminescent stability of SiNC clusters. Coexisting phases of varying nanoparticle density are identified in annealed SiNC-polymer nanocomposites, and the local photobleaching kinetics are measured under varied exposure to atmospheric oxygen. Increased particle packing and decreased oxygen exposure both contribute to improvements in cluster photostability, with Monte Carlo simulations of ensemble photobleaching clarifying the critical role of nanoparticle packing. The simulations further demonstrate the potential importance of nanoparticle interactions in dictating the photo-response of the self-assembled SiNC clusters.

1:39PM W44.00011 Utilizing photothermal heating by metal nanoparticles within polymer composites, SOMSUBHRA MAITY, JASON BOCHINSKI, LAURA CLARKE, NC State University — Photothermal heating by metal nanoparticles have been extensively researched in solution environments for applications such as cancer treatment and drug delivery, but very few have explored photothermal heating in solids, such as metal nanoparticle-polymer composites. When metal nanoparticles are excited by light resonant with the particle's surface plasmon, non-radiative relaxation efficiently generates heat. Thus, this photothermal effect facilitates *in situ* thermal processing of polymeric materials via externally-controllable light excitation. By embedding fluorophores in the composite, a sensitive relative fluorescence approach can be utilized to dynamically monitor the average temperature within the sample as it is thermally processed. With modest light intensities and dilute nanoparticle concentrations, controllable temperature changes of several hundred degrees Celsius have been achieved. We discuss various cooling mechanisms and their respective effect on the heating process. The spatial specificity and temperatures achieved can potentially be used for triggering phase transitions, cross-linking, or enabling region-specific chemical reactions within a polymeric material.

1:51PM W44.00012 What determines photoluminescence and quenching when fluorophores in a polymer matrix?, HYUNSOOK JANG, University of Connecticut, Institute of Materials Science, YING WANG, YU LEI, University of Connecticut, Chemical, Materials & Biomolecular Engineering, MU-PING NIEH, University of Connecticut, Institute of Materials Science, Chemical, Materials & Biomolecular Engineering — A model system composed of fluorophore (pyrene), dispersed in a polymer matrix (polystyrene, PS) is investigated in order to find the relation between the structure of pyrene assembly in the PS matrix and its fluorescence/quenching. It has been shown that the pyrene disperses differently in the polymer matrix as it is prepared by different processes (namely, electrospin, solution cast and spincoat) with same composition. The difference can result in drastically variation of fluorescence response and quenching efficiency in presence of DNT. Our preliminary data indicate that the salt (tetrabutylammonium hexafluorophosphate, TBAP) applied to electrospinning process plays a crucial role in excimer fluorescence in the emission spectra, while various polymer matrices (e.g., PS and poly-methyl methacrylate, PMMA) yield similar fluorescence without TBAP. X-ray diffraction data suggests that strong dimer fluorescence of the sample may relate to the alignment of pyrene crystal structure, with a lattice length of 8.4 Å. Moreover, a C^{13} solid-state NMR result seems to indicate that the mobility of pyrene in the PS matrix of electrospin system is lower for samples with higher quenching efficiency.

2:03PM W44.00013 Microtextured Omniphobic Surfaces by Solution Spraying of Fluorodecyl POSS/PMMA Blends, SIDDARTH SRINIVASAN, GARETH MCKINLEY, ROBERT COHEN, Massachusetts Institute of Technology — We present a simple technique to prepare various micro-structured surfaces by spray coating a polymer blend of poly(methyl methacrylate) (PMMA) and the low surface energy molecule 1H,1H,2H,2H-heptadecafluorodecyl polyhedral oligomeric silsesquioxane (fluorodecyl POSS) using an air brush with a pressurized nitrogen stream. The sprayed surface morphology can be systematically tuned from a spherical or corpuscular microstructure to beads-on-string and a fibrous non-woven mesh, nearly identical to structures obtained by electrospinning similar PMMA/fluorodecyl POSS solutions. A semi-empirical framework is used to develop an operating diagram to predict the surface morphology produced during the simple spraying technique based on the polymer solution concentration and molecular weight. The presence of the low-surface-energy POSS molecules at the surface combined with the re-entrant microtextured features confers super-liquid-repellent properties to the spray-coated substrate, which are characterized by advancing and receding contact angle measurements with liquids of a range of surface tensions.

Thursday, March 1, 2012 11:15AM - 2:15PM –
Session W45 DPOLY DBIO: Focus Session: Soft Matter Physics of Heterogeneous Membranes
- Theory and Simulation 159

11:15AM W45.00001 Hybrid Lipids as Line Active Molecules, TETSUYA YAMAMOTO, Weizmann Institute of Science — The lipid raft hypothesis suggests that stable nanoscopic domains in cellular membranes play an important role in several biological processes. Model membranes composed of saturated lipids, unsaturated lipids, and cholesterol (SUC membranes) exhibit coexisting chain-ordered and -disordered domains. However, these domains are unstable and the positive line tension at the interfaces between these domains drives coarsening until their size reaches of the order of the system size. This motivates the search for physical mechanisms that may reduce the line tension to zero and thus stabilize nanoscopic domains in biological membranes. There is a theoretical suggestion that the positive line tension at the interfaces between domains in SUC membranes results from the chain packing incompatibility between the ordered chains of saturated lipids and the disordered chains of unsaturated lipids. Hybrid lipids that have one saturated and one unsaturated chains may reconcile this chain packing incompatibility. We have used a phenomenological model to predict that a small concentration of hybrid lipids added to SUC membranes can reduce the line tension between coexisting domains to zero. However, this tends to occur only at low temperatures that may not be experimentally accessible, because localizing the hybrid lipids to the interfaces costs mixing entropy and this strongly suppresses the reduction of the line tension. Indeed, hybrid lipids are major components of biological membranes; unsaturated lipids are rather minor and uncommon. We have used a liquid crystal model to analyze the phase separation and line tension between domains in model membranes composed of saturated lipids, hybrid lipids, and cholesterol (SHC membranes). This model predicts that the line tension is reduced to zero at relatively higher in SHC membranes because the hybrid lipids are already at the interface and the mixing entropy of localization is no longer relevant.

11:51AM W45.00002 Turing Patterns on Curved Surfaces¹ , JOHN FRANK, MIT, JEMAL GUVEN, Instituto de Ciencias Nucleares, Universidad Nacional Autonoma de Mexico, MEHRAN KARDAR, MIT — Surface curvature modifies the emergence of Turing patterns in reaction-diffusion systems on two-dimensional interfaces. We adapt operator perturbation theory, familiar in quantum mechanics, to determine how curvature affects diffusion. When these modifications are taken into account in Turing's stability analysis, we observe new phenomena that may be relevant to patterning on cell membranes, neuron synapses, and fluid interfaces with reactive surfactants. A cylinder with longitudinal ripples illustrates how Turing patterns can lock into phase with the ripples when the most unstable mode is nearly commensurate with the ripples. The framework we introduce also sheds light on diffusion constrained to a rippled sphere, a Gaussian bump, and other shapes. More generally, it is relevant to any model that involves the Laplacian on a curved manifold.

¹Supported by the Hertz Foundation and NSF Grant No. DMR-08-03315

12:03PM W45.00003 2D Ising Model correlation function: Precise functional forms for comparison to membrane experiments , NATALIE PAQUETTE, BENJAMIN MACHTA, YAN-JIUN CHEN, JAMES SETHNA, LASSP, Cornell University — We find a precise form for the 2D Ising correlation function in the entire scaling regime as a function of external field H and temperature T . It is surprising that there is no functional form available, perhaps explained by the surprising complexity of the universal scaling function compared to other statistical mechanics models (e.g. 2D free energy or 3D Ising correlation function). We can use these results to test the hypothesis that heterogeneities found in a wide variety of membrane systems are manifestations of an underlying Ising critical point. We fit Monte Carlo lattice simulations in the (H, T) -plane with a functional form in parametric coordinates, while matching analytical results at $H = 0$ and $T = T_c$ to high accuracy. This functional form allows us to interpret FRET, NMR, or ESR data from membranes, where we can map experimentally controllable variables of composition and temperature onto the Ising axes of reduced temperature and magnetization.

12:15PM W45.00004 Fluctuating Lipid Bilayer Membranes With Diffusing Protein Inclusions: Hybrid Continuum-Particle Model , JON K. SIGURDSSON, Department of Mathematics, UC Santa Barbara, FRANK L.H. BROWN, Department of Chemistry, UC Santa Barbara, PAUL J. ATZBERGER, Department of Mathematics, UC Santa Barbara — Many proteins through their geometry and specific interactions with lipids induce changes in local membrane material properties. This can manifest in local stiffness variations and locally induced curvatures that track protein location. To study such phenomena we introduce a new hybrid continuum-particle description for the membrane-protein system that incorporates protein interactions, hydrodynamic coupling, and thermal fluctuations. We investigate how protein curvature and membrane stiffness influences protein diffusion. We discuss how collective protein effects influence membrane mechanical properties, such as the spectrum of membrane bending fluctuations and the effective elastic bending modulus of the heterogeneous protein-lipid membrane. Finally, we discuss possible roles of the membrane fluctuations influencing the distribution of proteins within the membrane.

12:27PM W45.00005 Influence of chain rigidity on the conformation of model lipid membranes in the presence of cylindrical nanoparticle inclusions , CHRIS DILORETO, ROBERT WICKHAM, Department of Physics, University of Guelph — We employ real-space self-consistent field theory to study the conformation of model lipid membranes in the presence of solvent and cylindrical nanoparticle inclusions ("peptides"). Whereas it is common to employ a polymeric Gaussian chain model for the lipids, here we model the lipids as persistent, worm-like chains. Our motivation is to develop a more realistic field theory to describe the action of pore-forming anti-microbial peptides that disrupt the bacterial cell membrane. We employ operator-splitting and a pseudo-spectral algorithm, using SpharmonicKit for the chain tangent degrees of freedom, to solve for the worm-like chain propagator. The peptides, modelled using a mask function, have a surface patterned with hydrophobic and hydrophilic patches, but no charge. We examine the role chain rigidity plays in the hydrophobic mismatch, the membrane-mediated interaction between two peptides, the size and structure of pores formed by peptide aggregates, and the free-energy barrier for peptide insertion into the membrane. Our results suggest that chain rigidity influences both the pore structure and the mechanism of pore formation.

12:39PM W45.00006 Mechanics, morphology, and mobility in stratum corneum membranes¹ , PETER OLMSTED, CHINMAY DAS, University of Leeds, School of Physics & Astronomy, MASSIMO NORO, Unilever Discover Port Sunlight — The stratum corneum is the outermost layer of skin, and serves as a protective barrier against external agents, and to control moisture. It comprises keratin bodies (corneocytes) embedded in a matrix of lipid bilayers. Unlike the more widely studied phospholipid bilayers, the SC bilayers are typically in a gel-like state. Moreover, the SC membrane composition is radically different from more fluid counterparts: it comprises single tailed fatty acids, ceramides, and cholesterol; with many distinct ceramides possessing different lengths of tails, and always with two tails of different lengths. I will present insight from computer simulations into the morphology, mechanical properties, and diffusion (barrier) properties of these highly heterogeneous membranes. Our results provide some clue as to the design principles for the SC membrane, and is an excellent example of the use of wide polydispersity by natural systems.

¹This work was funded by Yorkshire Forward and the European Regional Development Fund.

12:51PM W45.00007 Curvature-driven domain formation in ternary lipid membranes , MATTHEW DEMERS, RASTKO SKNEPNEK, MONICA OLVERA DE LA CRUZ, Northwestern University — We model vesicles formed by three-component fluid membranes whose components have differing spontaneous curvatures. We use Monte Carlo simulated annealing to find low energy configurations for a range of component characteristics. A wide variety of ordered structures are found, including highly symmetric structures with elongated domains resembling faceted edges. We also observe an effective attraction between components of highest and lowest spontaneous curvature. We relate these effects to the interplay of spontaneous curvature and underlying geometric constraints. Our results suggest that the composition-shape coupling can be an important mechanism in the formation of highly ordered structures in many-component membranes.

1:03PM W45.00008 Entropy driven aggregation of adhesion sites of supported membranes , ODED FARAGO, Ben Gurion Univ Beer Sheva — Supported lipid membranes are useful and important model systems for studying cell membrane properties and membrane mediated processes. One attractive application of supported membranes is the design of phantom cells exhibiting well defined adhesive properties and receptor densities. Adhesion of membranes may be achieved by specific and non-specific interactions, and typically requires the clustering of many adhesion bonds into "adhesion zones". One potential mediator of the early stages of the aggregation process is the Casimir-type forces between adhesion sites induced by the membrane thermal fluctuations. In the talk, I will present a theoretical analysis of fluctuation induced aggregation of adhesion sites in supported membranes. I will first discuss the influence of a single attachment point on the spectrum of membrane thermal fluctuations, from which the free energy cost of the attachment point will be deduced. I will then analyze the problem of a supported membrane with two adhesion points. Using scaling arguments and Monte Carlo simulations I will demonstrate that two adhesion points attract each other via an infinitely long range effective potential that grows logarithmically with the pair distance. Finally, I will discuss the many-body nature of the fluctuation induced interactions. I will show that while these interactions alone are not sufficient to allow the formation of aggregation clusters, they greatly reduce the strength of the residual interactions required to facilitate cluster formation. Specifically, for adhesion molecules interacting via a short range attractive potential, the strength of the direct interactions required for aggregation is reduced by about a factor of two to below the thermal energy kT .

1:39PM W45.00009 Membrane lateral structure: How immobilized particles can stabilize small domains¹, RICHARD VINK, TIMO FISCHER, Institute of Theoretical Physics, University of Goettingen, Germany — Membranes are two-dimensional fluid environments, consisting of lipids and proteins. In model membranes, macroscopic phase separation is routinely observed, but not so in biological membranes. Instead, the lateral structure of a biological membrane is characterized by small domains. This poses an interesting puzzle because a structure of small domains inevitably implies a large amount of interface, which is unfavorable because of line tension. In this contribution, it is shown that immobilized protein obstacles provide a mechanism to compensate the cost of line tension. The presence of such obstacles in biological membranes is known to occur (arising for instance from interactions with the underlying cytoskeleton). We present results from computer simulation, which indeed show that a structure of small domains becomes stable, already at a low concentrations of quenched obstacles. In addition, these results confirm a fundamental conjecture of de Gennes, stating that a fluid with quenched obstacles belongs to the universality class of the random-field Ising model.

¹Financed by the Emmy Noether program (VI 483/1-1) of the German Research Foundation (DFG).

1:51PM W45.00010 In-Plane Dynamics of Membranes with Immobile Inclusions, NAOMI OPPENHEIMER, HAIM DIAMANT, School of chemistry, Tel Aviv University — Cell membranes are anchored to the cytoskeleton via immobile inclusions. We investigate the effect of such anchors on the in-plane dynamics of a fluid membrane and mobile inclusions embedded in it. The immobile particles lead to a decreased diffusion coefficient of mobile ones and suppress the correlated diffusion of particle pairs. Due to the long-range, quasi-two-dimensional nature of membrane flows, these effects become significant at a low area fraction (below one percent) of immobile inclusions.

2:03PM W45.00011 Charge correlations in multicomponent ionic crystalline membranes, CREIGHTON THOMAS, MONICA OLVERA DE LA CRUZ, Northwestern University — We investigate the dissociation state of a polyelectrolyte membrane with charged head groups in solution. This state depends on the salt concentration and pH of the solution, but spatial correlations also highly influence it. Spatial correlations are typically neglected in these systems, as they are difficult to treat analytically, but they can qualitatively alter the results. We numerically incorporate charge correlations on both flat and curved membranes by simulating a multicomponent system on a fluctuating network with electrostatic interactions, using the replica exchange Monte Carlo approach. The salt-induced screening effects are modeled within the Debye-Huckel theory. For weak enough screening, we find a strong suppression of dissociation regardless of pH, and the membrane may exhibit a reentrant structural phase transition as pH is varied.

Thursday, March 1, 2012 11:15AM - 2:15PM –

Session W46 DCMP GQI: Invited Session: Silicon Spin Qubits: Relaxation and Decoherence

160AB

11:15AM W46.00001 Single-shot readout of spin qubits in Si/SiGe quantum dots¹, CHRISTIE SIMMONS, University of Wisconsin - Madison / Currently: Massachusetts Institute of Technology — Si/SiGe quantum dots are an attractive option for spin qubit development, because of the long coherence times for electron spins in silicon, arising from weak hyperfine interaction and low spin orbit coupling. I will present measurements of gate-defined single and double quantum dots formed in Si/SiGe semiconductor heterostructures. Control of the gate voltages on these dots enables tuning of the tunnel coupling to the leads and to other dots. Careful tuning of these tunnel rates, in combination with fast, pulsed-gate manipulation and spin-to-charge conversion, allow spin state measurement using an integrated quantum point contact as a local charge detector. Single spin qubit readout relies on the Zeeman energy splitting from an external magnetic field for spin-to-charge conversion. Two-electron singlet-triplet qubits, on the other hand, can be measured by using Pauli spin blockade of tunneling between the dots to readout the qubit even at zero magnetic field. I will present real-time, single-shot readout measurements of both individual spin [1] and singlet-triplet qubits [2] in gated Si/SiGe quantum dots. Work performed in collaboration with J. R. Prance, Zhan Shi, B. J. Van Bael, Teck Seng Koh, D. E. Savage, M. G. Lagally, R. Joynt, L. R. Schreiber, L. M. K. Vandersypen, M. Friesen, S. N. Coppersmith, and M. A. Eriksson.

[1] C. B. Simmons et al. Physical Review Letters 106, 156804 (2011).

[2] J. R. Prance, et al., e-print: <http://lanl.arxiv.org/abs/1110.6431>

¹This work was supported in part by ARO and LPS (W911NF-08-1-0482), by NSF (DMR-0805045), by DoD, and by DARPA (N66001-09-1-2021).

11:51AM W46.00002 Coherent manipulation of a Si/SiGe-based singlet-triplet qubit¹, MARK GYURE, HRL Laboratories, LLC — Electrically defined silicon-based qubits are expected to show improved quantum memory characteristics in comparison to GaAs-based devices due to reduced hyperfine interactions with nuclear spins. Silicon-based qubit devices have proved more challenging to build than their GaAs-based counterparts, but recently several groups have reported substantial progress in single-qubit initialization, measurement, and coherent operation. We report [1] coherent control of electron spins in two coupled quantum dots in an undoped Si/SiGe heterostructure, forming two levels of a singlet-triplet qubit. We measure a nuclei-induced T_2^* of 360 ns, an increase over similar measurements in GaAs-based quantum dots by nearly two orders of magnitude. We also describe the results from detailed modeling of our materials and devices that show this value for T_2^* is consistent with theoretical expectations for our estimated dot sizes and a natural abundance of ²⁹Si. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressly or implied, of the United States Department of Defense or the U.S. Government. Approved for public release, distribution unlimited.

[1] B. M. Maune et al., "Coherent Singlet-Triplet Oscillations in a Silicon-based Double Quantum Dot," accepted by Nature.

¹Sponsored by United States Department of Defense.

12:27PM W46.00003 Measurement and control of single electron spins in silicon MOS-based quantum dots, HONGWEN JIANG, UCLA — No abstract available.

1:03PM W46.00004 Simulating a solid state spin qubit in a spin bath, WAYNE WITZEL, Sandia National Laboratories, NM — Powerful computational methods have been developed in recent years for understanding decoherence induced by environmental spins. Specifically, the cluster correlation expansion [Phys. Rev. B 78, 085315 (2008)] and adaptations [Phys. Rev. Lett. 105, 187602 (2010)] provide successive approximations that approach the solution to the full quantum mechanical problem for small and large spin baths with good efficiency. With these methods, we are able to study the nature of spin-bath decoherence in various regimes, for different types of qubits (e.g., donors or quantum dots) and for different types of spin baths (e.g., nuclei or electrons). Our quantitative analyses have implications for solid state spin qubit prospects and materials choices. Sandia National Laboratories is a multiprogram laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

1:39PM W46.00005 Two-Spin Decoherence and Disentanglement in Semiconductor Nanostructures¹, XUEDONG HU, University at Buffalo, The State University of New York — A crucial issue in spin-based quantum information processing is spin coherence. Decoherence of a single electron spin confined in a quantum dot or to a donor ion has been studied extensively, with hyperfine interaction to the environmental nuclear spins being identified as the most important channel of spin decoherence [1]. Decoherence of two-spin-qubit states is inevitably affected by single-spin decoherence. Moreover, for exchange-coupled spin qubits, there are new decoherence channels beyond those for single spins because of the Coulombic nature of the exchange interaction. Here we discuss a series of studies of two-spin decoherence mechanisms [2-6], including both known single-spin decoherence and relaxation channels due to nuclear spins and new channels based on electrostatic coupling. More specifically, we examine two-spin relaxation due to hyperfine interaction and phonon emission [2], spin-orbit interaction and phonon emission [3], nuclear spin dynamics mediated by electrons, charge noise [4,5], and electron-phonon interaction [6]. We also analyze the associated disentanglement of the two spins as the decoherence processes go on. Our results show that while nuclear spins affect two-spin states in a qualitatively similar manner as for single spin states, there are interesting new twists because of the weaker hyperfine interaction due to the electron orbital symmetry. On the other hand, the charge noise and phonon induced dephasing depends strongly on the electrical features of the nanostructure, and could pose a significant constraint on two-qubit gates and quantum computing schemes based on two-spin encoding.

[1] L. Cywinski, W. Witzel, and S. Das Sarma, Phys. Rev. B **79**, 245314 (2009).

[2] M. Borhani and X. Hu, Phys. Rev. B **82**, 241302R (2010).

[3] M. Borhani and X. Hu, arXiv:1110.2193.

[4] X. Hu and S. Das Sarma, Phys. Rev. Lett. **96**, 100501 (2006).

[5] D. Culcer, X. Hu, and S. Das Sarma, Appl. Phys. Lett. **95**, 073102 (2009).

[6] X. Hu, Phys. Rev. B **83**, 165322 (2011).

¹We thank support by NSA/LPS through ARO, DARPA QuEST through AFOSR, and NSF PIF.

Thursday, March 1, 2012 11:15AM - 2:15PM –
Session W47 DPOLY DMP: Focus Session: Polymers for Energy Storage and Conversion -
Fundamentals of Ion Transport 160C

11:15AM W47.00001 Decoupling of Ionic Transport from Segmental Relaxation in Polymer Electrolytes, YANGYANG WANG, Oak Ridge National Lab, ALEXANDER AGAPOV, University of Akron, FEI FAN, University of Tennessee-Knoxville, KUNLUN HONG, XIANG YU, Oak Ridge National Lab, JIMMY MAYS, University of Tennessee-Knoxville, ALEXEI SOKOLOV, Oak Ridge National Lab — Polymer electrolytes provide elegant solutions to many difficulties in battery technology. However, their relatively low ionic conductivity has become the bottleneck for developing batteries with higher power density, shorter charging time, and better operations at low temperatures. In this work, we present detailed studies of the relationship between ionic conductivity and segmental relaxation in a set of specially-designed polymer electrolytes with systematic variation in chain rigidity. Our analysis shows that the ionic conductivity indeed can be decoupled from segmental dynamics in rigid polymers and the strength of the decoupling correlates with the fragility, but not with the glass transition temperature. These results call for a revision of the current picture of ionic transport in polymer electrolytes. We relate the observed decoupling phenomenon to frustration in packing of rigid polymers, which also affects their fragility. The principles demonstrated in this study may provide an alternative approach to design of highly conductive materials: by incorporating relatively rigid chain structures, it is possible to develop a new class of solid polymer electrolytes with strongly decoupled ionic conductivity.

11:27AM W47.00002 Ion Dynamics in Solid-State Polymer Electrolyte Electrochemical Cells using *in situ* Time-Resolved Infrared Spectroscopy, FRANCIS RICHEY, YOSSEF ELABD, Drexel University — Understanding ion transport in solid-state polymer electrochemical cells is of great interest for the advancement of cell efficacy. However, currently there is limited experimental knowledge of ion transport on a molecular level. In this study, we report a new spectroelectrochemical experimental technique that provides *in situ* molecular level detail about cation and anion transport of an ionic liquid in solid-state polymer electrolyte electrochemical cells. *In situ* time-resolved Fourier transform infrared attenuated total reflectance (FTIR-ATR) spectroscopy was utilized to measure the time dependent accumulation of ions at the cathode and anode interface under an applied potential. The results show that the cation and anion of the ionic liquid both transport and accumulate at the cathode under dry conditions, but only the cation accumulates at the cathode under humid conditions. This experiment was coupled with electrochemical impedance spectroscopy to simultaneously measure overall charge transport and cyclic voltammograms.

11:39AM W47.00003 Ion Transport in Polymerized Ionic Liquid Block and Random Copolymers, YOSSEF ELABD, YUESHENG YE, Drexel University, JAE-HONG CHOI, KAREN WINEY, University of Pennsylvania — Polymerized ionic liquid (PIL) block copolymers, a new type of solid-state polymer electrolyte, are of interest for energy conversion and storage devices, such as fuel cells, batteries, supercapacitors, and solar cells. In this study, a series of PIL diblock and random copolymers with various PIL compositions were synthesized. These consisted of an IL monomer and a non-ionic monomer, 1-[(2-methacryloyloxy)ethyl]-3-butylimidazolium bis(trifluoromethanesulfonyl)imide (MEBIm-TFSI) and methyl methacrylate (MMA), and 1-[(2-acryloyloxy)ethyl]-3-butylimidazolium bis(trifluoromethanesulfonyl)imide (AEBIm-TFSI) and styrene (S), respectively, were synthesized. The anion conductivity (ion transport) and morphology were measured in all of the polymers with EIS, SAXS/WAXS, and TEM. Ion transport in block copolymers are significantly higher than random copolymers at the same PIL composition and are highly dependent on the block copolymer nanostructure. The relationship between ion transport mechanisms and the phase behavior of these materials will be discussed.

11:51AM W47.00004 Ion conduction in phosphonium-polysiloxane ionomers, SIWEI LIANG, U. HYEOK CHOI, JAMES RUNT, RALPH COLBY, Penn State University — Low T_g ionomers with phosphonium cations covalently attached as side chains have potential application in energy conversion and storage devices. For example, alkaline fuel cells rely on membranes that transport hydroxide anions and some advanced batteries rely on membranes transporting fluoride anions. To better understand ion conduction in phosphonium-polysiloxane ionomers, allyl tributyl phosphonium bromide monomer was synthesized and, along with a vinyl ethylene oxide monomer, attached to polymethylhydrosiloxane by hydrosilylation. These ionomers maintain low T_g ≈ -74 °C with up to 10 mol% phosphonium and are fully water soluble, allowing easy anion exchange and purification. We report dielectric spectroscopy results for these ionomers with a variety of counter-anions. Electrode polarization at low frequencies is analyzed to determine the number density of simultaneously conducting counter ions and their mobility. This analysis reveals higher mobility and lower activation energy for conducting anions that are larger and more diffuse, such as bis(trifluoromethane sulfonyl)imide, contributing to better performance as anion-conducting membranes.

12:03PM W47.00005 Ion Conduction in Polymerized Ionic Liquid Thin Films, JAE-HONG CHOI, Department of Materials Science and Engineering, University of Pennsylvania, YUESHENG YE, Department of Chemical and Biological Engineering, Drexel University, MATTHEW D. GREEN, Department of Chemical Engineering, Macromolecules and Interfaces Institute, Virginia Tech, YOSSEF A. ELABD, Department of Chemical and Biological Engineering, Drexel University, TIMOTHY E. LONG, Department of Chemistry, Macromolecules and Interfaces Institute, Virginia Tech, KAREN I. WINEY, Department of Materials Science and Engineering, University of Pennsylvania — The ion conductivity in thin films is typically assumed to be isotropic. We have developed methods to measure in-plane and through-plane ionic conductivity in thin homopolymer and block copolymers. Specifically, we are studying the conductivity in imidazolium-containing polymerized ionic liquids as a function of film thickness. These data will be compared to conductivity measurements in a triblock copolymer with a polymerized ionic liquid midblock.

12:15PM W47.00006 Cross-linking of Ordered Pluronic/Ionic Liquid Blends for Solid Polymer Electrolytes, DANIEL MIRANDA, CRAIG VERSEK, MARK TUOMINEN, JAMES WATKINS, THOMAS RUSSELL, University of Massachusetts, Amherst — Ion gels were fabricated by cross-linking PPO-PEO-PPO triblock copolymers swollen in a room temperature ionic liquid (IL). The copolymers are modified by esterification to replace the terminal hydroxyl endgroups with methacrylate endgroups. This allows the copolymer/IL blends to be cross-linked by a UV cure, forming a gel. The strong interaction of the IL with the PEO block suppresses PEO crystallization which is necessary for good ion conduction. In addition, the interaction between the IL and PEO is strongly selective for PEO, strengthening microphase separation. Despite this, the low molecular weight copolymers remain disordered in the melt even when blended with the IL. However, high molecular weight copolymers are capable of microphase separating into highly ordered block copolymer morphologies. This difference allows the effect of microphase separation on ion transport to be studied. The effect of block copolymer composition is also studied, by varying the PEO fraction of the copolymer. The resultant gels show high ionic conductivity and solid-like behavior, indicating that these materials may be effective as solid polymer electrolytes.

12:27PM W47.00007 Ionomer Design Principles for Single Ion-Conducting Energy Materials¹, RALPH COLBY, SIWEI LIANG, WENJUAN LIU, U. HYEOK CHOI, JAMES RUNT, HUAI-SUEN SHIAU, MICHAEL JANIK, Penn State University — Single-ion conducting ionomers with low glass transition temperature, high dielectric constant and containing bulky ions with diffuse charge, are needed for polymer membranes that transport small counterions. Overarching design principles emerging from quantum chemistry calculations suggest that diffuse charge can be attained from simple considerations of atomic electronegativity. For lithium or sodium batteries, perfluorinated tetraphenyl borate ionomers with solvating polar comonomers are proposed. For fluoride or hydroxide batteries and for iodide transporting solar cells, tetra-alkyl phosphonium ionomers with anion receptors are proposed. First attempts to construct such ionomers to test these ideas will be discussed, with results from dielectric spectroscopy to measure conductivity, dielectric constant and number density of simultaneously conducting ions.

¹support from DOE-BES DE-FG02-07ER46409

12:39PM W47.00008 Ion Dynamics in Model Ionomer Melts as a Function of Polymer Architecture, LISA M. HALL, MARK J. STEVENS, AMALIE L. FRISCHKNECHT, Sandia National Laboratories — Ionomers, polymers with a small fraction of covalently bound ionic groups, have potential advantages as solid, single ion conducting electrolytes in future batteries. However, the strong electrostatic interactions in these materials can make counterion diffusion unacceptably slow. Understanding how controllable molecular properties affect ionomer dynamics could spur design of improved materials. With this goal, we perform molecular dynamics simulations of ionomers of various architectures and evaluate their dynamic behavior. Our model of coarse-grained polymers with explicit counterions captures the fundamental physics while allowing access to the long time and length scales relevant to ionomer melts. The simulated structure factors reproduce the trends found in experimental scattering of recently synthesized ionomers with controlled precise or pseudorandom spacing of charged groups along the chain. We calculate counterion diffusion constants and other dynamic properties, which can change significantly depending on the location and spacing of charges along the chain. Randomly spaced materials can have slower or faster dynamics than periodically spaced materials, depending on whether the sequence is completely random or pseudorandom, which will be discussed.

12:51PM W47.00009 Ion Conduction and Dielectric Response of Imidazolium-based Single-ion Conductors¹, U. HYEOK CHOI, Penn State University, MINJAE LEE, ANUJ MITTAL, Virginia Polytechnic Institute & State University, YUESHENG YE, YOSSEF ELABD, Drexel University, HARRY GIBSON, Virginia Polytechnic Institute & State University, JAMES RUNT, RALPH COLBY, Penn State University — We synthesized ionomers with imidazolium cations covalently attached as side groups with various ionic liquid counter-anions. Since these ionic polymers are single-ion conductors that are potentially useful for ionic actuators, it is of great interest to understand structure-property relations, such as the effect of different counterions and different imidazolium pendant structures, including tail and side chain lengths. Conductivities and dielectric properties of a range of monomers and polymers containing ionic liquid moieties are compared. The effects of counterions and side chain length are clearly observed in the T_g and ionic conductivity: larger anions and/or longer side chains lead to lower T_g and higher conductivity than smaller anions and/or shorter side chains. However, if the tail becomes too long (12 carbons) it facilitates - ion aggregation with a significantly lower dielectric constant and lower mobility for the conducting ions. Our study of counter-anions and polymer structural variations leads to insight regarding optimal design of imidazolium single-ion conductors for facile ion transport.

¹This work is supported in part by the U.S. Army Research Office under Grant No. W911NF-07-1-0452 Ionic Liquids in Electro-Active Devices (ILEAD) MURI.

1:03PM W47.00010 Effect of matrix crystallinity on the ionic conductivity in microstructured block copolymer solid electrolytes, NICHOLAS YOUNG, NITASH BALSARA, University of California, Berkeley — Polyethylene oxide (PEO)-based block copolymers have been studied extensively for use as solid electrolytes for rechargeable lithium metal batteries. Previous work has concentrated on block copolymers containing an amorphous second block, such as polystyrene, for which the modulus is sufficiently high to resist growth of dendrites that would lead to short circuiting. In this work, we instead focus on using semicrystalline polyethylene as the mechanically robust component. Polyethylene-polyethylene oxide (EEO) block copolymers doped with lithium bis(trifluoromethanesulfone) imide (LiTFSI) were characterized using AC impedance spectroscopy over a range of temperature, molecular weight, and composition values in order to determine the effect of crystallinity in the structural microphase on the conductivity of this material.

1:15PM W47.00011 Solvation Effects on Counterion Transport in Single-Ion Conducting Ionomers, JING-HAN HELEN WANG, Chemical Engineering, The Pennsylvania State University, University Park PA 16802, RALPH COLBY, Chemical Engineering and Materials Science and Engineering, The Pennsylvania State University, University Park PA 16802 — Ionomers with short ethylene oxide side chains are synthesized by free radical polymerization, to systematically test effects of solvating anion and cation, including directly substituting the ion attached to the polymer with its counterion. Dielectric relaxation spectroscopy is used to measure the conductivity, dielectric constant and segmental relaxations in these ionomers and the electrode polarization at very low frequencies is used to assess the number density of simultaneously conducting ions and their mobility. Conductivity and conducting ion content are larger for polyanions than their corresponding polycation because the counterion can be more effectively solvated by the ether oxygens. Changing ester linkages to amide linkages in polycations boosts conductivity and conducting ion content by solvating the anionic counterion. Such findings point a clear path toward design of superior single-ion conductors.

1:27PM W47.00012 Correlation between superionic behavior and ion aggregation in PEO-based single-ion conductors¹, KAN-JU LIN, JANNA MARANAS, Pennsylvania State University — PEO-based ionomers as solid polymer electrolytes offer the advantage of preventing reverse polarization in batteries by covalently bonding the anion to the PEO backbone. These ionomers form ion aggregates, which reduces the polymer mobility. Since ion transport is coupled to polymer dynamics, these systems have low conductivity. We therefore need a mechanism that decouples ion conduction and PEO dynamics to improve conductivity. We investigate these conduction mechanisms using different models in MD simulations of PEO based benzene sulfonate ionomers. The study shows that these ionomers are capable of showing superionic behavior. The geometry of benzene rings helps aligning the anions, assisting in the formation of chain-like aggregates. The simulations show that the chain-like aggregates result in ionomer conductivity greater than its self-diffusion limits. The superionic behavior is attributed to a charge transfer between two chain ends (conduction sites): a cation hopping to one chain end and the cation at the other end hopping to a nearby site. This allows long range positive charge transfer while the cations only move locally. The results suggest that the superionic behavior depends on the length and lifetime of the chain aggregates. While a long chain reduces the overall number of conduction sites, a short chain prevents long range charge transfer. If the lifetime of an aggregate is shorter than the hopping time for cations, the hopping will not occur and the self-diffusion dominates conductivity.

¹This work is supported by the Department of Energy, Office of Basic Energy Sciences, under Grant DEFG02-07ER46409.

1:39PM W47.00013 Simulation of Ionic Aggregation and Ion Dynamics in Model Ionomers, AMALIE L. FRISCHKNECHT, Sandia National Laboratories — Ionomers, polymers containing a small fraction of covalently bound ionic groups, are of interest as possible electrolytes in batteries. A single-ion conducting polymer electrolyte would be safer and have higher efficiency than the currently-used liquid electrolytes. However, to date ionomeric materials do not have sufficiently high conductivities for practical application. This is most likely because the ions tend to form aggregates, leading to slow ion transport. A key question is therefore how molecular structure affects the ionic aggregation and ion dynamics. To probe these structure-property relationships, we have performed molecular simulations of a set of recently synthesized poly(ethylene-co-acrylic acid) copolymers and ionomers, with a focus on the morphology of the ionic aggregates. The ionomers have a precise, constant spacing of charged groups, making them ideal for direct comparisons with simulations. *Ab initio* calculations give insight into the expected coordination of cations with fragments of the ionomers. All-atom molecular dynamics (MD) simulations of the ionomer melt show aggregation of the ionic groups into extended string-like clusters. An extensive set of coarse-grained molecular dynamics simulations extend the results to longer times and larger length scales. The structure factors calculated from the MD simulations compare favorably with x-ray scattering data. Furthermore, the simulations give a detailed picture of the sizes, shapes, and composition of the ionic aggregates, and how they depend on polymer architecture. Implications for ion transport will be discussed. [Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.]

Thursday, March 1, 2012 11:15AM - 2:15PM –
Session W48 DPOLY: New Experimental, Theoretical, and Computational Methods in Polymer and Soft Matter Physics 161

11:15AM W48.00001 Coherent States Formulation of Polymer Field Theory¹, XINGKUN MAN, Department of Chemical Engineering and the Materials Research Laboratory, University of California, Santa Barbara, KRIS DELANEY, Department of the Materials Research Laboratory, University of California, Santa Barbara, GLENN FREDRICKSON, Department of Chemical Engineering and the Materials Research Laboratory, University of California, Santa Barbara, HENRI ORLAND, Institut de Physique Theorique, CEA-Saclay, France — We developed a coherent-states formulation of equilibrium polymer field theory. Compared with the traditional Edwards' auxiliary field framework that underpins both field-theoretic simulation (FTS) and self-consistent field theory (SCFT) methods, this formulation has a number of attractive features, including much more local operators and a finite order polynomial action. The formalism is developed in the grand canonical ensemble for the Edwards model of polymers in an implicit solvent, and we show how to derive a numerically tractable scheme. We explore the efficiency and stability of the method in mean-field and fully fluctuating simulations for a polymer solution confined to a slit in one dimension.

¹This work made use of MRL Central Facilities supported by the MRSEC Program of the National Science Foundation under Award DMR-0520415.

11:27AM W48.00002 How Reliable Are Soft Potentials? Ensuring Thermodynamic Consistency Between Hierarchical Models of Polymer Melts, JAMES MCCARTY, MARINA GUENZA, University of Oregon — The use of soft effective potentials to represent macromolecular systems has become widespread in the areas of biophysics and materials science. A survey of the field reveals a vast array of various phenomenological potentials whose ability to provide quantitative information about several different properties of the same system is not evident. This talk will present a formally sound approach to obtain soft potentials for realistic models of simple linear polymer melts which reproduce the correct center of mass distribution of particles as well as the correct equation of state of the underlying system of interest. Furthermore, an analytical potential allows us to rigorously address the implications of coarse-graining on the entropy and free energies of the system and to account for the reduced degrees of freedom and smoothed energy landscape implicit to coarse-grained models. Finally, the transferability of the method to other systems and potential applications will be discussed.

11:39AM W48.00003 Simulation of Stress Induced Polymer-Polymer Interfacial Slip, ANDREW GUSTAFSON, DAVID MORSE, University of Minnesota — The phenomena of stress-induced tangential slip at polymer-polymer interfaces is studied via a slip-link simulation technique. Simulations combine a slip-link model of entanglement with a self-consistent field description of the chemical potential landscape near an interface. We consider how the slip velocity depends upon shear stress, interfacial entanglement density, and polymer chain length. Our model is based on the idea that the strongly non-linear shear thinning of the interface observed in experiment is a result of stress-induced convective release (pulling-out) of entanglements across the interface.

11:51AM W48.00004 Tumbling dynamics of isolated polymer chains in strong shear flows and the effects of chain resolution, RONALD LARSON, INDRANIL SAHA DALAL, ALEX ALBAUGH, University of Michigan, NAZISH HODA, ExxonMobil Upstream Research — Using Brownian dynamics simulations, without hydrodynamic and excluded volume interactions, on polymer chain models encompassing a wide range of resolutions, we present a detailed investigation on the behavior of isolated chains in shear flow. We find a highly non-monotonic behavior for all models, with chain compression occurring at ultra-high shear rates that is consistent with the recent simulation studies. However, results obtained using highly refined models, with resolutions lower than a Kuhn step, reveal that this transition is an artifact of the level of chain discretization. Also, our results clearly indicate that, at high shear rates, the chain thickness in the shear-gradient direction is independent of the chain length, which differ from previously reported scaling law. We show that the chain thickness is fixed by the distance a sub-section of the chain can diffuse in the shear-gradient direction before convection stretches it out and suppresses further diffusion. Simple physical arguments are then used to derive the correct scaling laws for the coil width and the tumbling time at high shear rates. We believe that our findings presented here will provide the foundation for a better understanding of this basic problem in polymer dynamics.

12:03PM W48.00005 ABSTRACT WITHDRAWN —

12:15PM W48.00006 A Mesoscale Simulation Method for High Salt Concentrations, STEFAN MEDINA¹, Caltech, USA / University of Mainz, Germany, FRIEDERIKE SCHMID, University of Mainz, Germany — In mesoscale simulations of electrolyte solutions the interplay between electrostatics and hydrodynamics plays the critical role for computational efficiency and accuracy. In the past it became apparent that high salt concentrations are too costly, if every salt ion is treated explicitly as a separate particle. On the other hand, charges are highly screened at high salt concentrations and ion-ion correlations are less important than in the low-salt limit. Therefore, we have developed a dynamic mean-field treatment of charges which is expected to be perfectly sufficient in many cases leading to applications in controlled manipulation of polyelectrolytes and charged colloids by external electric fields.

¹Graduate School Materials Science in Mainz, Germany

12:27PM W48.00007 Molten Salt Eutectics from Atomistic Alchemical Simulations, SAIVENKATARAMAN JAYARAMAN, AIDAN THOMPSON, Advanced Device Technologies department, Sandia National Laboratories, Albuquerque, NM, O. ANATOLE VON LILIENFELD, Leadership Computing Facility, Argonne National Laboratory, Argonne, IL — Molten salt mixtures are gaining importance in solar thermal power applications. Unfortunately, their phase diagrams cannot be easily computed from first principles calculations. The eutectic mixture composition and temperature are located using the liquid mixture free energy and the pure component solid-liquid free energy differences. The liquid mixture free energy is obtained using thermodynamic integration of alchemical transformations of one atom to another. Numerical results for binary and ternary mixtures of alkali nitrates agree well with experimental measurements [1]. Some results involving mixtures of monovalent and divalent cations will also be presented.

[1] Jayaraman, Thompson, and von Lilienfeld, PRE, 84, 030201 (2011).

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

12:39PM W48.00008 ABSTRACT WITHDRAWN —

12:51PM W48.00009 An $[N]PT$ Ensemble for Studying the Intricate Thermodynamics of Cluster Crystals, KAI ZHANG, PATRICK CHARBONNEAU, Duke University — Exotic soft matter systems such as certain dendrimers can overlap with only a finite energy penalty. Systems governed by steep, bounded repulsive interactions, such as the penetrable sphere model (PSM), indeed form cluster crystals with multiple particles per lattice site under compression. Standard simulation approaches that keep NVT , NPT , or μVT constant cannot directly equilibrate cluster crystals, because either N or lattice constant is not free to relax. It is tempting to allow all fields to fluctuate by keeping " μPT " constant, but basic thermodynamics indicates that infinite fluctuations then result. We avoid this caveat by using a $[N]PT$ ensemble, in which P and T are fixed but N is allowed to fluctuate within bounds $[N_{\min}, N_{\max}]$ under a conjugate field analogous to μ . The approach provides the equilibrium properties of neighboring state points through histogram reweighting. We solve the phase diagram of the PSM, and confirm that the FCC crystal lattice occupancy linearly increases with ρ at high T . At low T the occupancy plateaus at integer values, but the transitions remain continuous and the crystal does not phase separate. We also examine the critical behavior of another related model.

1:03PM W48.00010 From nucleus to phase: Growing dynamics of critical nucleus in polymer blends¹, DADONG YAN, XINGHUA ZHANG, Department of Physics, Beijing Normal University, Beijing 100875 — In metastable system, nonclassical critical nucleus is not a drop of stable bulk in core wrapped with a sharp interface, but a diffuse structure depending on the metastability. Thus, forming a critical nucleus does not mean the birth of a new phase. Also, the dynamics of nucleus' growing before the phase is born is still unknown. In present work, the nonclassical growing dynamics of the critical nucleus is addressed in the metastable polymer blends by incorporating self-consistent field theory and external potential dynamics theory, and leads to an intuitionistic description for the results of scattering experiments. Our results suggest that the growth of nonclassical critical nucleus is not self-similarly, but forms shell structure, which gives the scattering peak at nonzero wavenumber in the experiments. This phenomenon comes from the spinodal-decomposition-like behaviors constrained within the critical nucleus. The growing dynamics of the critical nucleus can be considered as a spinodal-assistant nucleation process.

¹Finacial support by NSFC.

1:15PM W48.00011 An Interactive 3D Interface to Model Complex Surfaces and Simulate Grazing Incidence X-ray Scatter Patterns, ELIOT GANN, North Carolina State University, Jema Science Inc., SLIM CHOUROU, ABHINAV SARJE, Lawrence Berkeley National Laboratory, HARALD ADE, North Carolina State University, CHENG WANG, ELAINE CHAN, Lawrence Berkeley National Laboratory, XIAODONG DING, Jema Science Inc., ALEXANDER HEXEMER, Lawrence Berkeley National Laboratory — Grazing Incidence Scattering is becoming critical in characterization of the ensemble statistical properties of complex layered and nano structured thin films systems over length scales of centimeters. A major bottleneck in the widespread implementation of these techniques is the quantitative interpretation of the complicated grazing incidence scatter. To fill this gap, we present the development of a new interactive program to model complex nano-structured and layered systems for efficient grazing incidence scattering calculation.

1:27PM W48.00012 Numerical Computation of Diffusion Properties in Molecular Systems on a Topology-Conforming Grid¹, IVAN TEO, KLAUS SCHULTEN, Department of Physics, University of Illinois at Urbana-Champaign, Beckman Institute for Advanced Science and Technology — Multiscale problems involving diffusion in molecular systems are a mainstay of computational biophysics. Given a molecular system, the local diffusion coefficient $D(\mathbf{r})$ as well as the equilibrium distribution function $P(\mathbf{r})$ that characterizes the local free energy are computed to describe the kinetics of diffusing particles at each point in space through the Smoluchowski equation (SE). An irregular grid of space-varying fineness conforming to $P(\mathbf{r})$ is generated via the method of topology-representing networks and a subsequent Voronoi tessellation. The discretized SE produces a rate matrix which describes the probabilities of particles hopping from point to point on the grid. We demonstrate the calculation of the rate matrix for ions diffusing through the balloon-like structure of the mechanosensitive channel of small conductance (MscS) and thence the determination of mean first-passage times that characterize conduction of ions through balloon and channel.

¹Supported by NIH grants P41-RR005969 and R01-GM067887 and NSF grant PHYS0822613. XSEDE supercomputer time provided by NSF grant MCA93S028. High performance computing resources provided by Texas Advanced Computing Center, University of Texas at Austin.

1:39PM W48.00013 Fluorescent excitation transfer as a tool for the phase transition studies ,

ALEXEI GOUN, Postdoctoral researcher — The use of the fluorescent resonant excitation transfer technique (FRET) to study the phase transition kinetics is demonstrated. The laser temperature jump is applied to the water/2,6-lutidine mixture and causes the demixing. Coumarin 480 and hydroxypyrene laser dyes form excitation transfer that interrogates the spatial structure of the system. Due to the differential solubility of these dyes in the components of the mixture, the excitation transfer ceases once the phase separation occurs. The spatial resolution of the method is determined by the Forster distance of the excitation transfer pair, and in this case is equal to 3 nm. The phase separation is completed within 1 microsecond. The rising edge of the fluorescence is consistent with polynomial growth of the phase separated domains, and not with Cahn-Hilliard fixed length instability. The theoretical model for the excitation transfer in a variety of systems such as separation of binary mixture, phase reorganization of membranes, formation of lamellar structure is developed.

1:51PM W48.00014 The Physics of Phase-Separation Fronts ,

ALEXANDER WAGNER, ERIC FOARD, Department of Physics, North Dakota State University, Fargo, ND 58108 — When phase separation does occur in a sequential manner, e.g. due to the diffusion of a control parameter into the system, the resulting phase-separation structures have a markedly different appearance than homogeneous phase-separation patterns. The reason lies in the influence the already phase-separated material and the recent phase-separation dynamics exert on the newly phase-separating material. We call the region where phase-separation first occurs the phase-separation front. In this talk we will consider the simplest possible phase-separation front, i.e. a sharp transition in the control parameter moving through the system with a prescribed velocity inducing phase-separation. We show numerical and analytical solutions for the structures that are formed by such a front as a function of the front speed and the composition of the overtaken material.

2:03PM W48.00015 Protected TERS Probes for the Study of Polymer Surfaces ,

REBECCA AGAPOV, The University of Akron, Dept. of Polymer Science, Akron, OH, ALEXEI SOKOLOV, Chemical Sciences Division, ORNL and Department of Chemistry, University of Tennessee, Knoxville, TN, MARK FOSTER, The University of Akron, Dept. of Polymer Science, Akron, OH — The chemistry of polymer surfaces can potentially be imaged with high (~20nm) lateral resolution using Tip Enhanced Raman Spectroscopy (TERS). The method's applicability can be tremendously broadened if the metallized tips central to the technique can be made more robust. Protecting the TERS probes with alumina coatings reduces chemical, mechanical, and thermal degradation, prolonging the use lifetime. Most recently we have focused on the detailed effect of the protective coating for cases in which the enhancement is particularly strong. "Blinking", which is characteristic of extreme enhancement, has been observed with TERS on polymer films for the first time. An alumina coating prolongs the duration of blinking from 20 min to 30 h, greatly extending the experimental window of extreme enhancement. The protective coating is also helpful for illuminating the mechanism behind blinking. Our results are consistent with thermal diffusion of molecules as the major mechanism facilitating blinking.

Thursday, March 1, 2012 11:15AM - 2:15PM –

Session W49 DMP DPOLY: Focus Session: Organic Electronics and Photonics - Thin Film Transistors 162A

11:15AM W49.00001 Pressure effect on organic field-effect transistors ,

YUGO OKADA, KEN-ICHI SAKAI, SHIN KITAOKA, TAKAFUMI UEMURA, JUN TAKEYA, ISIR, Osaka University — Macroscopic transport in organic semiconductors is governed by intermolecular charge transfer, necessarily resulting in its sensitivity to molecular arrangement. The effect of external pressure in such soft materials is fundamentally important because of vulnerability in molecular displacement against relatively small force. Here, we introduce a method of measuring the effect of hydrostatic pressure on the conductivity in organic semiconductor crystals inducing high-mobility charge with the application of electric field. We performed four-terminal conductivity measurement to exclude extrinsic influence of the metal/semiconductor contact resistance. In addition, Hall coefficients are simultaneously measured to deduce the pressure coefficient properly. Using rubrene single-crystal transistors, variation of mobility under pressure turned out to be about 7 times larger than in the typical experiments reported for silicon and other inorganic semiconductors. Interestingly, the mobility starts to decrease with further increasing pressure above 600 MPa. The anomalous negative pressure effect indicate that the application of pressure not only diminishes distance between centers of adjacent molecules but relative positions of equivalent atoms in the two molecules.

11:27AM W49.00002 Determining the elastic constants of rubrene single-crystals¹ ,

MARCOS REYES-MARTINEZ, Polymer Science & Engineering, University of Massachusetts Amherst, ASHWIN RAMASUBRAMANIAM, Mechanical & Industrial Engineering, University of Massachusetts Amherst, ALEJANDRO BRISENO, ALFRED CROSBY, Polymer Science & Engineering, University of Massachusetts Amherst — Organic single crystals have opened the doors to a new generation of high-performance organic electronic devices. Exceptional charge-transport properties combined with the advent of large-area patterning techniques make organic single crystals excellent candidates for flexible electronics applications. However, in order to effectively employ organic single crystals on mechanically flexible architectures, their mechanical properties need to be understood and characterized. In this presentation, the mechanical properties of rubrene single-crystals are investigated. Given the limited dimensions of as-grown crystals and associated handling difficulty, the elastic buckling instability is chosen as a metrology tool for determining the in-plane elastic constants. Our results show that ultrathin (200nm - 1000nm) rubrene crystals exhibit anisotropic wrinkling wavelengths as a function of crystallographic direction, which can be correlated to the anisotropic nature of its molecular packing. An adaptive intermolecular reactive bond order potential (AIREBO) is employed to calculate the nine elastic constants corresponding to orthorhombic rubrene.

¹US Department of Energy, Office of Basic Energy Sciences as part of Polymer-Based Materials for Harvesting Solar Energy, an Energy Frontier Research Center (EFRC)

11:39AM W49.00003 Tuning contorted hexabenzocoronene crystal structure and texture for organic field-effect transistors ,

ANNA HISZPANSKI, Chemical and Biological Engineering Department, Princeton University, ARTHUR WOLL, Cornell High Energy Synchrotron Source, Cornell University, YUEH-LIN LOO, Chemical and Biological Engineering Department, Princeton University — Crystallography conducted on single crystals reveals contorted hexabenzocoronene (HBC) can adopt either herringbone (Pbcn) or slip-stack (P21/c) packing motifs. By adjusting the molecule-solvent interactions during solvent-vapor annealing (SVA), we can controllably crystallize thin films of HBC and access both packing motifs. In HBC films annealed with dichloromethane (DCM) vapor, molecule-solvent interactions are strong and yield highly oriented Pbcn crystals. However, in films annealed with hexanes vapor, molecule-solvent interactions are weaker and randomly oriented P21/c crystals form. In addition to tuning the molecule-solvent interactions via solvent choice, the interactions may also be modulated by selectively fluorinating the peripheral aromatic rings of HBC. With increased fluorination, we decrease molecule-solvent interactions during SVA. As such, we can coax these HBC derivatives to adopt the P21/c crystal structure even with DCM SVA. Further, more fluorinated HBCs form more oriented crystals when exposed to DCM vapors. Transistors fabricated with crystalline HBC active layers suggest that the mobilities of these devices are, to first order, determined by the extent of crystal orientation and less so by the crystal structure. The ability to independently access both crystal structures with varying degrees of orientation has allowed us to decouple their relative contributions to device performance.

11:51AM W49.00004 Quantitative assessments of the effect of microstructure on transport in organic semiconductors, ALBERTO SALLEO, Stanford University — From the fundamental standpoint, organic semiconductors are fascinating as they are neither crystalline nor amorphous and their microstructure plays a central role in governing charge transport. I will show that understanding disorder is the key to determining charge transport mechanism. We are particularly interested in cumulative disorder (paracrystallinity), where the lattice parameter takes on a Gaussian distribution about its mean value. The disorder parameter g allows us to rank materials quantitatively on a continuous scale, from a perfectly crystalline material ($g < 1\%$) to an amorphous one ($g > 10\%$). Surprisingly, even the polymers that are considered to have the highest crystallinity (PBTBT) have a g in the π -stacking direction close to that of an amorphous material ($\sim 7\%$). Furthermore, comparison of X-ray diffraction data and optical absorption data provides insight into the nature of the disordered phase as well. Using first principle calculations and tight binding methods, I will show that paracrystallinity in the π -stacking direction provides a fundamental mechanism for the existence of an exponential distribution of localized tail states in the gap. The larger the degree of disorder the higher the trap density and the deeper their energy. Using disorder as a ranking parameter, I will discuss the differences in transport between small molecule and polymer films as well as their respective inherent limitations and bottlenecks.

12:27PM W49.00005 Air-Stable Solution-Processed Thin-Film Transistors with Hole Mobilities of $3.5 \text{ cm}^2/\text{Vs}$, YAOCHUAN MEI, KATELYN GOETZ, Department of Physics, Wake Forest University, Winston-Salem, NC, MARSHA LOTH, JOHN ANTHONY, Department of Chemistry, University of Kentucky, Lexington, KY, OANA JURCHESCU, Department of Physics, Wake Forest University, Winston-Salem, NC — We report on organic thin-film transistors fabricated on a novel soluble small molecule organic semiconductor difluoro bis(triethylgermyl) anthradithiophene. Fabrication techniques are all applicable at room temperature and ambient pressure, and include drop-casting, spin-coating, and spray deposition. Devices exhibit remarkable electronic properties, including charge carrier mobilities as high as $3.5 \text{ cm}^2/\text{Vs}$, on/off current ratios of 10^5 , and good environmental and operational stability. Chemical treatment of the contact surface with self-assembled monolayers allows us great control of the crystalline order within the organic semiconductor layer. Because thin-film microstructure defects such as grain boundaries reduce the charge transport capabilities of the active layer, high quality single crystals are grown by physical vapor transport for comparison. By correlating the electrical properties with the structural data obtained from X-ray diffraction, we find that a good $\pi - \pi$ overlap is responsible for this superior electronic behavior.

12:39PM W49.00006 Variable-range hopping transport and Hall effect measurements in electrolyte-gated P3HT, SHUN WANG, MINGJING HA, MICHAEL MANNO, C. DANIEL FRISBIE, C. LEIGHTON, Department of Chemical Engineering and Material Science, University of Minnesota — Extensive charge transport measurements ($1.5 - 250 \text{ K}$) at gate-tuned hole concentrations between 1×10^{20} and $9 \times 10^{20} \text{ cm}^{-3}$ have been made on a single ion-gel gated poly-(3-hexylthiophene) (P3HT) thin film transistor. We report observation of a robust Hall effect, having rational trends with magnetic field, gate voltage, and temperature, and yielding hole concentrations close to those measured via the charging current. At high doping we observe transitions from apparent band transport, to 3D Mott variable range hopping (VRH), to Efros-Shklovskii (ES) VRH on cooling. At lower doping ES VRH is observed at all temperatures. A detailed analysis of the temperature and field-dependence of the VRH resistivity provides information on the localization length and dielectric constant as a function of doping, providing significant insights into the approach to the insulator-metal transition in this system and the nature of the Coulomb-gapped density of states. Work at UMN supported by NSF MRSEC

12:51PM W49.00007 Charge Density Dependent Hole Mobility and Density of States Throughout the Entire Finite Potential Window of Conductivity in Ionic Liquid Gated Poly(3-hexylthiophene), BRYAN D. PAULSEN, C. DANIEL FRISBIE, Department of Chemical Engineering & Materials Science, University of Minnesota — Ionic liquids, used in place of traditional gate dielectric materials, allow for the accumulation of very high 2D and 3D charge densities ($>10^{14} \text{ \#}/\text{cm}^2$ and $>10^{21} \text{ \#}/\text{cm}^3$ respectively) at low voltage ($<5 \text{ V}$). Here we study the electrochemical gating of the benchmark semiconducting polymer poly(3-hexylthiophene) (P3HT) with the ionic liquid 1-ethyl-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate ([EMI][FAP]). The electrochemical stability of [EMI][FAP] allowed the reproducible accumulation of $2 \times 10^{21} \text{ hole}/\text{cm}^3$, or one hole (and stabilizing anion dopant) per every two thiophene rings. A finite potential/charge density window of high electrical conductivity was observed with hole mobility reaching a maximum of $0.86 \text{ cm}^2/\text{V s}$ at $0.12 \text{ holes per thiophene ring}$. Displacement current measurements, collected versus a calibrated reference electrode, allowed the mapping of the highly structured and extremely broad density of states of the P3HT/[EMI][FAP] doped composite. Variable temperature and charge density hole transport measurements revealed hole transport to be thermally activated and non-monotonic, displaying an activation energy minimum of $\sim 20 \text{ meV}$ in the region of maximum conductivity and hole mobility. To show the generality of this result, the study was extended to an additional four ionic liquids and three semiconducting polymers.

1:03PM W49.00008 Conductivity Maxima on the Surface of Organic Semiconductor Crystals at High Charge Densities¹, WEI XIE, C. DANIEL FRISBIE, Department of Chemical Engineering and Materials Science, University of Minnesota — We have previously achieved effective carrier mobility up to $3.2 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ at charge densities larger than 10^{13} cm^{-2} in rubrene electrical double layer transistors (EDLTs) gated with ionic liquids (ILs). At lower temperatures when a larger gate bias can be applied, the maximum attainable charge density reaches $6.5 \times 10^{13} \text{ cm}^{-2}$ ($0.34 \text{ holes per rubrene molecule}$), and more remarkably, two pronounced maxima in channel conductivity have been reproducibly and stably observed. This feature, which has not been reported for any EDLTs gated with electrolytes, is independent of ionic liquid composition, current-voltage sweep rate, and crystallographic directions of rubrene crystals. We have identified that the first and second conductivity peaks occur at charge densities of $2.0 \times 10^{13} \text{ cm}^{-2}$ and $5.2 \times 10^{13} \text{ cm}^{-2}$, respectively. Capacitance-voltage (C-V) measurements at different frequencies have also revealed two maxima at the same gate voltages as in current-voltage measurements. Collectively, these observations imply that the conductivity maxima at high charge densities are very likely related to the electronic band structure on the surface of rubrene crystals.

¹This work is funded by NSF MRSEC at the University of Minnesota

1:15PM W49.00009 Solvent-Resistant Organic Transistors and Thermally-Stable Organic Photovoltaics Based on Crosslinkable Conjugated Polymers, H.J. KIM, C.-H. CHO, B.J. KIM, KAIST, A.-R. HAN, J.H. OH, UNIST, J.M.J. FRECHET, UC Berkeley — Conjugated polymers in general are unstable when exposed to air, solvent, or thermal treatment, and these challenges limit their practical applications. Herein we have developed a simple, but powerful approach to achieve solvent-resistant and thermally stable organic electronic devices with improved air-stability, by introducing a crosslinkable group into a conjugated polymer. To demonstrate this concept, we have synthesized polythiophene with crosslinkable groups attached to the end of alkyl chain. Photo-crosslinking of crosslinkable P3HT dramatically improves the solvent resistance of the active layer without disrupting the molecular ordering and charge transport. This is the first demonstration of solvent-resistant organic transistors. Furthermore, the bulk-heterojunction organic photovoltaics (BHJ OPVs) containing crosslinkable P3HT show an average efficiency higher than 3.3% after 40 h annealing at an elevated temperature of 150°C , which represents one of the most thermally-stable OPV devices reported to date. This enhanced stability is due to an in-situ compatibilizer that forms at the P3HT/PCBM interface and suppresses macrophase separation.

1:27PM W49.00010 Surface enhanced Raman spectroscopic studies of the metal-semiconductor interface in organic field effect transistors¹, DANISH ADIL, SUCHI GUHA, Departemnt of Physics and Astronomy, University of Missouri, Columbia, MO 65211 — The performance of organic field-effect transistors (FETs) largely depends on the nature of interfaces of dissimilar materials. Metal-semiconductor interfaces, in particular, play a critical role in the charge injection process. Here, Raman spectroscopy is used to investigate the nature of the Au-semiconductor interface in pentacene based FETs. A large enhancement in the Raman intensity (SERS) is observed from the pentacene film under the Au layer. The enhancement is evidence of a nano-scale roughness in the morphology of the interface, which is further confirmed by electron microscopy images. The morphology of the interface is investigated by SERS as a function of the pentacene layer thickness and the Au layer thickness. The Raman spectra are found to be extremely sensitive in detecting small changes in the morphology of the interface in the sub-nanometer range. Changes in the Raman spectra are further tracked after biasing and ageing the devices. Evolution of these Raman spectra is correlated with degradation in device performance. Finally, FETs based on other donor-acceptor semiconductors are probed by Raman scattering and contrasted with those of the pentacene-based devices.

¹This work was supported by NSF-ECCS # 0823563.

1:39PM W49.00011 Ultra-thin body poly(3-hexylthiophene) transistors with improved short-channel performance, CHENCHEN WANG, Applied Physics, Stanford University, JONATHAN RIVNAY, SCOTT HIMMELBERGER, Department of Materials Science and Engineering, Stanford Univerity, KIARASH VAKHSOURI, ENRIQUE D. GOMEZ, Department of Chemical Engineering, The Pennsylvania State University, ALBERTO SALLEO, Department of Materials Science and Engineering, Stanford Univerity — The microstructure and charge transport properties of binary blend of regioregular (rr) and regiorandom(RRa) poly(3-hexylthiophene) (P3HT) are investigated. X-ray diffraction study shows vertical phase separation in the blend films, with rr-P3HT crystallized at the semiconductor/dielectric interface. These thin film transistors with layered structure preserve high field effect mobility when rr-P3HT contents are reduced to as low as 5.6% where the channel thickness is only a few nanometers. As a result of this ultra-thin active layer at interface, short channel effects due to bulk currents are eliminated, suggesting a new route to fabricate high performance, small size and reliable electronic devices.

1:51PM W49.00012 Physical Characterization of Functionalized Silk Material for Electronic Application and Devices¹, EDEN STEVEN, National High Magnetic Field Laboratory, USA, ERIC JOBILIONG, University of Pelita Harapan, Indonesia, JIN GYU PARK, ANANT PARAVASTU, MICHAEL DAVIDSON, MICHELLE BAIRD, RUFINA ALAMO, PAPATYA KANER, JAMES BROOKS, THEO SIEGRIST, National High Magnetic Field Laboratory, USA — Naturally harvested spider silk fibers are investigated for their physical properties under ambient, humidified, iodine-doped, pyrolyzed, sputtered gold and carbon nanotube coated conditions. The functional properties include: humidity activated conductivity; enhanced flexibility and carbon yield of pyrolyzed iodized silk fibers; full metallic conductivity and flexibility of micron-sized gold-sputtered silk fibers; and high strain sensitivity of carbon nanotube coated silk fibers. Magic angle spinning nuclear magnetic resonance (MAS-NMR) and Fourier transform infrared spectroscopy (FTIR) are used to explore the nature of ambient and functionalized spider silk fiber, and significant changes in amino acid-protein backbone signature are correlated with gold sputtering, and iodine-doped conditions. The application of gold-sputtered neat spider silk fibers for making four terminal flexible, clean, ohmic contacts to organic superconductor samples and carbon nanotube coated silk fibers for heart pulse monitoring sensor are demonstrated. The role of silk thin film in organic thin film transistor will be briefly discussed.

¹E.S. is supported by NSF-DMR 1005293.

2:03PM W49.00013 Spectroscopic signatures of ambipolar injection in narrow gap donor-acceptor polymer transistors, OMAR KHATIB, UCSB, JONATHAN D. YUEN, UCSB, JIM WILSON, UCSB, RAJEEV KUMAR, Nanoterra, FRED WUDL, UCSB, MASSIMILIANO DI VENTRA, UCSB, ALAN J. HEEGER, UCSB, DIMITRI N. BASOV, UCSB — Donor-Acceptor (D-A) copolymers have recently emerged as versatile materials for use in a large variety of device applications. Specifically, these systems possess extremely narrow bandgaps, enabling ambipolar charge transport when integrated in solution-processed field-effect transistors (OFETs). However, the fundamentals of electronic transport in this class of materials remain unexplored. We present a systematic investigation of ambipolar charge injection in D-A conjugated polymers polybenzobisthiadiazole-dithienopyrrole (PBBTPD) and polybenzobisthiadiazole-dithienocyclopentane (PBBTCD) using infrared spectroscopy. We observed a significant modification of the absorption edge in both PBBTPD- and PBBTCD-based OFETs under the applied electric field. The absorption edge reveals hardening under electron injection and softening under hole injection. The most straightforward interpretation of the observed band edge modification is in terms of the linear Stark effect, implying the existence of a built-in electrical dipole moment in these polymers. Additionally, we carried out microscopic IR measurements to characterize the ambipolar injection profile between electrodes.

Thursday, March 1, 2012 11:15AM - 2:15PM —

Session W50 DPOLY DFD: Focus Session: Micro and Nano Fluidics I: Devices and Applications

162B

11:15AM W50.00001 Self-Sorting of Deformable Particles in a Microfluidic Circuit¹, MARCO A. CARTAS-AYALA, MOHAMMED RAAFAT, ROHIT KARNIK, MIT — Sorting of cells, droplets, and particles based on physical characteristics including size and deformability is important for bioseparation, diagnostics, and two-phase microfluidics. While several methods have been developed to sort particles based on size, few techniques exist for sorting of particles based on deformability. Here, we present a microfluidic circuit that enables self-sorting of deformable particles based on the hydraulic resistance that the particle induces in a microchannel, which directly relates to the particle deformability. The present method employs a feed-forward circuit that biases a microfluidic Y-junction based on the hydraulic resistance induced by the particle as it enters a sensing channel. Since particles encountering a symmetric junction follow the branch with the higher flow rate, the resulting modulation of fluid flow at the junction switches the particle into one of two output channels depending on the resistance induced by the particle. Since hydraulic resistance can be influenced by particle-wall interactions, it also opens possibilities for functionalizing the sensing channel for sorting based on specific interactions. This technique may find use in cell sorting and analysis and in two-phase microfluidics.

¹This work was partially supported by CONACYT (Mexican Science and Technology Council), grant 205899.

11:27AM W50.00002 Accelerating Yeast Prion Biology using Droplet Microfluidics¹, LLOYD UNG, ASSAF ROTEM, Harvard School of Engineering and Applied Sciences, DANIEL JAROSZ, Whitehead Institute for Biomedical Research, MANOSHI DATTA, Whitehead Institute for Biomedical Research, MIT Computational and Systems Biology, SUSAN LINDQUIST, Whitehead Institute for Biomedical Research, Howard Hughes Medical Institute, MIT Department of Biology, DAVID WEITZ, Harvard School of Engineering and Applied Sciences, Department of Physics — Prions are infectious proteins in a misfolded form, that can induce normal proteins to take the misfolded state. Yeast prions are relevant, as a model of human prion diseases, and interesting from an evolutionary standpoint. Prions may also be a form of epigenetic inheritance, which allow yeast to adapt to stressful conditions at rates exceeding those of random mutations and propagate that adaptation to their offspring. Encapsulation of yeast in droplet microfluidic devices enables high-throughput measurements with single cell resolution, which would not be feasible using bulk methods. Millions of populations of yeast can be screened to obtain reliable measurements of prion induction and loss rates. The population dynamics of clonal yeast, when a fraction of the cells are prion expressing, can be elucidated. Furthermore, the mechanism by which certain strains of bacteria induce yeast to express prions in the wild can be deduced. Integrating the disparate fields of prion biology and droplet microfluidics reveals a more complete picture of how prions may be more than just diseases and play a functional role in yeast.

¹LU acknowledges funding from NSERC

11:39AM W50.00003 Microfluidic devices for droplet injection, DONALD AUBRECHT, ILKE AKARTUNA, DAVID WEITZ, Harvard University — As picoliter-scale reaction vessels, microfluidic water-in-oil emulsions have found application for high-throughput, large-sample number analyses. Often, the biological or chemical system under investigation needs to be encapsulated into droplets to prevent cross contamination prior to the introduction of reaction reagents. Previous techniques of picoinjection or droplet synchronization and merging enable the addition of reagents to individual droplets, but present limitations on what can be added to each droplet. We present microfluidic devices that couple the strengths of picoinjection and droplet merging, allowing us to selectively add precise volume to our droplet reactions.

11:51AM W50.00004 Microfluidic devices for label-free separation of cells through transient interaction with asymmetric receptor patterns¹, S. BOSE, R. SINGH, M.H. HOLLATZ², C.-H. LEE, MIT, J. KARP, Brigham & Women's Hospital, R. KARNIK, MIT — Cell sorting serves an important role in clinical diagnosis and biological research. Most of the existing microscale sorting techniques are either non-specific to antigen type or rely on capturing cells making sample recovery difficult. We demonstrate a simple; yet effective technique for isolating cells in an antigen specific manner by using transient interactions of the cell surface antigens with asymmetric receptor patterned surface. Using microfluidic devices incorporating P-selectin patterns we demonstrate separation of HL60 cells from K562 cells. We achieved a sorting purity above 90% and efficiency greater than 85% with this system. We also present a mathematical model incorporating flow mediated and adhesion mediated transport of cells in the microchannel that can be used to predict the performance of these devices. Lastly, we demonstrate the clinical significance of the method by demonstrating single step separation of neutrophils from whole blood. When whole blood is introduced in the device, the granulocyte population gets separated exclusively yielding neutrophils of high purity (<10% RBC contamination). To our knowledge, this is the first ever demonstration of continuous label free sorting of neutrophils from whole blood. We believe this technology will be useful in developing point-of-care diagnostic devices and also for a host of cell sorting applications.

¹Funding: NSF CAREER award 0952493 (R.K.), NIH grants HL-095722 and HL-097172 (J.M.K.)

²Current affiliation: California Institute of Technology, Pasadena, USA

12:03PM W50.00005 Role of Structural Asymmetry in Controlling Drop Spacing in Microfluidic Ladder Networks, WILLIAM WANG, JEEVAN MADDALA, SIVA VANAPALLI, RAGHUNATHAN RENGASAMY, Texas Tech University — Manipulation of drop spacing is crucial to many processes in microfluidic devices including drop coalescence, detection and storage. Microfluidic ladder networks —where two droplet-carrying parallel channels are connected by narrow bypass channels through which the motion of drops is forbidden—have been proposed as a means to control relative separation between pairs of drops. Prior studies in microfluidic ladder networks with vertical bypasses, which possess fore-aft structural symmetry, have revealed that pairs of drops can only undergo reduction in drop spacing at the ladder exit. We investigate the dynamics of drops in microfluidic ladder networks with both vertical and slanted bypasses. Our analytical results indicate that unlike symmetric ladder networks, structural asymmetry introduced by a single slanted bypass can be used to modulate the relative spacing between drops, enabling them to contract, synchronize, expand or even flip at the ladder exit. Our experiments confirm all the behaviors predicted by theory. Numerical analysis further shows that ladders containing several identical bypasses can only linearly transform the input drop spacing. Finally, we find that ladders with specific combinations of vertical and slanted bypasses can generate non-linear transformation of input drop spacing, despite the absence of drop decision-making events at the bypass junctions.

12:15PM W50.00006 Synchronized Reinjection and Coalescence of Droplets in Microfluidics, MANHEE LEE, Department of Physics, Harvard University, JESSE COLLINS, DONALD AUBRECHT, SHINHYUN KIM, TINA LIN, ASSAF ROTEM, School of Engineering and Applied Sciences, Harvard University, LAURA SOLOMON, College of Engineering, Temple University, DAVID WEITZ, School of Engineering and Applied Sciences, Harvard University, VINOTHAN MANOHARAN, Department of Physics & School of Engineering and Applied Sciences, Harvard University, DAVID A. WEITZ COLLABORATION — In droplet-based microfluidics, one of the essential techniques is controlled addition of desired materials into the droplets. This is best achieved through the coalescence of pairs of droplets, and therefore various methods of coalescence have been developed over the last decade. However, the coalescence of two different droplets made independently in different devices still remains a challenging problem, primarily because it is difficult to synchronize the reinjection of the different droplets before their coalescence. In addition, typical coalescers require some specific conditions such as uniform droplet-droplet distances and constant flow rate, which hinders the flexible use of coalescers in practical applications. Here we present a straightforward method for synchronizing reinjection of two kinds of droplets and coalescing them. We employ a home-made emulsion collector operated by hydrostatic pressure to reinject droplets into a device, where two kinds of droplets are driven into two opposing T-junction alternatively and then pairs of droplets are merged at the new coalescer proposed here. We use the technique to create droplets with a controlled number of colloidal particles inside, so that we can observe their self-assembly into a cluster.

12:27PM W50.00007 Probing cell mechanical properties with microfluidic devices, AMY ROWAT, University of California, Los Angeles — Exploiting flow on the micron-scale is emerging as a method to probe cell mechanical properties with 10-1000x advances in throughput over existing technologies. The mechanical properties of cells and the cell nucleus are implicated in a wide range of biological contexts: for example, the ability of white blood cells to deform is central to immune response; and malignant cells show decreased stiffness compared to benign cells. We recently developed a microfluidic device to probe cell and nucleus mechanical properties: cells are forced to deform through a narrow constrictions in response to an applied pressure; flowing cells through a series of constrictions enables us to probe the ability of hundreds of cells to deform and relax during flow. By tuning the constriction width so it is narrower than the width of the cell nucleus, we can specifically probe the effects of nuclear physical properties on whole cell deformability. We show that the nucleus is the rate-limiting step in cell passage: inducing a change in its shape to a multilobed structure results in cells that transit more quickly; increased levels of lamin A, a nuclear protein that is key for nuclear shape and mechanical stability, impairs the passage of cells through constrictions. We are currently developing a new class of microfluidic devices to simultaneously probe the deformability of hundreds of cell samples in parallel. Using the same soft lithography techniques, membranes are fabricated to have well-defined pore distribution, width, length, and tortuosity. We design the membranes to interface with a multiwell plate, enabling simultaneous measurement of hundreds of different samples. Given the wide spectrum of diseases where altered cell and nucleus mechanical properties are implicated, such a platform has great potential, for example, to screen cells based on their mechanical phenotype against a library of drugs.

1:03PM W50.00008 Droplet Microfluidics for Virus Discovery , ASSAF ROTEM, Department of Physics and SEAS Harvard University, SHELLEY COCKRELL, Department of Biological Sciences University of Pittsburgh, MIRA GUO, Department of Physics and SEAS Harvard University, JAMES PIPAS, Department of Biological Sciences University of Pittsburgh, DAVID WEITZ, Department of Physics and SEAS Harvard University, WEITZ LAB TEAM, PIPAS LAB TEAM — The ability to detect, isolate, and characterize an infectious agent is important for diagnosing and curing infectious diseases. Detecting new viral diseases is a challenge because the number of virus particles is often low and/or localized to a small subset of cells. Even if a new virus is detected, it is difficult to isolate it from clinical or environmental samples where multiple viruses are present each with very different properties. Isolation is crucial for whole genome sequencing because reconstructing a genome from fragments of many different genomes is practically impossible. We present a Droplet Microfluidics platform that can detect, isolate and sequence single viral genomes from complex samples containing mixtures of many viruses. We use metagenomic information about the sample of mixed viruses to select a short genomic sequence whose genome we are interested in characterizing. We then encapsulate single virions from the same sample in picoliter volume droplets and screen for successful PCR amplification of the sequence of interest. The selected drops are pooled and their contents sequenced to reconstruct the genome of interest. This method provides a general tool for detecting, isolating and sequencing genetic elements in clinical and environmental samples.

1:15PM W50.00009 Creating 3D chemical gradients with self-folding microfluidic networks , MUSTAPHA JAMAL, YEVGENIY KALININ, AASIYEH ZARAFSHAR, DAVID GRACIAS, Chemical and Biomolecular Engineering, Johns Hopkins University — We describe the reversible self-folding of polymeric films into intricate three-dimensional (3D) microfluidic networks and investigate their utility as bio-inspired synthetic vasculature for in vitro tissue culture models. Our fabrication methodology relies on patterning of channels inside the films at the planar microfabrication stage followed by programmable self-folding of the two-dimensional patterned structures. Here self-folding action is enabled by stress gradients which develop in the films due to differential ultraviolet cross-linking and subsequent solvent conditioning. We achieved wafer-scale assembly of micropatterned geometries including helices, polyhedra and corrugated sheets. To demonstrate utility of such self-folded microfluidic devices we present localized chemical delivery of biochemicals in 3D to discrete regions of cells cultured on the curved self-assembled surfaces and in a thick, surrounding hydrogel. We believe that the devices can be used to mimic such natural self-assembled systems as leaves and tissues. Reference: M. Jamal et al., Nature Communications (2011; in press).

1:27PM W50.00010 Control of Mass Transport and Chemical Reaction Kinetics in Ultrasmall Volumes , CHARLES COLLIER, ORNL — This talk will describe means for triggering chemical reactions for studying reaction kinetics under extreme confinement with sub-millisecond temporal resolution, including on-demand generation and fusion of femtoliter (10^{-15} L) volume water-in-oil droplets, and triggering reactions in femtoliter chambers microfabricated in poly(dimethylsiloxane) (PDMS). We demonstrated a reversible chemical toggle switch, which lays the groundwork for exploring more complex chemical and biochemical reaction sequences triggered and monitored in real time in discrete ultrasmall reactors, such as sequential and coupled enzymatic reactions. We are also developing methods to vary confinement and macromolecular crowding in ultrasmall, water-in-oil droplets and chambers micromolded in PDMS as biomimetic reaction vessels containing minimal synthetic gene circuits, in order to better understand how confinement, reduced dimensionality and macromolecular crowding affect molecular mechanisms involved in the operation and regulation of genetic circuits in living cells.

1:39PM W50.00011 Thin Polymer Films as Microvalves in Microfluidic Devices , CLEMENCE VERGNE, FABRICE MONTI, PATRICK TABELING, UMR 7083 CNRS ESPCI, YVETTE TRAN, LUCIE DEVYS, UMR 7615 CNRS ESPCI, MMN TEAM, PPMD TEAM — We report on a novel technology allowing the integration of microvalves and micropumps in lab-on-a-chips made of either soft or hard materials. The approach is based on the grafting of responsive hydrogels onto the microchannel walls. These gels undergo large volume variations by absorbing or expelling water when subjected to external stimuli (here, temperature is used as the stimulus). The hydrogel thin films we study here are chemical polymer networks that are covalently bound to the surface. The first step of the elaboration of that valves is the development of the surface-attached hydrogel thin films. The objective is to obtain hydrogel films with a wide range of thicknesses. The second step is the completion of the microfluidic system by bonding a channel on the active surface. The polymer used is thermoresponsive, at room temperature the swollen gel forms a thick layer, measuring typically several micrometers. When the system is heated above the LCST (Low Critical Solution Temperature), the gel collapses, forming a submicrometric film. In this work we introduce two different applications. In the first situation, the gel layer constitutes a variable resistance. In the second situation the polymer entirely closes the channel after swelling, thus forming a valve.

1:51PM W50.00012 Nanofluidic Transistor Circuits¹ , HSUEH-CHIA CHANG, LI-JING CHENG, YU YAN, ZDENEK SLOUKA, SATYAJYOTI SENAPATI, University of Notre Dame — Non-equilibrium ion/fluid transport physics across on-chip membranes/nanopores is used to construct rectifying, hysteretic, oscillatory, excitatory and inhibitory nanofluidic elements. Analogs to linear resistors, capacitors, inductors and constant-phase elements were reported earlier (Chang and Yossifon, BMF 2009). Nonlinear rectifier is designed by introducing intra-membrane conductivity gradient and by asymmetric external depletion with a reverse rectification (Yossifon and Chang, PRL, PRE, Europhys Lett 2009-2011). Gating phenomenon is introduced by functionalizing polyelectrolytes whose conformation is field/pH sensitive (Wang, Chang and Zhu, Macromolecules 2010). Surface ion depletion can drive Rubinstein's microvortex instability (Chang, Yossifon and Demekhin, Annual Rev of Fluid Mech, 2012) or Onsager-Wien's water dissociation phenomenon, leading to two distinct overlimiting I-V features. Bipolar membranes exhibit an S-hysteresis due to water dissociation (Cheng and Chang, BMF 2011). Coupling the hysteretic diode with some linear elements result in autonomous ion current oscillations, which undergo classical transitions to chaos. Our integrated nanofluidic circuits are used for molecular sensing, protein separation/concentration, electrospray etc.

¹This work is supported by NSF CBET 1060652 and NSF EFRI 0937997.

2:03PM W50.00013 The Lab-on-a-Disc: Miniature Counterpart to the Lab-on-a-CD for Driving Chip-Based Microcentrifugation , LESLIE YEO, NICK GLASS, RICHARD SHILTON, PEGGY CHAN, JAMES FRIEND, Micro/Nanophysics Research Laboratory, RMIT University — The Lab-on-a-CD concept has opened up the powerful possibility of carrying out a range of microfluidic operations simply by using a compact disc (CD) player to spin a disc on which microchannels are fabricated. Nevertheless, the bulk rotation of the entire CD structure is cumbersome, expensive and unreliable - the antithesis of microfluidic philosophy. Fluid transfer on and off the chip can also be difficult. We have instead developed a miniaturized centrifugal microfluidic platform for lab-on-a-chip applications that employs surface acoustic waves to drive the rotation of a 10 mm SU-8 disc on which microfluidic structures are patterned. Unlike its macroscopic Lab-on-a-CD counterpart, the Lab-on-a-Disc does not require moving parts, and is inexpensive, disposable, and significantly smaller both in terms of the disc itself and the portable palmtop battery-operated circuit used to power the chip-sized device. In the first proof of concept, we show the capability of the Lab-on-a-Disc platform to drive capillary-based valving, mixing and size-based concentration/separation of aqueous particle suspensions in microchannels on the disc. To the best of our knowledge, the miniature Lab-on-a-Disc concept is the first microcentrifugation platform small enough to comprise a handheld device.

Thursday, March 1, 2012 11:15AM - 2:15PM —
Session W52 GSNP DFD: Focus Session: Extreme Mechanics - Fluid-Structure Interactions and Swelling 153C

11:15AM W52.00001 Capillary rise between exible walls¹ , JOSÉ BICO, THOMAS CAMBAU, ETIENNE REYSSAT, PMMH-ESPCI — We report experimental work on capillary rise of a liquid in a cell formed by parallel plates, one of which is flexible. We show that above a critical width, the cell collapses under the negative capillary pressure in the liquid. This collapse allows the liquid to rise virtually without limit between the plates. The height of the rising front is found to increase with time as $t^{1/3}$, a characteristic of capillary imbibition in a wedge.

¹funding: ANR MecaWet-Paris 7 University-CNRS-ESPCI

11:27AM W52.00002 Motion of a rigid sphere through an elastic tube , THOMAS CAMBAU, JOSE BICO, ETIENNE REYSSAT, PMMH ESPCI PARISTECH — The transport of soft objects through small rigid channels is a common problem in the biological world : red blood cells are deformed when passing through small capillaries and polymer coils can make their way through minute pores. We study the opposite model problem of a rigid sphere moving in a narrower elastic tube. Geometry, mechanical properties of the tube and friction or lubrication conditions determine the dynamics of the entrapped sphere. We present experimental results on this problem, together with scaling law analysis.

11:39AM W52.00003 Equilibrium and stability of an elastic meniscus¹ , MARCO RIVETTI, ARNAUD ANTKOWIAK, Institut Jean le Rond d'Alembert, UPMC & CNRS — A liquid-air interface touching a solid wall gives rise to a liquid meniscus, whose shape has been well known for two centuries and results from the balance between capillarity and gravity. We investigate the case in which a portion of the liquid interface has been replaced by a soft strip, adding the elastic ingredient to this physical problem. We experimentally study the equilibrium configurations, from small to high non-linear deformations, and we compare to a 2D theoretical model. Stability of the system involving 3D corrections is also addressed.

¹This work is supported by ANR grant ANR-09-JCJC-0022- 01 and “La Ville de Paris - Programme Emergence.”

11:51AM W52.00004 Capillary-Induced Self-Organization of Soft Pillar Arrays into Moiré Patterns by Dynamic Feedback Process , SUNG KANG, NING WU, ALISON GRINTHAL, JOANNA AIZENBERG, School of Engineering and Applied Sciences, Harvard University — We report a self-organized pattern formation of polymer nanopillar arrays by dynamic feedback: two nanopillar arrays collectively structure a sandwiched liquid and pattern the menisci, which bend the pillars into Moiré patterns as it evaporates. Like the conventional Moiré phenomenon, the patterns are deterministic and tunable by mismatch angle, yet additional behaviors—chirality from achiral starting motifs and preservation of the patterns after the surfaces are separated—appear from the feedback process. Patterning menisci based on this mechanism provides a simple, scalable approach for making a series of complex, long-range-ordered structures. Reference: Sung H. Kang, Ning Wu, Alison Grinthal, and Joanna Aizenberg, Phys. Rev. Lett., **107**, 177802 (2011).

12:03PM W52.00005 Study of waving of grass using a soap film model , RAVI SINGH, Brown University, MAHESH BANDI, Okinawa Institute of Science and Technology, L. MAHADEVAN, Harvard University, AMALA MAHADEVAN, Woods Hole Oceanographic Institution, SHREYAS MANDRE, Brown University — Wind blowing over a grass field incites synchronized response from the grass blades, which appear as waves. This effect is called Mo-nami in a terrestrial setting, while in an aquatic setting it is termed as Ho-nami. We use a combination of experimental observations, numerical simulations and theoretical analysis to understand this effect. The experiment is conducted in two-dimensional realization of these phenomena in a gravity driven soap film tunnel. Nylon filaments attached to the boundaries of the soap film play the role of the grass. We provide a preliminary characterization of this analog model for the synchronized oscillations of grass.

12:15PM W52.00006 Direct measurements of flow and deformation of a free reed , PETER BUCHAK, University of Massachusetts Amherst, JOHN BUSH, Massachusetts Institute of Technology — The free reed, responsible for producing sound in a family of air-driven musical instruments, is an example of a coupled fluid-structure system engineered to vibrate efficiently at a controllable frequency. In Western free reed instruments, a flexible metal plate is clamped at one end above a slot cut into a rigid support plate. This geometry allows a constant driving pressure to produce and sustain large-amplitude vibrations. The mechanism behind this has been discussed by several investigators. However, it has yet to be verified experimentally with direct measurements of the flow speed. We present simultaneous measurements of the reed motion and the flow speed in the downstream jet, which enable characterization of the relationship between the finite-amplitude deformation of the reed and the flow.

12:27PM W52.00007 Control and Manipulation of Fluid Flow Using Elastic Deformations , BEHROUZ TAVAKOL, DOUGLAS HOLMES, Virginia Tech, GUILLAUME FROELICHER, HOWARD STONE, Princeton University — In this work, we utilize elastic deformations within a flexible microfluidic device via mechanical actuation to control and direct fluid flow. The device consists of a microchannel with a flexible arch prepared by buckling a thin elastic film. The deflection of the arch can be predicted and controlled using the classical theory of Euler buckling. We controlled the fluid flow rate by coupling the elastic deformation of the arch to the gap within the microchannel, and matched these experimental results analytically with a perturbation of lubrication theory and with computational simulations. These results illustrate an experimental design paradigm for the preparation of portable microchannels for chemical mixing, self-healing, and in situ diagnostics.

12:39PM W52.00008 Curling paper , ETIENNE REYSSAT, PMMH-ESPCI, L. MAHADEVAN, Harvard University — As many soft materials, paper is mechanically sensitive to humidity. Owing to its hygroscopic cellulose-based structure, it is known to wrinkle when subject to humidity fluctuations. Here, we present experimental results on the more extreme deformations observed when a sheet of tracing paper is put on a bath of water. After contact with the liquid surface, water diffuses into the hygroscopic material from below and induces differential swelling, resulting in the curling of the paper. Within seconds, a spectacular roll-up motion follows. We explain the observed shapes and curling dynamics.

12:51PM W52.00009 Walking and jumping spores , PHILIPPE MARMOTTANT, University of Grenoble and CNRS, Lab. Interdisciplinaire de Physique, France — The Equisetum plants, more commonly called “horsetail,” emit 50-microns spores that are spherical in shape and present four hygroscopic arms. Under high humidity, the arms are retracted. But under lower humidity, less than 70%, the four arms deploy beautifully. With time-lapse image recordings, we show that under repeated cycles of dry and high humidity, the spores behave as random walkers, since they move by about their size in a different direction at every cycle. The process is apparently stochastic because of the complex shape of the arms and hysteretic friction of the arms on the ground. For some spores, a decrease in humidity level results in very fast jumps, the spores taking off at a typical velocity of a meter per second, as recorded on high-speed camera. With these jumps, they reach centimetric elevations, much larger than their size. The physical mechanism at the root of these “Levy-flight” jumps is still under investigation. The walking and jumping phenomena thus provide motility, which we believe is helpful for the understanding of the biological dispersion of the spores. It could also bring biomimetic inspiration to engineer new motile elastic structures.

1:03PM W52.00010 Mechanic instabilities of swelling gels , MARTINE BEN AMAR, JULIEN DERVAUX, Ecole Normale Supérieure — While the study of gels takes undoubtedly its roots within the field of physico-chemistry, the interest for gels has flourished and they progressively became an important object in the study of the mechanics of polymeric materials and volumetric growth, rising some fascinating problems, some of them remaining unsolved. Because gels are multiphase objects, their study represents an important step in the understanding of the mechanics of complex soft matter as well as for the process of shape generation in biological bodies. I will present here experiments and models of swelling gels mainly in the cylindrical geometry which mimic various growth instabilities from tumors up to the morphogenesis of tubular organs.

1:15PM W52.00011 Patterns formed by swelling-induced folding of films¹, SACHIN VELANKAR, VICTORIA LAI, University of Pittsburgh, RICHARD VAIA, Wright Patterson Air Force Base — The solvent swelling of a thin polymer film attached to a rigid substrate is known to induce a creasing pattern on the free surface of the film. Here we show that if the film is weakly attached to the substrate, the swelling-induced compressive stress nucleates buckle delamination of the film from the substrate. Surprisingly, the buckles do not have a sinusoidal profile, instead, the film near the delamination buckles slides towards the buckles causing growth of sharp folds of high aspect ratio. The folds persist even after the solvent evaporates. Such fold formation depends on the size of the region of the film exposed to solvent. A very small region of exposure (realized by placing a small drop of solvent on the film) does not induce delamination. Remarkably, with moderate sized drops, the delamination and folding occurs around the perimeter of the drop, thus culminating in a corral with tall walls. We quantify the parameters (drop volume, film thickness) which demarcate the transitions between no fold formation, corral formation, and multiple fold formation.

¹Funding support from AFOSR Grant number FA9550-10-1-0329 is acknowledged.

1:27PM W52.00012 Swelling-Driven Shaping of Thermally Responsive Photo-Patterned Gel Sheets, MYUNGHWAN BYUN, JUNGWOOK KIM, RYAN HAYWARD, Polymer Science and Engineering Department, University of Massachusetts Amherst, JAMES HANNA, CHRISTIAN SANTANGELO, Physics Department, University of Massachusetts Amherst — Swelling-mediated shaping of patterned non-Euclidean plates offers a powerful route to design and engineer complex 3-D structures, with possible applications in biomedicine, robotics, and tunable micro-optics. We have studied the behavior of poly(N-isopropyl acrylamide) (PNIPAm) copolymers containing pendent benzophenone units that allow the degree of crosslinking to be tuned by varying the dose of ultraviolet light. A halftone (gray) gel lithography approach, wherein two photomasks enable patterning of highly-crosslinked domains within a lightly-crosslinked matrix, is shown to provide effectively continuous variations in swelling in truly two-dimensional patterns. We show how this technique can be harnessed to form complex, reversibly actuating, 3-D structures through patterned growth.

1:39PM W52.00013 Dynamical Actuation and Pattern Formation with Local Swelling in Microgels¹, HOWON LEE, KIN HUNG FUNG, NICHOLAS FANG, MIT — In this invited talk, we present a set of study on swelling-induced actuation and pattern formation in hydrogels of three dimensional microstructures. For example, rapid actuation of a micro hydrogel device is observed by exploiting swelling-induced snap-buckling. Utilizing its fast actuation speed, the device can even jump by itself upon wetting. It is demonstrated that elastic energy is effectively stored and quickly released from the device by incorporating elastic instability. In our experiment, the micro device could generate a snapping motion within 12 milliseconds, releasing power at a rate of 34 mW/g. We also captured the evolution circumferential buckling of tubular shaped microgels. Inhomogeneous stress develops as gel swells under mechanical constraints, which gives rise to buckling instability. A simple analytical model is developed using elastic energy to predict stability and post-buckling patterns upon swelling. Our experiment demonstrates that circumferential buckling of desired mode can be created in a prescribed manner. Our study on the mechanics of three-dimensionally microstructured gels might provide new insights for in morphogenesis in tissue engineering, and provide new gateways in many emerging fields such as soft robotics and tunable matamaterials.

¹partially supported by NSF and LLNL LDRD

1:51PM W52.00014 Separating Viscoelasticity and Poroelasticity of Gels with Different Length and Time Scales, ANIRUDH MOHAN, XUANHE ZHAO, Soft Active Materials Laboratory, Duke University, SOFT ACTIVE MATERIALS LABORATORY, DUKE UNIVERSITY TEAM — Viscoelasticity and poroelasticity commonly coexist in polymer gels. We propose a method capable of separating the viscoelasticity and poroelasticity of gels in various mechanical tests. The viscoelastic characteristic times and the poroelastic diffusivities of a gel can define intrinsic material length scales of the gel. The experimental setup can give sample length scales, over which the solvent migrates in the gel. By setting the sample lengths to be much larger or smaller than the material lengths, the viscoelasticity and poroelasticity of the gel will manifest at different time scales in a test. Therefore, the viscoelastic and poroelastic properties of the gel can be probed separately at different time scales of the test.

2:03PM W52.00015 A constitutive theory for visco-hyperelastic gels, SHAWN CHESTER, Lawrence Livermore National Laboratory — Many gels operate in chemically saturated environments in a variety of applications. Most constitutive theories for gels are formulated using large deformation hyperelasticity coupled with fluid transport. However, in most cases the mechanical response of such gels show hysteresis and other dissipative effects which are not accounted for in present constitutive theories. We have recently developed a three dimensional continuum level theory to describe the coupled fluid permeation and large deformation response of visco-hyperelastic materials. In this work, we apply our theory and numerical simulation capability to study the indentation response among others of visco-hyperelastic gels.

Thursday, March 1, 2012 11:15AM - 2:15PM —
Session W53 GSNP: Focus Session: Common Features of Soft Materials: Polymers, Colloids and Granular Media I 153B

11:15AM W53.00001 Athermal Jamming Vs Thermalized Glassiness in a Simple Model of Soft-Core Interacting Particles¹, STEPHEN TEITEL, University of Rochester, PETER OLSSON, Umeå University — Numerical simulations of soft-core frictionless disks in two dimensions are carried out to study shear viscosity η and pressure p of a simple model liquid, as a function of thermal temperature T , packing fraction ϕ , and uniform applied shear strain rate $\dot{\gamma}$. We find that viscosity in the athermal hard-core limit, $\lim_{\dot{\gamma} \rightarrow 0} [\lim_{T \rightarrow 0} \eta]$, is singularly disconnected from viscosity in the hard-core thermal limit, $\lim_{T \rightarrow 0} [\lim_{\dot{\gamma} \rightarrow 0} \eta]$, demonstrating that thermal glassy behavior is not governed by the athermal jamming critical point, “point J”.

¹Work supported by Department of Energy Grant No. DE-FG02-06ER46298 and Swedish Research Council Grant No. 2010-3725. Simulations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at PDC and HPC2N.

11:27AM W53.00002 Spontaneous formation of permanent shear bands in a mesoscopic model of flowing disordered matter¹, KIRSTEN MARTENS, LYDÉRIC BOCQUET, LPMCn, Université Lyon 1, JEAN-LOUIS BARRAT, LiPhy, Université Joseph Fourier, Grenoble — In this presentation we propose a coherent scenario of the formation of permanent shear bands in the flow of yield stress materials. Within a minimalistic mesoscopic model we investigate the spatial organisation of plasticity. The most important parameter is the typical time needed to regain the original structure after a local rearrangement. In agreement with a recent mean field study [Coussot *et al.*, *Eur. Phys. J. E*, 2010, **33**, 183] we observe a spontaneous formation of permanent shear bands, when this restructuring time is large compared to the typical stress release time in a rearrangement. This heterogeneous flow behaviour is different in nature from the transient dynamical heterogeneities that one observes in the small shear rate limit in flow without shear-banding [Martens *et al.*, *Phys. Rev. Lett.*, 2011, **106**, 156001]. We analyse the dependence of the shear bands on system size, shear rate and restructuring time. Further we rationalise the scenario within a mean field version of the model, that explains the instability of the homogeneous flow below a critical shear rate. Our study therefore strongly supports the idea that the characteristic time scales involved in the local dynamics are at the physical origin of permanent shear bands.

¹ANR - SYSCOMM, Marie Curie FP7-PEOPLE-2009-IEF

11:39AM W53.00003 Creep and critical scaling in random spring networks¹, BRIAN TIGHE, Delft University of Technology — Random networks of springs are a minimal model for physical, biological, and engineered materials ranging from foams and emulsions to biopolymer and bar-joint networks. Near the central force isostatic point, the creep response of damped networks is intimately tied to the presence or absence of floppy motions in the long time limit. We show that nearly isostatic networks display dynamical critical scaling, and that this scaling connects viscous flow and elastic deformation via a critical creep regime. We give scaling arguments for the critical exponents and confirm our predictions with numerics.

¹Supported by the Dutch Organization for Scientific Research (NWO).

11:51AM W53.00004 Rheology of particle assemblies close to a jamming transition, CLAUD HEUSSINGER, University of Goettingen, Germany — The jamming paradigm aims at providing a unified view for the elastic and rheological properties of materials as different as foams, emulsions, suspensions or granular media. Structurally, these systems can all be viewed as dense assemblies of particles, and the particle volume fraction ϕ plays the role of the coupling constant that tunes the distance to the jamming transition. Enhanced experimental techniques allow to visualize the dynamics of these systems on the level of the individual particles, generating huge amount of information. Several interesting, and partially conflicting, results have emerged. It therefore seems necessary to ask in how far the experimental results reveal genuine aspects of a universal jamming transition, or just system-specific properties that depend on microscopic details, the driving mechanism or the preparation protocol. By comparing different computational models we will discuss the question of universality on the macroscopic level of rheological observables as well as on the microscopic level of single particle trajectories and collective particle motion.

12:03PM W53.00005 Inhomogeneous structure and position-dependent dynamics in complex fluids, JAMES CARMER, Department of Chemical Engineering, University of Texas at Austin, GAURAV GOEL, Department of Chemical Engineering, Indian Institute of Technology, Delhi, JEFFREY ERRINGTON, Department of Chemical and Biological Engineering, University at Buffalo, THOMAS TRUSKETT, Department of Chemical Engineering, University of Texas at Austin — We present computer simulation results of model complex fluids, quantifying how inhomogeneous structuring and dynamics of particles can be tuned through interactions. We first illustrate how a tracer particle's interactions can be tuned to significantly modify its long-time diffusivity. We use a recently proposed propagator-based formalism to address how this enhancement can be understood in terms of the local dynamics of neighboring particles. We then discuss how these results compare to related behaviors of model confined colloidal and molecular fluids.

12:15PM W53.00006 Demonstration of Secondary Currents in the Pressure-Driven Flow of a Concentrated Suspension Through a Square Conduit, ARUN RAMCHANDRAN, ADAM ZREHEN, University of Toronto — It has been known for several decades now that the pressure-driven flow of polymer melts in non-axisymmetric conduits is not unidirectional; the main flow through the channel is accompanied by secondary currents, whose origin can be attributed to second normal stress differences. However, only recently was it realized [Ramachandran and Leighton, *J. Fluid Mech.* (2008)] that the same may be true for concentrated suspensions, which, upon shearing, exhibit strong second normal stress differences. This work confirms the existence of these secondary flows by carrying out pressure-driven suspension flow experiments through a square (non-axisymmetric) duct. By tracking the motion of a thin stream of a contrastingly-dyed suspension introduced into the bulk flow of another, it is demonstrated that the suspension flows out of the sidewalls of the geometry towards the corners of the square cross-section, and then flows towards the center. This is found to be qualitatively consistent with calculations based on the suspension balance model of Nott and Brady [*J. Fluid Mech.* (1994)]. Secondary currents have been predicted to be the dominant mechanism determining particle distribution in suspension flows, and this work lends support to that idea.

12:27PM W53.00007 Understanding entangled polymers: What we can learn from athermal chain packings¹, NIKOS KARAYIANNIS, Institute of Optoelectronics and Microsystems (ISOM) and ETSII, Universidad Politécnica de Madrid (UPM) — The study of random and ordered packings (from atoms and colloidal particles to sand grains) has been the focus of extensive research. This is not surprising since an understanding of the mechanisms that control morphology and packing is the key to the design and synthesis of novel “smart” materials and functionalities. In particular, the study of packings of chain molecules presents challenges but also insights which are absent in monatomic systems and further allows for a direction comparison with them. In this contribution we give an overview of our work on very dense and nearly jammed packings of athermal polymers. We show that chain molecules can be as efficiently and as densely packed as monatomic analogs up to the same maximally random jammed state. We also show that an exact correspondence can be established between the statistical-mechanical ensembles of packings of monatomic, and chain systems, which yields insights on the universality of jamming. By studying the effect of concentration on polymer size and on the underlying network of topological hindrances we precisely identify the distinct universal scaling regimes and the corresponding exponents. An unsuspected connection, valid from dilute up to very dense assemblies, is established between knots (of intermolecular origin) and entanglements (intermolecular constraints). We finally show that, against expectations, entropy-driven crystallization can occur in dense systems of athermal polymers once a critical volume fraction is reached. Such phase transition is driven by the increase in translational entropy: ordered sites exhibit enhanced mobility as their local free volume becomes more spherical and symmetric. Incipient nuclei develop well defined, stack-faulted layered crystal morphologies with a single stacking direction. The ordering transition and the resulting complex morphologies are analyzed, highlighting similarities and differences with respect to monatomic crystallization.

¹We acknowledge support by the Spanish Ministry of Science and Innovation (MICINN) through project “Ramon y Cajal” and by MICINN and Comunidad de Madrid through project “I3.”

1:03PM W53.00008 Sudden Chain Energy Transfer Events in Vibrated Granular Media , NICOLÁS

RIVAS, University of Twente, SUOMI PONCE, RODRIGO SOTO, PATRICIO CORDERO, NICOLÁS MUJICA, Departamento de Física, FCFM, Universidad de Chile, Santiago, Chile, DINO RISSO, Departamento de Física, Universidad del Bío-Bío, Concepción, Chile, BASILLE GALLET, Laboratoire de Physique Statistique, CNRS, Ecole Normale Supérieure, Paris, France — In a mixture of two species of grains of equal size but different mass, placed in a vertically vibrated shallow box, there is spontaneous segregation. Once the system is at least partly segregated and clusters of the heavy particles have formed, there are sudden peaks of the horizontal kinetic energy of the heavy particles, that is otherwise small. Together with the energy peaks the clusters rapidly expand and the segregation is partially lost. The process repeats once segregation has taken place again, either randomly or with some regularity in time depending on the experimental or numerical parameters. An explanation for these events is provided based on the existence of a fixed point for an isolated particle bouncing with only vertical motion. The horizontal energy peaks occur when the energy stored in the vertical motion is partly transferred into horizontal energy through a chain reaction of collisions between heavy particles.

1:15PM W53.00009 Equation of state and jamming density for equivalent bi-, tri- and poly-disperse, smooth, elastic sphere systems¹ , VITALIY OGARKO, STEFAN LUDING, University of Twente — We study binary, ternary and polydisperse mixtures of hard particle fluids as models for granular matter, colloids and other soft matter. Size ratios between 1 and 100 are studied for different size distributions. Simulation results are compared with previously found analytical equations of state by looking at the compressibility factor, Z , and agreement is found with much better than 1% deviation in the fluid regime. A slightly improved empirical correction to Z is proposed. When the density is further increased, the behavior of Z changes and there is a close relationship between many-component mixtures and their two- and three-component equivalents (where our contribution is to define the term “equivalent”). We determine the size ratios for which the liquid-solid transition exhibits crystalline, amorphous or mixed system structure. Near the jamming density, Z is independent of the size distribution and follows a -1 power law as function of the difference from the jamming density. In this limit, Z depends only on one free parameter, the jamming density itself, as reported for several different size distributions with a wide range of widths.

¹This research is supported by the Dutch Technology Foundation STW, which is the applied science division of NWO, and the Technology Programme of the Ministry of Economic Affairs, project Nr. STW-MUST 10120.

1:27PM W53.00010 Recovery of polymer glasses from mechanical perturbation , ANTON SMESSAERT, JÖRG RÖTTLER, The University of British Columbia — There is a longstanding debate about the nature and extent of mechanical rejuvenation in aging glasses and most related studies have concentrated on the impact of aging during plastic deformation. Here we study the time period after nonlinear creep where the glass recovers, using molecular dynamics simulations of a bead-spring model for a wide range of stress amplitudes and glass ages. We compute α -relaxation times as well as several quantities that characterize structural changes. From an analysis of the recovery paths we find a transition from memory effects to mechanical rejuvenation that is controlled by the total strain and not the stress amplitude. Although strong mechanical perturbation can make the dynamics appear very similar to that of a freshly quenched glass, various measures of short range order as well as inherent structure energies reveal systematic differences in the underlying thermodynamic state.

1:39PM W53.00011 Spatiotemporal stress/strain correlations in a quasi-2D jammed emulsion , KENNETH DESMOND, ERIC R. WEEKS, Emory University — We flow quasi-2D emulsions in a flow geometry analogous to pure shear to better understand the microscopic events within jammed materials during the straining process. Our quasi-2D system serves as an experimental model system of jamming and consists of oil-in-water emulsion droplets confined between two parallel plates. Using a technique we have developed, we can determine the forces between pairs of droplets in contact based on each droplet's deformation. By imaging the motion and deformation of the droplets during the flowing process, we quantify the microscopic events using spatiotemporal correlations in strain and stress. We study these spatiotemporal correlations at various droplet concentrations to understand how the microscopic events change as we approach the jamming point.

1:51PM W53.00012 Low- k behavior in Structure Factor and Compressibility Factor for Monodisperse and Bidisperse Packings of Frictionless Spheres , JAIME BOHORQUEZ-BALLEN, LEONARDO SILBERT, Southern Illinois University - Carbondale — One particular structural signature of jamming transition has emerged in studies of large systems: *hyperuniformity*, which is the suppression of the long wavelength density fluctuations. Also, it has been observed an unusual linear dependence ($S(k) \sim k$) of the structure factor in the low k limit, in monodisperse systems. The small wavenumber region of the static structure factor $S(k)$ for monodisperse systems and the compressibility factor $\theta(k)$ for bidisperse mixtures, are investigated for jammed packings of frictionless spheres with Hooke and Hertz force model, using a high precision data analysis. We have found that the zero-wavenumber intercept $S(k=0)$ and $\theta(k=0)$, as a function of the pressure, are non-zero constant, revealing a finite compressibility. This behavior is relatively insensitive to the force model but shows a dependence on the bidispersity. We have studied also zero-temperature Lennard-Jones glasses which exhibit a finite compressibility that depend weakly on the density of the glass.

2:03PM W53.00013 Jamming and Unjamming of the Rigid Amorphous Fraction , PEGGY CEBE, QIAN MA, Tufts University, GEORGI GEORGIEV, Assumption College — Semicrystalline polymers obey a three-phase model comprising crystalline, mobile amorphous (MAF), and rigid amorphous fractions (RAF) as an interphase. Using quasi-isothermal temperature modulated differential scanning calorimetry (QI-TMDSC), we investigate the formation behavior of these fractions in poly(trimethylene terephthalate), PTT. PTT was quasi-isothermally cooled step-wise from the melt which causes its crystalline fraction to be fixed below 451K, and RAF is determined as a function of temperature. For PTT, most of the RAF vitrifies between 451K and T_g step-by-step during QI cooling. With lamellar crystals acting as topological constraints, a model is proposed in which the vitrification and devitrification of RAF are interpreted using the concepts of “jamming” and “unjamming.” Constraints of the crystal surfaces reduce the mobility of the highly entangled polymer chains attached to the lamellae, and the layers which constitute RAF are formed one after another in the manner of successive jamming. In this way, several features of the RAF temperature dependence are explained for the first time, with implications in other research areas, such as topological constraints exerted on the polymer melt through effects of inclusions in polymer-based nanocomposites.

For support of this research, the authors thank the NSF, Polymers Program of the Division of Materials Research through DMR-0602473, and the MRI Program under DMR-0520655 for thermal analysis instrumentation. A portion of this work was conducted at the BNL, National Synchrotron Light Source, supported by the DoE. G. Georgiev thanks Assumption College for continuous research support.

Thursday, March 1, 2012 2:30PM - 5:42PM –

Session X1 GIMS: Focus Session: Advances in Scanned Probe Microscopy IV: New Instrumentation & Techniques 203

2:30PM X1.00001 ezAFM: A low cost Atomic Force Microscope(AFM) , UMIT CELIK, KUBRA CELIK, Department of Material Science and Engineering, Istanbul Technical University, HUSNU ASLAN, IHSAN KEHRIBAR, Faculty of Engineering & Natural Sciences, Sabanci University, MUNIR DEDE, NanoMagnetics Instruments Ltd., H. OZGUR OZER, Department of Physics Engineering, Istanbul Technical University, AHMET ORAL, Faculty of Engineering & Natural Sciences, Sabanci University — A low cost AFM, ezAFM is developed for educational purposes as well as research. Optical beam deflection method is used to measure the deflection of cantilever. ezAFM scanner is built using voice coil motors (VCM) with $\sim 50 \times 50 \times 6 \mu\text{m}$ scan area. The microscope uses alignment free cantilevers, which minimizes setup times. FPGA based AFM feedback Control electronics is developed. FPGA technology allows us to drive all peripherals in parallel. ezAFM Controller is connected to PC by USB 2.0 interface as well as Wi-Fi. We have achieved $< 5\text{nm}$ lateral and $\sim 0.01\text{nm}$ vertical resolution. ezAFM can image single atomic steps in HOPG and mica. An optical microscope with $< 3 \mu\text{m}$ resolution is also integrated into the system. ezAFM supports different AFM operation modes such as dynamic mode, contact mode, lateral force microscopy. Advanced modes like magnetic force microscopy and electric force microscopy will be implemented later on. The new ezAFM system provides, short learning times for student labs, quick setup and easy to transport for portable applications with the best price/performance ratio. The cost of the system starts from \$15,000, with system performance comparable with the traditional AFM systems.

2:42PM X1.00002 Compact Scanning Tunneling Microscope for Spin Polarization Measurements¹ , SEONG HEON KIM, LEUJEN CHEN, ALEX DE LOZANNE, Department of Physics, The University of Texas at Austin — We have built a low temperature scanning tunneling microscope for spin-polarized studies. An important aspect of our design philosophy is to keep everything small, starting with a one-inch STM body that fits in the UHV bore of a small superconducting solenoid that provides up to 8 Tesla parallel to the tip. This, in turn, makes the liquid helium and liquid nitrogen dewars smaller and leads to a compact UHV chamber. The largest flange in the system is 10 inches in outer diameter. The benefits of a smaller system include lower consumption of cryogenics and a reduced footprint. The STM has been tested from 300K to 77K and has achieved atomic resolution. A test at 4.2K will be done soon. We have imaged cobalt clusters deposited in situ using a simple and compact design for an electron-beam evaporator. We have developed new electronics for z-approach and a novel magnetically-coupled manipulator with an actuated grabber for tip and sample exchange.

¹Supported by NSF DMR-0923231

2:54PM X1.00003 Development of Molecular Beam Epitaxy/Pulsed Laser Deposition/Low Temperature Spin-Polarized Scanning Tunneling Microscopy System¹ , JEONGIHM PAK, WENZHI LIN, KANGKANG WANG, ANDREW FOLEY, TIANJIAO CHEN, YINGHAO LIU, ABHIJIT CHINCHORE, DANIEL BERGMAN, MENG SHI, ARTHUR R. SMITH, Ohio University Nanoscale and Quantum Phenomena Institute — Spin-polarized scanning tunneling microscopy and spectroscopy have shown tremendous abilities to obtain detailed spin information about surfaces down to the atomic scale. In order to take full advantage of this method for studying pristine, as-prepared sample surfaces, we couple an SP-STM system to a sophisticated ultra-high-vacuum growth facility. The hybrid molecular beam epitaxy/pulsed laser deposition/spin-polarized STM system is home-designed and constructed with many unique features. A wide variety of engineered spintronic materials can be grown in the 8 source growth chamber, or using the 9 source laser deposition system. Samples may be heated during growth to as high as 1300 K or cooled using LN₂ to temperatures below 195 K, while being simultaneously probed using reflection high energy electron diffraction. The system is currently configured for nitride systems as well as transition metal or rare earth ultra-thin films. Prepared samples are transferred through a central distribution chamber to the LHe-cooled, spin-polarized STM operating inside an integral superconducting magnet (0-4.5 T). The system is outfitted with magnetic tip preparation. The magnetic field allows us to manipulate the magnetic structure of samples during SP-STM experiments.

¹National Science Foundation and Department of Energy

3:06PM X1.00004 ABSTRACT WITHDRAWN —

3:18PM X1.00005 A Dual Tip STM for Imaging the Superconducting Phase Difference¹ , ANITA ROYCHOWDHURY, Laboratory for Physical Sciences and Physics Dept., University of Maryland, College Park, M.A. GUBRUD, Department of Physics and Astronomy, University of North Carolina, Chapel Hill, D. SULLIVAN, NASA - Goddard, MICHAEL DREYER, Laboratory for Physical Sciences and Physics Dept., University of Maryland, College Park, J. R. ANDERSON, C.J. LOBB, F.C. WELLSTOOD, Physics Dept., University of Maryland, College Park — We have built a dual tipped millikelvin STM with each tip capable of independently scanning a sample. We will use the STM to measure spatial variations of the gauge-invariant phase difference at the atomic scale. The two tips along with the superconducting sample constitute a SQUID. This configuration is designed to minimize fluctuations in the superconducting phase of one of the tips as it scans the sample, hence inhibiting supercurrent suppression. We are currently developing a technique to fabricate superconducting Niobium tips for use with this system.

¹This project was funded in part by NSF and the Laboratory for Physical Sciences

3:30PM X1.00006 mK-Scanning Probe Microscope(mK-SPM) operating in a Cryogen-Free Dilution Refrigerator at 20mK , MUNIR DEDE, Nanomagnetics Instruments Ltd. Suite 290 266 Banbury Road OX2 7DL. Oxford, UK, OZGUR KARCI, Hacettepe University, Dept. of Nanotechnology and Nanomedicine, Beytepe, 06800, Ankara, Turkey, CHRIS SNELLING, Oxford Instruments plc Tubney Woods, Abingdon, Oxon OX13 5QX, UK, AHMET ORAL, Sabanci University, Faculty of Science and Engineering, Orhanli - Tuzla, 34956, Istanbul, Turkey — Dramatic increase in liquid helium price limits the usage of cryogenic equipment. Dry cryogen-free dilution refrigerators(DR) systems are promising platforms to run mK-Scanning Probe Microscopes(mK-SPM) systems with a number of operating modes: STM, AFM, MFM, EFM, SSRM, PFM, etc. We present the design of a mK-Scanning Probe Microscope (mK-SPM) operating in a cryogen-free DR. An Oxford Instrument cryogen-free DR(Triton DR200) with 200uW cooling power and 7mK base temperature is used for the experiments. A 1W Pulse Tube cryocooler is integrated into the DR. After wiring and attaching the microscope we achieved 20mK base temperature. Piezo driven Stick slip coarse approach mechanism is used to bring the sample in to close proximity of the sample. In these initial results we deliberately did not take any precautions to isolate the pumping lines, attached to the DR and the DR itself. The turbomolecular pump was attached directly to the top plate of the DR. We first tested our mK-SPM in Scanning Tunnelling Microscope (STM) mode as it is the most sensitive of the SPM techniques. An image, using a gold coated $6 \mu\text{m}$ period calibration grating at 20mK, obtained under these rudimentary conditions.

3:42PM X1.00007 Atom-Specific Interaction Quantification and Identification by 3D-SPM

TODD C. SCHWENDEMANN, Southern Connecticut State University, MEHMET Z. BAYKARA, HARRY MONIG, Dept. of Mech. Eng & Mat. Sci., Yale University, MILICA TODOROVIC, Dept. de Física Teórica de la Materia Condensada, JAN GOTZEN, OZHAN UNVERDI, Dept. of Mech. Eng & Mat. Sci., Yale University, RUBEN PEREZ, Dept. de Física Teórica de la Materia Condensada, ERIC I. ALTMAN, Dept. of Chem. & Env. Eng., Yale University, UDO D. SCHWARZ, Dept. of Mech. Eng & Mat. Sci., Yale University — Entire scientific disciplines such as mechanics and chemistry are governed by the interactions between atoms and molecules. On surfaces, forces extending into the vacuum direct the behavior of phenomena such as thin film growth, nanotribology, and surface catalysis. To advance our knowledge of the fundamentals governing these topics, it is desirable to simultaneously map electron densities and quantify force interactions between the surface of interest and a probe with atomic resolution. Using the oxygen-reconstructed copper (100) surface as a model system, we demonstrate that much of this information can be derived from combining three-dimensional atomic force microscopy (3D-AFM) with simultaneous STM. The three-dimensional scanning probe microscopy (3D-SPM) variant resulting from this combination provides complementary information in the various interaction channels recorded. The surface oxide layer of copper (100) features defects and a distinct structure of the Cu and O sublattices that is ideally suited for such model investigations. The analysis of our experimental results allows for the identification of atomic species and defects on the sample surface through the comparison of simultaneously recorded force and current data.

3:54PM X1.00008 Laser Scanning Microscopy for Quantitative Measurement of the Local Microwave-Photonic Properties of Advanced Materials and Devices¹

BEHNOOD GHAMSARI, JACOB TOSADO, MAHITO YAMAMOTO, JINGLEI PING, DANIEL LENSKE, MICHAEL FUHRER, STEVEN ANLAGE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park — We present laser scanning microscopy (LSM) as a non-contact and non-invasive instrumentation technique for quantitative measurement of the local microwave, optoelectronic, and optical properties of advanced materials including superconductors and graphene. Since an LSM setup may be configured in different modes of operation, we will focus on the photoresponse and reflectivity imaging modes. It will be discussed how an LSM, in the photoresponse measurement mode, may be used to image the distribution of rf/microwave currents at the surface of a superconducting device, such as a resonator. In addition, relevant techniques for distinguishing the kinetic and resistive parts of the superconductor's photoresponse as well as imaging its possible anisotropic microwave properties are addressed. With regard to the reflectivity mode, we will present how this method enables precise measurement of the topological features and optical properties of non-opaque samples. As an example, we will show how the thickness of few-layer graphene flakes may be measured by this method.

¹B.G.G and S.M.A would like to acknowledge technical help from Dr. Alexander Zhuravel. This work is, in part, supported by the DOE grant number DESC0004950 and ONR/AppEl, Task D10, through grant number N000140911190.

4:06PM X1.00009 Torsional tapping atomic force microscopy for molecular resolution imaging of soft matter

JAMIE HOBBS, NIC MULLIN, University of Sheffield — Despite considerable advances in image resolution on challenging, soft systems, a method for obtaining molecular resolution on 'real' samples with significant surface roughness has remained elusive. Here we will show that a relatively new technique, torsional tapping AFM (TTAFM), is capable of imaging with resolution down to 3.7 Angstrom on the surface of 'bulk' polymer films [1]. In TTAFM T-shaped cantilevers are driven into torsional oscillation. As the tip is offset from the rotation axis this provides a tapping motion. Due to the high frequency and Q of the oscillation and relatively small increase in spring constant, improved cantilever dynamics and force sensitivity are obtained. As the tip offset from the torsional axis is relatively small (typically 25 microns), the optical lever sensitivity is considerably improved compared to flexural oscillation. Combined these give a reduction in noise floor by a factor of 12 just by changing the cantilever geometry. The ensuing low noise allows the use of ultra-sharp 'whisker' tips with minimal blunting. As the cantilevers remain soft in the flexural axis, the force when imaging with error is also reduced, further protecting the tip. We will show that this combination allows routine imaging of the molecular structure of semicrystalline polymer films, including chain folds, loose loops and tie-chains in polyethylene, and the helical conformation of polypropylene within the crystal, using a standard, commercial AFM.

[1] N Mullin, JK Hobbs, PRL 107, 197801 (2011)

4:18PM X1.00010 Reference system for scanning probe tip fingerprinting¹

ROBERT TURANSKY, Institute of Physics, Slovak Academy of Sciences, JOSEPH BAMIDELE, Dept. of Physics, King's College London, YASUHIRO SUGAWARA, Dept. of Applied Physics, Osaka University, LEV KANTOROVICH, Dept. of Physics, King's College London, IVAN STICH, Institute of Physics, Slovak Academy of Sciences — Knowledge of the chemical structure of the tip asperity in Non-Contact Atomic Force Microscopy (NC-AFM) is crucial as controlled manipulation of atoms and/or molecules on surfaces can only be performed if this information is available. However, a simple and robust protocol for ensuring a specific tip termination has not yet been developed. We propose a procedure for chemical tip fingerprinting and an example of a reference system, the oxygen-terminated Cu(110) surface, that enables one to ensure a specific tip termination with Si, Cu, or O atoms. To follow this up and unambiguously determine tip types, we performed a theoretical DFT study of the line scans with the tip models in question and found that the tip characterization method based on experimental results (Cu/O-terminated tip imaging Cu/O atoms) is in fact incorrect and the opposite is true (Cu/O-terminated tip imaging O/Cu atoms). This protocol allows the tip asperity's chemical structure to be verified and established both before as well as at any stage of the manipulation experiment when numerous tip changes may take place.

¹Financial support from APVT (ESF-EC-0007-07) under the Nanoparma ESF FANAS project is gratefully acknowledged. This research was supported in part by ERDFOP&D, Project CE QUTE ITMS 26240120009, and via CE SAS QUTE.

4:30PM X1.00011 Micromolding fabrication of "T" cross section SiC SPM probes

CHIAYUN WU, Physics U. Mass Lowell, SHIHANG WANG, DANIEL SCHMIDT, Plastics Eng U. Mass Lowell, JOEL THERRIEN, ECE U. Mass Lowell — Micromolding techniques using pre-ceramic polymers have been demonstrated for the creating silicon carbide based AFM cantilevers. In an attempt to reach higher resonance frequencies without significantly increasing the spring constant of the cantilevers, a "T" cross section cantilever was fabricated. The resonant frequency and spring constant have been compared to the standard rectangular cross section cantilevers of both SiC and commercially available silicon cantilevers.

4:42PM X1.00012 Single molecule and single atom sensors for atomic resolution imaging of chemically complex surfaces

F. STEFAN TAUTZ, GEORGY KICHIN, CHRISTIAN WEISS, CHRISTIAN WAGNER, RUSLAN TEMIROV, Peter Gruenberg Institute (PGI-3), Forschungszentrum Juelich, Germany — To resolve single atoms has always been a major goal of surface science. Mapping forces with a dynamic AFM, it is possible to reconstruct atomic resolution of various surfaces and of large organic molecules [1]. At the same time scanning tunneling hydrogen microscopy (STHM) reaches atomic scale resolution and reveals intermolecular interactions with much less technical effort [2]. Besides H₂ and D₂, also individual Xe atoms, single CO and CH₄ molecules adsorbed at the tip apex of an STM function as microscopic force sensors that change the tunneling current in response to the forces acting from the surface. An STM equipped with any of these sensors is able to image the Pauli repulsion and thus resolve the inner structure of organic adsorbates. The more rigidly bounded CO yields the strongest, least distorted contrast. Thus, the sensor functionality can be tailored by tuning the interaction between sensor particle and STM tip. Hence, STHM belongs to a wider family of atomic-sensor microscopy techniques.

[1] L. Gross et al., Science 325, 1110 (2009)

[2] R. Temirov et al., New J. Phys. 10, 053012 (2008); C. Weiss et al., Phys. Rev. Lett. 105, 086103 (2010), C. Weiss et al., J. Am. Chem. Soc. 132, 11864 (2010); G. Kichin et al., J. Am. Chem. Soc. 133, 16847 (2011)

4:54PM X1.00013 Detection of cantilever thermal motion and feedback cooling using a quantum point contact, MICHELE MONTINARO, University of Basel, Switzerland, SARAH HELLMÜLLER, KLAUS ENSSLIN, ETH Zuerich, Switzerland, MARTINO POGGIO, University of Basel, Switzerland — Nanomechanical oscillators enable ultrasensitive detection of force, mass and displacement. In particular, recent measurements of oscillator displacement have achieved an imprecision below that at the standard quantum limit (SQL), using optical [1] or microwave techniques [2]. A quantum point contact (QPC) has been employed as a transducer of nanomechanical motion, thanks to the sensitive dependence of its conductance on electrostatic fields. Such an approach has been demonstrated in combination with an off-board micromechanical cantilever in a versatile design compatible with nanoscale oscillators and, in principle, with a variety of force-sensing applications, including magnetic resonance force microscopy [3]. The aim of the research we present here is to improve this technique and to approach the SQL by accessing a regime in which, due to the one-dimensional electron transport, quantum mechanical back-action effects emerge on the mechanical resonator. We demonstrate the use of different types of QPCs as sensitive detectors of the low-temperature thermal motion of an off-board cantilever and their ability to cool the cantilever oscillation mode through feedback.

[1] Phys. Rev. A 82, 061804 (2010)

[2] Nat. Nano. 4, 820 (2009)

[3] Nat. Phys. 4, 635 (2008)

5:06PM X1.00014 Design of a Self-Aligned, High Sensitivity Fiber Fabry-Perot Interferometer for Low Temperature Atomic Force Microscope/Magnetic Force Microscope, OZGUR KARCI, Hacettepe University, MUNIR DEDE, NanoMagnetics Instruments Ltd., AHMET ORAL, Sabanci University — We describe the design of a high sensitivity fiber Fabry-Perot interferometer for low temperature atomic force microscope/magnetic force microscope. This is a self-aligned system utilizing an alignment chip and eliminating all tedious alignment procedures. Our interferometer cavity is composed of a cleaved fiber, which is coated using dielectric to increase the reflectivity of laser from fiber-air interface, and a cantilever. 50 percent of the incident laser beam is reflected at the end of the fiber. The transmitted light propagates from the fiber end and hits the cantilever. Multiple reflections occur between cantilever and the fiber then the beams go into the fiber again. These two beams interfere and generate a photocurrent at the PD which is used for deflection measurement. We designed a special stick-slip coarse approach mechanism using piezoelectric tube scanner of the microscope. We have measured 8fm per square root Hz noise level at 300K, while the shot noise limit was 2fm per square root Hz. Our previous Michelson interferometer design had 20 fm per square root Hz noise level and gave better than 10nm MFM resolution on hard disk. Our goal is to further enhance the noise levels and achieve 6 nm resolution for LT-MFM with this new interferometer.

5:18PM X1.00015 Next Generation SPM Control System with ppm precision, ALESSANDRO PIODA, SPECS Surface Nano Analysis GmbH — Novel scanning probe microscopy techniques, modes of operation, and advances in microscope hardware are pushing the boundary for signal resolution and flexibility in SPM measurements. Here we present a new state of the art SPM control system, which improves signal precision, resolution, bandwidth and noise performance by about one order of magnitude compared to current generation controllers. The controller incorporates the performance of expensive dedicated instruments in a compact modular multichannel package. In combination with the well proven and flexible Nanonis SPM control software, this next generation controller is the ideal platform for the most demanding microscopy, spectroscopy and transport measurements tasks, opening the door to a larger range of applications compared to current systems. Furthermore, the flexible and easily configurable user interface of the controller and the large number of measurement channels allows its operation as a high performance DC and AC source and measurement interface with ppm precision and multiple lock-in amplifiers, opening new perspectives for materials research.

5:30PM X1.00016 Conical spin-spiral ground state of a Mn double layer on W(110) driven by higher-order exchange interactions, YASUO YOSHIDA, University of Hamburg / The University of Tokyo, SILKE SCHROEDER, PÁOLO FERRIANI, University of Kiel, DAVID SERRATE, Universidad de Zaragoza, KIRSTEN VON BERGMANN, ANDRE KUBETZKA, University of Hamburg, STEFAN HEINZE, University of Kiel, ROLAND WIESENDANGER, University of Hamburg — The magnetic properties of transition-metal nanostructures are commonly explained based on the interplay of Heisenberg exchange, Dzyaloshinskii-Moriya (DM) interaction and magnetocrystalline anisotropy while higher order terms such as the biquadratic exchange and the four-spin interaction are typically neglected due to their small strength. Here, we demonstrate that higher-order terms can play a crucial role for the magnetic ground state and report as an example a transverse conical spin-spiral state in an ultra-thin film composed of two atomic layers of Mn on W(110). This spin structure is characterized by magnetic moments rotating on a cone that is perpendicular to the [001] propagation direction of the spin-spiral with a periodicity of 2.4 nm. The cones of nearest-neighbor Mn atoms point into opposite directions which results in nearly antiferromagnetic alignment. This intriguing spin structure has been resolved on the atomic-scale using spin-polarized scanning tunneling microscopy and confirmed to be the ground state by first-principles calculations based on DFT. Our calculations also reveal that the canting of the spins is induced by higher-order exchange interactions while the spiraling along the [001]-direction is due to frustrated Heisenberg exchange and DM interaction.

Thursday, March 1, 2012 2:30PM - 5:30PM –

Session X2 FHP: Invited Session: History of Metrology and Today's Frontiers of Measurement
204AB

2:30PM X2.00001 Dreams of a Final System: Origins of the Quest for an Absolute Standard, ROBERT CREASE, Stony Brook University — The first attempts to find unchanging phenomena that could be used to evaluate the accuracy of standards and recreate them if lost predated the metric system. As early as the seventeenth century, members of the French Academy and British Royal Society sought to use the seconds pendulum and the Earth's meridian as tethers for length standards. These efforts ultimately failed. The vision of an absolute standard was revived in the 1870s, when C. S. Peirce was the first to experimentally tie a unit, the meter, to a natural standard, the wavelength of a spectral line, using a diffraction grating. This work inspired A. Michelson and E. Morley, in the 1880s, to apply the interferometer with which they were attempting to detect ether drift to this purpose. Michelson further pursued this work at the BIPM in 1892, which set the stage for the later redefinition, in 1960, of the meter in terms of the wavelength of a spectral line.

3:06PM X2.00002 Beller Lectureship: From Artefacts to Atoms: The Origins and Early Years of the International Bureau of Weights and Measures (BIPM), TERRY QUINN¹, Retired — The BIPM was founded by the Metre Convention in 1875. Its main task was to maintain and disseminate the units of length and mass using the new International Prototypes of the Metre and Kilogram. My talk will be based on the opening chapters of my book "From Artefacts to Atoms" which recount the story of the Metre Convention and the creation of the BIPM at the Pavillon de Breteuil in Sèvres on the outskirts of Paris, as the first international scientific institute. I shall include a brief outline of the sometimes acrimonious discussions at the Diplomatic Conference of the Metre, which opened on 1 March 1875 and concluded with the signing of the Convention on 20 May, of the construction of a new laboratory building, recruitment of staff, purchase of instruments and equipment and the beginning of scientific work. There was no precedent for any of this, success was due to the wisdom and foresight of those who drafted the Convention and to the founder Members of the International Committee for Weights and Measures overseeing the BIPM and to the high quality of the original scientific staff. However, success came at a price, the decision to define the Metre at 0 °C, for example, led to much ill health in the early years among the staff from working in cold damp laboratories, an aspect of metrology that is easy to forget these days.

¹The author is Emeritus Director of the BIPM

3:42PM X2.00003 Measurement of the gravitational quantities g and G : How ideas for precision measurement experiments come about, JAMES FALLER, JILA (CU and NIST), University of Colorado, and University of Glasgow — I will talk about g and G whose determinations go back to some of the earliest measurements in the history of metrology. Although today's measurement accuracy for g , the free-fall acceleration due to the Earth's gravity, has improved by nearly nine orders of magnitude, the measurement accuracy of G , the Newtonian Constant of Gravitation, has improved by only two orders of magnitude over its 300 year measurement history. I will discuss what has driven (and impeded) this progress, and how ideas for improvements in these measurements have helped advance the frontiers of measurement science. Finally, I will point out the interconnectedness of all precision measurement experiments.

4:18PM X2.00004 The Odyssey of the Frequency Measurements of Visible Light at NBS/NIST, HOWARD LAYER, National Institute of Standards and Technology — The long term goal of defining the length standard based on a constant of nature rather than an artifact was pursued at the National Bureau of Standards/National Institute of Standards and Technology during the period of 1968 to 1983. With the invention of the laser it became possible to measure the frequency of lasers, stabilized on atoms or molecules, with the cesium atomic clock as the time standard. Using lasers, high speed MIM (metal insulator metal) diodes, and summing the radiation from three lasers in a He-Ne plasma the frequency of the iodine stabilized HeNe laser at 633 nm was measured by direct frequency counting to an accuracy of 1.6 parts in 10^{10} . The major consequences of this accomplishment were the adoption of a fixed value for the speed of light and the redefinition of the SI meter based on the speed of light. After a brief historical review, the milestones of the research will be outlined and the principle researches indicated.

4:54PM X2.00005 Evolving Planck Constant Measurements into the SI Kilogram Standard, RICHARD STEINER, National Institute of Standards and Technology — This is a very brief 100 year history of measuring $2e/h$ (pre-and post-Josephson), with a little on e^2/h (quantum Hall Effect, QHE), and then on to a direct measure of Planck constant h , where the watt balance technique combines four basic standards, i.e., physical constants of time, length, voltage, and resistance into a mass redefinition. There are parallels between old and new controversies. In the 1970's and 80's the controversy was in the changeover from standard cells to the Josephson effect as voltage reference. A slightly similar and briefer one concerned the ohm and QHE. Today's discussion is about changing definitions from an artifact mass standard to the Planck constant (or Avogadro constant) using the different methods as realization. The mass redefinition concerns are two orders of magnitude down from those of voltage, and the discrepancies between h are probably more systemic rather than artifact related (or not) as compared to the Josephson effect testing. This shows how far electronic metrology has progressed but also that it is not completed research. The conclusion summarizes the latest efforts on the watt balances.

Thursday, March 1, 2012 2:30PM - 5:30PM –
Session X3 DCMF: Invited Session: Full Counting Statistics, Fluctuation Theorems, and Many-Body Entanglement 205AB

2:30PM X3.00001 Towards Measuring the Many-Body Entanglement from Fluctuations¹, KARYN LE HUR, CNRS and Center For Theoretical Physics, Ecole Polytechnique, 91128 Palaiseau France; Yale University, Physics Department, New Haven CT 06520 USA — The degree of entanglement in a many-body quantum system is often characterized using the bipartite entanglement entropy. We propose that bipartite fluctuations are also an effective tool for studying many-body physics [1] particularly its entanglement properties, in the same way that noise and full counting statistics have been used in mesoscopic transport and cold atoms. We apply some concepts underlying the field of full counting statistics to the study of the ground states of many-body Hamiltonians, with the boundary introduced by the bipartition playing the role of the scattering or interacting region. For systems that are equivalent to non-interacting fermions, we show that fluctuations and higher-order cumulants fully encode the information needed to determine the entanglement entropy [1-3]. In the context of quantum point contacts, measurement of the second charge cumulant showing a logarithmic dependence on time [2] then would constitute a strong indication of many-body entanglement [1]. Here, the measurability of the entanglement entropy, while suggestive, is particular to the nature of non-interacting particles [4,5].

- [1] H. Francis Song, S. Rachel, C. Flindt, I. Klich, N. Laflorencie and K. Le Hur, arXiv:1109.1001. 30 pages + 25 pages supplementary information.
- [2] I. Klich and L. Levitov, Phys. Rev. Lett. 102, 100502 (2009).
- [3] H. F. Song, C. Flindt, S. Rachel, I. Klich and K. Le Hur, Phys. Rev. B 83, 161408R (2011).
- [4] B. Hsu, E. Grosfeld and E. Fradkin, Phys. Rev. B 80, 235412 (2009).
- [5] H. Francis Song, Stephan Rachel and Karyn Le Hur, Phys. Rev. B 82, 012405 (2010).

¹This work is done in collaboration with H. Francis Song, Stephan Rachel, Christian Flindt, Israel Klich and Nicolas Laflorencie. We acknowledge the financial supports from NSF and DOE.

3:06PM X3.00002 Charge sensing and real-time electron counting in quantum dots, THOMAS IHN, ETH Zurich — The charge state of a Coulomb blockaded quantum dot can be sensed at the single-electron level using charge sensors integrated on-chip [1]. Quantum point contacts or quantum dots have proven to work as reliable charge sensors. Coupling between the quantum dot's charge state and the sensor is provided by Coulomb interactions between electrons in the two systems. The technique is therefore independent of the material of quantum dot and sensor, and works for diverse systems such as GaAs [1] and graphene [2]. Different materials, such as InAs and GaAs have even been combined. Time-resolved charge sensing is of fundamental interest for studying the statistical properties of charge flow, like the full counting statistics. Single-shot charge and spin read-out schemes are also needed for the measurement of qubits. Some of our recent work has focused on the exploration and optimization of the read-out bandwidth limits. Towards this goal, we learned how to influence the dot-detector coupling [3], and how to employ high-frequency techniques in the range of a few hundred megahertz [4], or even up to a few gigahertz for improved performance. New experiments using the slower conventional sensing schemes have allowed us to explore non-equilibrium statistics and the fluctuation theorem. In our measurements, rare events can be detected, where electrons flow against the applied source-drain bias direction thereby consuming entropy in agreement with theoretical predictions.

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3:42PM X3.00003 High-order counting statistics and interactions , CHRISTIAN FLINDT, University of Geneva

— Full counting statistics concerns the stochastic transport of electrons in mesoscopic structures [1]. Recently it has been shown that the charge transport statistics for noninteracting electrons in a two-terminal system is always generalized binomial: it can be decomposed into independent single-particle events, and the zeros of the generating function are real and negative [2]. In this talk I show how the zeros of the generating function move into the complex plane due to interactions and demonstrate how the positions of the zeros can be detected using high-order factorial cumulants [3]. As an illustrative example I discuss electron transport through a Coulomb blockade quantum dot for which the interactions on the quantum dot are clearly visible in the high-order factorial cumulants. These findings are important for understanding the influence of interactions on counting statistics, and the characterization in terms of zeros of the generating function provides a simple interpretation of recent experiments, where high-order statistics have been measured [4].

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4:18PM X3.00004 Hidden correlations in the zero-point motion of electrons revealed by non-Gaussian quantum noise , BERTRAND REULET, Université de Sherbrooke

— We have performed the measurement of the correlation between the low frequency voltage fluctuations and the power fluctuations of the high frequency electromagnetic field generated by a tunnel junction at very low temperature. Our experiment provides the first observation of the correlation between the electron transport at low frequency and the photon field at high frequency, both when real photons are emitted ($eV > hf$, with V the dc voltage and f the frequency) and when the electromagnetic field is solely due to vacuum fluctuations. In terms of electrons only, our observations indicate that the intrinsic current fluctuations in a tunnel junction are given by $S_3(0, f) = e^2 I$, regardless of the frequency f . Despite its classical look, this result expresses that the high frequency current fluctuations, caused by the zero-point motion of electrons, are correlated with their low frequency counterpart, associated with "real" motion of electrons. In terms of photons only, we observe that the electromagnetic field exhibits a discontinuity at $eV = hf$, not in the amplitude of the fluctuations but in their relative phases.

4:54PM X3.00005 Noise and fluctuation statistics in mesoscopic heat transport , DMITRI AVERIN, Department of Physics and Astronomy, Stony Brook University, SUNY

— Fluctuations play important role in thermodynamics of small systems. In the talk, I will discuss two recent results on fluctuations in mesoscopic heat transport. One is the demonstration [1] that the fluctuation-dissipation theorem for thermal conductance of a mesoscopic junction is not valid at non-zero frequencies ω . Finite relaxation energy creates fluctuations of the energy flux in the junction even at vanishing temperature, $T=0$, when the conductance vanishes. This suggests that in contrast to electrical conductance, there is no "Kubo-Green formula" for equilibrium thermal conductance at $\omega \neq 0$. Non-equilibrium heat transfer satisfies general "fluctuation relations" of non-equilibrium thermodynamics. Recently, we have established the conditions of applicability of these relations to single-electron tunneling (SET), and calculated explicitly the statistics of dissipated energy in driven SET transitions [2], which gives an example of general statistics of energy dissipation in reversible information processing. An interesting consequence of this statistics is the possibility of implementing the electronic version of Maxwell's demon in the SET structures [3].

[1] D.V. Averin and J.P. Pekola, Phys. Rev. Lett. **104**, 220601 (2010).

[2] D.V. Averin and J.P. Pekola, arXiv:1105.041.

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Thursday, March 1, 2012 2:30PM - 5:30PM –

Session X4 DAMOP: Focus Session: Quantum Quench Dynamics in Cold Atom Systems 205C

2:30PM X4.00001 Integrability versus Thermalizability in Isolated Quantum Systems¹ , MAXIM OLSHANII, University of Massachusetts Boston

— The purpose of this presentation is to assess the status of our understanding of the transition from integrability to thermalizability in isolated quantum systems. In Classical Mechanics, the boundary stripe between the two is relatively sharp: its integrability edge is marked by the appearance of finite Lyapunov's exponents that further converge to a unique value when the ergodicity edge is reached. Classical ergodicity is a universal property: if a system is ergodic, then every observable attains its microcanonical value in the infinite time average over the trajectory. On the contrary, in Quantum Mechanics, Lyapunov's exponents are always zero. Furthermore, since quantum dynamics necessarily invokes coherent superpositions of eigenstates of different energy, projectors to the eigenstates become more relevant; those in turn never thermalize. All of the above indicates that in quantum many-body systems, (a) the integrability-thermalizability transition is smooth, and (b) the degree of thermalizability is not absolute like in classical mechanics, but it is relative to the class of observables of interest. In accordance with these observations, we propose a concrete measure of the degree of quantum thermalizability, consistent with the expected empirical manifestations of it. As a practical application of this measure, we devise a unified recipe for choosing an optimal set of conserved quantities to govern the after-relaxation values of observables, in both integrable quantum systems and in quantum systems in between integrable and thermalizable.

¹Supported by ONR, NSF, and IFRAF.

3:06PM X4.00002 Chaos and statistical relaxation in quantum systems of interacting particles , LEA SANTOS, Yeshiva University, USA, FAUSTO BORGONOV, Università Cattolica, FELIX IZRAILEV, Universidad Autónoma de Puebla, Mexico

— Recent experimental progresses in the studies of quantum systems of interacting particles with optical lattices have triggered the interest in basic problems of many-body physics. One of the issues that has been widely discussed in the literature is the onset of thermalization in an isolated quantum system caused by interparticle interactions. A prerequisite for thermalization is the statistical relaxation of the system to some kind of equilibrium and its viability has been associated with the onset of quantum chaos. We propose a method to study the transition to chaos in isolated quantum many-body systems, which is based on the concept of delocalization of eigenstates in the energy shell. We show that although the fluctuations of energy levels and delocalization measures in integrable and non-integrable systems differ, global properties of the eigenstates may be quite similar, provided the interaction between particles exceeds some critical value. In this case the quench dynamics can be described analytically, demonstrating the universal statistical relaxation of the systems irrespectively of whether they are chaotic or not.

3:18PM X4.00003 Non-adiabatic ramps in quantum many-particle systems , MASUD HAQUE, Max Planck Institute (PKS), Dresden

— A change of system parameter can be neither truly instantaneous nor truly adiabatic in real life. For several quantum many-particle systems, I will consider non-equilibrium dynamics induced by finite-rate ramps. The ramp rate extrapolates between an instantaneous quench and an adiabatic sweep. I will characterize the deviation from adiabaticity through the excess energy or "heating" of the system. For cold-atom systems in a harmonic trapping potential, I will show that the non-adiabatic heating in finite-time ramps has universal features common to a wide range of systems.

3:30PM X4.00004 Entropy of Isolated Quantum Systems after a Quench¹ , MARCOS RIGOL, Georgetown University, LEA SANTOS, Yeshiva University, ANATOLI POLKOVNIKOV, Boston University — A diagonal entropy, which depends only on the diagonal elements of the system's density matrix in the energy representation, has been argued to be the proper definition of thermodynamic entropy in out-of-equilibrium quantum systems. We study this quantity after an interaction quench in lattice hardcore bosons and spinless fermions, and after a local chemical potential quench in a system of hard-core bosons in a superlattice potential. The former systems have a chaotic regime, where the diagonal entropy approaches the equilibrium microcanonical entropy, coinciding with the onset of thermalization. The latter system is integrable. We show that its diagonal entropy is additive and different from the entropy of a generalized Gibbs ensemble, which has been introduced to account for the effects of conserved quantities at integrability [1].

[1] Lea F. Santos, Anatoli Polkovnikov, and Marcos Rigol, Phys. Rev. Lett. 107, 040601 (2011).

¹This work was supported by ONR and NSF under Grant No. PHY05-51164 (M.R.), by the Research Corporation (L.F.S.), by DMR-0907039, AFOSR under Grant No. FA9550-10-1-0110, and by the Sloan Foundation (A.P.)

3:42PM X4.00005 Mode coupling induced dissipative and thermal effects at long times after a quantum quench¹ , ADITI MITRA, New York University, THIERRY GIAMARCHI, University of Geneva — An interaction quench in a Luttinger liquid can drive it into an athermal steady state. We analyze the effects on such an out of equilibrium state of a mode coupling term due to a periodic potential. Employing a perturbative renormalization group approach we show that even when the periodic potential is an irrelevant perturbation in equilibrium, it has important consequences on the athermal steady state as it generates a temperature as well as a dissipation and hence a finite life-time for the bosonic modes.

[1] Supported by NSF DMR 1004589

3:54PM X4.00006 Random phase approximation study of one-dimensional fermions after a quantum quench¹ , JARRETT LANCASTER, New York University, THIERRY GIAMARCHI, DPMC-MaNEP, University of Geneva, ADITI MITRA, New York University — The effect of interactions on a system of fermions that are in a nonequilibrium steady state due to a quantum quench is studied employing the random phase approximation. As a result of the quench, the distribution function of the fermions is greatly broadened. This gives rise to an enhanced particle-hole spectrum and overdamped collective modes for attractive interactions between fermions. On the other hand, for repulsive interactions, an undamped mode above the particle-hole continuum survives. The sensitivity of the result to the nature of the nonequilibrium steady state is explored by also considering a quench that produces a current-carrying steady state.

[1] Supported by NSF-DMR1004589

4:06PM X4.00007 Ballistic expansion of interacting fermions in one-dimensional optical lattices , FABIAN HEIDRICH-MEISNER, STEPHAN LANGER, LMU Munich, MARTIN J.A. SCHUETZ, MPQ Garching and LMU Munich, IAN MCCULLOCH, U Queensland, Brisbane, Australia, ULRICH SCHOLLWOECK, LMU Munich — In most quantum quenches, no net particle currents arise. Access to studying transport properties can be gained by letting a two-component Fermi gas that is originally confined by the presence of a trapping potential expand into an empty optical lattice. In recent experiments, this situation was addressed in 2D and 3D optical lattices [1]. We focus on the 1D case in which an exact numerical simulation of the time-evolution is possible by means of the DMRG method. Concretely, we study the expansion in the 1D Hubbard model with repulsive interactions, driven by quenching the trapping potential to zero, and we concentrate on the most direct experimental observable, namely density profiles [2]. In the strict 1D case, we identify conditions for which the expansion is ballistic, characterized by an increase of the cloud's radius that is linear in time. This behavior is found whenever initial densities are smaller or equal to one, both for the expansion from box and harmonic traps. We make quantitative predictions for the expansion velocity as a function of onsite repulsion and initial density that can be probed in experiments.

[1] Schneider et al., arXiv:1005.3545
[2] Langer et al., arXiv:1109.4364

4:18PM X4.00008 Quenching across a quantum critical point: dependence of scaling laws on spatial periodicity , SMITHA VISHVESHVARA, University of Illinois at Urbana-Champaign, MANISHA THAKURATHI, Indian Institute of Science, Bangalore, India, WADE DEGOTTARDI, University of Illinois at Urbana-Champaign, DIPTIMAN SEN, Indian Institute of Science, Bangalore, India — We study the quenching dynamics of a quantum many-body system in one dimension described by a Hamiltonian having spatial periodicity. Specifically, we consider a spin-1/2 XX chain subject to a periodically varying magnetic field in the $\hat{z}$ direction or, equivalently, a tight-binding model of spinless fermions having a periodic local chemical potential. If the strength of the magnetic field (or chemical potential) is varied slowly in time at a rate $1/\tau$ so as to take the system across a quantum critical point, we find that the density of excitations thereby produced scales as a power of $1/\tau$. Remarkably, the power depends on the spatial periodicity of the field and deviates from the $1/\sqrt{\tau}$ scaling that is ubiquitous to a range of systems. This behavior is analyzed by mapping the slow quenching problem to a collection of fermionic two-level systems, labeled by the lattice momentum k , for which the effective Hamiltonians vary as a power of the time close to the quantum critical point. For a magnetic field described by multiple periodicities, the power depends on the smallest period for very large values of τ . Finally, we find that if there are interactions between the fermions, the power varies continuously with the interaction strength.

[1] Schneider et al., arXiv:1005.3545
[2] Langer et al., arXiv:1109.4364

4:30PM X4.00009 Kibble-Zurek Scaling: Universality and scaling , ANUSHYA CHANDRAN, Princeton University, AMIR EREZ¹, Ben-Gurion University, SHIVAJI L. SONDHI, STEVEN S. GUBSER, Princeton University — Near a critical point, the equilibrium relaxation time of a system diverges and any change of control/thermodynamic parameters leads to non-equilibrium behavior. The Kibble-Zurek (KZ) problem is to determine the dynamical evolution of the system parametrically close to its critical point when the change is parametrically slow. We formulate the KZ problem as a scaling limit and compute its universal content analytically (critical exponents+scaling functions) in a few classical and quantum models. We also use gauge-gravity duality to compute KZ response functions in more exotic critical theories.

[1] Equal contribution

4:42PM X4.00010 Universal Quantum Dynamics of the Transverse-Field Ising Model , MICHAEL KOLODRUBETZ, BRYAN CLARK, DAVID HUSE, Princeton University — The one-dimensional transverse field Ising model is a prototypical example of a quantum phase transition. While its equilibrium scaling has been known for more than half a century, we discuss the non-equilibrium quantum dynamics as the system is swept slowly through the critical point (a Kibble-Zurek ramp). Scaling is well understood for Kibble-Zurek ramps that end at the quantum critical point or deep in the ferromagnetic regime. We solve for the full finite-size scaling forms of excess heat and spin-spin correlation function for an arbitrary point along the ramp. We also confirm the postulated universality of the dynamic scaling forms by numerically simulating Mott insulating bosons in a tilted potential, an experimentally realizable model in the same universality class [Simon et. al., Nature 472, 372 (2011)]. Our numerics indicate that the time-scales necessary to see non-equilibrium scaling should already be within the reach of experiment.

[1] Equal contribution

4:54PM X4.00011 Self-consistent theory of instabilities in the spin-1 Bose gas, AUSTEN LAMACRAFT, University of Virginia, RYAN BARNETT, University of Maryland — We discuss instabilities of a spin-1 Bose condensate using a Hartree-Fock-Bogoliubov approximation to account for the interactions between the unstable modes. There is a close analogy to the “S-theory” that describes parametric excitation of magnons in solid state systems. We particularly emphasize the pair-breaking effect of phase fluctuations in the parent condensate and their role in inhibiting the instability.

5:06PM X4.00012 Decay of classical quasiperiodic state and emergence of prethermalization in quenched Fermi-Pasta-Ulam system, RAFAEL HIPOLITO, City University of New York, College of Staten Island, IPPEI DANSHITA, Computational Condensed Matter Physics Laboratory, RIKEN, VADIM OGANESYAN, City University of New York, College of Staten Island, ANATOLI POLKOVNIKOV, Boston University — We will discuss the relaxation of the Fermi Pasta Ulam system in the presence of quantum fluctuations. In order to make comparisons with the classical relaxation, we strongly excite a single normal mode, while the rest of the modes are initially in the quantum ground state. We confine ourselves to the quasiperiodic regime where the classical system never thermalizes. We show that the short time dynamics of the quantum problem are very different from classical evolution, with the quantum zero point energy playing a key role. The short time dynamics can be viewed as an enhancement of zero point energy, parametrically driven by the classical degrees of freedom. This introduces nontrivial off-diagonal correlations in the low momentum sector and dampens the classical oscillations eventually leading to both dephasing and decay, and we identify the time scales associated with these processes. Eventually the system reaches a nontrivial very long lived quasistationary regime where off-diagonal correlations disappear and the energy remains mostly localized in the low q sector while the high q sector relaxes to a uniform effective temperature. In this regime, correlations are very well described by a generalized Gibbs ensemble.

5:18PM X4.00013 Fisher zeroes and non-analytic real time evolution for quenches in the transverse field Ising model, STEFAN KEHREIN, University of Goettingen, MARKUS HEYL, University of Munich, ANATOLI POLKOVNIKOV, Boston University — We study quenches of the magnetic field in the transverse field Ising model. For quenches across the quantum critical point, the boundary partition function in the complex temperature-time-plane shows lines of Fisher zeroes that intersect the time axis, indicating non-analytic real time evolution in the thermodynamic limit (analogous to well-known thermodynamic phase transitions). We obtain exact analytical results for these dynamic transitions and show that the dynamic behavior cannot be obtained from a naive analytic continuation of the thermal equilibrium partition function: Real time evolution across this quantum critical point generates a new non-equilibrium energy scale. We argue that this behavior is expected to be generic for interaction quenches across quantum critical points in other models as well.

Thursday, March 1, 2012 2:30PM - 5:30PM – Session X5 DCMP: Structure and Formation of Oxide Surfaces and Interfaces 206A

2:30PM X5.00001 Quasi-long range ordered hole-adatoms pairs on SrTiO₃(110)-(4×1) surface¹, JIANDONG GUO, FENGMAO LI, ZHIMING WANG, SHENG MENG, ZHIQIANG ZHANG, Institute of Physics, Chinese Academy of Sciences — The surface structure of transition metal oxides (TMOs) has been an important issue for chemistry and photocatalysis. We studied the surface of SrTiO₃, which is a wide-gap semiconductor and has been believed useful for photo-induced water splitting. Specifically we focused on the (110) surface that bears intrinsic instability of reconstruction due to the surface polarity. The monophased (4×1)-reconstructed surface was obtained with the treatment of argon ion sputtering followed by annealing in ultra high vacuum. More interestingly, we observed a (4×10) quasi-long range ordered hole-adatom structure. The atomic configuration was identified by both experimentally adsorbing additional Sr atoms and density functional calculations. The ordering of the hole-adatom pairs was robust since its formation effectively released the stress on (4×1)-reconstructed SrTiO₃(110) surface. Such a surface with ordered defects served as a good template for the guided growth of noble metal nanoclusters with controlled size and density.

¹This work was supported by CMOST.

2:42PM X5.00002 Growth modes of multiferroic BiFeO₃ (001) thin films on SrTiO₃ – Real time X-ray synchrotron study, PRIYA V. CHINTA, RANDALL HEADRICK, ASHRAFI ALMAMUN, Dept. of Physics & Materials Science, University of Vermont, SARA CALLORI, MATTHEW DAWBER, Dept. of Physics, Stony Brook University — Real time X-ray scattering measurements during heteroepitaxial film deposition provide details of initial nucleation and growth, thus giving insight into atomic-scale processes and growth mechanisms. In this work the growth of pulsed laser deposited (PLD), and RF-magnetron sputter deposited multiferroic BiFeO₃ (001) thin films on SrTiO₃ substrates are studied using *in-situ* X-ray specular and diffuse scattering. Both the out-of-plane (height distribution) and lateral (surface mounds and correlations) information is obtained from these measurements. Specular X-ray intensity monitored at (00 1/2) shows unit-cell growth oscillations during the first few monolayers, while both diffuse scattering width and intensity oscillate out-of-phase with specular, characteristic of 2D layer-by-layer growth for PLD deposited films. The coarsening process is consistent with growth and coalescence of islands - identified as key fundamental processes in epitaxial growth. Beyond several monolayers oscillations decay and the diffuse intensity increases indicating rapid growth of mounds. However, the mounds themselves subsequently merge after a few more deposited layers, leaving arrays of mesas with some holes due to incomplete coalescence. This behavior was corroborated with ex-situ Atomic Force Microscopy (AFM) at each stage. Results for sputter deposited films showed unusually strong specular and diffuse oscillations; implications for interface structure and formation will be discussed.

2:54PM X5.00003 Polarization Dependent Reconstructions of Ferroelectric Surfaces¹, JOHN MARK MARTIREZ, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, WISSAM AL-SAIDI, Department of Chemical and Petroleum Engineering, University of Pittsburgh, ANDREW RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania — We present an *ab initio* density-functional study of the surface structures and the thermodynamic stability of ferroelectric tetragonal (001)-oriented slabs of BaTiO₃ and PbTiO₃, including both cases where the bulk polarization is directed towards (positive) and away (negative) from the surface. We analyzed systematically the total energies of surfaces with different reconstruction symmetries and stoichiometries. The thermodynamic stability diagrams show that the stable surface compositions for the positive and negative surfaces are different, which are in turn different from those of the paraelectric phase. We show that the prevalence of certain surface reconstructions can be understood in the light of the ability of ions to passivate ferroelectric surface charges.

¹The authors acknowledge support from the AFOSR under Grant FA9550-10-1-0248, from the DOE under Grant DE-FG02-07ER15920, and computational support from the HPCMO.

3:06PM X5.00004 STM study of the Mn-dopants on the surface of $\text{Sr}_3(\text{Ru}_{1-x}\text{Mn}_x)_2\text{O}_7$ ($x=6\%$, 16%)¹, WARD PLUMMER, GUORONG LI, Louisiana State University, QING LI, MINGHU PAN, Oak Ridge National Laboratory, BIAO HU, VON BRAUN NASCIMENTO, JIANDI ZHANG, RONGYING JIN, Louisiana State University — The double-layered $\text{Sr}_3\text{Ru}_2\text{O}_7$ is a paramagnetic metal, but the substitution of Mn for Ru ($\text{Sr}_3(\text{Ru}_{1-x}\text{Mn}_x)_2\text{O}_7$) results in a metal-to-insulator transition at T_{MIT} and antiferromagnetic (AF) ordering at T_M (the two transitions are closely coupled for $x < 6\%$). STM measurements at 4.2 K and 100 K on the surface of $\text{Sr}_3(\text{Ru}_{1-x}\text{Mn}_x)_2\text{O}_7$ ($x = 6\%$, 16%) reveal a $(\sqrt{2} \times \sqrt{2})R45^\circ$ unit cell, consistent with the orthorhombic bulk structure. The Mn dopant has been identified through bias-dependent STM topography and dI/dV mapping. The Mn dopant equally occupies two sites which are anti-phase - one sitting at the center and the other on the corner of the $(\sqrt{2} \times \sqrt{2})R45^\circ$ unit cell. We have directly imaged the chirality of MnO_6 rotation at the anti-phase sites. In contrast to the bulk measurements, the surface is always metallic for $x=16\%$ and insulating only for 4.2K measurements on the $x = 6\%$ sample. The surface apparently suppresses the Mn-induced insulating (AF) phase observed in the bulk.

¹Research at LSU is supported by NSF DMR-1002622. Research at ORNL's CNMS was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. DOE.

3:18PM X5.00005 Morphology and Magnetism of Atomically Thin Layers of Chromia – An STM Investigation, XUMIN CHEN, DONNA KENKEL, GEOFFREY ROJAS, XI HE, CHRISTIAN BINEK, AXEL ENDERS, University of Nebraska-Lincoln, MSREC COLLABORATION — A low temperature scanning tunneling microscopy (LT-STM) study of ultrathin chromium oxide films on Cu(111) is presented. The (0001) surface of Cr_2O_3 (chromia) exhibits long-range antiferromagnetic ordering, and its usefulness for electric field control of exchange bias has been recently established [Xi He, Ch. Binek, et al., *Nature Materials* 9, 579 – 585 (2010)]. We deposited ultrathin chromium layers on Cu(111), followed by post-annealing in oxygen partial pressures to promote oxidation of the chromium films. We find that chromium grows on Cu(111) in the Volmer-Weber mode, resulting in small 3D islands. During annealing, the small islands coalesce to form large, flat terraces and the most stable oxide of chromium, Cr_2O_3 , is formed at 630°C . Spin-polarized scanning tunneling microscopy has been performed to image the layer-wise antiferromagnetism in different structural layers of the chromia films. Thin layers of cobalt have been deposited on the chromia so that the magnetism of the Co couples to that of the chromia. Imaging the magnetism of the Co islands on the Cr_2O_3 terraces with spin-polarized STM helped us distinguishing between magnetic and electronic contrast in the complex dI/dV maps of the chromia surface.

3:30PM X5.00006 Structures of Stoichiometric and Oxygen Deficient Sapphire Surfaces, HA-WOONG HONG, Argonne National Laboratory, AARON GRAY, T.-C. CHIANG, Department of Physics, University of Illinois at Urbana-Champaign, SHAWN HAYDN, MICHAEL GRAMLICH, YIYAO CHEN, PAUL MICELI, Department of Physics, University of Missouri — Sapphire, $\alpha\text{-Al}_2\text{O}_3$ is one of widely used oxide substrates. Its (0001) surface is presumed quite stable. However, when it is heat-treated under vacuum, the surface shows the variety of different surface structures, mostly due to oxygen deficiency. The initial surface structure could be also modified by covering the substrate with another sapphire substrate during air annealing above 1500°C . During the course of the heat-treatment under UHV condition, the x-ray reflectivity and crystal truncation rods were measured in addition to observing reflection high energy electron diffraction patterns. Metal films such as Pb, Ag, and Pd were deposited onto these various sapphire surfaces. Contrary to common belief that metal films would not grow well on insulating oxide substrates, metal films could be formed on some of the sapphire surfaces. The influence of the sapphire surface structure to the morphology of the metal films will be discussed.

3:42PM X5.00007 Crystallographic Orientation(s) of Vanadium Dioxide Nano-Grains on Various Single-Crystal Sapphire Substrates, FELIPE RIVERA, Brigham Young University, JOYEETA NAG, RICHARD HAGLUND, Vanderbilt University, ROBERT DAVIS, RICHARD VANFLEET, Brigham Young University — Vanadium dioxide (VO_2) is a material of particular interest due to its reversible structural semiconductor to metal phase transition near room temperature (68°C) and its accompanied hysteresis. Electron Back-Scattered Diffraction (EBSD) was used to study the orientation of the crystalline VO_2 grains deposited on three cuts of sapphire (a-, c-, and r-cuts) by pulsed laser deposition. EBSD showed a predominant family of crystallographic relationships present in all cuts of sapphire wherein the rutile VO_2 {001} planes tend to lie parallel to the substrate's {10-10} and the rutile VO_2 {100} planes lie parallel to the substrate's {1-210} and {0001}. This family of relationships accounts for the majority of the VO_2 grains observed on all the studied sapphire substrates. However, due to the symmetry of the substrate, there were variations of these same relationships that prevent a single epitaxy from taking place in these cuts as the VO_2 grains did orient themselves with equivalent out-of plane directions in the substrate.

3:54PM X5.00008 Growth of Vanadium Dioxide Thin Films Using Magnetron Sputtering, FANGFANG SONG, B.E. WHITE JR., Binghamton University — In this work, we present our experimental investigation of vanadium oxide thin film deposition. RF and DC magnetron sputtering are used for thin film deposition. Post deposition anneal are introduced to stabilize the vanadium dioxide phase. The impact of deposition conditions and anneal conditions on the structural and morphological properties of the thin films, as determined by x-ray diffraction and scanning electron microscopy, will be discussed. Results indicate that on the technologically relevant silicon dioxide surface, the transitional phase of vanadium dioxide can be stabilized by post deposition anneal at 550°C and oxygen partial pressures between 3.6×10^{-4} torr and 10^{-2} torr. The films obtained show a resistivity change of a factor of 200 at 350K. The shift in transition temperature is attributed to thin film stress.

4:06PM X5.00009 Studies of high coverage oxidation of the Cu(100) surface using low energy positrons, N.G. FAZLEE, W.B. MADDOX, A.H. WEISS, Department of Physics, University of Texas at Arlington — The study of oxidation of single crystal metal surfaces is important in understanding the corrosive and catalytic processes associated with thin film metal oxides. The structures formed on oxidized transition metal surfaces vary from simple adlayers of chemisorbed oxygen to more complex structures which result from the diffusion of oxygen into subsurface regions. In this work we present the results of theoretical studies of positron surface and bulk states and annihilation probabilities of surface-trapped positrons with relevant core electrons at the oxidized Cu(100) surface under conditions of high oxygen coverage. Calculations are performed for various high coverage missing row structures ranging between 0.50 and 1.50 ML oxygen coverage. The results of calculations of positron binding energy, positron work function, and annihilation characteristics of surface trapped positrons with relevant core electrons as function of oxygen coverage are compared with experimental data obtained from studies of oxidation of the Cu(100) surface using positron annihilation induced Auger electron spectroscopy (PAES).

4:18PM X5.00010 *In situ* TEM Studies of the Initial Oxidation stage of Cu and Cu Alloy Thin Films, JUDITH YANG, YIHONG KANG, University of Pittsburgh, LANGLI LUO, State University of New York at Binghamton, JAMES CISTON, Lawrence Berkeley National Laboratory, ERIC STACH, Brookhaven National Laboratory, GUANGWEN ZHOU, State University of New York at Binghamton — The fundamental understanding of oxidation at the nanoscale is important for the environmental stability of coating materials as well as processing of oxide nanostructures. Our previous studies show the epitaxial growth of Cu_2O islands during the initial stages of oxidation of Cu thin films, where surface diffusion and strain impact the oxide development and morphologies. The addition of secondary elements changes the oxidation mechanism. If the secondary element is non-oxidizing, such as Au, it will limit the Cu_2O island growth due to the depletion of Cu near the oxide islands. When the secondary element is oxidizing, for example Ni, the alloy will show more complex behaviour, where duplex oxide islands were observed. Nucleation density and growth rate of oxide islands are observed under various temperatures and oxygen partial pressures ($p\text{O}_2$) as a function of time by *in situ* ultra high vacuum (UHV)-transmission electron microscopy (TEM). Our initial results of Cu-Ni(001) oxidation is that the oxide epitaxy and morphologies change as function of Ni concentration. For higher spatial resolution, we are examining the atomic scale oxidation by aberration-corrected ETEM with $1\text{\AA}$ resolution.

4:30PM X5.00011 Quantum-Mechanical Investigations for the Oxidation Mechanism of Ti_3Al , WENHUA XUE, The University of Tulsa, SHI-YU LIU, Tianjin Normal University, SHIYANG LIU, Zhejiang Normal University, DEJUN LI, Tianjin Normal University, TARA DRWENSKI, SHUXIA YIN, SANWU WANG, The University of Tulsa — First-principles density-functional theory and thermodynamics calculations are combined to establish a microscopic mechanism for the oxidation of the $\alpha_2\text{-Ti}_3\text{Al}(0001)$ surface. The surface energies as functions of the chemical potentials, as well as structural relaxations and electronic densities of states, are determined. The surface phase diagram (SPD) of the $\alpha_2\text{-Ti}_3\text{Al}(0001)$ systems with different defects and at various oxygen coverages is constructed. It is found that the Al antisite defect prefers to segregate on the $\alpha_2\text{-Ti}_3\text{Al}(0001)$ surface and oxygen adsorption enhances the segregation with the formation of the surface with three Al antisites per unit surface cell (i.e., the top surface layer is full of Al atoms) at the initial stage of oxidation, accounting for the aluminum selective oxidation observed experimentally. After the initial stage of oxidation, the $\text{O}/\alpha_2\text{-Ti}_3\text{Al}(0001)$ system manifests itself with a non-uniform double-phase SPD, suggesting the competition between oxidations of the Al and Ti elements in the oxidation process. This result explains the experimentally observed second regime of oxidation in which both metal elements are oxidized.

4:42PM X5.00012 Site Specific Molecular Chemisorption of O_2 on $\text{TiO}_2(110)$: A Scanning Tunneling Microscopy Study, ZHITAO WANG, YINGGE DU, ZDENEK DOHNÁLEK, IGOR LYUBINETSKY, Pacific Northwest National Laboratory — The investigation of O_2 adsorption on TiO_2 is critical since it can help us to better understand the photooxidation mechanism of TiO_2 . In our work, molecularly chemisorbed O_2 were directly imaged on reduced $\text{TiO}_2(110)$ at 50 K with scanning tunneling microscopy (STM). Two O_2 adsorption channels, one at bridging oxygen vacancies (V_O) and another at five-fold coordinated Ti atoms (Ti_{5c}), have been identified. While O_2 at Ti_{5c} appears as a single protrusion, the O_2 at V_O manifests itself by a disappearance of the V_O feature. It is found that STM tip can easily dissociate O_2 and the dissociation details strongly depend on the tunneling conditions and the type of the O_2 adsorption site. The chemisorbed O_2 at these two distinctive sites are the most likely precursors for the two previously established O_2 dissociation channels, observed at temperatures above 150 and 230 K at the V_O and Ti_{5c} sites, respectively

4:54PM X5.00013 Hard x-ray photoemission studied and band alignment in $\text{TiO}_2/\text{HfO}_2/\text{Ge}$ heterojunctions, ABDUL RUMAIZ, NSLS, Brookhaven National Laboratory, JOSEPH WOICK, NIST, QI XIE, University of Ghent, PETER SIDONS, NSLS, Brookhaven National Laboratory, CONAN WEILAND, NIST, CHRISTOPHE DETAVERNIER, University of Ghent — Novel high K oxides such as hafnium oxide and zirconium oxide have replaced silicon dioxide as gate oxide. Although titanium oxide has a high dielectric constant, the poor conduction band offset between titanium oxide and Si/Ge makes it a poor choice for gate oxide. One way to address this issue is to have a thin intermediate layer with appropriate band alignment between titanium oxide and the semiconductor. Here we present hard x-ray photoelectron spectroscopy (HAXPES) study on the band alignment between atomic layer deposited (ALD) $\text{TiO}_2/\text{HfO}_2/\text{Ge}$ heterojunctions. The exact position of the valence band maximum was determined by convoluting theoretical calculated density of states from first-principles calculations and comparing with experimental valence band data. We will also discuss the dependence of the band alignment on the thickness of the intermediate layer.

5:06PM X5.00014 Synchrotron Photoemission Characterization of Process Dependent Oxidation Control in InGaAs/High-k Film Systems, CONAN WEILAND, JOSEPH WOICK, National Institute of Standards and Technology, JIMMY PRICE, PAT LYSAGHT, JEFF HUANG, SEMATECH — To continue CMOS scaling, higher mobility substrates, such as III-V semiconductors, are being investigated. However, certain technological barriers must be overcome before high-mobility devices can be employed; notably, defects at the semiconductor/high-k interface need to be well controlled. Here, we investigate the role of an AlN interlayer between InGaAs and ALD ozone deposited ZrO_2 using synchrotron source X-ray photoemission spectroscopy (XPS). XPS is able to quantify the relative levels of oxidation from the In, Ga and As signals. Also, by comparing the relative As 3d_{3/2}: As 3d_{5/2} peak intensities, it is possible to quantify the level of As-As bond formation, which is common to coarse As-O reduction processing and consistent with mobility degradation. To elucidate the role of the AlN interlayer, XPS spectra of InGaAs/AlN/ ZrO_2 , InGaAs/ ZrO_2 and InGaAs/AlN films will be presented and compared. We will demonstrate that an AlN interlayer is effective in reducing In, Ga and As interfacial oxides, as well as As-As bonding, yet is not sufficient to passivate the interface against further oxidation from ozone based ALD processing.

5:18PM X5.00015 Engineering an epitaxial dielectric/metal/dielectric trilayer system¹, JISUN KIM, Department of Physics, The University of Texas at Austin, YANG MENG, Z.Q. QIU, Department of Physics, University of California at Berkeley, CHIH-KANG SHIH, Department of Physics, The University of Texas at Austin — Ag is a favorable material platform for plasmonic applications. Most plasmonic devices to date have been based on granular polycrystalline metal films, which suffer from scattering due to surface roughness. Recently, superior plasmonic properties have been demonstrated by using atomically smooth epitaxial Ag(111) films grown on Si(111), illustrating the advantages of an epitaxial approach. For further device applications of the above example, it is desirable to create epitaxially grown dielectric/metal/dielectric multi-layer systems. Here we report successful epitaxial growth of a $\text{MgO}(001)/\text{Ag}(001)/\text{MgO}(001)$ trilayer system which can be used as a material platform for creating multi-layered (dielectric/metal)_N heterostructures with any desired number, N. This type of new structure can be utilized for plasmonic devices with a wider wavelength range due to the transparency of MgO substrates in visible light. Moreover, it can open a door to new integrated devices with high quality atomically smooth films.

¹NSF Grants No. DMR-0906025, CMMI-0928664, Welch Foundation F-1672

Thursday, March 1, 2012 2:30PM - 5:30PM – Session X6 DMP: Carbon Nanotube Optics II: Absorption and Raman Spectroscopy 206B

2:30PM X6.00001 Measurement of Absolute Absorption Cross-section of Individual Carbon Nanotubes on a Substrate, LIHONG HERMAN, ADAM TSEN, JIWOONG TSEN, Cornell University — The absorption cross-section is one of the central parameters that determine the efficiency of most optical and optoelectronics processes in single-walled carbon nanotubes (SWNT), including photoluminescence, photodetection, and photovoltaic energy conversion. While absorption measurements on SWNT ensembles in solution provide a reliable estimate, the absolute absorption cross-sections of individual carbon nanotubes on and off resonance have not been reported. Here, we measure the absorption cross-section of SWNTs on chip with spatial resolution using lock-in technique with a spatial modulation of a focused laser spot near SWNTs. We measure the absorption cross-section of SWNTs near resonance to be on the order of 10^{-17} cm^2 per carbon atom, which is consistent with on-chip Rayleigh measurements as well as recent time-resolved photoluminescence measurements. Since our measurement is performed on SWNTs on chip, it can be directly applied to various optoelectronic devices made with SWNTs, thus allowing quantitative analysis of the fundamental performance limits of SWNT photovoltaic devices.

2:42PM X6.00002 Measurement of Absorption Cross-section for Single-walled Carbon Nanotubes, XIAOPING HONG, KAIHUI LIU, FENG WANG, University of California Berkeley — Optical absorption is the most fundamental optical property. Quantitative knowledge of absorption cross-section provides valuable information on the material electronic structure, and is necessary for evaluating quantum efficiency of other important optical processes, such as photoluminescence and photocurrent generation. However, absorption measurement of individual single-walled carbon nanotubes (SWCNTs) is quite challenging. Here we used an efficient interferometric method to obtain the absorption cross-section of individual chirality-defined SWCNTs. We will discuss how the absorption cross-section varies in different carbon nanotubes.

2:54PM X6.00003 Enhancement of photoluminescence from single-walled carbon nanotubes by photonic crystal microcavities¹, R. WATAHIKI, T. SHIMADA, P. ZHAO, S. CHIASHI, S. IWAMOTO, Y. ARAKAWA, S. MARUYAMA, Y.K. KATO, The University of Tokyo — Single-walled carbon nanotubes are bright nanoscale emitters, while photonic crystal microcavities offer the possibility for efficient optical coupling at the nanoscale because of their small mode volumes and high quality factors. Here we report on the enhancement of photoluminescence from single-walled carbon nanotubes by L3 cavities in hexagonal lattice photonic crystals. Free-standing photonic-crystal membranes are fabricated from silicon-on-insulator substrates, and micelle-encapsulated carbon nanotubes are dispersed on the devices. We observe sharp peaks with a typical spectral width of 0.4 nm which corresponds to a quality factor of ~3000. As the peaks appear at wavelengths longer than those of Si photoluminescence, they are attributed to carbon nanotube emission coupled to the microcavity modes. We find that the photoluminescence intensity is enhanced by more than a factor of four compared to luminescence from an unpatterned area.

¹This work is supported by SCOPE, Casio Science Promotion Foundation, Global COE and Photon Frontier Network Programs of MEXT, Japan.

3:06PM X6.00004 Can we look into carbon nanotubes by infrared light?¹, KATALIN KAMARAS, ARON PEKKER, ZSOLT SZEKRENYES, Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, Budapest, FERENC SIMON, Budapest University of Technology and Economics, BEA BOTKA, RUDI HACKL, Walther-Meissner-Institute, Garching, AKOS BOTOS, ANDREI KHLOBYSTOV, University of Nottingham — Individual molecules filled into carbon nanotubes exhibit Raman activity but very weak, if any, infrared absorption. We will present infrared (transmission and ATR), Raman and transmission electron microscopy data of various filled nanotubes (sorted by diameter and metallicity; encapsulating organometallic, aromatic and fullerene-based molecules) to illustrate this puzzling behavior. In the infrared spectra of double-walled carbon nanotubes, however, vibrational signatures of the inner and outer tubes are clearly discernible. A strong proof for this assignment is the shift of the inner-tube modes with ¹³C isotope content in samples where the inner tube is enriched with ¹³C.

¹Supported by OTKA Grant No. 75813 and ERC-259374-Sylo grant

3:18PM X6.00005 ABSTRACT WITHDRAWN —

3:30PM X6.00006 Intersubband Edge Singularity in Metallic Nanotubes, EUGENE MISHCHENKO, OLEG STARYKH, University of Utah — Tunneling density of states of both the massless and massive (gapped) particles in metallic carbon nanotubes is known to have anomalous energy dependence. This is the result of coupling to multiple low-energy bosonic excitation (plasmons). For both kinds of particles the ensuing effect is the suppression of the density of states by electron-electron interactions. We demonstrate that the optical absorption between gapless and gapped states is affected by the many-body effects in the opposite way. The absorption probability is enhanced compared with the non-interacting value and develops a power-law frequency dependence, with the -0.2 exponent for typical nanotubes.

3:42PM X6.00007 Indication of Long Lived States in Decay Associated Spectra of Single-Walled Carbon Nanotubes¹, VASUDEV LAL, ROSEANNE SENSION, DUNCAN STEEL, University of Michigan, Ann Arbor — The direct bandgap nature of Single-Walled Carbon Nanotubes(SWCNTs) along with the quantized energy level structure due to reduced dimensionality makes them useful elements in chip-based photonic devices for sensing and communications. However, their fundamental linear and nonlinear optical properties remain poorly understood. Using various nonlinear optical spectroscopy techniques with micelle encapsulated SWCNTs, we have measured carrier dynamics at both the picosecond, and tens of nanosecond timescale. We measure a fast 20ps timescale decay that agrees well with the lifetime of the lowest excited state measured before for such samples but surprisingly we also obtain an optical double-resonance signal on the slow timescale (10nsec). Such slow timescale signals due to artifacts such as thermal effects have been ruled out. Decay associated spectra shows striking differences between the spectral lineshapes arising from the fast and slow components of the nonlinear optical signal which might indicate the creation of a long-lived state by the pump pulse that changes the subsequent probe spectra. This indicates the possibility of the presence of either a trap state or possibly a more complex energy level structure for the SWCNT involving the presence of a metastable state.

¹The authors would like to acknowledge financial support from DTRA.

3:54PM X6.00008 Asymmetric resonance Raman excitation profiles and violation of the Condon approximation in single-wall carbon nanotubes, STEPHEN DOORN, JUAN DUQUE, HAGEN TELG, Los Alamos National Laboratory, HANG CHEN, ANNA SWAN, Boston University, ERIK HAROZ, JUNICHIRO KONO, Rice University, XIAOMIN TU, MING ZHENG, NIST — DNA wrapping-based ion exchange chromatography and density gradient ultracentrifugation provide nanotube samples highly enriched in single chiralities. We present resonance Raman excitation profiles for the G-band of several single chirality semiconducting and metallic species. The expected incoming and outgoing resonance peaks are observed in the profiles, but contrary to long-held assumptions, the outgoing resonance is always significantly weaker than the ingoing resonance peak. This strong asymmetry in the profiles arises from a violation of the Condon approximation [1]. Results will be discussed in the context of theoretical models that suggest significant coordinate dependence in the transition dipole (non-Condon effects). The generality of the behavior across semiconducting and metallic types, nanotube family, phonon mode, and Eii will be demonstrated.

[1] J. Duque et. al., ACS Nano, 5, 5233 (2011).

4:06PM X6.00009 Raman Spectroscopy characterization of individual triple-walled carbon nanotubes, THOMAS HIRSCHMANN, PAULO ARAUJO, MILDRED DRESSELHAUS, Massachusetts Institute of Technology, USA, KORNELIUS NIELSCH, University of Hamburg, Germany — The characterization of individual triple-walled carbon nanotubes (TWCNT) was studied in detail by using Raman spectroscopy resonant signals taken with various laser excitation energies. TWCNTs are in fact an assembly of three concentric weakly coupled single-walled carbon nanotubes (SWCNTs) or, equivalently, a double-walled carbon nanotube (DWCNT) concentric to an external SWCNT. An isolated TWCNT consists of an inner, middle and outer tube, each of which can be either metallic or semiconducting. All of the eight possible combinations provide a multitude of information about the electrical and optical properties. Among numerous applications, TWCNTs offer an ideal structure to study and understand how an interacting medium influences the properties of both, SWCNTs and DWCNTs structures. The measured spectra show exceptionally distinctive radial breathing modes, G-, G'-band and further modes of the three concentric tubes. All of the Raman three bands described above are very sensitive to changes in the structure of each tube. By following the spectral changes of these frequency modes, we can extract important information about, for example, the respective tube distances, inter-tube interaction in TWCNTs systems and its consequences on their related SWCNTs and DWCNTs counterparts.

4:18PM X6.00010 Resonance Raman Spectroscopy of Separated Single-Wall Carbon Nanotube¹, J.R. SIMPSON², Towson University, J.A. FAGAN, X. TU, M. ZHENG, A.R. HIGHT WALKER, National Institute of Standards and Technology, J.G. DUQUE, J. CROCHET, S.K. DOORN, Los Alamos National Laboratory — The heterogeneity of single-wall carbon nanotubes (SWCNTs) produced by typical techniques complicates characterization and presents a barrier for technological applications. Improvements in separation and purification techniques enable detailed studies of specific nanotube properties by providing samples of unique chirality, length, metallicity, bundling, and interior filling. We report resonant Raman spectroscopy (RRS) measurements on these samples over a wide range of excitation wavelengths using a series of discrete and continuously tunable laser sources coupled to a triple-grating spectrometer. RRS of these homogeneous samples reveals unique spectral features and affords interpretation of intrinsic nanotube optical properties. Of particular interest are the G-band of chirally-pure armchair metallic SWCNTs and shifts of the radial breathing mode and excitation energy with water filling. Additionally, we will compare Raman results with other optical characterization techniques.

¹JRS acknowledges support from the Research Corporation CCSA.

²Towson University and NIST.

4:30PM X6.00011 Optical properties of single-walled carbon nanotube aerogels¹, GORDANA OSTOJIC, Northwestern University — A network of connected single-walled carbon nanotubes (SWNT) is created by a novel DNA-protein complex directed assembly. Due to a point-like nature of connectors, the SWNT aerogel represents a network of self-suspended nanotubes with a record ultra-low density of less 0.75 mg/cm³. The assembly method and low density enables a direct comparison of optical properties of nanotubes in solvent and air to surfactant solubilized nanotubes. Optical properties of SWNT gels are investigated using optical absorption, photoluminescence and Raman spectroscopy. Gelled nanotubes in water and in the low population regime behave similar to solubilized nanotubes. In contrast, photoluminescence of SWNT aerogels exhibit nonlinear effects and a phonon-induced broadening. In addition, aerogels show a previously unobserved photoluminescence peak at 1.3 eV that corresponds to a phonon-assisted recombination of photoexcited charges. Raman spectra of carbon nanotube aerogels display narrow peaks due to the phonon decoupling of suspended SWNTs in air and a redistribution of G phonon population due to nonlinear effects.

¹This work was supported by the Northwestern University EECS Department and McCormick School of Engineering.

4:42PM X6.00012 ABSTRACT WITHDRAWN —

4:54PM X6.00013 Coupled Radial Breathing Oscillation in Double-Walled Carbon Nanotubes, KAIHUI LIU, XIAOPING HONG, UC Berkeley, ENGE WANG, Peking University, China, FENG WANG, UC Berkeley, UC BERKELEY COLLABORATION, PEKING UNIVERSITY, CHINA COLLABORATION — Double-walled carbon nanotubes (DWNTs) provide a model system for quantitative study of electronic and vibrational couplings in the nanoscale. Here we investigate coupled radial breathing mode (RBM) oscillations in structurally defined DWNTs by combining electron diffraction, Rayleigh scattering, and Raman scattering spectroscopy on the same individual nanotubes. We find that the two RBM oscillations in DWNTs are strongly coupled, with vibration energies significantly higher than those of constituent inner- and outer-wall nanotubes. In addition, the oscillation strength of these two coupled modes shows an interesting quantum interference behavior between the inner- and outer-wall electronic resonance channels.

5:06PM X6.00014 Observation of Optical Phonon Emission Threshold in the Current-Voltage Characteristics of Suspended Carbon Nanotubes, MOH AMER, University of southern california, ADAM BUSHMAKER, The Aerospace Corporation, IKAI HSU, STEVE CRONIN, University of southern california — Electrically-heated suspended, nearly defect-free, carbon nanotubes (CNTs) exhibiting negative differential conductance in the high bias regime experience a sudden drop in current (or “kink”). The bias voltage at the kink (V_{kink}) is found to depend strongly on the applied gate voltage, substrate temperature, pressure, and gas environment. After subtracting the voltage drop across the contacts, however, the kink bias voltages converge around 0.2V, independent of gate voltage and gas environment. Due to the ballistic nature of these defect free carbon nanotubes, this bias voltage of 0.2V corresponds to the threshold energy of optical phonon emission. This phenomenon is corroborated by simultaneously monitoring the Raman spectra of these nanotubes as a function of bias voltage. At the kink bias voltage, the Gband Raman modes experience a sudden downshift, further indicating threshold optical phonon emission. A Landauer model is used to fit these kinks in various gas environments where the kink is modeled as a sudden change in the optical phonon lifetime, which corresponds to a change in the non-equilibrium factor that describes the existence of hot phonons in the system.

5:18PM X6.00015 The Electronic and Vibrational Properties of Carbon Nanorings, HANG CHEN, ANNA SWAN, Electrical and Computer Engineering Department and Photonics Center, Boston University — [n]-Cycloparaphenylenes ([n]-CPPs), carbon nanorings with n benzene units reminiscent of a single unit of a (n, n) armchair carbon nanotubes, show unusual optical behaviors: the absorption maximum is almost size independent at 340 nm, while the lower energy fluorescence exhibits multiple peaks with strong size dependence, opposite of quantum confinement behavior [1]. The energy levels for CPPs with various sizes are calculated using time-dependent density functional theory (TDDFT) and compared to the experimental results. Moreover, we calculate the Raman modes of various [n]-CPPs and propose that the multiple peaks observed in the fluorescence spectra could be due to the electron-phonon coupling effects. We also consider possible excitonic effects in these carbon nanorings, and discuss their similarities as well as differences to carbon nanotubes. [1] T. Iwamoto, Y. Watanabe, Y. Sakamoto, T. Suzuki, S. Yamago. *J. Am. Chem. Soc.*, 133, 2011;

Thursday, March 1, 2012 2:30PM - 5:30PM —

Session X7 DCMP: Electronic, Structural and Chemical Properties of Non-Carbon Nanotubes and Nanowires 207

2:30PM X7.00001 Electronic properties of fluorine passivated silicon nanowires: density functional calculations, KEENAN ZHUO, MEI-YIN CHOU, Georgia institute of technology — Arrays of silicon nanowire (SiNWs) have recently gained attention as a promising new photovoltaic technology. Previous studies show that halogen passivated SiNWs have good chemical stability and also form a critical pathway towards organic group functionalization. Yet, surface halogens are known to alter the SiNW electronic structure, most notably by reducing the band gap. We explore the fundamental physics behind this effect through first principles calculations on hydrogen and fluorine passivated (110) SiNWs. Electronic structure analysis reveals that the highly electronegative fluorine passivation modifies the quantum confinement potential and induces changes in the energy level ordering. Furthermore, we show how a modified cylindrical potential well model can demonstrate a link between this quantum confinement modification and the shift in energy levels responsible for the band gap reduction.

2:42PM X7.00002 Molecular Hydrogen and Oxygen Interactions with Armchair Si Nanotubes¹

, HAOLIANG CHEN, ASOK RAY, Physics Department, University of Texas at Arlington, Arlington, Texas 76019 — First principles calculations based on hybrid density functional theory have been used to study the electronic structure properties of armchair silicon nanotubes from (3, 3) to (12, 12). Full geometry and spin optimizations have been performed without any symmetry constraints with an all electron 3-21G* basis set and the B3LYP functional. The largest silicon nanotube studied has a cohesive energy of 3.47eV/atom. Molecular hydrogen and oxygen adsorptions on a (6, 6) tube have been studied by optimizing the distances of the ad molecules from both inside and outside the tube. The molecule is originally placed perpendicular or parallel to the tube axis. The on-top external site is the most preferred site for the hydrogen molecule with adsorption energy of 3.71eV and an optimized distance of 3.31 Å when it is perpendicular to the tube axis. For oxygen, the molecule dissociates into two atoms with adsorption energy of 7.45eV, the optimized distances being 1.65/1.68Å. The buckling of the nanotubes increased significantly indicating structural deformation and an increase of sp³ structure. The band gap increases from 0.98eV of bare nanotube to 1.26eV after adsorption of hydrogen molecule. For oxygen molecule, the band gap slightly increases from 0.98eV to 1.01eV.

¹Work partially supported by the Welch Foundation. (Grant No. Y-1525)

2:54PM X7.00003 Modeling Earle-Stage Kinking during VLS Ge Nanowire Growth , SEUNGHWA

RYU, Mechanical Engineering, Stanford University, Stanford, CA, United States, YANYING LI, Applied Physics, Stanford University, Stanford, CA, United State, ANN F. MARSHALL, Geballe Laboratory for Advanced Materials, Stanford University, Stanford, CA, United State, WEI CAI, Mechanical Engineering, Stanford University, Stanford, CA, United State, PAUL C. MCINTYRE, Materials Science Engineering, Stanford University, Stanford, CA, United State — The catalyzed growth of Ge nanowires from gold nanoparticles via the vapor-liquid-solid (VLS) mechanism has been the subject of intense research worldwide, due to their potential applications in nanotechnology. Understanding the fundamental mechanisms underlying kinking during Ge nanowire growth, especially at the early-stage, is helpful for better control of Ge nanowire growth for technological applications. We report an investigation of wire morphology before and during Ge nanowire kinking in early stage growth under typical nucleation conditions. The Ge nanowires grew either along the vertical [111] direction or kinked away onto inclined <111> axes early on during their growth. We found that most kinked Ge nanowire deposited under these conditions kinked at similar height, and had similar sidewall facet structure in the kinked region. High-resolution transmission and scanning electron microscopy investigations also showed that the typical kinking-structure was bounded by (111) and other relatively stable Ge surface facets. We construct 3D phase field model of the nanowire based on the transmission and scanning electron microscopy and compare the evolution of the droplet and nanowire with experimental observations.

3:06PM X7.00004 Detection of bio-molecules of different polarities by Boron Nitride Nan-

otube , SAIKAT MUKHOPADHYAY, Michigan Technological University, RALPH SCHEICHER, Department of Physics and Astronomy, Uppsala University, RAVINDRA PANDEY, Michigan Technological University, SHASHI KARNA, U.S. Army Research Laboratory, Weapons and Materials Research Directorate, DEPARTMENT OF PHYSICS, MICHIGAN TECHNOLOGICAL UNIVERSITY COLLABORATION, DEPARTMENT OF PHYSICS AND ASTRONOMY, UPPSALA UNIVERSITY COLLABORATION, U.S. ARMY RESEARCH LABORATORY, WEAPONS AND MATERIALS RESEARCH DIRECTORATE COLLABORATION — The effect of molecular polarity on the interaction between a boron nitride nanotube (BNNT) and amino acids is investigated with density functional theory. Three representative amino acids, namely, tryptophane (Trp), a nonpolar aromatic amino acid, and aspartic acid (Asp) and arginine (Arg), both polar amino acids are considered for their interactions with BNNT. The polar molecules, Asp and Arg, exhibit relatively stronger binding with the tubular surface of BNNT. The binding between the polar amino acid molecules and BNNT is accompanied by a charge transfer, suggesting that stabilization of the bioconjugated complex is mainly governed by electrostatic interactions. The results show modulation of the BNNT band gap by Trp. Interestingly, no change in band gap of BNNT is seen for the polar molecules Asp and Arg. The predicted higher sensitivity of BNNTs compared to carbon nanotubes (CNTs) toward amino acid polarity suggests BNNTs to be a better substrate for protein immobilization than CNTs.

3:18PM X7.00005 Quantum Confinement and Surface Relaxation Effects in Rutile TiO₂

Nanowires¹ , ABRAHAM HMIEL, YONGQIANG XUE, College of Nanoscale Science and Engineering, State University of New York at Albany — Recent developments in synthesis of TiO₂ nanowires with diameters on the atomic scale have opened up new grounds for studying structure-property relationships in the regime where quantum confinement effects are important. In the sub-nanometer range, the properties of nanowires can be sensitive to atomic-level control of surface morphology, functionalization, and nanowire stoichiometry during the growth and fabrication processes, thereby opening the way for new applications. First-principles density functional theory calculations have been applied to investigate the size- and shape-dependent properties of [001]-oriented rutile TiO₂ nanowires of rectangular cross section. We find that the pronounced oscillation in the formation energy and band structure of the nanowires as a function of the number of TiO₂ trilayers is largely connected to the presence or absence of a mirror Ti-O plane along each confinement direction. We demonstrate that the relative stability and the indirect or direct character of the band structure of the rutile TiO₂ nanowires arise from the interplay between surface relaxation and quantum confinement effects that depend on the even-odd parity of the number of TiO₂ trilayers.

¹This work was partially supported by the New York State Energy Research and Development Authority (NYSERDA), computations were performed at the Cornell Nanoscale Science and Technology Facility (CNF).

3:30PM X7.00006 Simulation of Nanowires on Metal Vicinal Surfaces: Effect of Growth Parameters and Energetic Barriers , AJMI B.H. HAMOUDA, University of Maryland & Univ. of Monastir, SONIA BLEL, Univ. of Monastir,

T.L. EINSTEIN, University of Maryland, MRSEC, MARYLAND TEAM, LAB. OF QUANTUM PHYSICS OF MONASTIR TEAM — Growing one-dimensional metal structures is an important task in the investigation of the electronic and magnetic properties of new devices. We used kinetic Monte-Carlo (kMC) method to simulate the formation of nanowires of several metallic and non-metallic adatoms on Cu and Pt vicinal surfaces. We found that mono-atomic chains form on step-edges due to energetic barriers (the so-called Ehrlich-shwoebel and exchange barriers) on step-edge. Creation of perfect wires is found to depend on growth parameters and binding energies. We measure the filling ratio of nanowires for different chemical species in a wide range of temperature and flux. Perfect wires were obtained at lower deposition rate for all tested adatoms, however we notice different temperature ranges. Our results were compared with experimental ones [Gambardella et al., Surf. Sci. 449, 93-103 (2000), PRB 61, 2254-2262, (2000)]. We review the role of impurities in nanostructuring of surfaces [Hamouda et al., Phys. Rev. B 83, 035423, (2011)] and discuss the effect of their energetic barriers on the obtained quality of nanowires. Our work provides experimentalists with optimum growth parameters for the creation of a uniform distribution of wires on surfaces.

3:42PM X7.00007 Escape of an axial dislocation from a thin rod , ZHAOXUAN WU, YONG-WEI ZHANG, MARK

JHON, DAVID SROLOVITZ, Institute of High Performance Computing — Whiskers, nanowires and nanorods have been supposed to grow by preferential attachment to the atomic step formed from a screw dislocation intersecting the surface. This is expected to leave behind an axial screw dislocation, as has been observed in ionic nanowires such as NaCl, PbS and PbSe. However, we are not aware of any studies that have directly observed axial dislocations in pure FCC metal nanowires. To explain this, we speculate that thermal vibrations will be enough to kick out dislocations due to their high mobility. We consider two models of how a dislocation might escape from a nanowire. The first model is that the dislocation vibrates inside the nanowire. The second is that the nanowire itself vibrates, causing deformations of the nanowire that push the dislocation out. Analysis of these models imply that dislocations in thin nanowires are remarkably thermally stable. We test this prediction with molecular dynamics calculations on Cu nanowires, and find that the preparation of these systems is critical to the dislocation stability. Preparing the sample by simply raising the MD temperature will cause the dislocation to run out.

3:54PM X7.00008 Ensemble Measurements of Temperature Dependence in High-Q GaN Nanowire Mechanical Resonators¹, JOSHUA MONTAGUE, University of Colorado, KRIS BERTNESS, NORMAN SANFORD, NIST Quantum Electronics and Photonics Division, VICTOR BRIGHT, CHARLES ROGERS, University of Colorado — We report on measurements of c-axis oriented, single crystal, gallium nitride nanowire (GaN NW) mechanical resonators. Our measurements use a capacitively-coupled, microwave homodyne reflectometer that allows for simultaneous detection of large ensembles of the as-grown, GaN NW resonators. The NWs - grown via molecular beam epitaxy - behave as singly clamped beams, have lengths near 15 microns, and radii near 100 nm. We observe, respectively, typical resonance frequencies and mechanical quality factors (defined as the ratio of resonance frequency to full width at half maximum power), Q, near 1 MHz and above 10,000, near room temperature [1]. At lower temperatures, we observe increases in resonance frequencies consistent with temperature-dependent elastic moduli. Measured Q factors demonstrate a minimum near 150 K and typically increase an order of magnitude - to above 100,000 - below 100 K.

[1] S.W. Hoch et al., Appl. Phys. Lett. 99(5), 053101 (2011).

¹We acknowledge support from NSF and DARPA (iMINT Center).

4:06PM X7.00009 ABSTRACT WITHDRAWN —

4:18PM X7.00010 Low-frequency noise in gallium nitride nanowire mechanical resonators, JASON GRAY, University of Colorado, KRIS BERTNESS, NORMAN SANFORD, National Institute of Standards and Technology, CHARLES ROGERS, University of Colorado — We report on the low-frequency 1/f (flicker) parameter noise displayed by the resonance frequency and resistance of doubly clamped c-axis gallium nitride nanowire (NW) mechanical resonators. The resonators are electrostatically driven and their mechanical response is electronically detected via NW piezoresistance. With an applied dc voltage bias, an NW driven near its mechanical resonance generates a dc and Lorentzian rf current that both display 1/f noise. The rf current noise is proportional to the square of the derivative of the Lorentzian lineshape with a magnitude highly dependent on NW dc bias voltage conditions, consistent with noise in the NW's resistance leading to temperature noise from local Joule heating, which in turn generates resonance frequency noise. An example device with a 27.8 MHz resonance frequency and 220 k Ω resistance experiences an approximate resonance frequency shift of -5.8 Hz/nW. In terms of NW resistance change, this corresponds with shifts of 0.1 Hz/ Ω and 2.6 Hz/ Ω at 1 V bias and 4 V bias, respectively, with an average resistance fluctuation of 1 k Ω in a 1-second bandwidth.

4:30PM X7.00011 Unusual Germanium Nanowire Crystal Structures Formed During Low Temperature Catalytic Growth¹, ANDREW GAMALSKI, Dep. of Engineering, University of Cambridge, JERRY TERSOFF, IBM T. J. Watson Research Center, CATERINA DUCATI, Dep. of Materials Science and Metallurgy, University of Cambridge, RENU SHARMA, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, STEPHAN HOFMANN, Dep. of Engineering, University of Cambridge — Implementing bottom-up grown semiconductor nanowires (NW) in technological applications will require a detailed understanding of the electronic/physical properties of the NWs, which are closely related to their crystal structure. We present environmental transmission electron microscopy video data of Au catalyzed Ge NW growth under digermane exposure at 240 – 320 °C. The catalyst particles are initially liquid after gas exposure [1], and Ge NWs temporarily grow by step flow from the liquid AuGe alloy [2] before the liquid catalyst crystallizes into a metastable solid phase. Nucleating solid Ge at low temperatures requires a considerable supersaturation in the liquid catalyst, which drives the formation of a NW with a non-equilibrium crystal structure [3]. We explore how nanoscale systems with high supersaturations lead to the formation of metastable phases whose properties can be dramatically different from those of the common bulk phases. [1] A. D. Gamalski et al., Nano Lett., 10, 2972 (2010) [2] A. D. Gamalski et al., J. Phys. Chem. C, 115, 4413 (2011) [3] A. D. Gamalski et al., in preparation

¹A. D. G. acknowledges funding from the Marshall Aid Commemoration Commission and NSF's GRFP.

4:42PM X7.00012 Strong Spin-Orbit Interaction and Helical Hole States in Ge/Si Nanowires, CHRISTOPH KLOEFFEL, University of Basel, MIRCEA TRIF, University of California, Los Angeles, DANIEL LOSS, University of Basel — We study theoretically the low-energy hole states of Ge/Si core/shell nanowires. The low-energy valence band is quasidegenerate, formed by two doublets of different orbital angular momenta, and can be controlled via the relative shell thickness and via external fields. We find that direct (dipolar) coupling to a moderate electric field leads to an unusually large spin-orbit interaction of Rashba type on the order of meV which gives rise to pronounced helical states enabling electrical spin control. The system allows for quantum dots and spin qubits with energy levels that can vary from nearly zero to several meV, depending on the relative shell thickness [1].

[1] C. Kloeffer, M. Trif, and D. Loss, Phys. Rev. B 84, 195314 (2011).

4:54PM X7.00013 Spontaneous Formation of A Nanotube From A Square Ag Nanowire: An Atomistic View¹, MINE KONUK ONAT, Department of Physics, Istanbul Technical University, Istanbul, Turkey, SONDAN DURUKANOGLU, Nanotechnology Research and Application Center, and Faculty of Engineering and Natural Sciences, Sabanci University, Istanbul, Turkey — We have performed molecular static calculations to investigate the recently observed phenomenon of the spontaneous formation of a nanotube from a regular, square Ag nanowire[1]. In the simulations, atoms are allowed to interact via the model potential obtained from the modified embedded atom method. Our simulations predict that this particular type of structural phase transformation is controlled by the nature of applied strain, length of the wire and initial cross-sectional shape. For such a perfect structural transformation, the <100> axially oriented fcc nanowire needs (1) to be formed by stacking A and B layers of an fcc crystal, both possessing the geometry of two interpenetrating one-lattice-parameter-wide squares, containing four atoms each, (2) to have an optimum length of eight layers, and (3) to be exposed to a combination of low and high stress along the length direction. The results further offer insights into atomistic nature of this specific structural transformation into a nanotube with the smallest possible cross-section. [1] M.J. Lagos et al., Nature Nanotech. 4, 149 (2009).

¹This work was supported by TUBITAK under Grant No. 109T105. Computations were carried out through UYBHM at Istanbul Technical University, under Grant No. 20132007.

5:06PM X7.00014 Crossed Andreev Reflection in Quantum Wires with Strong Spin-Orbit Interaction, KOJI SATO, University of California, Los Angeles, DANIEL LOSS, University of Basel, YAROSLAV TSERKOVNYAK, University of California, Los Angeles — We theoretically study tunneling of Cooper pairs from an s-wave superconductor into two semiconductor quantum wires with strong spin-orbit interaction under magnetic field, which approximate helical Luttinger liquids. The entanglement of the two electrons within a Cooper pair can be detected by the electric current cross correlations in the wires. By controlling the relative orientation of the wires, either lithographically or mechanically, on the substrate, the ensuing current correlations can be tuned, as dictated by the initial spin entanglement. This proposal of a spin-to-charge readout of quantum correlations is alternative to a recently proposed utilization of the quantum spin Hall insulator.

5:18PM X7.00015 A Microscopic View of Repeated Polytypism in Self-organization of Hierarchical Nanostructures¹, MU WANG, MING LIU, GUO-BIN MA, ZHAO-WU WANG, RU-WEN PENG, Natl. Lab. Solid State Microstructures, Nanjing University, China — We demonstrate that the stacking-fault-induced repeated polytypism of wurtzite (WZ) and zinc-blend (ZB) phases may lead to a hierarchical nanostructure of ZnO possessing a hexagonal central trunk decorated with thin blades. Each blade keeps a fixed angle to the central trunk, resembling propellers with seemingly six-fold symmetry. The blades epitaxially nucleate on the ZB stripe assisted by the defect-induced reentrant corners at the interface of ZB-WZ phases. Our experiments reveal a unique approach to assemble hierarchical nanostructures, and the mechanism could be general to many materials.

¹the project supported by MOST and NSF of China

Thursday, March 1, 2012 2:30PM - 5:18PM – Session X8 DMP GMAG: Focus Session: Frustrated Magnetism - Theory 208

2:30PM X8.00001 Spin wave theory study of neutron intensity, magnetic field, and anisotropy of Type IIA FCC antiferromagnet¹, TRINANJAN DATTA, Augusta State University, DAO-XIN YAO, State Key Lab of Optoelectronic Materials and Technologies, School of Physics and Engineering, Sun Yat-sen University — We study the spin dynamics in a 3D quantum antiferromagnet on a face-centered cubic (FCC) lattice. The effects of magnetic field, single-ion anisotropy, and biquadratic interactions are investigated using linear spin wave theory with Dyson-Maleev transformation for spins in a canted basis. We calculate the expected finite frequency neutron scattering intensity and give qualitative criteria for typical FCC materials MnO and CoO. The magnetization reduction due to quantum zero point fluctuations is also analyzed.

¹Sun Yat-sen University and Fundamental Research Funds for the Central Universities, Augusta State University, NSFC-11074310.

2:42PM X8.00002 Lifetime of gapped excitations in antiferromagnets¹, SASHA CHERNYSHEV, UC Irvine, MICHAEL ZHITOMIRSKY, CEA Grenoble — We show that local modulations of magnetic couplings may have a profound effect on the temperature-dependence of the relaxation rate of gapped excitations in a class of antiferromagnets in which gapless modes are also present. Considering a prototypical 2D XY antiferromagnet with random disorder we find that the disorder-induced relaxation rate of the gapped mode should greatly exceed the effect of conventional magnon-magnon scattering, which becomes negligible at low temperatures. Our results compare favorably with the available experimental data. Generalizations to the other systems are discussed.

¹Supported by the DoE.

2:54PM X8.00003 Effect of Interlayer Coupling on Field-Induced Magnon Decays in Square-Lattice Antiferromagnet¹, WESLEY FUHRMAN, UC Irvine, MARTIN MOURIGAL, Johns Hopkins, MICHAEL ZHITOMIRSKY, CEA Grenoble, SASHA CHERNYSHEV, UC Irvine — We study the high-field magnon dynamics in the quasi-2D tetragonal Heisenberg antiferromagnet. Within spin-wave theory, we show that non-zero interlayer coupling mitigates singular corrections to the excitation spectrum occurring above the threshold field that would otherwise require a self-consistent approach beyond the Born approximation. Increasing field yields widening two-magnon sidebands with significant shifting of the spectral weight away from the quasi-particle peak. We examine the dynamic structure factor with interlayer coupling corresponding to realistic materials.

¹Supported by DoE

3:06PM X8.00004 Detecting non-magnetic excitations in quantum magnets¹, ZHIHAO HAO, Department of Physics and Astronomy, University of Waterloo — Many unconventional quantum phases host special non-magnetic excitations such as photons and visons. We discuss two possible ways to detect these excitations experimentally. Firstly, spin-lattice coupling mixes the excitations with phonons. The phonon spectral function acquires new features that can be detected by neutron or X-ray scattering. Secondly, valence-bond fluctuations translate into charge density fluctuations on non-bipartite lattices. Such charge fluctuations can be characterized by conventional spectroscopies such as Terahertz spectroscopy. Observation of exotic singlet excitations would provide positive identification of unconventional quantum phases in frustrated antiferromagnets.

¹The work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-FG02-08ER46544 and NSERC of Canada.

3:18PM X8.00005 Finite temperature phase diagram of quantum compass model¹, FEI LIN, VITO SCAROLA, Virginia Tech — The quantum compass model has been proposed as a simplified model to study Mott insulators with orbital degeneracy and, more recently, as a candidate model to study protected non-local qubits. In this talk we will show that in addition to well known bond-directional ordering, there is additional ordering associated with long range string operators. We will discuss quantum Monte Carlo results that explore the thermodynamics of non-local order in the quantum compass model.

¹This work is supported by AFOSR (FA9550-11-1-0313) and DARPA-YFA (N66001-1-1-4122).

3:30PM X8.00006 Order by geometrical disorder in a 2D quantum antiferromagnet, ANURADHA JAGANNATHAN, Universite Paris-Sud, Orsay, BENOIT DOUCOT, Universite Pierre et Marie Curie, Paris 6, ATTILA SZALLAS, S3 nanoscience Institute- CNR, Modena, Italy, STEFAN WESSEL, Institute for Theoretical Solid State Physics, RWTH Aachen University — We consider the effects of random fluctuations in the local geometry on the ground state properties of a two-dimensional quantum antiferromagnet. We analyse the behavior of spins described by the Heisenberg model as a function of what we call “phason flip disorder,” following a terminology used for aperiodic systems. The calculations were carried out both within linear spin wave theory and using quantum Monte Carlo simulations. An “order by disorder” phenomenon is observed in this model, wherein antiferromagnetism is found to be enhanced by phason disorder. The value of the staggered order parameter increases with the number of defects, accompanied by an increase in the ground state energy of the system. We furthermore find a long-ranged attractive Casimir-like force between two domain walls of defects separated by a finite distance.

3:42PM X8.00007 From Popov-Fedotov case to universal fermionization¹, BORIS SVISTUNOV, NIKOLAY PROKOF'EV, University of Massachusetts, Amherst — We show that Popov-Fedotov trick of mapping spin-1/2 lattice systems on two-component fermions with imaginary chemical potential readily generalizes to bosons with a fixed (but not limited) maximal site occupation number, as well as to fermionic Hamiltonians with various constraints on the site Fock states. In a general case, the mapping—fermionization—is on multi-component fermions with many-body non-Hermitian interactions. Additionally, the fermionization approach allows one to convert large many-body couplings into single-particle energies, rendering the diagrammatic series free of large expansion parameters; the latter is essential for the efficiency and convergence of the diagrammatic Monte Carlo method.

¹Supported by NSF and DARPA

3:54PM X8.00008 Universality of modulation length exponents, SAURISH CHAKRABARTY, ALEXANDER SEIDEL, ZOHAR NUSSINOV, Department of Physics, Washington University in St Louis — We study systems (classical or quantum) with general pairwise interactions. Our prime interest is in frustrated spin systems. First, we focus on systems with a crossover temperature T^* across which the correlation function changes from exhibiting commensurate to incommensurate modulations. We report on a *new exponent*, ν_L , characterizing the universal nature of this crossover. Near the crossover, the characteristic wave-vector k on the incommensurate side differs from that on the commensurate side, q by $|k - q| \propto |T - T^*|^{\nu_L}$. We find, in general, that $\nu_L = 1/2$, or in some special cases, other rational numbers. We discuss applications to the axial next nearest neighbor Ising model, Fermi systems (with application to the metal to band insulator transition) and Bose systems. Second, we obtain a universal form of the high temperature correlation function in general systems. From this, we show the existence of a diverging correlation length in the presence of long range interactions. Such a correlation length tends to the screening length in the presence of screening. We also find a way of obtaining the pairwise interaction potentials in the high temperature phase from the correlation functions.

4:06PM X8.00009 Restricted Spin Set Lattice Models: A Route to Topological Order¹, R. ZACHARY LAMBERTY, Cornell University, STEFANOS PAPANIKOLAOU, Yale University, C.L. HENLEY, Cornell University — A typical lattice gauge model configuration consists of elements of a finite symmetry group G placed on directed edges of a two-dimensional lattice. We consider generalized models² which are defined by instead only allowing elements from a subset $S \subset G$ consisting of certain classes of group elements. The subset restriction can be regarded as a new (but discrete) tunable model parameter, providing a novel pathway to topologically ordered phases. Taking a small allowed set S , we can realize well understood critical models (e.g. the square lattice ice model or dimer covering); in contrast, for large enough S the configuration ensemble realizes a form of topological order. Using a sequence of sets $S_1 \subset S_2 \subset \dots$, we can “interpolate” from one kind of state to the other. This is confirmed by Monte Carlo simulations, measuring two characteristic properties: (1) the distribution of separations between two (possibly deconfined) topological defects, and (2) the relative probabilities of different sectors (sub-ensembles with inequivalent products of the group elements around the periodic boundary conditions). We also discuss how to construct quantum-mechanical extensions of these models.

¹Supported by the National Science Foundation through a Graduate Research Fellowship to R. Zach Lamberty, as well as grant DMR-0552461.

²C. L. Henley, J. Phys. Condens. Matter. 23, 164212 (2011).

4:18PM X8.00010 Stability of the quantum Lifshitz model in 2+1 Dimensions, BENJAMIN HSU, Princeton University, EDUARDO FRADKIN, University of Illinois, Urbana Champaign — Magnetic and electric perturbations to the quantum Lifshitz model in 2+1 dimensions are examined in this paper. The quantum Lifshitz model is an effective field theory for quantum critical systems that include generalized 2D quantum dimer models in bipartite lattices. Magnetic perturbations break the dimer conservation law. Electric excitations have been studied extensively both in the classical 3D model and in the quantum 2D model, but magnetic vortex excitations have been ignored. While they are forbidden in classical 3D statistical mechanics, they are allowed in the quantum version. To study the interplay of both excitations, we perform a perturbative renormalization group study to one loop order. This is done by generalizing the operator product expansion to anisotropic models. The relation with recent classical Monte Carlo simulations will be discussed.

4:30PM X8.00011 Supersymmetry in strongly correlated fermion models, DIMITRIOS GALANAKIS, Nanyang Technological University, STEFANOS PAPANIKOLAOU, Yale University, CHRIS HENLEY, Cornell University — We investigate the Fendley and Schoutens¹ model of hard core fermions on a lattice which have hopping elements t , and potential terms V which include a second-neighbor repulsion with some multi-particle terms. At the special point $t = V$, the Hamiltonian is $H = \{Q^\dagger(r), Q\}$ with $Q = \sum_r q(r) = \sum_r c(r)P(r)$, where $c(r)$ is an annihilation operator and $P(r)$ enforces the hard core. That means the system acquires an exact non-relativistic supersymmetry, and for a range of fillings has a large number of zero-energy ground states¹. To better understand the nature of the zero-energy states and excitations, we perform exact diagonalizations on finite clusters for the square and triangular lattice, different fillings and center of mass momenta. In momentum sectors with unique zero energy ground states we find a menagerie of symmetry breaking patterns in the density-density correlation functions and we investigate them further by evaluating the entanglement spectrum. In momentum sectors with degenerate ground states we search for topological ground states using the numerical Berry matrix method².

¹ P. Fendley and K. Schoutens, Phys. Rev. Lett. 90, 120402 (2003).

² E. Kapit, P. Ginsparg, and E. Mueller, arXiv:1109.4561

4:42PM X8.00012 First-principles study on electronic properties of the pyrochlore oxide Cd₂Os₂O₇¹, HIROSHI SHINAOKA, NRI, AIST, TAKASHI MIYAKE, SHOJI ISHIBASHI, NRI, AIST — The pyrochlore oxide Cd₂Os₂O₇ is one of 5d pyrochlore oxides in which the interplay of geometrical frustration, electron correlation, and spin-orbit coupling is expected. This compound exhibits a metal-insulator transition at 227 K, below which the emergence of a magnetic order has been suggested by experiments. Despite extensive studies for over thirty years, however, the nature of the low-temperature phase remains to be clarified. We depict the ground-state phase diagram based on the LSDA+ U method (LSDA denotes local spin density approximation). We find that the all-in/all-out non-collinear magnetic order is stable in a wide range of U . We show that the easy-axis anisotropy arising from the spin-orbit coupling plays a significant role in stabilizing the all-in/all-out magnetic order. A pseudo gap extending up to high energy is found to appear near a continuous metal-insulator transition between an antiferromagnetic metallic phase and an antiferromagnetic insulating phase. Based on the computed results, we discuss possible origins of peculiar low-temperature properties observed in experiments.

¹This study has been funded by JST-CREST.

4:54PM X8.00013 Exchange and Magnetic Anisotropic Interactions of Magnetic Ions in Antiferromagnetic Materials, ALEXANDER BAZHAN, P.L. Kapitza Institute for Physical Problems, RAS, Kosygin str, 2, Moscow, Russia — Investigations of exchange and magnetic anisotropic interactions, based on materials crystallographic and magnetic symmetry, introducing quadratic forms of thermodynamic potentials, invariant with respect to operations of magnetic symmetry groups and presented in irreducible representations of interacting ions magnetic moments, are in discussions in connection with considerations of symmetric, Anderson exchange interactions, based on Hubbard Hamiltonians, that indicates dependencies of symmetric exchange on electrons transferings between magnetic, nonmagnetic ions, electrons kinetic energy, Coulomb interactions and, determined by crystal fields, energy levels. As example, according to symmetry for some rhombohedral structures, spin Hamiltonians of symmetric, Anderson and antisymmetric, Dzyaloshinskii-Moria exchange, $H_{ex} = \sum_{ij} J_{ij}(\mathbf{S}_i \mathbf{S}_j) - \sum_{ij} D_{ij,z}(\mathbf{S}_{ix} \mathbf{S}_{jy} - \mathbf{S}_{iy} \mathbf{S}_{jx})$, with $D_{ij,z}$ in abs values. Magnetic field dependencies of separate, three components of samples magnetic moments of vector v.s. magnetometer, indicating magnetic moments orientations, present direct information about interactions of magnetic ions, especially with high spin orbit interactions.

5:06PM X8.00014 ABSTRACT WITHDRAWN —

Thursday, March 1, 2012 2:30PM - 5:18PM —

Session X9 DMP GMAG: Focus Session: Complex Bulk Oxides: Magnetic Phase Transitions

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2:30PM X9.00001 Temperature and pressure induced Cu-Fe intermetallic charge transfer in $\text{LaCu}_3\text{Fe}_4\text{O}_{12}$ ¹, YOUWEN LONG, ICR, Kyoto Univ., Kyoto 611-0011, Japan; IOP, CAS, Beijing 100190, China, T. KAWAKAMI, IQS, Nihon Univ., Tokyo 101-8308, Japan, Y. SHIMAKAWA, ICR, Kyoto Univ., Kyoto 611-0011, Japan — An A-site ordered double perovskite $\text{LaCu}_3\text{Fe}_4\text{O}_{12}$ was prepared at high pressure and high temperature. At ambient condition, the charge combination was proved to be $\text{LaCu}_3^{3+}\text{Fe}_4^{3+}\text{O}_{12}$. When the temperature was increased to 393 K, however, an intermetallic charge transfer was found to occur between the A-site Cu and the B-site Fe ions, giving rising to the change of charge combination from the low-temperature $\text{LaCu}_3^{3+}\text{Fe}_4^{3+}\text{O}_{12}$ to the high-temperature $\text{LaCu}_3^{2+}\text{Fe}_4^{3.75+}\text{O}_{12}$. [1,2] Similarly, at room temperature, if high pressure was applied, the Cu-Fe intermetallic charge transfer could also be induced. This charge transfer led to a first-order isostructural phase transition with sharp reduction in unit cell, negative thermal expansion and unusual softening (decreased bulk modulus). Moreover, the material experienced antiferromagnetism-to-paramagnetism and insulator-to-metal transitions accompanying with the charge-transfer transition.

[1] Y. W. Long *et al*, Nature, 458, 60-63 (2009).

[2] Y. W. Long and Y. Shimakawa, New J. Phys. 12, 063029 (2010).

¹Youwen Long thanks the support of the “100 Talents Project” of Chinese Academy of Sciences.

2:42PM X9.00002 Spin-phonon coupling effect in AMnO_3 ($A=\text{Ca, Sr, Ba}$) and LaMO_3 ($M=\text{Cr, Fe, Cr/Fe}$) from DFT+ U and hybrid functional methods, JIAWANG HONG, Rutgers University, ALESSANDRO STROPPA, CNR-SPIN, Italy, JORGE INIGUEZ, ICMA-B-CSIC, Spain, SILVIA PICOZZI, CNR-SPIN, Italy, DAVID VANDERBILT, Rutgers University — Spin-phonon coupling effects, as reflected in phonon frequency shifts between ferromagnetic (FM) and G-type antiferromagnetic (AFM) configurations in cubic CaMnO_3 , SrMnO_3 , BaMnO_3 , LaCrO_3 , LaFeO_3 and $\text{La}_2(\text{CrFe})\text{O}_6$, are investigated using density-functional methods. The calculations are carried out using the DFT+ U method with a U that has been extracted by comparing with hybrid-functional (HSE) calculations. The phonon frequency shifts $\Delta\omega = \omega_{\text{AFM}} - \omega_{\text{FM}}$ obtained in this way agree well with those computed directly from the more accurate HSE approach, but are obtained with much less computational effort. We find that in the AMnO_3 materials class with ($A=\text{Ca, Sr, Ba}$), the Γ (R) phonon frequency shift $\Delta\omega$ decreases (increases) as the A^{2+} size increases. In LaMO_3 ($M=\text{Cr, Fe, Cr/Fe}$), the phonon frequencies at Γ decrease as spin order changes from AFM to FM for LaCrO_3 and LaFeO_3 , but they increase for double perovskite $\text{La}_2(\text{CrFe})\text{O}_6$. We discuss the prospects for bulk and superlattice forms of these materials to be useful as multiferroics.

2:54PM X9.00003 Nd magnetic order in $\text{NdFe}_x\text{Ga}_{1-x}\text{O}_3$, FERNANDO BARTOLOME, ICMA - CSIC, MARIA PARRA-BORDERIAS, Centro de Astrobiologia - CSIC, JOSE ALBERTO RODRIGUEZ-VELAMAZAN, JUAN BARTOLOME, BURZURI ENRIQUE, FERNANDO LUIS, MARCO EVANGELISTI, ICMA - CSIC — The Nd magnetic order in $\text{NdFe}_x\text{Ga}_{1-x}\text{O}_3$ has been studied as a function of Fe content along the whole $0 < x < 1$ range, both experimental and theoretically. In NdGaO_3 , where Nd-Nd exchange interaction is in isolation, Nd sublattice orders antiferromagnetically at $T_N = 1$ K. In NdFeO_3 , the Nd sublattice is polarized at low temperatures by Fe-Nd exchange, and a competition between Nd-Nd and Nd-Fe interactions is established, but Nd still orders cooperatively at $T_N = 0.95$ K. The evolution of the magnetic ordering of Nd with the Fe content is studied by low-temperature specific-heat, ac susceptibility and neutron scattering measurements. In the Fe-rich side of the phase diagram, Nd order is inhibited by Fe-Nd internal field at very low Ga content, while in the Fe-poor side, Nd order is more robust, reaching the Fe magnetic percolation concentration ($x_c = 0.33$). We have used a mean field model as well as MonteCarlo simulations to clarify the interpretation of the results. The introduction of Ga ions induces discompensation of the ordered ferromagnetic Fe sublattice which strongly inhibits Nd order. However, this is only effective at every temperature if the Fe sublattice is long range ordered, while below Fe percolation, Nd is able to orders at sufficiently low T.

3:06PM X9.00004 Magnetic phase transitions in single crystalline $\text{Mn}_{0.68}\text{Ni}_{0.32}\text{TiO}_3$ ¹, SONGXUE CHI, HUIBO CAO, FENG YE, JAIME A. FERNANDEZ-BACA, Oak Ridge National laboratory, HAIDONG ZHOU, National High Magnetic Field Laboratory, Florida State University — The magnetoelectric MnTiO_3 has the ilmenite structure and order antiferromagnetically with neighboring Mn^{2+} spins antiparallel to each other both within the ab-plane and along the c-axis. We have observed a magnetic field induced electric polarization in the 32%Ni-doped MnTiO_3 . To understand the origin of this magnetoelectric effect, we have carried out neutron diffraction study on single crystalline $\text{Mn}_{0.68}\text{Ni}_{0.32}\text{TiO}_3$. The Mn^{2+} spins order below 27 K and arrange in the same antiparallel manner as the parent compound, but with different spin direction. On cooling the magnetic phase goes through a second transition at 15 K, below which the spins lock into a new direction. We have also determined the spin structure under a magnetic field applied along the c-axis.

¹This work was partially supported by the Division of Scientific User Facilities of the Office of Basic Energy Sciences, U.S. Department of Energy.

3:18PM X9.00005 Electron energy loss spectroscopy study of $\text{Sr}_{2-x}\text{Gd}_x\text{TiMnO}_6$ ¹, NEVENKO BISKUP, INMACULADA ALVAREZ-SERRANO, MARIA LUISA VEIGA, Universidad Complutense Madrid, Spain, MAR GARCIA-HERNANDEZ, ICMM, CSIC, Spain, MARIA LUISA LOPEZ, Universidad Complutense Madrid, Spain, MARIA VARELA, Oak Ridge National Laboratory — The newly synthesized double perovskite family $\text{Sr}_{2-x}\text{Gd}_x\text{TiMnO}_6$ ($0 < x < 1$) is magnetically frustrated system that orders magnetically at $T=40\text{K}$. In spite of the probable double exchange interaction around $x=0.5$, no metallic state is established and the magnetoresistance is weak in the whole family. The most interesting feature in this material is the giant electroresistance that persists even at room temperature. We have studied the microscopic composition of these polycrystals by the electron energy loss spectroscopy. We find that, in spite of some precipitations of Mn and Ti rich regions that exist in $0.25 \leq x \leq 0.75$, the manganese and titanium ions are generally well intermixed in both interior of the grains and on the grain boundaries. We discuss these results in the frame of highly non-linear electrical conductivity found in these materials.

¹Research sponsored by the European Research Council Starting Investigator Award (NB) and the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division (MV).

3:30PM X9.00006 Density functional modeling for a perovskite $\text{SrTi}_{1-x}\text{Co}_x\text{O}_3$ system: Beyond GGA+U functional¹, JUAN MANUEL FLOREZ, Massachusetts Institute of Technology and Universidad Técnica Federico Santa María, SHYUE PING ONG, GERBRAND CEDER, GERALD F. DIONNE, Massachusetts Institute of Technology, PATRICIO VARGAS, Universidad Técnica Federico Santa María, CAROLINE A. ROSS, Massachusetts Institute of Technology — Understanding the exact mechanisms of spin-stabilization according to the oxygen stoichiometry and substituting metal-transition ions is essential to finding new perovskites-based technologies to augment silicon-based devices with room-temperature spintronic materials. We perform ab-initio modeling for the $\text{SrTi}_{1-x}\text{Co}_x\text{O}_3$ system with $x = 0.0, 0.25, 1.0$, and by using a HSE06 hybrid functional. Electronic structure for $x=(0.0,1.0)$ predicts 3.1 eV band gap and a metallic behavior, respectively, predicting lattice parameters in agreement with experiments. Different positions for the cobalt ions are taken into account for $x=0.25$, and predicted ground states and Co energy-correlations suggest the structurally stabilized Co-site positions as fingerprints of whether possible intrinsic magnetic ordering or other phenomena is giving rise to the macroscopic magnetism. Passing from Stoichiometric $\text{SrTi}_{0.75}\text{Co}_{0.25}\text{O}_3$ to 1-O-vacancy $\text{SrTi}_{0.75}\text{Co}_{0.25}\text{O}_{3-\delta}$ produces a lattice parameter expansion due to the valence state distribution of the substituting B (ABO_3) ions, which is turn lead us to a band gap expansion. The stabilized valence spin states of the magnetic ions are discussed in comparison with the ligand-field theory.

¹National Science Foundation, Fondecyt, DGIP

3:42PM X9.00007 Role of cooperative structural distortions in the metal–insulator transitions of perovskite ferrates¹, ANTONIO CAMMARATA, JAMES RONDINELLI, Drexel University — Transition-metal oxides within the perovskite crystal family exhibit strong electron–electron correlation effects that coexist with complex structural distortions, leading to metal-insulator (MI) transitions. Using first-principles density functional calculations, we investigate the effects of cooperative octahedral rotations and dilations/contractions on the charge-ordering MI-transition in CaFeO_3 . By calculating the evolution in the lattice phonons, which describe the different octahedral distortions present in the low-symmetry monoclinic phase of CaFeO_3 with increasing electron correlation, we show that the MI-transition results from a complex interplay between these modes and correlation effects. We combine this study with group theoretical tools to disentangle the electron–lattice interactions by computing the evolution in the low-energy electronic band structure with the lattice phonons, demonstrating the MI-transition in CaFeO_3 proceeds through a symmetry-lowering transition driven by a cooperative three-dimensional octahedral dilation/contraction pattern. Finally, we suggest a possible route by which to control the charge ordering by fine-tuning the electron–lattice coupling.

¹A.C. and J.M.R. were supported by the U.S. Office of Naval Research, under grant number N00014-11-1-0664

3:54PM X9.00008 Far infrared spectroscopy of magnons and phonons in TbFeO_3 single crystal¹, T.N. STANISLAVCHUK, E.C. STANDARD, A.A. SIRENKO, Department of Physics, New Jersey Institute of Technology, Newark, NJ, USA, G.L. CARR, National Synchrotron Light Source, Brookhaven National Laboratory, Upton, NY, USA, A.A. MUKHIN, Prokhorov General Physics Institute, Moscow, Russia, M.V. MOSTOVOY, Zernike Institute for Advanced Materials, University of Groningen, The Netherlands, N. LEE, S-W. CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, USA — Far-infrared spectra of TbFeO_3 single crystals have been studied in the temperature range between 1.6 K and 300 K using transmission in high magnetic field and rotating analyzer ellipsometry. The symmetry of the IR optical phonons and their oscillator strengths were determined. Polarization and frequencies of two AFM resonances at around 18 and 23 cm^{-1} were analyzed around the spin reorientation (SR) transition at $\sim 8\text{K}$ and magnetic fields up to 9 T. Intensity of the AFM resonances exhibit an unusual oscillator dependence on both temperature and magnetic field. The observed effects are analyzed taking into account main magnetic interactions in the system including exchange of the Fe^{3+} spins with Tb^{3+} paramagnetic moments as well as the geometry of the measurements.

¹Work at NJIT and Rutgers was supported by DOE DE-FG02-07ER46382. Use of NSLS-BNL was supported by DOE DE-AC02-98CH10886.

4:06PM X9.00009 Optical properties of iron oxides¹, JANICE MUSFELDT, University of Tennessee — Magnetoelectric coupling in materials like multiferroics, dilute magnetic semiconductors, and topological insulators has attracted a great deal of attention, although most work has been done in the static limit. Optical spectroscopy offers a way to investigate the dynamics of charge-spin coupling, an area where there has been much less effort. Using these techniques, we discovered that charge fluctuation in LuFe_2O_4 , the prototypical charge ordered multiferroic, has an onset well below the charge ordering transition, supporting the “order by fluctuation” mechanism for the development of charge order superstructure. Bragg splitting and large magneto-optical contrast suggest a low temperature monoclinic distortion that can be driven by both temperature and magnetic field. At the same time, dramatic splitting of the LuO_2 layer phonon mode is attributed to charge-rich/poor proximity effects, and its temperature dependence reveals the antipolar nature of the W layer pattern. Using optical techniques, we also discovered that $\alpha\text{-Fe}_2\text{O}_3$, a chemically-similar parent compound and one of the world's oldest and most iconic antiferromagnetic materials, appears more red in applied magnetic field than in zero field conditions. This effect is driven by a field-induced reorientation of magnetic order. The oscillator strength lost in the color band is partially transferred to the magnon side band, a process that also reveals a new exciton pattern induced by the modified exchange coupling. Analysis of the exciton pattern exposes $C2/c$ monoclinic symmetry in the high field phase of hematite. Taken together, these findings advance our understanding of iron-based materials under extreme conditions.

Collaborators include: X. S. Xu, P. Chen, Q. -C. Sun, T. V. Brinzari (Tennessee); S. McGill (NHMFL); J. De Groot, M. Angst, R. P. Hermann (Julich); A. D. Christianson, B. C. Sales, D. Mandrus (ORNL); A. P. Litvinchuk (Houston); J. -W. Kim (Ames); Z. Islam (Argonne); N. Lee, S. -W. Cheong (Rutgers).

¹We thank the Materials Science Division, Basic Energy Sciences, U. S. Department of Energy for support of this research.

4:42PM X9.00010 Theory of Spectroscopy and Transport in Half-metallic Double Perovskites¹

JULIA JANCZAK, OINAM NGANBA MEETEI, MOHIT RANDERIA, NANDINI TRIVEDI, The Ohio State University — Half-metallic double perovskites hold great promise in spintronics applications, hence we are motivated to understand the spectroscopy and charge transport in these materials. We present theoretical calculations of the temperature and disorder dependence of the spin-resolved density of states of the conduction electrons, the optical conductivity $\sigma(\omega)$, and the anomalous Hall conductivity for $\text{Sr}_2\text{FeMoO}_6$ (SFMO), a half-metal with 100% spin-down polarized charge carriers at $T = 0$. We build on the recent progress [1] in modeling magnetic properties of SFMO by using an exact diagonalization plus Monte Carlo scheme. We obtain $\sigma(\omega)$ as a function of disorder as well as temperature using the Kubo formula for linear response in the exact eigenstate basis. In agreement with experiment, we find a secondary peak in $\sigma(\omega)$ at $\omega \sim 0.5 \text{ eV}$, and attribute it to a spin-up density of states at the chemical potential induced by disorder and/or thermal fluctuations. We propose that the size of the secondary peak can be used to determine the polarization of conduction electrons at the chemical potential, facilitating experimental measurements. [1] O. Erten et al, arXiv:1107.0983; Phys. Rev. Lett. (to appear)

¹This work was supported by the Center for Emergent Materials and NSF MRSEC, DMR-0820414

4:54PM X9.00011 High T_c Ferrimagnetism, Multiband Mott Transition and Spin-Orbit Coupling in Double Perovskites¹

ONUR ERTEN, O. NGANBA MEETEI, The Ohio State University, ANAMITRA MUKHERJEE, University of British Columbia, MOHIT RANDERIA, NANDINI TRIVEDI, PATRICK M. WOODWARD, The Ohio State University — The ferrimagnetic insulator $\text{Sr}_2\text{CrOsO}_6$ (SCOO), which has the highest $T_c = 725\text{K}$ among all double perovskites, raises several questions. Why is this material an insulator? What sets the scale for the high T_c ? Why is there a net moment given that both Cr and Os have d^3 configurations? What is the role of spin-orbit coupling in Os? Finally, why does SCOO show a highly unusual, non-monotonic magnetization $M(T)$ as a function of temperature? We address all of these questions. First, we describe the charge sector using slave-rotor mean field theory and obtain an analytic Mott criterion $\sqrt{U_{Cr}U_{Os}} > 2.5W$ relating the Hubbard U 's to the bandwidth W . We argue that SCOO is a multiband Mott insulator. Next, we argue that the orbital moment on Os is quenched in SCOO and spin-orbit coupling does not play a major role in this material. Finally, we show that the effective spin Hamiltonian for SCOO has both Cr-Os and Os-Os superexchange interactions that are frustrated. This leads to a canted ground state with a net moment at $T = 0$ and a nonmonotonic magnetization $M(T)$. Our results are in excellent agreement with available data and we make predictions to test our theory.

¹Supported by the NSF-MRSEC grant DMR-0820414.

5:06PM X9.00012 Magnetically driven metal-insulator transition in NaOsO_3 ¹

STUART CALDER, VASILE GARLEA, ORNL, DESMOND MCMORROW, UCL, MARK LUMSDEN, MATHEW STONE, ORNL, JONATHAN LANG, JONG-WOO KIM, JOHN SCHLUETER, ANL, YOUGUO SHI, CAS, YING SUN, YOSHIRA TSUJIMOTO, KAZUNARIA YAMAURA, NIMS, ANDREW CHRISTIANSON, ORNL — The metal-insulator transition (MIT) is one of the most dramatic manifestations of electron correlations in materials, enjoying interest both for its fundamental nature and technological application. Various mechanisms producing MITs have been extensively considered over the years associated with the names of their originators, including most especially Mott (electron localization through Coulomb repulsion) and Anderson (localization through disorder). An alternative route due to Slater dating back to 1951, in which long-range magnetic order in a three dimensional system drives the MIT, has received relatively little attention, particularly from an experimental viewpoint. Using neutron and X-ray scattering we have shown that the MIT in NaOsO_3 is coincident with the onset of long-range commensurate three dimensional magnetic order at 410 K. NaOsO_3 thus encompasses all of the expected features of the long predicted Slater transition. Our results are the first definitive experimental example of a Slater MIT and we discuss them in the light of recent reports of a Mott spin-orbit insulating state in other 5d oxides.

¹Work at ORNL was supported by the scientific User Facilities Division, Office of Basic Energy Sciences, U. S. Department of Energy and use of the APS was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.

Thursday, March 1, 2012 2:30PM - 5:30PM —

Session X10 DCOMP: Invited Session: Thermal Properties and Electron-Phonon Coupling from First Principles 210A

2:30PM X10.00001 Competition between electron-phonon coupling and spin fluctuations in superconductors

SILKE BIERMANN, Ecole Polytechnique — No abstract available.

3:06PM X10.00002 Phonon Raman scattering from first principles

CLAUDIA AMBROSCH-DRAXL, University of Leoben — Light propagating through a crystal can be inelastically scattered by lattice vibrations. Thereby the exciting light beam experiences a frequency shift which is detected in the Raman experiment. This *Raman shift* is caused by the modulation of the material's polarizability upon time-dependent ionic displacements. Experimental Raman data thus contain a wealth of information about phonons, electronic structure, as well as their interplay. For instance, temperature-dependent lineshapes and overtone spectra can be related to the extent of anharmonic effects, and strong electron-phonon interaction is expressed in terms of large scattering intensities. The assignment of frequencies to specific vibrations typically relies on comparison with reference systems by considering atomic masses and the symmetry of the crystal. For an in-depth understanding of the measured features and an unambiguous assignment of modes, *ab initio* theory can provide valuable insight. In the Raman spectra, the peak positions correspond to the phonon frequencies and thus can be solely determined from frozen-phonon or linear-response calculations. The scattering intensities, however, involve the change of the frequency-dependent complex dielectric tensor with atomic displacements along the phonon eigenvector. All these quantities can be obtained from density-functional theory (DFT) in combination with time-dependent DFT or many-body perturbation theory. In this talk, I will review how to compute Raman spectra from first principles. Selected examples will demonstrate the effects of isotope substitution, anharmonicity, temperature, and excitation energy, as well as the role of symmetry. They reveal that Raman scattering is a beautiful technique as it reflects basic principles of quantum mechanics as much as complex excitations of complex matter.

3:42PM X10.00003 Pushing the limits of first-principles electron-phonon calculations: from photoemission kinks to band gaps, FELICIANO GIUSTINO, Department of Materials, University of Oxford — The electron-phonon interaction is key to some of the most intriguing and technologically important phenomena in condensed matter physics, ranging from superconductivity to charge density waves, electrical resistivity, and thermoelectricity. Starting from the late nineties first-principles calculations of electron-phonon interactions in metals have become increasingly popular, mainly in connection with the study of conventional superconductors and with the interpretation of angle-resolved photoemission experiments. In contrast, progress on first-principles calculations of electron-phonon interactions in insulators has been comparatively slower. This delay is arguably due to the conventional wisdom that the signatures of electron-phonon interactions in semiconductor band structures are so small that they fall within the error bar of the most accurate electronic structure calculations. In order to fill this gap we developed, within the context of state-of-the-art density-functional techniques, a theory proposed by Allen and Heine for calculating the temperature dependence of band gaps in semiconductors [P. B. Allen, V. Heine, J. Phys. C: Solid State Phys. 69, 2305 (1976)]. This methodology allows us to calculate both the temperature dependence of the quasiparticle energies and the renormalization due to zero-point quantum fluctuations. In order to demonstrate this technique an application to the intriguing case of diamond will be discussed [F. Giustino, S. G. Louie, M. L. Cohen, Phys. Rev. Lett. 105, 265501 (2010)]. In this case the calculated temperature dependence of the direct band gap agrees well with spectroscopic ellipsometry data, and the renormalization due to the electron-phonon interaction is found to be spectacularly large (>0.6 eV). This unexpected finding might be only the tip of the iceberg in a research area which remains largely unexplored and which, from a first glimpse, appears rich of surprises.

4:18PM X10.00004 Phonon-assisted Auger recombination and optical absorption in semiconductors, EMMANOUIL KIOUPAKIS, University of Michigan — The coupling of charge carriers to lattice vibrations is an important process in materials that enables higher-order electronic transitions. We employed first-principles methods based on density functional theory to study various phonon-assisted electronic processes in semiconductors, such as Auger recombination and optical absorption. Auger recombination is a three-particle non-radiative recombination process that affects optoelectronic devices at high carrier densities. Phonon-assisted Auger recombination, in particular, is expected to be important in wide-band-gap materials. We describe the computational formalism to study phonon-assisted Auger recombination in semiconductors. We show that these indirect Auger processes are strong in the group-III nitrides and affect the high-power performance of visible light-emitting diodes. Moreover, the electron-phonon interaction facilitates the absorption of light by free carriers in doped semiconductors and transparent conducting oxides, which limits the output power of optoelectronic devices. We describe how first-principles techniques can be used to calculate the phonon-assisted free-carrier absorption coefficient in semiconductors and discuss our results for the group-III nitrides. In addition, the electron-phonon coupling enables indirect interband optical transitions in indirect-gap materials such as silicon. These processes are instrumental for the absorption of visible light and the operation of silicon solar cells. We present our first-principles formalism and calculated results for the phonon-assisted absorption of visible light in silicon. Our calculated results are in very good agreement with experiment. Our work highlights the significance of first-principles methods in understanding key microscopic quantum phenomena in technologically important materials and devices. Work done in collaboration with C. G. Van de Walle, P. Rinke, K. Delaney, A. Schleife, F. Bechstedt, D. Steiauf, H. Peelaers, J. Noffsinger, S. G. Louie, and M. L. Cohen. Support was provided by CEEM, SSLEC, NERSC, and Teragrid.

4:54PM X10.00005 Large scale atomistic approaches to thermal transport and phonon scattering in nanostructured materials¹, IVANA SAVIC, Department of Chemistry, University of California at Davis, Davis, California, USA — Decreasing the thermal conductivity of bulk materials by nanostructuring and dimensionality reduction, or by introducing some amount of disorder represents a promising strategy in the search for efficient thermoelectric materials [1]. For example, considerable improvements of the thermoelectric efficiency in nanowires with surface roughness [2], superlattices [3] and nanocomposites [4] have been attributed to a significantly reduced thermal conductivity. In order to accurately describe thermal transport processes in complex nanostructured materials and directly compare with experiments, the development of theoretical and computational approaches that can account for both anharmonic and disorder effects in large samples is highly desirable. We will first summarize the strengths and weaknesses of the standard atomistic approaches to thermal transport (molecular dynamics [5], Boltzmann transport equation [6] and Green's function approach [7]). We will then focus on the methods based on the solution of the Boltzmann transport equation, that are computationally too demanding, at present, to treat large scale systems and thus to investigate realistic materials. We will present a Monte Carlo method [8] to solve the Boltzmann transport equation in the relaxation time approximation [9], that enables computation of the thermal conductivity of ordered and disordered systems with a number of atoms up to an order of magnitude larger than feasible with straightforward integration. We will present a comparison between exact and Monte Carlo Boltzmann transport results for small SiGe nanostructures and then use the Monte Carlo method to analyze the thermal properties of realistic SiGe nanostructured materials. This work is done in collaboration with Davide Donadio, Francois Gygi, and Giulia Galli from UC Davis.

[1] See e.g. A. J. Minnich, M. S. Dresselhaus, Z. F. Ren, and G. Chen, Energy Environ. Sci. 2, 466 (2009).

[2] A. I. Hochbaum et al, Nature 451, 163 (2008).

[3] R. Venkatasubramanian, E. Siivola, T. Colpitts, and B. O'Quinn, Nature 413, 597 (2001).

[4] B. Poudel et al, Science 320, 634 (2008).

[5] See e.g. Y. He, D. Donadio, and G. Galli, Nano Lett. 11, 3608 (2011).

[6] See e.g. A. Ward and D. A. Broido, Phys. Rev. B 81, 085205 (2010).

[7] See e.g. I. Savic, N. Mingo, and D. A. Stewart, Phys. Rev. Lett. 101, 165502 (2008).

[8] I. Savic, D. Donadio, F. Gygi, and G. Galli (in preparation).

[9] See e.g. J. E. Turney, E. S. Landry, A. J. H. McGaughey, and C. H. Amon, Phys. Rev. B, 79, 064301 (2009).

¹Work supported by DOE-SciDAC-e, DE-FC02-06ER25777.

Thursday, March 1, 2012 2:30PM - 5:30PM –
Session X11 DMP: Focus Session: Graphene Structure, Stacking, Interactions: Twisting, Stretching, Folding, Wrinkling 210B

2:30PM X11.00001 Graphene Origami, MELINA BLEES, Department of Physics, Cornell University, ARTHUR BARNARD, School of Applied and Engineering Physics, Cornell University, SAMANTHA ROBERTS, Department of Physics, Cornell University, PEIJIE ONG, Materials Science and Engineering, Cornell University, ALIAKSANDR ZARETSKI, Florida International University, SI PING WANG, School of Electrical and Computer Engineering, Cornell University, PAUL MCEUEN, Department of Physics, Kavli Institute at Cornell for Nanoscale Science, Cornell University — Graphene, which features unparalleled in-plane strength and low out-of-plane bending energy, is an ideal material with which to tackle the challenge of building three-dimensional structures and moving parts at the nanoscale. Here we demonstrate laser-induced folding and scrolling of large-area monolayer graphene in solution. Monolayer graphene is typically well-adhered to its substrate, but we have achieved control of the adhesion using a combination of an aluminum sacrificial layer and surfactants. Once the graphene can move, local heating with an infrared laser and the interfacial tension of laser-nucleated bubbles allow us to lift, fold, and scroll the graphene. We have also formed a regular array of polymer dots on the graphene surface which can be easily imaged in three dimensions, allowing us to optically track the shape of the graphene as it moves. And finally, we establish graphene's viability as a strong but flexible sheet hinge by building and manipulating structures of rigid metallic panels connected by strips of graphene.

2:42PM X11.00002 Twisting Graphene into Carbon Nanotubes¹ , OLEG O. KIT, University of Jyväskylä, Finland, TUOMAS TALLINEN, L. MAHADEVAN, Harvard University, JUSSI TIMONEN, PEKKA KOSKINEN, University of Jyväskylä, Finland — Carbon nanotubes are usually described as being rolled up from graphene sheets; this process, however, have never been realized experimentally. We showed that graphene can indeed be transformed into nanotube by twisting [1]. Further, we showed that tube formation can be well-explained within classical theory of elasticity—in fact the very mechanism of tube formation can be observed by twisting a strap from one's backpack (try now!). Furthermore, we showed that nanotube chirality may not only be predicted, but can also be controlled externally. The quantum molecular dynamic simulations at T=300K were achieved thanks to the revised periodic boundary conditions (RPBC) approach [2-3]. The structures similar to simulated have been recently observed experimentally [4]. This novel route for nanotube formation opens new opportunities in nanomaterial manipulation not restricted to carbon alone. In the presentation, I will describe tube formation, as well as outline the easy and efficient technique for distorted nanostructures simulation, the RPBC approach.

[1] O. O. Kit et al. arXiv:1108.0048

[2] P. Koskinen & O. O. Kit PRL 105, 106401 (2010)

[3] O. O. Kit, L. Pastewka, P. Koskinen PRB 84, 155431 (2011)

[4] A. Chuvilin et al. Nature Materials 10, 687 (2011)

¹Computational resources provided by the Finnish IT Center for Science (CSC).

2:54PM X11.00003 Wrinkling instability in graphene supported on nanoparticle-patterned SiO₂ , WILLIAM CULLEN, MAHITO YAMAMOTO, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742-4111, OLIVIER PIERRE-LOUIS, LPMC, Université Lyon 1, France, THEODORE EINSTEIN, MICHAEL FUHRER, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742-4111 — Atomically-thin graphene is arguably the thinnest possible mechanical membrane: graphene's effective thickness (the thickness of an isotropic continuum slab which would have the same elastic and bending stiffness) is significantly less than 1 Å, indicating that graphene can distort out-of-plane to conform to sub-nanometer features. Here we study the elastic response of graphene supported on a SiO₂ substrate covered with SiO₂ nanoparticles. At a low density of nanoparticles, graphene is largely pinned to the substrate due to adhesive interaction. However, with increasing nanoparticle density, graphene's elasticity dominates adhesion and strain is relieved by the formation of wrinkles which connect peaks introduced by the supporting nanoparticles. At a critical density, the wrinkles percolate, resulting in a wrinkle network. We develop a simple elastic model allowing for adhesion which accurately predicts the critical spacing between nanoparticles for wrinkle formation. This work has been supported by the University of Maryland NSF-MRSEC under Grant No. DMR 05-20471 with supplemental funding from NRI, and NSF-DMR 08-04976.

3:06PM X11.00004 Molecular Dynamics Study of Ripples in Graphene and Bilayer Graphene , ARUNIMA SINGH, RICHARD G. HENNIG, Department of Materials Science and Engineering, Cornell University — Transmission electron microscopy experiments have shown that suspended graphene is not perfectly flat, but displays ripples such that the surface normal of graphene varies by several degrees [1,2]. For multi-layered graphene, the ripples are suppressed with increasing numbers of layers. Recent experiments demonstrated that ripples in suspended graphene can also be controlled by mechanical and thermally induced strain [3]. Knowledge of and control over the ripples in graphene is desirable for fabricating and designing of strain-based devices. We show using molecular dynamics simulation that thermally induced ripples in suspended single and multi-layer graphene at room temperature result in deviations of the local surface normal by $\pm 7^\circ$ and $\pm 4^\circ$ for single and bilayer graphene, respectively. These angular deviations are in excellent agreement with transmission electron microscopy results [2] and confirm that these ripples can be dynamic and thermally induced. We also study how these angles change as a function of applied tensile and shear strain. [1] Meyer J. C., Geim A. K., et al. Solid State Communications, 143, 101 (2007). [2] Meyer J.C., Geim A.K., et al. Nature, 446, 60 (2007). [3] Bao W., Miao F., et al. Nature Nanotechnology, 4 (9), 562 (2009).

3:18PM X11.00005 Ideal strength of graphene¹ , SUNGJONG WOO, YOUNG-WOO SON, Korea Institute for Advanced Study — We have investigated the ideal strength of graphene by calculating the response under strain based on density functional theory. The strength of materials with usual contaminations and impurities is typically weaker than the ideal one. However, we have considered realistic factors and calculated several electromechanical properties of perturbed graphene showing that under certain conditions graphene can endure more strain than the pristine one. The interpretation of our result will be presented in the context of competitions among different energy scales under mechanical strains that eventually leads to the structure failure.

¹Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2011-C1-21).

3:30PM X11.00006 Determination of Young's Modulus of Graphene by Raman Spectroscopy , JAE-UNG LEE, DUHEE YOON, HYEONSIK CHEONG, Department of Physics, Sogang University, Seoul, Korea — The mechanical properties of graphene are interesting research subjects because its Young's modulus and strength are extremely high. Values of ~ 1 TPa for the Young's modulus have been reported [Lee et al. Science, 321, 385 (2008), Koenig et al. Nat. Nanotech. 6, 543 (2011)]. We made a graphene sample on a SiO₂/Si substrate with closed-bottom holes by mechanical exfoliation. A pressure difference across the graphene membrane was applied by putting the sample in a vacuum chamber. This pressure difference makes the graphene membrane bulge upward like a balloon. By measuring the shifts of the Raman G and 2D bands, we estimated the amount of strain on the graphene membrane. By comparing the strain estimated from the Raman measurements with numerical simulations based on the finite element method, we obtained the Young's modulus of graphene.

3:42PM X11.00007 Role of the effective tensile strain in the electromechanical response of helical graphene nanoribbons with open and closed edges , TRAIAN DUMITRICA, DONG-BO ZHANG, University of Minnesota — There is a growing need to understand the electronic properties of non-ideal graphene nanoribbons. Using objective molecular dynamics [1] and a density-functional based tight-binding model, we investigate the effects of torsion on the electromechanical properties of graphene nanoribbons with armchair edges. We propose to characterize with an effective tensile strain scalar [2] the torsional mechanical response, including a reverse Poynting effect, and the fundamental band gap modulations. The demonstrated utility of this concept in both the mechanical and electrical domains provides a perspective for understanding electromechanical response in a unified way, and for designing NEMS devices with graphene components. [1] T. Dumitric? and R.D. James, J. Mech. Phys. Sol. 55, 2206-2236 (2007). [2] D.-B. Zhang and T. Dumitric?, Small 7, 1023 (2011) .

3:54PM X11.00008 Failure mechanisms of graphene under tension , CHRIS MARIANETTI, Columbia University — Recent experiments established pure graphene as the strongest material known to mankind, further invigorating the question of how graphene fails. Using density functional theory, we reveal the mechanisms of mechanical failure of pure graphene under a generic state of tension at zero temperature. One failure mechanism is a novel soft-mode phonon instability of the K_1 -mode, whereby the graphene sheet undergoes a phase transition and is driven towards isolated hexagonal rings resulting in a reduction of strength. The other is the usual elastic instability corresponding to a maximum in the stress-strain curve. Our results indicate that finite wave vector soft modes can be the key factor in limiting the strength of monolayer materials.

4:06PM X11.00009 Characterization of strain in CVD graphene on copper substrates¹, RUI HE, University of Northern Iowa, LIUYAN ZHAO, NICHOLAS PETRONE, Columbia University, MICHAEL ROTH, University of Northern Iowa, JAMES HONE, PHILIP KIM, ABHAY PASUPATHY, ARON PINCZUK, Columbia University — Strain plays an important role in controlling graphene's properties and induces significant changes in the electronic band structure. Strain and morphology of CVD (chemical vapor deposition) graphene layers grown on Cu substrates are studied by Raman spectroscopy and scanning tunneling microscopy (STM). We find that CVD graphene on Cu surfaces are subject to strain which depends on the orientation of the underlying Cu surfaces. The strain is compressive on Cu (111) surface and estimated to be on the order of 0.5 percent by molecular dynamics (MD) simulations. For graphene grown on Cu (100) surface the strain is highly nonuniform and includes both compressive and tensile components. MD simulations of graphene on Cu (100) show highly nonuniform strain patterns including linear superstructures, consistent with the patterns seen in STM. For graphene grown on Cu foil the strain is partially released after graphene is removed from Cu surfaces and transferred onto oxidized Si substrate.

¹Supported by ONR and NSF

4:18PM X11.00010 Local nanoscale frictional variations of graphene investigated with lateral force microscopy¹, PATRICK HUNLEY, TYLER FLYNN, TOM DODSON, ABHISHEK SUNDARARAJAN, DOUGLAS STRACHAN, University of Kentucky — Lateral force microscopy is used to investigate the local nanoscale frictional variations on single- and multi-layered graphene films. Employing novel calibration methods, quantitative frictional measurements are taken for a range of normal loads. The coverage of specific high-friction regions with a single layer of graphene shows a significant reduction in the frictional characteristics.

¹Supported in part by the Kentucky NSF EPSCoR program through award EPS-0814194 and the University of Kentucky Center for Advanced Materials.

4:30PM X11.00011 Adsorption-induced Pore Expansion and Contraction in Activated Carbon, MATTHEW CONNOLLY, CARLOS WEXLER, University of Missouri Physics Department — Adsorbent materials such as activated carbon and Metal-Organic Frameworks (MOFs) have received significant attention as a potential storage material for hydrogen and natural gas. Typically the adsorbent material is assumed to consist of rigid slit- or cylindrical-shaped pores. Recent work has revealed the importance of the mechanical response of the adsorbent in the presence of an adsorbate. Here, we first demonstrate the flexibility of pore walls in activated carbon and the effect this has on the pore structure of the bulk samples. The interaction is modeled as a competition between Van der Waals interactions between neighboring walls and a resistance to bending due to the rigidity of graphene. Minimal energy configurations were calculated analytically for a simplified potential and numerically for a more realistic potential. The pore structures are discussed in the context of pore measurements on activated carbon samples. Following recent work by Cole and Neimark, large pressures due to an adsorbed film are predicted in the narrow pores of activated carbon. The coverage-dependent nature of adsorbed-film pressure, indicating a pressure-variant pore structure, is discussed in terms of adsorption isotherms.

4:42PM X11.00012 Hierarchical graphene materials: from monolayers to papers and nanocomposites, ZHIPING XU, Tsinghua University — Macroscopic graphene materials such as papers and nanocomposites consist of chemically modified graphene sheets and intersheet crosslinks of various types, which hold great promises in high-performance, multifunctional and light-weighted applications. In this talk, we will present a multiscale approach (density functional theory, molecular dynamics and continuum mechanics) to understand simultaneously atomistic mechanisms, microscale structures and microscopic performance of these hierarchical graphene materials, and provide general principles for materials design that are supported by experimental evidence. Hierarchical structures of graphene-based materials will be also discussed comparably with biological materials that are widely studied recently, such as bones, nacre and collagen fibrils, which possess similar materials hierarchies and inspire many novel concepts in new materials development.

4:54PM X11.00013 Layer Effects in Graphene NEMS Resonators, BRITTON BAUGHER, TCFEOR NDUKUM, KEVIN FISCHER, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — In this talk we will present new data on mono, bi, and tri-layer graphene nanoelectromechanical (G-NEMS) resonators. G-NEMS resonators utilize graphene's high mobility, high Young's modulus, Dirac-like dispersion relation, and other unique qualities to produce unusual physical phenomena at the intersection of electronics and mechanics on the quantum scale. We extend the work done on these devices with a study into the effects of layer number on temperature dependence, quality factor, tunability, and frequency amongst others.

5:06PM X11.00014 Ultrastrong Adhesion of Graphene Membranes, STEVEN P. KOENIG, NARASIMHA G. BODDETI, MARTIN L. DUNN, J. SCOTT BUNCH, Department of Mechanical Engineering, University of Colorado at Boulder — As mechanical structures enter the nanoscale regime, the influence of van der Waals forces increases. Graphene is attractive for nanomechanical systems because its Young's modulus and strength are both intrinsically high, but the mechanical behavior of graphene is also strongly influenced by the van der Waals force. For example, this force clamps graphene samples to substrates, and also holds together the individual graphene sheets in multilayer samples. Here we use a pressurized blister test to directly measure the adhesion energy of graphene sheets with a silicon oxide substrate. We find an adhesion energy of 0.45 ± 0.02 J m⁻² for monolayer graphene and 0.31 ± 0.03 J m⁻² for samples containing two to five graphene sheets. These values are larger than the adhesion energies measured in typical micromechanical structures and are comparable to solid-liquid adhesion energies. We attribute this to the extreme flexibility of graphene, which allows it to conform to the topography of even the smoothest substrates, thus making its interaction with the substrate more liquid-like than solid-like.

5:18PM X11.00015 Graphene coatings: An efficient protection from oxidation, MEHMET TOPSAKAL, HASAN SAHIN, SALIM CIRACI, UNAM-Institute of Materials Science and Nanotechnology — We demonstrate that graphene coating can provide an efficient protection from oxidation by posing a high energy barrier to the path of oxygen atom, which could have penetrated from the top of graphene to the reactive surface underneath. Graphene bilayer, which blocks the diffusion of oxygen with a relatively higher energy barrier provides even better protection from oxidation. While an oxygen molecule is weakly bound to bare graphene surface and hence becomes rather inactive, it can easily dissociate into two oxygen atoms adsorbed to low coordinated carbon atoms at the edges of a vacancy. For these oxygen atoms the oxidation barrier is reduced and hence the protection from oxidation provided by graphene coatings is weakened. Our predictions obtained from the state of the art first-principles calculations of electronic structure, phonon density of states and reaction path will unravel how a graphene can be used as a corrosion resistant coating and guide further studies aiming at developing more efficient nanocoating materials.

Thursday, March 1, 2012 2:30PM - 5:30PM –

Session X12 DMP: Focus Session: Graphene: Growth, Mechanical Exfoliation, and Properties - Morphology and Interactions 210C

2:30PM X12.00001 Atomic Scale Properties of Chemically Doped Graphene, ABHAY PASUPATHY, Columbia University — In monolayer graphene, substitutional doping during growth can be used to alter its electronic properties. We used scanning tunneling microscopy, Raman spectroscopy, x-ray spectroscopy, and first principles calculations to characterize individual nitrogen dopants in monolayer graphene grown on a copper substrate. Individual nitrogen atoms were incorporated as graphitic dopants, and a fraction of the extra electron on each nitrogen atom was delocalized into the graphene lattice. The electronic structure of nitrogen-doped graphene was strongly modified only within a few lattice spacings of the site of the nitrogen dopant. These findings show that chemical doping is a promising route to achieving high-quality graphene films with a large carrier concentration. Ref: L. Zhao et al, *Science* **333**,999 (2011).

3:06PM X12.00002 Quantum Hall Effect in Graphene Bilayers Grown on Copper by Chemical Vapor Deposition¹, BABAK FALLAHAZAD, The Microelectronics Research Center, The University of Texas at Austin, YUFENG HAO, The University of Texas at Austin, KAYOUNG LEE, SEYOUNG KIM, The Microelectronics Research Center, The University of Texas at Austin, RODNEY RUOFF, The University of Texas at Austin, EMANUEL TUTUC, The Microelectronics Research Center, The University of Texas at Austin — We report an investigation of quantum Hall effect in graphene bilayers grown on Cu substrates by chemical vapor deposition. Raman spectroscopy of the as grown graphene bilayers reveals a position dependent full width half maximum of the 2D peak, ranging from 22 to 55 cm⁻¹, suggesting the bilayer is a mixture of Bernal stacked and decoupled graphene monolayers. Using scanning Raman spectroscopy we identify areas with either wide (45-55 cm⁻¹), as well as narrow (22-26 cm⁻¹) 2D peaks, in order to fabricate back-gated Hall bars on such grains. Magnetotransport measurements in bilayer regions characterized by a wide 2D peak reveal quantum Hall states (QHS) at filling factors $\nu = \pm 4, 8, 12$ consistent with a Bernal stacked bilayer, which develop at magnetic fields higher than 15 T. In contrast, magnetotransport measurements in bilayer regions defined by a narrow 2D peak shows QHSs down to 3 T, and with a sequence consisting of the superposition of the QHSs of two independent monolayers. We compare the QHS energy gaps extracted from activation measurements with the theoretical Landau level (LL) separation, and estimate the LL broadening.

¹We appreciate support from the SWAN NRI and the ONR.

3:18PM X12.00003 Layer Number and Stacking Order Imaging of Few-layer Graphenes by Transmission Electron Microscopy, JINGLEI PING, MICHAEL FUHRER, Center for Nanophysics and Advanced Materials, University of Maryland, College Park — A method using transmission electron microscopy (TEM) selected area electron diffraction (SAED) patterns and dark field (DF) images is developed to identify graphene layer number and stacking order by comparing intensity ratios of SAED spots with theory. Graphene samples are synthesized by ambient pressure chemical vapor deposition and then etched by hydrogen in high temperature to produce samples with crystalline stacking but varying layer number on the nanometer scale. Combined DF images from first- and second-order diffraction spots are used to produce images with layer-number and stacking-order contrast with few-nanometer resolution. This method is proved to be accurate enough for quantitative stacking-order-identification of graphenes up to at least four layers. This work was partially supported by Science of Precision Multifunctional Nanostructures for Electrical Energy Storage, an Energy Frontier Research Center funded by the U.S. DOE, Office of Science, Office of Basic Energy Sciences under Award Number DESC0001160.

3:30PM X12.00004 Metal surface melting effect on the formation of graphene wrinkles, TEREZA PARONYAN, ELENA PIGOS, AVETIK HARUTYUNYAN, Honda Research Institute, USA Inc., Columbus, OH, 43212, USA, HONDA RESEARCH INSTITUTE TEAM — The synthesis of high quality large area graphene is a significant challenge that needs to be overcome for practical applications of this material. Therefore, understanding the growth mechanism of graphene is crucial in order to explain the origin of defects on it. Different thickness of Copper and Nickel films deposited on silica substrates, and foils with various degrees of purity were used in this study. We investigated the changes in the surface morphology of the thin films and foils with temperature at 860-1100°C with and without growth of graphene by Chemical Vapor Deposition method. Detailed investigation by Raman spectroscopy, SEM and AFM analysis revealed that thermal treatment of the metal substrates at high temperatures ~1000°C causes formation of dendritic like structures on the surface. We attributed these structures to the non-equilibrium solidification of the melted surface of the metal during the cooling, which are also present in the case of graphene growth. We concluded that the reconstruction of the metal surface morphology in the case of graphene growth, due to the surface melting, significantly affects on the final topography of the graphene wrinkles and, thereby on the quality of graphene.

3:42PM X12.00005 Growth and Characterization of Graphene-Boron Nitride Heterostructures¹, PETER SUTTER, Brookhaven National Laboratory — Graphene has been used to explore the fascinating properties of two-dimensional sp² carbon, and shows great promise for applications. Heterostructures of graphene (G) and hexagonal boron nitride (h-BN) have the potential for extended functionality, e.g., providing high carrier mobilities in graphene devices supported on h-BN and giving rise to emergent electronic behavior near in-plane G/h-BN junctions. While significant progress has been made recently in separate graphene and boron nitride growth on transition metals, the controlled synthesis of high-quality G/h-BN heterostructures poses new challenges. We discuss the fundamental growth mechanisms underlying the synthesis of G/h-BN heterostructures, studied by a combination of in-situ surface microscopy methods. Real-time low-energy electron microscopy (LEEM) provides a mesoscale view of the nucleation and growth of h-BN in the presence of graphene, and vice-versa. LEEM imaging together with diffraction and angle resolved photoemission spectroscopy (micro-ARPES) gives insight into the interaction between graphene and h-BN. Scanning tunneling microscopy has been used to probe intermixing and the atomic-scale structure of interfacial boundaries. Combining real-time and atomic-resolution imaging, we identify successful approaches for achieving atomically sharp G/h-BN junctions.

¹Research carried out at the Center for Functional Nanomaterials, Brookhaven National Laboratory, supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

4:18PM X12.00006 Physical and electrical properties of graphene folds grown by Chemical Vapor Deposition, WENJUAN ZHU, TONY LOW, YU ZHU, AGEETH BOL, HUGEN YAN, XUESONG LI, YU-MING LIN, YANQING WU, FENGNIAN XIA, VASIL PEREBEINOS, PHAEDON AVOURIS, IBM T.J. Watson Research Center — We found that there is a large density of wrinkles on CVD graphene transferred to a SiO₂/Si substrate. At these graphene wrinkles, the SEM signal intensity is lower, the AFM height is higher, and the Raman G-band intensity is stronger as compared to the surrounding single-layer graphene, due to extra layers of graphene at the wrinkles. TEM images confirmed that wide wrinkles are folds instead of ridges. The channel resistance near the Dirac point along graphene folds is significantly lower than the resistance without folds. However, as the gate field or the carrier density is increased, the difference between graphene channel along the fold and without the fold is reduced, due to carrier screening.

4:30PM X12.00007 Superior Mobility in Chemical Vapor Deposition Synthesized Graphene by Grain Size Engineering, NICHOLAS PETRONE, CORY DEAN, INANC MERIC, AREND VAN DER ZANDE, Columbia University, PINSHANE HUANG, Cornell University, LEI WANG, Columbia University, DAVID MULLER, Cornell University, KENNETH SHEPARD, JAMES HONE, Columbia University — Chemical vapor deposition (CVD) offers a promising method to produce large-area films of graphene, crucial for commercial realization of graphene-based applications. However, electron transport in CVD grown graphene has continued to fall short of the performance demonstrated by graphene derived from mechanical exfoliation. Lattice defects and grain boundaries developed during growth, structural defects and chemical contamination introduced during transfer, and charged scatterers present in sub-optimal dielectric substrates have all been identified as sources of disorder in CVD grown graphene devices. We grow CVD graphene and fabricate field-effect transistors, attempting to minimize potential sources of disorder. We reduce density of grain boundaries in CVD graphene by controlling domain sizes up to 250 microns. By transferring CVD graphene onto h-BN utilizing a dry-transfer method, we minimize trapped charges at the interface between graphene and in the underlying substrate. We report field-effect mobilities up to 110,000 cm²V⁻¹s⁻¹ and oscillations in magnetotransport measurements below 1 T, confirming the high quality and low disorder in our CVD graphene devices.

4:42PM X12.00008 Transfer-Free, Wafer-Scale, and Patterned Synthesis of Graphene on Dielectric Substrates, HOSSEIN SOJOURDI, SAMUEL GRAHAM, Woodruff School of Mechanical Engineering, Georgia Institute of Technology, 771 Ferst Dr Atlanta, GA 30332-0405 — We report a method for the direct, wafer-scale synthesis of graphene on dielectric substrates using a solid carbon source. Graphene films were synthesized through the thermal decomposition of poly(methyl methacrylate) on copper coated quartz and Si/SiO₂ substrates in a low pressure H₂/Ar environment. The Cu film partially evaporated during growth, leaving a graphene layer directly on the dielectric substrate. Polyacrylamide was used for synthesis of N-doped graphene due to its nitrogen content. A similar method with process optimization was utilized to grow graphene without any external carbon source. Trace amounts of carbon in metal films result in direct formation of graphene on insulators through a segregation process. A wet etch step allowed complete removal of the metal film, leading to continuous graphene coverage of the surface. This technique utilized for patterned synthesis of graphene and can be used in Si-wafer compatible device fabrication.

4:54PM X12.00009 Transport studies of dual-gated ABA- and ABC-stacked trilayer graphene, K. ZOU, Department of Physics, The Pennsylvania State University, University Park, PA 16802, F. ZHANG, Department of Physics, The University of Texas at Austin, Austin, TX 78701, C. CLAPP, Department of Chemistry, Amherst College, Amherst, MA 01002, A.H. MACDONALD, Department of Physics, The University of Texas at Austin, Austin, TX 78701, J. ZHU, Department of Physics, The Pennsylvania State University, University Park, PA 16802 — We present electrical transport studies of dual-gated ABA- and ABC-stacked trilayer graphene field effect transistors. Employing high-quality thin HfO₂ layers as the top and back gate dielectrics, we independently tune the carrier density and control the band structure of trilayer graphene via the application of a perpendicular electric field E_{perp} . The large gating efficiency of the two gates (5.53×10^{12} /cm² per Volt) and their high breakdown voltage (> 6 V) enable us to reach exceedingly large carrier densities and E_{perp} values, which results in wide tuning of the conductivity of the trilayer devices. Results on ABA-stacked trilayer graphene confirm its semi-metallic nature and reveal evidence of the band structure changes induced by E_{perp} . The resistance at the charge neutrality point of ABC-stacked trilayer graphene increases by many orders of magnitude with increasing E_{perp} due to the gradual opening of a band gap. Our results suggest a saturation of the gap size at perpendicular displacement fields greater than 3.5 V/nm, in agreement with theoretical calculations.

5:06PM X12.00010 Graphene growth by CVD using liquid precursors, JESSICA CAMPOS DELGADO, ANDRÉS BOTELLO-MÉNDEZ, BENOIT HACKENS, JEAN-CHRISTOPHE CHARLIER, THOMAS PARDOEN, JEAN-PIERRE RASKIN, Université Catholique de Louvain — Chemical vapor deposition (CVD) represents an attractive route to synthesize large-area graphene. Its catalytic growth using metals has been studied in recent years, the most popular being nickel and copper. We have successfully grown graphene on copper by CVD at ambient pressure using alcohols as the carbon feedstock. The produced materials are analyzed by SEM, TEM, Raman spectroscopy and transferred onto Si/SiO₂ substrates using standard methods. Raman fingerprint of monolayer graphene is present in our samples. This technique represents a safer and more versatile alternative to the production of graphene compared to the synthesis of graphene using methane at low pressure.

5:18PM X12.00011 Vibrational properties in graphene-on-metal systems: A scanning tunneling microscopy study and density functional theory calculations, HAIGANG ZHANG, YUYANG ZHANG, WENDE XIAO, SHIXUAN DU, HONGJUN GAO, Institute of Physics, Chinese Academy of Science, PROF. HONGJUN GAO'S NANO RESEARCH GROUP TEAM — Combining inelastic electron tunneling microscopy (IETS) measured by scanning tunneling microscopy and quantum mechanical calculations based on density functional theory, we investigate and compare the vibrational properties of graphene on various transition metal substrates. The observed dI/dV spectra and mappings indicate there is a mode dependant spatial localization for graphene on Ru(0001) surface. In contrast, vibrations of graphene on Pt(111) surface and Ni(111) surface is homogeneous. Out-of-plane vibration modes of graphene are tuned by the different interactions on these three substrates. Vibrational density of states of graphene and graphene/Ni(111) system are calculated and make comparison to the IETS experiments. We also calculate the inelastic and elastic tunneling coefficients in Graphene/Ni(111) system to understand the missing peak in IETS experiments. Our results point to the importance of interfacial bonding on phonon properties and, consequently, electronic and thermal transport properties of graphene based devices.

Thursday, March 1, 2012 2:30PM - 5:30PM –

Session X13 DMP GMAG: Focus Session: Magnetic Nanostructures-Hard Magnetic Materials and Magnetocaloric Materials 211

2:30PM X13.00001 Thermal Fluctuation and Finite- Temperature Performance of Hard-Soft Composite Magnets¹, ALEXANDER BELEMUK, S.T. CHUI, University of Delaware — The demagnetization behavior of exchange-coupled hard/soft magnets was studied by finite temperature Monte Carlo simulation. Hard phase cube inclusions (Nd₂Fe₁₄B, SmCo₅ and Sm₂Fe₁₇N₃) into a soft matrix (FeCo) and hard/soft multilayer structure were studied. The easy axis of the hard and soft phase and the initial magnetization are parallel to the applied field. We found significant thermal fluctuations and lowering of the remnant magnetization with increasing soft magnet content than is anticipated from zero-temperature models, especially at higher temperatures. This greatly diminishes the expected performances of composites. For cube inclusions there is a boundary mismatch of the magnetization on the hard/soft interface. We investigated this mismatch as function of the soft phase content and temperature. The spin wave spectrum due to the mismatched dipolar interaction will be discussed.

¹Supported by ARPAE

2:42PM X13.00002 Control of Size and Magnetic Properties of L_{10} FePt islands by DC sputtering¹, XIAO CAO HU, Department of Materials Science and Engineering, University of DE, Newark, DE, 19716, USA, OZAN AKDOGAN, WANFENG LI, GEORGE HADJIPANAYIS, Department of Physics and Astronomy, University of DE, Newark, DE, 19716, USA — FePt particles with the tetragonal L_{10} structure are attractive for high density recording media. In this study, we have fabricated well-ordered and separated L_{10} FePt islands on MgO (100) substrates by DC sputtering at temperatures varying from room temperature to 700 °C. The dependence of particle size, degree of ordering and magnetic properties on sputtering time (5-20s), power (5-20W) and substrate temperature (300-1000K) were investigated. Electron diffraction patterns from TEM showed that the islands had the L_{10} tetragonal structure. TEM data revealed that a higher substrate temperature significantly increased the size of the islands from 2 to 20 nm whereas a higher sputtering power and longer sputtering times did not change the island size much but made the islands more connected with each other. Larger size islands and inter-connected islands showed a higher degree of ordering with an ordering parameter of 0.8 achieved at 600 °C. The magnetic properties are currently being measured and the results will be reported.

¹Work is supported by DOE ARPA-E DE-AR0000046.

2:54PM X13.00003 Nano-granular FePt thin films for thermally-assisted magnetic recording, TIFFANY SANTOS, OLEKSANDR MOSENDZ, SIMONE PISANA, JAMES REINER, GREGORY PARKER, BARRY STIPE, DIETER WELLER, Hitachi Global Storage Technologies — In order to extend the data storage density in hard disk drives beyond 1 Tb/in², nano-size grains of a high crystalline anisotropy (K_u) material are required to obtain these high densities and maintain thermal stability. A promising approach to recording using high- K_u materials is thermally-assisted magnetic recording (TAR), in which the media is locally heated above the Curie temperature while a magnetic field is applied in order to write a bit. FePt with L_{10} crystalline order is a potential candidate for TAR media. We deposit FePt nano-granular films with carbon as the segregant material, by co-sputtering on glass substrates at elevated temperature. Underlayer materials are selected for heat-sinking and to attain high out-of-plane L_{10} order. Characterization of the media by x-ray diffraction, magnetometry and transmission electron microscopy show that we can achieve properties that are promising for TAR media, such as an average grain size < 7.5nm, size distribution as low as 16%, coercivity as high as 5 tesla and $K_u > 4.5 \times 10^7$ erg/cm³. Recording densities exceeding 600 Gb/in² have been demonstrated for our FePt granular films using a static tester.

3:06PM X13.00004 Confined stripe structure in periodically grooved NdCo Films with perpendicular magnetic anisotropy¹, JOSE I. MARTIN, AURELIO HIERRO-RODRIGUEZ, ROSALIA CID, GABRIEL RODRIGUEZ-RODRIGUEZ, MARIA VELEZ, LUIS M. ALVAREZ-PRADO, JOSE M. ALAMEDA, Depto. Fisica, Universidad de Oviedo and CINN (CSIC - U.Oviedo - P.Asturias), Spain — Magnetic multilayers are broad research field with many interesting phenomena depending on interlayer coupling. Also, since the development of nanolithography techniques, magnetic nanowires and dots have been intensively investigated [1]. Recently, as a combination of these two fields, the concept of magnetic lateral superlattice has emerged: continuous magnetic films with a lateral modulation of their magnetic properties at submicrometric length scale [2]. In this work, we have fabricated amorphous Nd-Co films with perpendicular magnetic anisotropy and a periodic thickness modulation by e-beam lithography and ion milling. Lateral periods range from 2 μ m - 500 nm and groove depths from 10 to 30 nm. MFM and Kerr magnetometry have been used for characterization. Lateral patterning modifies the interplay between magnetostatic energy, perpendicular and in plane anisotropy and exchange interaction resulting in confined magnetic stripe structures. The different regimes that appear depending on the size of the periodic thickness modulation relative to the magnetic stripe period will be discussed. [1] J.I Martin et al, JMMM, 256 (2003) 449 [2] S. P. Li et al, PRL 88 (2002) 087202; N. Martin et al, PRB 83 (2010) 174423

¹Work supported by Spanish MICINN

3:18PM X13.00005 Intrinsic Magnetic Properties of fct FePt Nanocubes and Rods by Cluster Beam Deposition¹, OZAN AKDOGAN, WANFENG LI, GEORGE HADJIPANAYIS, Department of Physics and Astronomy, University of DE, Newark, DE, 19711 USA, RALPH SKOMSKI, DAVID SELLMYER, Department of Physics and Astronomy, University of Nebraska, Lincoln, NE 68588 USA — In this work, single crystal fct FePt nanocubes have been successfully produced by a cluster beam deposition technique without the need of post annealing. Particles have been deposited by DC magnetron sputtering using high Ar pressures (0.5 to 2 Torr) on both single crystal Si substrates and Au grids for the measurement of magnetic and structural properties, respectively. The nanocubes have a uniform size distribution with an average size of 6.5 nm. At 1 Torr, the particles have the fct structure with an order parameter of 0.5 and a RT coercivity of 2 kOe with high switching fields seen in the hysteresis loop. Particle size was controlled by changing the pressure and power and also by ex-situ annealing. In addition to these nanocubes, micron size rods (which consist of 20 nm nanoparticles) with the fct structure have been observed near the cluster gun. These particles show a room temperature coercivity of 8 kOe with an order parameter of 0.85. Intrinsic magnetic properties (Curie temperature, H_A , M_S and magnetic viscosity) of the nanocubes and the nanoparticles (separated from the rods) have been extensively studied and the results will be reported.

¹Work is supported by DOE DE-FG02-04ER4612.

3:30PM X13.00006 Confinement Effect on the Phase Transformation of FePt from $A1$ to $L1_1$, ANDREW GALLAGHER, LEVENT COLAK, OZAN AKDOGAN, GEORGE HADJIPANAYIS, Department of Physics and Astronomy, University of DE, Newark, DE, 19711, USA — The major challenge for the application of chemically synthesized FePt nanoparticles (NPs) in magnetic storage media is the sintering problem encountered during the required high temperature annealing to obtain the high anisotropy L_{10} phase. In this work, we have used two methods to avoid sintering: coating the NPs with a protective layer of silica (SiO_2) and using porous aluminum oxide (Al_2O_3) as a template to hold the NPs. The NPs were synthesized via the synthesis method of Sun *et al.*^[1] The NPs were added to the Al_2O_3 by in-situ suctioning of the reaction solution into the porous Al_2O_3 template. Monodispersed FePt NPs with a size of 5.8 and 15 nm were coated with SiO_2 shells using a water-in-oil microemulsion method. High room temperature coercivities were only obtained after annealing the samples at 900 °C for long times (24-48 h) under forming gas flow as compared to the usual 600-700 °C. Values of 4.7 and 7.8 kOe were observed in SiO_2 and Al_2O_3 samples, respectively after annealing for 24 h at 900 °C. This behavior suggests that the restricted geometry of the samples suppresses the phase transformation drastically.

[1] S. Sun, C. B. Murray, D. Weller, L. Folks, A. Moser *Science* **2000**, 287, 1989.

¹Work supported by DOE DE-FG02-04ER4612.

3:42PM X13.00007 Towards high strength nanocomposite magnets — Approaches from the bottom¹, J. PING LIU, University of Texas at Arlington — Exchange-coupled nanocomposite magnets are regarded as the next generation of permanent magnetic materials, based on the theoretical predictions. However, many fundamental questions and technical challenges remain in understanding the inter-phase exchange interactions and in processing bulk nanocomposite magnets with enhanced energy products. We will review recent advancements in both the fundamental research and the materials processing technologies. New findings about the effects of soft-phase properties and interface conditions on the hard/soft phase exchange interactions will be presented. Particularly, the development of the bottom-up approaches in materials processing will be discussed. Novel methodology for nanoparticle synthesis including the salt-matrix annealing, surfactant-assisted ball milling and severe plastic deformation will be described. Unconventional compaction techniques including warm compaction and dynamic compaction are recommended because they can be used to retain desired nanoscale morphology for effective exchange coupling in bulk nanocomposite magnets. A perspective on fabrication of anisotropic nanocomposite magnets will be also given.

¹Work supported by DoD/DARPA, MURI, ARO, and NSF.

4:18PM X13.00008 NdCo₅ Nanoflakes and Nanoparticles Produced by Surfactant-Assisted High Energy Ball Milling¹, NILAY GUNDUZ AKDOGAN, WANFENG LI, GEORGE HADJIPANAYIS, Department of Physics and Astronomy, University of Delaware, Newark, DE, U.S.A. — The study of size and surface effects in rare earth transition metal nanoparticles is scientifically very important. In this work our studies were focused on NdCo₅ which is interesting because of its complex magnetic ordering behavior at different temperatures. Anisotropic NdCo₅ nanoparticles have been produced by surfactant-assisted high-energy ball milling (HEBM) of nanocrystalline precursor alloys. A two-stage ball milling method has been employed to produce the NdCo₅ nanoflakes and nanoparticles. NdCo₅ flakes have a thickness below 150 nm and an aspect ratio as high as 10² - 10³; the nanoparticles have an average size of 7 nm. Both the nanoparticles and nano-flakes showed high coercivities at low temperatures, with values at 50 K of 3 kOe and 3.7 kOe, respectively. The high values of coercivity observed in a planar anisotropy phase can be attributed to the large surface anisotropy of nanoparticles that leads to an effective uniaxial-type of behavior. The nanoparticles also showed spin reorientation temperatures which are lower when compared to the bulk values.

¹Work supported by NSF DMR-1005871.

4:30PM X13.00009 Magnetic Studies on Nd₂Fe_{14-x}Mn_xB Nanoflakes and Nanoparticles Produced by Surfactant-Assisted High Energy Ball Milling¹, GEORGE HADJIPANAYIS, NILAY GUNDUZ AKDOGAN, WANFENG LI, Department of Physics and Astronomy, University of Delaware, Newark, DE, U.S.A. — High temperature magnetic ordering studies on rare earth transition-metal nanoparticles and nanoflakes present a great challenge due to the very high reactivity of these materials. It is well known that Mn substitution for Fe in Nd₂Fe₁₄B compound decreases the Curie temperature to a temperature range that allows for reliable measurements to be made. In this work, we have studied the magnetic properties of Mn substituted Nd₂Fe₁₄B particles in the temperature range of 50-400 K. Nd₂Fe_{14-x}Mn_xB nanoparticles and nanoflakes have been produced by surfactant-assisted high-energy ball milling (SA-HEBM). Different size nanoparticles have been obtained by varying the milling conditions. Anisotropic Nd₂Fe_{14-x}Mn_xB nanoparticles have been found with a size from 13 to 25 nm. Both the nanoparticles and nano-flakes showed high coercivities at low temperatures, with values at 50 K of 2.4 kOe and 5.5 kOe, respectively. The Curie temperature was determined from the temperature dependence of magnetization. We have observed a different magnetic ordering behavior in the nanoparticles with Curie temperatures that are higher when compared to the bulk values.

¹Work supported by NSF DMR-1005871.

4:42PM X13.00010 Giant Coercive Fields of 2.5 Tesla in Nanostructured Mn_xGa Films¹, STEVEN BENNETT, THOMAS NUMMY, THOMAS CARDINAL, WELVILLE NOWAK, DON HEIMAN, Northeastern University — There is a growing interest in designing new magnetic materials that are free of rare-earth elements. The magnetism of the Heusler ferrimagnet Mn_xGa [1] was found to be enhanced when fabricated with nanoscale structural disorder. Films of Mn_xGa (x=2 to 3) with thicknesses of 20 to 40 nm were grown using molecular beam epitaxy at 100 °C then annealed at 400 °C. Disordered films were grown on lattice mismatched Si (001) substrates, then compared to epitaxially grown films on desorbed GaAs (001) substrates. While the epitaxial films have small hysteresis in the magnetization with coercive fields in the range $\mu_0 H_C = 10^{-2}$ - 10^{-1} T, the disordered films exhibited surprisingly wide hysteresis with record high coercive fields as large as $\mu_0 H_C = 2.5$ T. These magnitudes are comparable to those of rare-earth-based magnets. This hysteresis was also present in the anomalous Hall effect. The enhanced coercive field in the disordered material arises from a combination of the exceptionally large magnetocrystalline anisotropy and nanoscale structural disorder. These results point out a new opportunity for developing rare-earth-free magnetic materials. Discovery of this unusually high coercive field is outlined and its sources discussed. [1] J. Winterlik, et al., Phys. Rev. B **77**, 054406 (2008).

¹Work supported by NSF-DMR-0907007

4:54PM X13.00011 Tunable exchange length in laminate exchange coupled composite media, B.J. KIRBY, National Institute of Standards and Technology, HAO-CHENG HOU, CHIH-HUANG LAI, National Tsing Hua University, Taiwan — Exchange coupled composites - with a hard layer (HL) to anchor against thermal instabilities, and a soft layer (SL) to assist magnetization reversal - have been proposed for advanced recording applications. The reversal assist relies on a non-coherent rotation between the HL and SL, - the exchange-spring (ES) - in which the interfacial domain wall traverses the hard/soft interface, and promotes switching. Typically, the soft region is a single layer, with the emergent composite properties mainly determined by the choice of soft material. We are pursuing a more sophisticated approach, using a hard CoPtCr-SiO₂ layer adjacent to a multilayer of the same material, [CoPtCr-SiO₂/Pt]N, softened by lamination with Pt layers. Simulations predict that when the SL thickness exceeds a critical exchange length, a significant portion should decouple from the HL, becoming a domain wall nucleation site. Thus, ES behavior should be tunable via the Pt thickness. To test this, we have used polarized neutron reflectometry to measure the field-dependent magnetic depth profiles - and directly characterize ES formation - for a series of samples with varying Pt laminate thickness. The experimentally determined relationship between laminate thickness and ES formation will be discussed.

5:06PM X13.00012 Impact of Size Reduction on the Magnetocaloric Effect in Single- and Multi-Phase Manganites¹, N.S. BINGHAM, P. LAMPEN, A. PURI, S. CHANDRA, M.H. PHAN, H. SRIKANTH, University of South Florida, C.L. ZHANG, S.W. CHEONG, Rutgers University, T.H. HOANG, H.D. CHINH, Hanoi University of Technology — Mixed-valent manganites of the form $R_{1-x}M_x\text{MnO}_3$ ($R=\text{La, Pr, Nd, Sm}$ and $M=\text{Sr, Ca, Ba, Pb}$) are of interest as low-cost materials for potential application in the area of active magnetic refrigeration (AMR). An important parameter to optimize for AMR is the refrigerant capacity (RC), which depends on both the magnitude and breadth of the magnetic entropy change peak. Reducing the dimensions of a system to the nanoscale has the potential to enhance the RC by broadening a transition, but can also lead to a drop in entropy change. In this study, we contrast the impact of size reduction on the magnetic and magnetocaloric properties of single-phase $\text{La}_{0.4}\text{Ca}_{0.6}\text{MnO}_3$ (LCMO) and phase-separated $\text{La}_{0.35}\text{Pr}_{0.275}\text{Ca}_{0.375}\text{MnO}_3$ (LPCMO). Nanoparticles of LCMO and LPCMO were prepared by a sol-gel method; single crystals were grown in an optical floating zone furnace. XRD, SEM, and TEM were used to characterize the samples and DC magnetometry measurements were performed using a Quantum Design VSM. We find that size reduction negatively impacts both magnetization and the magnetocaloric properties in LCMO, while enhancing RC and entropy change simultaneously in LPCMO.

¹Support: DOE-BES Grant No. DEFG02-07ER46438 and FCASST

5:18PM X13.00013 Enhancement of magnetic refrigerant capacity in nanocrystalline LaMnO_3 ¹, ANIS BISWAS, SAYAN CHANDRA, M.H. PHAN, H. SRIKANTH, University of South Florida, FUNCTIONAL MATERIALS LABORATORY TEAM — Manganites are considered as potential magnetic refrigerants owing to their large magnetocaloric effect (MCE). However, the effective temperature span of large MCE (δT) is quite small in their bulk form resulting in small refrigerant capacity (RC). We have studied the magnetocaloric property of LaMnO_3 in its polycrystalline bulk and nanocrystalline form with particle size $\sim 50\text{nm}$. MCE is quantified as the change in magnetic entropy ($-\Delta S_M$), which is calculated from the isothermal magnetization curves using Maxwell relation. The samples exhibit large $-\Delta S_M$ associated with their paramagnetic to ferromagnetic transition. Relative to the bulk sample, δT increases significantly in the nanocrystalline form giving rise to more than 63% enhancement in RC. The calculated values of $-\Delta S_M(\text{RC})$ for bulk and nanocrystalline samples are $\sim 2.6\text{J/KgK}$ (173J/Kg) and 2.4J/KgK (282J/Kg) respectively for magnetic field change of 50 kOe. From present study, it can be inferred that reduction of particle size to the nanoscale may be an effective way to increase δT and hence improve RC of a material.

¹DOE-BES Grant No. DEFG02-07ER46438 and FCASST

Thursday, March 1, 2012 2:30PM - 5:06PM –
Session X14 GMAG DMP FIAP: Focus Session: Spins in Semiconductors - Spin-Orbit Interaction and Relaxation in Si and Ge 212

2:30PM X14.00001 Field-induced negative differential spin lifetime in silicon, JING LI, University of Maryland, LAN QING, HANAN DERY, University of Rochester, IAN APPELBAUM, University of Maryland — Using experimental measurements of spin transport in undoped silicon, we show that the electric field-induced thermal asymmetry between the electron and lattice systems substantially impacts the identity of the dominant spin relaxation mechanism. In contrast to the Elliott-Yafet theory where intraband phonon absorption leads to spin relaxation, here we induce phonon *emission* during which electrons are scattered between conduction band valleys that reside on different crystal axes. This leads to anomalous behavior, where reduction of the transit time between spin-injector and spin-detector with larger electric field is accompanied by a counterintuitive reduction in spin polarization and an apparent *negative* spin lifetime.

Work at UMD is supported by the Office of Naval Research and the National Science Foundation. We acknowledge the support of the Center for Nanophysics and Advanced Materials and Maryland NanoCenter and its FabLab. Work at UR is supported by AFOSR and NSF (No. FA9550-09-1-0493 and No. DMR 1124601).

2:42PM X14.00002 Decrease of electron spin lifetime in external electric field due to intervalley phonon scattering in silicon¹, LAN QING, HANAN DERY, University of Rochester, Rochester, New York 14627, JING LI, IAN APPELBAUM, University of Maryland, College Park, Maryland 20742 — We derive a simple approximate expression of the spin lifetime of drifting electrons in silicon. This expression agrees well with elaborate Monte Carlo simulations of the charge transport and spin relaxation of conduction electrons heated by the electric field. Already at low temperatures, the drifting electrons become hot enough to undergo *f*-processes (scattering between valleys of different crystal axes following emission of a shortwave phonon). Such a process involves a direct coupling of valence and conduction bands and dominates the spin relaxation. A sharp decrease of spin lifetime can then be expected in intermediate electric fields in between $\sim 100\text{V/cm}$ and $\sim 1\text{kV/cm}$. When electrons are transported between a spin injector and a spin-resolved detector, the decrease of both transit time and spin lifetime results in a non-monotonic behavior of the detected spin polarization with the electric field. The theory shows excellent agreement with empirical results.

¹This work is supported by AFOSR Contract No. FA9550-09-1-0493, NSF Contract No. ECCS-0824075 and No. DMR-1124601.

2:54PM X14.00003 Spin-Polarized Luminescence Across the Indirect Band-Gap of Strained Ge, Si and Their Alloys¹, DHARA TRIVEDI, Department of Physics & Astronomy, University of Rochester, PENGKE LI, HANAN DERY², Department of Electrical and Computer Engineering, University of Rochester — We study optical orientation and circularly polarized photoluminescence in germanium, silicon and their alloys. We focus on phonon-assisted optical transitions across the indirect band-gap under conditions of biaxial strain (either compressive or tensile). The signature of strain on the band structure and phonon dispersion is observed in the luminescence spectra where spin properties are better resolved from the change in intensity ratio between left and right circularly polarized emission. The spectra is simulated using the combined results of a spin-dependent empirical pseudopotential method, adiabatic bond charge model, electric-dipole approximation, and rigid-ion model. An additional strain tensor has been introduced in calculating the strain effect. We have used group theory extensively to account for all possible transitions and to provide concise selection rules.

¹This work is supported by AFOSR Contract No. FA9550-09-1-0493 and NSF Contract No. DMR-1124601 (NEB 2020).

²Also at Department of Physics & Astronomy, University of Rochester

3:06PM X14.00004 Spin-orbit interaction and spin relaxation of conduction band electrons in Si and Ge¹, PENGKE LI, University of Rochester — Group IV element semiconductors, silicon and germanium, are promising material candidates in spintronics due to their intrinsic long electron spin lifetimes. To describe the spin properties of conduction electrons in these indirect band-gap multivalley semiconductors, the method of invariants is employed to build 8×8 (for Si) and 10×10 (for Ge) spin-dependent Hamiltonians that capture the symmetries of the zone edge states (X-point of Si [1] and L-point of Ge) and their spin dependent parameters. Concise expressions of the energy bands, and more importantly, of the spin mixed states are derived and verified by numerical results of an empirical pseudopotential method. These analytical state expressions are powerful tools to study the behavior of electron spins similar to the way that the Kane model in being used in direct band-gap semiconductors. Mechanisms of spin relaxation by electron-phonon scattering are studied based on this model. We reveal fundamental differences between spin and momentum relaxation mechanisms. In the case of silicon, intravalley spin flipping is governed by scattering with transverse acoustic (TA) phonons via the interband deformation potential that couples the upper and lower conduction bands (this deformation potential would also break the degeneracy of the conduction band at the X point if off-diagonal stress is applied). The intervalley g-process spin flipping couples the lowest conduction bands of different irreducible representations in opposite valleys via acoustic phonons; the intervalley f-process spin flipping, which is the dominant contribution of spin relaxation in a wide temperature range, couples the conduction and valence band components of the states by scattering with Σ_1 and Σ_3 phonons. In the case of germanium, intervalley spin-flip scattering, which is also the main contribution of spin relaxation, couples the lowest and upper conduction bands of different valleys by X-phonons. The intravalley spin flip scattering, which is about two orders of magnitude smaller, couples the conduction and valence bands mostly via TA phonons.

[1] Pengke Li and Hanan Dery, Phys. Rev. Lett. 107, 107203 (2011)

¹This work is supported by AFOSR and NSF (No. FA9550-09-1-0493 and No. DMR 1124601).

3:42PM X14.00005 Group theory analysis of phonon-induced spin relaxation in silicon¹, YANG SONG, Department of Physics and Astronomy, University of Rochester, HANAN DERY², Department of Electronic and Computer Science, University of Rochester — Selection rules and leading order matrix element expressions are derived for all important spin flip processes in the multivalley conduction band of bulk silicon. All results are generalized to arbitrary spin orientation directions. Intervalley *f*-process scattering induced by all phonon modes are analyzed using double group irreducible representation matrices of the Δ axis and independent integrals are identified for transitions between states of either spin. Intervalley *g*-process and intravalley spin flips are analyzed using the *X* point single group and detailed selection rules are derived using a four-band basis. Together with electronic states obtained by a spin-dependent *k*-*p* expansion, wavevector dependent spin-flip matrix elements are derived for all phonon modes in intravalley and for the leading order phonon mode in *g*-process scattering. Higher order matrix elements are qualitatively studied. Comparison with deformation potential theory in momentum scattering is made. Integrations for spin relaxation rate are carried out. Symmetry breaking mechanisms such as stress and electric field are discussed and quantified. We benchmark all of our analysis with numerical results of strain-dependent empirical pseudopotential and adiabatic-bond-charge models.

¹This work is supported by AFOSR Contract No. FA9550-09-1-0493 and NSF Contract No. DMR-1124601 (NEB 2020)

²also at Department of Physics and Astronomy

3:54PM X14.00006 Influence of spin polarization on resistivity of a two-dimensional electron gas in Si MOSFET at metallic densities¹, I. SHLIMAK, A. BUTENKO, D.I. GOLOSOV, Dept. of Physics, Bar-Ilan University, Israel, K.-J. FRIEDLAND, Paul Drude Institute, Berlin, Germany, S.V. KRAVCHENKO, Physics Dept., Northeastern University, Boston, MA, U. S. A. — Positive magnetoresistance (PMR) of a silicon MOSFET in parallel magnetic fields *B* has been measured at high electron densities $n \gg n_c$ where n_c is the critical density of the metal-insulator transition (MIT). It turns out that the normalized PMR curves, $R(B)/R(0)$, merge together when the field is scaled according to $B/B_c(n)$ where B_c is the field in which electrons become fully spin polarized. The values of B_c have been calculated from the simple equality between the Zeeman splitting energy and the Fermi energy taking into account the experimentally measured dependence of the spin susceptibility on the electron density. This extends the range of validity of the scaling all the way to a deeply metallic regime far away from MIT. The subsequent analysis of PMR for low $n \gtrsim n_c$ demonstrated that the merging of the initial parts of curves can be achieved only with taking into account the temperature dependence of B_c . It is shown that the shape of the PMR curves at strong magnetic fields is affected by a crossover from a purely two-dimensional (2D) electron transport to a regime where out-of-plane carrier motion becomes important (quasi-three-dimensional regime).

¹Supported by the BSF under grant 2006375

4:06PM X14.00007 Spin phase coherence of donor nuclear spins in silicon: the influence of electrical readout, DANE MCCAMEY, School of Physics, University of Sydney, Australia, JOHAN VAN TOL, National High Magnetic Field Laboratory and Florida State University, Tallahassee, GAVIN MORLEY, Department of Physics, University of Warwick, UK, CHRISTOPH BOEHME, Department of Physics and Astronomy, University of Utah — Storing information in spin underpins the operation of a wide range of emerging technologies. However, the ability to interact with, and thus control electron spin implies a reasonable coupling to the environment, and a correspondingly limited spin coherence time. This problem can be overcome by using nuclear spins for long term information storage, and significant experimental progress in this direction has been seen recently. Readout of stored information can be achieved in a variety of ways, with electrical approaches offering substantial benefit with regard to integration of spintronic and classical electronic applications. Here, we discuss electrical readout of coherent nuclear spin states of donor nuclei in silicon. By utilizing nuclear Hahn echo sequences, we are able to demonstrate that nuclear spin phase coherence can exceed 3 ms with electrical readout. We find that the spin phase coherence is in this case limited by the spin lifetime of the donor electron which mediates our readout scheme, and discuss approaches to ameliorate this effect.

4:18PM X14.00008 ABSTRACT WITHDRAWN —

4:30PM X14.00009 Optical Orientation and Spin Relaxation of electrons and holes in Strained Germanium Quantum Wells¹, FABIO PEZZOLI, Università degli Studi di Milano-Bicocca, FEDERICO BOTTEGONI, FRANCO CICCACCI, STEFANO CECCHI, Politecnico di Milano, EMANUELE GRILLI, MARIO GUZZI, GIOVANNI ISELLA, Università degli Studi di Milano-Bicocca, DHARA TRIVEDI, PENGKE LI, YANG SONG, HANAN DERY, University of Rochester — We demonstrate optical orientation in strained Ge/SiGe quantum wells and study their spin properties. The energy proximity between the center of the Brillouin zone to its edge allows us to achieve high spin-polarization efficiency and to resolve the spin dynamics of holes and electrons. The circular polarization degree of the direct-gap photoluminescence is 37% and 86% for transitions with heavy and light holes states, respectively. Considering the ultrafast transition of electrons to L valleys, the extracted spin lifetime of holes at the top of the valence band is found to be 0.5 ps. This lifetime is governed by transitions between heavy and light hole states. The indirect-gap photoluminescence via the no-phonon line and its LA phonon replica allows us to study spin properties of electrons at the bottom of the conduction band. Taking into account the recombination lifetime of electrons (radiative and non-radiative channels), we find that their spin lifetime exceeds 5 ns below 150 K. Theoretical analysis of the electrons spin relaxation indicates that phonon-induced intervalley scattering by the X point phonon modes dictates the spin lifetime.

¹This work is supported by PRIN Project No. 20085JEW12, by Regione Lombardia through Dote ricercatori, by AFOSR Contract No. FA9550-09-1-0493, and by NSF Contract No. ECCS-0824075.

4:42PM X14.00010 Infrared Kerr measurements in ferromagnetic silicon carbide, ALOK MUKHERJEE, CHASE ELLIS, NADA TESAROVA, JOHN CERNE, Physics Dept., University at Buffalo, Buffalo, NY, YU LIU, SHUNCHONG WANG, GANG WANG, Institute of Physics, Chinese Academy of Sciences, China — We measure the infrared (100-1000 meV) polar Kerr angle in ferromagnetic silicon carbide (SiC). The Kerr angle is sensitive to the Hall conductivity σ_{xy} and measures the difference of optical responses for left and right circularly polarized light, which makes it a sensitive spectral probe for small changes in the symmetry of the system due to magnetic order. Both neutron-irradiated and Al-doped samples are studied in the 10-300K temperature range. This study provides new insights into the mechanisms by which non-magnetic impurities and defects can produce magnetic order. Strong frequency dependence and hysteresis are observed in the Kerr measurements. Work supported by NSF-DMR1006078.

4:54PM X14.00011 Low-temperature scattering-Scanning Near-field Optical Microscopy of Strongly Correlated Materials, MOLLY MAY, JOANNA ATKIN, MARKUS RASCHKE, University of Colorado at Boulder — Strongly correlated electron materials display diverse complex phenomena such as metal-insulator transitions and ferroelectric and ferromagnetic ordering, with characteristic lengths on the nanometer scale. In order to directly access and study the associated nano-phase behavior and domains for a wide range of materials, we have developed a low temperature tip-enhanced scattering-type scanning near-field optical microscope (s-SNOM). A microscopy flow cryostat reservoir is coupled to a shear-force atomic force microscope, with illumination of electrochemically etched Au tips provided by an on-axis high numerical aperture parabolic mirror. We will discuss the use of this system for the study and imaging of ferroic ordering in multiferroic and ferroelectric materials through the symmetry selectivity provided by tip-enhanced second harmonic generation (SHG) and nano-Raman crystallography via the tensor based selection rules.

Thursday, March 1, 2012 2:30PM - 5:18PM –
Session X15 DMP FIAP GMAG: Focus Session: Spin and Dynamics in Metal, Resonance Phenomena II: FMR in Magnetic Nanostructures 213

2:30PM X15.00001 Two dimensional spectroscopic imaging of individual ferromagnetic nanostripes, ROBERT MCMICHAEL, HAN-JONG CHIA, Center for Nanoscale Science and Technology, NIST, Gaithersburg MD, LYUBA BELOVA, Dept. of Matls. Science & Eng., Royal Institute of Technology, Stockholm — We report on high resolution imaging of the center and edge modes of individual Permalloy nanostripes using ferromagnetic resonance force microscopy (FMRFM). Fabrication of future spintronic devices requires an understanding of how edge damage affects a device's magnetic properties, and the highly localized edge modes of a nanostripe provide a direct method to investigate edge properties. While previous studies have measured spectra of the edge modes in large arrays of stripes, in this work we use FMRFM to image and probe the center and edge modes in individual NiFe stripes, 400 and 700 nm in width and 20 nm in thickness. Our spectroscopic measurements reveal different resonance fields for opposite edges of a stripe, which also exhibit different structural profiles. 2-D spatial imaging of the bulk and edge mode resonances demonstrates the inhomogeneity of the edge modes along their lengths with a resolution of 300 nm.

2:42PM X15.00002 Size dependent nonlinear effects of magnetization dynamics in Permalloy disks, FENG GUO, HAN-JONG CHIA, National Institute of Standards and Technology, University of Maryland, LYUBA BELOVA, Royal Institute of Technology, ROBERT MCMICHAEL, National Institute of Standards and Technology — We use ferromagnetic resonance force microscopy (FMRFM) to probe nonlinear magnetization dynamics in individual $\text{Ni}_{80}\text{Fe}_{20}$ disks with diameters ranging from 100 nm to 500 nm. The nonlinear behavior of magnetic nanostructures has important implications for rapid switching of memory devices and for frequency stability of spin torque oscillators. In the studied size range, micromagnetic modeling predicts a transition from complex power dependent behavior in the larger disks to simple behavior in the smallest disks where only a few modes are observed. At low power levels in the measurements, precession produces a force-detected signal that is linear in power and that displays a Lorentzian line shape. At higher powers, we observe nonlinear effects, including asymmetric line shapes and foldover where the resonance shifts with power. In addition, complex, jagged line shapes appear at high powers. We report that the onset power level of the nonlinear regime was found to be size dependent. In smaller disks, higher microwave power is required to drive nonlinear precession, and we see fewer complex peaks. Furthermore, the direction of foldover also depends upon the disk size. We have modeled our results using micromagnetic simulations and they display good correspondence with our experimental data.

2:54PM X15.00003 Electrically Detected Broadband Ferromagnetic Resonance in Individually Defined Permalloy Nanowires, ZHENG DUAN, CARL BOONE, ILYA KRIVOROTOV, UC Irvine, NATHALIE RECKERS, SVEN STIENEN, JUERGEN LINDNER, University of Duisburg-Essen, UC IRVINE TEAM, UNIVERSITY OF DUISBURG-ESSEN TEAM — We report measurements of electrically detected broadband ferromagnetic resonance (FMR) in lithographically defined Permalloy nanowires. For these measurements, the Permalloy nanowire is placed in close proximity to the short of a gold coplanar strip waveguide. The microwave power applied to the waveguide drives the magnetization precession in the wire and the four-point resistance of the wire is measured as a function of DC external magnetic field. The time-averaged resistance of the wire depends on the amplitude of the magnetization precession via anisotropic magnetoresistance (AMR), and thus peaks and dips with resistance dependence on the bias magnetic field arise from resonant excitation of spin wave modes in the wire. Using this electrically detected FMR technique, we measure the frequency and linewidth of the quasi-uniform mode of magnetization precession as well as bulk modes and edge modes that exist for the magnetic field applied in the plane of the sample perpendicular to the wire. We will present measurements of the resonance frequency and linewidth of various modes for several values of the wire width and compare our results to theoretical predictions of the field dependence of the mode frequency.

3:06PM X15.00004 Spin torque phenomena originating from the spin Hall effect: resonance, magnetic switching, and magnetic dynamics¹, LUQIAO LIU, Cornell University — The spin Hall effect (SHE) generates a transverse spin current with the passage of a current through a non-ferromagnetic metal (NM) film. Quite different results have been obtained for the magnitude of this effect. Here I will discuss a new technique where, by applying an RF current to a NM/FM thin film bilayer, the spin current onto the FM layer can induce a spin torque ferromagnetic resonance (ST-FMR). This enables the determination of the SHE strength with precision and without the need to assume the values of unmeasured parameters. The large magnitude of the SHE that we have established in several types of NM is sufficient to reversibly switch the magnetic orientation of a FM layer and I will discuss two different implementations of this. In the first the FM layer has a perpendicular-to-plane magnetic moment at equilibrium and the SHE injected spins are orthogonal to the moment. The spin torque can overcome the anisotropy (coercive) field restoring torque, with the polarity of the current-induced switching being determined by the sign of a small external field applied along the current direction. In the second approach, the FM moment lies in plane and the spins injected by the SHE exert a negative damping just as in conventional ST switching of a spin valve or magnetic tunnel junction (MTJ). We have fabricated three-terminal devices that incorporate a MTJ and a SHE layer to induce in-plane reversal switching. The simple architecture of this three terminal device and the high efficiency of the SHE induced switching made it a promising technique for future memory and non-volatile logic applications. We have also used this three terminal device to demonstrate DC induced dynamics in the magnetic layer due to the SHE.

¹With Chi-Feng Pai, O. J. Lee, T. J. Gudmundsen, D. C. Ralph and R. A. Buhrman

3:42PM X15.00005 Magnetostatics and magnetodynamics in single crystal Ni on MgO¹, MICHAEL PECHAN, BRIAN KASTER, MICHAEL SINKO, Department of Physics, Miami University, DAN DAHLBERG, Department of Physics and Astronomy, University of Minnesota, C.A. ROSS, GYE HYUN KIM, CARL V. THOMPSON, Department of Materials Science and Engineering, Massachusetts Institute of Technology — We present an investigation of the magnetic properties of 120 nm thick (100) and (110) oriented single crystal Ni films grown on MgO via evaporative deposition. X-ray diffraction analysis was used to confirm the single crystal nature and crystallographic orientations of the films. Magnetization measurements reveal anisotropy and magnetic moment consistent with bulk Ni values. Ferromagnetic resonance measurements have been made as a function of in-plane angle and temperature at 36 GHz. Resonance field maps confirm the anisotropy expected for high quality single crystal films. Both the anisotropy and damping are presented at temperatures ranging from 50 K to room temperature. Additional FMR results at 10 GHz are also presented from 4 K to room temperature. These results are discussed in the context of the temperature-dependent magnetocrystalline anisotropy of Ni and magnetoelastic anisotropy resulting from thermal mismatch between the Ni and MgO.

¹U.S. Dept. of Energy (MU), U.S. National Science Foundation MRSEC Program (MN) and U.S. National Science Foundation (MIT)

3:54PM X15.00006 Localized Edge Modes in Permalloy Square Antidot Arrays, J.B. KETTERSON, J. SKLENAR, Northwestern University, V.S. BHAT, L. DELONG, University of Kentucky, Lexington, O. HEINONEN, Northwestern University, Argonne National Laboratory — We have carried comprehensive experiments on and simulations of the ferromagnetic resonance spectrum of various thin films of permalloy patterned with a periodic array of holes on a square lattice. These so-called antidot lattices show a rich multi-line spectrum covering a wide range of frequencies and magnetic fields; they also exhibit striking angular dependences. One mode that is predicted in our simulations is highly localized at the edges of the holes. Our simulations further show that for a fixed field or excitation frequency the angular dependence of this mode strongly depends on the shape of the holes in the antidot array. It has been suggested¹ that, in comparison to other more extended modes, this localized mode would be difficult to find experimentally due to: i) the effects of varying shape and roughness present in an actual array, and ii) the fact that the mode is concentrated within a small fraction of the unit cell of the sample. Our experiments, performed with a broadband meanderline-based ferromagnetic resonance (FMR) spectrometer,² show a very weak resonance (requiring extensive signal averaging) that is in rough agreement with the simulations, which we propose as a candidate for this elusive edge mode.

¹S. Neusser, B. Botters and D. Grundler, Phys. Rev. B, 78, 054406 (2008).

²C. C. Tsai, J. Choi, S. Cho, B. K. Sarma, C. Thompson, O. Chernyashevskyy, I. Nevirkovets, and J. B. Ketterson, Rev. of Sci. Instr. **80**, 023904 (2009).

4:06PM X15.00007 Topological Localization of FMR Modes by Antidot Arrays Patterned into Permalloy Thin Films¹, VINAYAK BHAT, JUSTIN WOODS, LANCE DE LONG, University of Kentucky, JOSEPH SKLENAR, JOHN KETTERSON, Northwestern University, OLLE HEINONEN, Argonne National Laboratory — We have observed novel broad-band FMR spectra for 25-nm-thick Permalloy films patterned with square arrays of diamond antidots with axes $D_x = 1430$ nm and $D_y = 860$ nm. The y-axis lattice spacing was held constant at $d_y = 2000$ nm, and variable x-axis lattice spacings $d_x = 1730, 2000, 2267$ and 2730 nm. The applied DC magnetic field H (in-plane at angle θ with respect to x-axis) spanned the hysteretic regime $|H| \leq 150$ Oe, to $|H| = 3$ kOe in the saturated regime, corresponding to mode frequencies $f \approx 250$ MHz to 14 GHz. In spite of hysteretic evolution of domain walls in the low-field regime, highly reproducible absorption peaks appear at $f < 3$ GHz. Static and dynamic micromagnetic simulations agree with DC magnetization and FMR dispersion curves, and show domain pinning by the antidot edges is responsible for the reproducible spectra in the hysteretic regime. For $H = 1$ kOe along the x-axis, we observe two localized modes: one ($f = 9$ GHz) in a narrow gap between the acute vertices, and another ($f = 10.25$ GHz) between the oblique vertices, of adjacent diamonds. For $\theta = 45^\circ$, one mode ($f = 8.7$ GHz) extends along the (-1,1) direction with strong angular variation of f , and a standing mode ($f = 9.87$ GHz) is localized between nearly parallel edges of adjacent antidots.

¹Research at Kentucky supported by U.S. DoE Grant #DE-FG02-97ER45653.

4:18PM X15.00008 Ferromagnetic Resonance Studies of Individual Ferromagnetic Nanowires, ROHAN ADUR, INHEE LEE, The Ohio State University, STEFAN PHILIPPI, THOMAS MUHL, IFW Dresden, DENIS V. PELEKHOV, P. CHRIS HAMMEL, The Ohio State University — We investigate magnetization dynamics in ferromagnetic nanowires using two techniques: Ferromagnetic Resonance Force Microscopy (FMRFM) and Vector Network Analyzer Ferromagnetic Resonance (VNA-FMR). Using FMRFM we report our attempts at scanned probe FMR imaging of individual ferromagnetic nanowires. By placing ferromagnetic nanowires on permalloy we can use the capability of localized mode imaging (I. Lee et. al, Nature 2010) to measure local fields both in and around the ferromagnetic nanowire. In addition, we use VNA-FMR to study dipolar interactions in densely packed nanowire arrays. The dipolar fields between neighboring nanowires introduce an anisotropy field that can dominate over the shape anisotropy expected for isolated nanowires, and this effect is observed in the angular dependence of VNA-FMR spectra.

4:30PM X15.00009 Damping Dependence in Microwave Assisted Magnetization Reversal, YUNPENG CHEN, XIN FAN, QI LU, JOHN XIAO, University of Delaware — Microwave assisted magnetization reversal (MAMR) is one possible technique to mitigate the writability problem in ultrahigh density magnetic recording. In the presence of microwaves, the magnetization reversal of a magnetic recording material could be triggered at significantly reduced switching field. The damping constant is one of the critical parameters in magnetization switching for the magnetization precession spiraling down to the direction along the external field. We demonstrate microwave assisted magnetization reversal (MAMR) in a CoFeB film and the damping dependence in MAMR through the measurement of ferromagnetic resonance (FMR). Spin-pumping in non-ferromagnetic/ferromagnetic films provides a large range variation of Gilbert damping constants in magnetic samples when changing the thickness of non-ferromagnetic layers without changing the ferromagnetic film. An evident dependence of switching fields on the damping constant is observed in the presence of microwaves. The trend of the experiment data is well reproduced by a numerical simulation based on the Landau-Lifshitz-Gilbert equation. The result indicates that the large damping decreases the efficiency of microwaves in reducing the magnetization switching field.

4:42PM X15.00010 Theory of the ac spin valve effect: a new method to measure spin relaxation time¹, DENIS KOCHAN, MARTIN GMITRA, JAROSLAV FABIAN, University Regensburg — Parallel (P) and antiparallel (AP) configurations of FNF junctions have, in a dc regime, different resistivities ($R_{AP} > R_P$), giving rise to the giant magnetoresistance (GMR) effect, which can be explained within the spin injection drift-diffusion model. We extend the model to include ac phenomena and predict new spin dynamical phenomenon; the resonant amplification and depletion of spin accumulation in the P and AP configurations, respectively. As the major new effect, the spin valve magnetoimpedance of the FNF junction oscillates with the driving ac frequency, which leads to negative GMR effect ($|Z_{AP}| < |Z_P|$). We show that from the spin-valve oscillation periods, measured all electrically in the GHz regime, the spin relaxation times could be extracted without any magnetic field and sample size changes (contrary to other techniques). For thin tunnel junctions the ac signal becomes pure Lorentzian, also enabling one to obtain the spin relaxation time of the N region from the signal width. This work, was published in Physical Review Letters,¹⁰, 176604 (2011).

¹This work was supported by DFG SFB 689

4:54PM X15.00011 Vortex Resonance in Coupled Ferromagnetic Disks, SHIKHA JAIN, HELMUT SCHULTHEISS, JOHN PEARSON, FRANK FRADIN, SAMUEL BADER, VALENTYN NOVOSAD, Argonne National Laboratory — Advances in nanolithography and thin film growth techniques offer the unique opportunity to prepare a variety of laterally confined nanostructured magnets. Of particular interest are lithographically patterned micron and submicron disk-shaped particle arrays. The magnetic ground state in confined geometries consists of a curling spin configuration, known as a vortex state. Studies of vortex dynamics have mainly focused on circular or elliptical dots at remanence. In this work, we investigate the dynamic response of vortex gyration in interacting systems where two circular dots are statically exchange coupled. The induced coupling due to the interacting area forces the disks to have antiparallel chirality of magnetization. Apart from different vortex polarity combinations, various frequency modes were observed as a function of external magnetic field and contact length. Moreover, due to the induced configurational anisotropy in the system, vortex resonance in the two disks was found to be strongly dependent on the orientation of the static magnetic field.

5:06PM X15.00012 Study of the coupling of vortices in magnetic nanodisks, ALBERTO GUIMARAES, Brazilian Center for Physical Research (CBPF), Rio de Janeiro, Brazil, GABRIEL FIOR, FLAVIO GARCIA, LNLs, Campinas, Brazil — There is a marked interest nowadays in the dynamic behavior of magnetic nanodisks that present magnetic vortices [1]. The tailoring of vortex features, including their gyrotropic frequency, critical vortex core switching velocity and strength of the coupling between nanodisks, is very desirable for future applications, such as vortex magnetic memories (VRAMs) and spin transfer nanooscillators (STNOs) [2]. An original way to tune some of the static vortex properties (specially the vortex core diameter) is simply to introduce a uniaxial perpendicular magnetic anisotropy, as has been recently shown [3]. Here we have studied the coupling between vortices as a function of the magnetic properties of the disks and their separation, using micromagnetic simulations. We analyzed the motion of a vortex core caused by the motion of the second one, excited by static or rotating magnetic fields. A splitting of the gyrotropic frequency is also observed. Exciting one of the disks, it is possible to switch the core polarity of the other. These results open new possibilities for applications of magnetic vortices.

[1] Ruotolo et al. *Nat Nano*, 4(8):528-532, (2009);

[2] Jung et al. *Sci. Rep.* 1, 59; DOI:10.1038/srep00059 (2011);

[3] Garcia et al. *APL*, 97, 022501 (2010).

Thursday, March 1, 2012 2:30PM - 5:06PM – Session X16 DCMF: Manganites: Perovskite and Bilayer 251

2:30PM X16.00001 Persistence of Jahn-Teller Distortion up to the Insulator to Metal Transition in LaMnO_3 , MARIA BALDINI, HpSynC, Carnegie Institution of Washington, Argonne, Illinois USA, VIKTOR STRUZHNIKIN, ALEX GONCHAROV, Geophysical lab. Carnegie Institution of Washington, Washington D.C. USA, PAOLO POSTORINO, Dipartimento di Fisica, Università "Sapienza," Roma Italy, WENDY MAO, Geological and Environmental Science, Stanford University, California USA — High pressure, low temperature Raman measurements performed on LaMnO_3 up to 34 GPa provide the first evidence for the persistence of the Jahn-Teller distortion over the entire stability range of the insulating phase. This result resolves the ongoing debate about the nature of the pressure driven insulator to metal transition (IMT), demonstrating that LaMnO_3 is not a classical Mott insulator. The formation of domains of distorted and regular octahedra, observed from 3 to 34 GPa, suggests that LaMnO_3 becomes metallic when the fraction of undistorted octahedra domains increases beyond a critical threshold. In this scenario, it is interesting to consider whether or not the CMR effect may be induced in LaMnO_3 by applying pressure. Preliminary results obtained performing high pressure resistivity measurements in a magnetic field will be reported.

[1] I. Loa, et al., *Phys. Rev. Lett.* 87, 125501 (2001).

[2] A.Y. Ramos et al., *Phys. Rev. B* 75, 052103(2007).

[3] A.Y. Ramos et al., *J. Phys. Conf. Ser.* 190, 012096 (2009).

[4] A. Yamasaki et al., *Phys. Rev. Lett.* 96, 166401 (2006).

[5] J. D. Fuhr et al., *Phys. Rev. Lett.* 100, 216402 (2008).

[6] M. Baldini et al., *Phys. Rev. Letter* 106, 066402 (2011).

2:42PM X16.00002 Influence of Gd-doping in $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ on its structural and Magnetoelectrical Properties, SEVGI POLAT ALTINTAS, Abant Izzet Baysal University, ABDERREZAK AMIRA, Université de Jijel, CABIR TERZIOGLU, Abant Izzet Baysal University — We present a study of the structural and electrical properties of lanthanum-based manganite, $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ with $x=0.0$ and 0.1 . The samples synthesized by the conventional solid state reaction method. The samples are characterized by X-ray diffraction, scanning electron microscope and energy dispersive X-ray spectrometer. The electrical and magneto-transport properties of bulk samples have been investigated in the temperature range 5-300 K and a magnetic field up to 7 T. Although the replacement of La ion by Gd results a decrease in metal-insulator transition temperature TMI, the magnetoresistance and resistivity are found to be increased. The electrical resistivity in the entire temperature range fit well with the phenomenological percolation model, which is based upon an approach that the system consists of the phase separated ferromagnetic metallic and paramagnetic insulating regions.

2:54PM X16.00003 Size control of Magnetism, Charge and Orbital Order in Half-Doped Manganite, $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ ¹, TANUSRI SAHA-DASGUPTA, S.N.Bose National Centre for Basic Sciences, HENA DAS, Cornell University, G. SANGIOVANNI, A. VALLI, K. HELD, Institute for Solid State Physics, Vienna University of Technology, 1040 Wien, Austria — Motivated by recent experimental results, we study the effect of size reduction on half-doped manganite, $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$, using the combination of density functional theory (DFT) and dynamical mean field theory (DMFT). We find that upon size reduction, the charge-ordered antiferromagnetic phase, observed in bulk, to be destabilized, giving rise to the stability of a ferromagnetic metallic state. Our theoretical results, carried out on defect-free nanocluster in isolation, establish the structural changes that follow upon size reduction to be responsible for this. Our study further points out the effect of size reduction to be distinctively different from application of hydrostatic pressure. Interestingly, our DFT+DMFT study, additionally, reports the correlation-driven stability of charge-orbitally ordered state in bulk $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$, even in absence of long range magnetic order.

¹To appear in Physical Review Letters

3:06PM X16.00004 Measuring Coexisting Phases in $\text{La}_{0.35}\text{Pr}_{0.275}\text{Ca}_{0.375}\text{MnO}_3$ ¹, MARK H. BURKHARDT, SIMES, SLAC National Accelerator Laboratory and Stanford University, M.A. HOSSAIN, S. SARKAR, H.A. DÜRR, J. STÖHR, SIMES, SLAC National Accelerator Laboratory, Y.-D. CHUANG, A.G. CRUZ GONZALEZ, A. DORAN, A. SCHOLL, A.T. YOUNG, Advanced Light Source, Lawrence Berkeley National Laboratory, Y.J. CHOI, S.-W. CHEONG, Rutgers Center for Emergent Materials and Department of Physics & Astronomy — Manganite compounds in the $\text{La}_{0.625-y}\text{Pr}_y\text{Ca}_{0.375}\text{MnO}_3$ series are known for exhibiting phase separation over a large temperature range. We combined the x-ray photoemission electron microscopy (PEEM) and resonant elastic soft x-ray scattering (RSXS) techniques to study the interplay between the low-temperature ferromagnetic and intermediate temperature charge-ordered/antiferromagnetic phases, respectively, in $\text{La}_{0.35}\text{Pr}_{0.275}\text{Ca}_{0.375}\text{MnO}_3$. We found that the system is driven by glassy polarons, which are present above the curie temperature T_C in many ferromagnetic metallic manganites. They stunt the growth of the ferromagnetism on cooling: we clearly observe the onset of small, strained ferromagnetic domains almost 30 K above the temperature where ferromagnetism fully sets in, and the ferromagnetism has a very unconventional temperature dependence even below T_C . This relationship could explain the need for such high magnetic fields to induce colossal magnetoresistance.

¹This research and the ALS are supported by U.S. Department of Energy, Office of Basic Energy Science.

3:18PM X16.00005 Oxygen Vacancy Induced Metal Insulator Transition in Epitaxial $\text{Pr}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ Thin Films¹, JINGDI ZHANG, KEBIN FAN, Boston University, RYUHEI KINJO, WEIMING XU, IWAO KAWAYAMA, MASAYOSHI TONOUCHI, Osaka University, XIN ZHANG, RICHARD AVERITT, Boston University — We report the metal-insulator transition in epitaxial $\text{Pr}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ thin film by introducing oxygen vacancies, which assist the nucleation of ferromagnetic metallic domains in an antiferromagnetic insulating matrix. The hysteresis of the resistivity indicates the transition is first-order, and covers a broad temperature range from 80K to 220K. Such novel transport properties of the $x=0.3$ doped manganite may result from strong spin-lattice coupling which stabilizes the system to a metallic metastable state at low temperature.

¹We acknowledge DOE BES support.

3:30PM X16.00006 Search for Multi-Ferroic Manganites with Elongated Mn-O bonds, BOGDAN DABROWSKI, JAMES MAIS, STANISLAW KOLESNIK, Department of Physics, Northern Illinois University, DeKalb, IL — Development of multi-ferroic materials, where magnetism and ferroelectricity are strongly coupled near room temperature, is of fundamental technological and theoretical importance. Typically, both phenomena tend to be mutually exclusive because ferroelectricity is usually present for d^0 and magnetism for non- d^0 transition metals. By analogy to perovskite $\text{Ba}^{2+}\text{Ti}^{4+}\text{O}_3$ (d^0) for which [Ti-O] bonds are highly elongated beyond their equilibrium lengths resulting in Ti distortion out of the center of the TiO_6 octahedral unit, resulting in $T_F \sim 400$ K ferroelectricity, we have projected that similar effect should be observed for the non- d^0 insulating and antiferromagnetic ($T_N \sim 240$ K) perovskites of Mn^{4+} (d^3). I will describe our search for such compounds guided by our “tolerance factor design rules” in the (Sr,Ba)MnO₃ system for which strong multi-ferroic behavior was achieved near room temperature.

3:42PM X16.00007 Formation of mesoscopic metallic filaments in manganite thin films imaged by microwave impedance microscopy, WORASOM KUNDHIKANJANA, KEJI LAI, YONGLIANG YANG, YUE MA, MICHAEL KELLY, ZHI-XUN SHEN, Stanford University, MASAO NAKAMURA, ZHIGAO SHENG, MASASHI KAWASAKI, YOSHI TOKURA, RIKEN, Japan, STANFORD UNIVERSITY COLLABORATION, RIKEN, JAPAN COLLABORATION — We study the ferromagnetic metallic domains from the charge-order insulating background at mesoscopic length scale in a $\text{Pr}_{0.55}\text{Ca}_{0.75}\text{Sr}_{0.25}\text{MnO}_3$ thin film using a variable temperature microwave impedance microscope (MIM). The metallic state in this compound can be easily induced at a moderate magnetic field as low as 2 T observed by both the transport and MIM. The temperature dependent transport under 1.2 T shows a large hysteresis loop. MIM allows us to observe the formation and melting of metallic domains at different temperatures during the cooling and warming processes. At higher temperatures, the metallic domains first emerge in small isolated filaments along certain crystal axes of the LSAT(110) substrate, suggesting that the local strain plays an important role. Surprisingly, small insulating islands remain in the metallic ground state and persist up to very high magnetic fields, indicating strong pinning sites. Lastly, the sizes of the insulating islands at the ground state increase when the film is field cooled at lower speeds, suggesting a glassy order in this compound.

3:54PM X16.00008 Imaging of nano domain fluctuations in manganites¹, MIRIAN GARCIA FERNANDEZ, STUART WILKINS, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA, HONG ZHENG, JOHN MITCHELL, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA — We present a soft x-ray resonant diffraction study of the electronic spatial nano-scale domains present in manganites. We explain the details of our new set up that allow us to perform this diffraction contrast microscopy in the nano regime. We will present preliminary results on the nanoscale domains in the bilayer manganite $\text{LaSr}_2\text{Mn}_2\text{O}_7$. The structural reflection (002) and the A-type antiferromagnetic reflection (001) have been investigated with soft x-rays in the vicinity of the manganese L_3 edge. A resolution of ~ 150 -200 nm has been achieved by implementing a zone plate focusing optic in our diffraction set up. These two reflections have been mapped in the same region of the sample. This region has dimensions of 20×20 microns. We will present measurements comparing the magnetic nano scale domains in $\text{LaSr}_2\text{Mn}_2\text{O}_7$ probed directly by measuring the (001) antiferromagnetic reflection, with crystallographic inhomogeneities that are observed in the mapping of the (002) crystallographic reflection. Finally, future directions using this setup will be discussed for the study of strongly correlated systems.

¹Work performed at BNL was supported by the US Department of Energy, Division of Materials Science, under Contract No.DEAC02-98CH10886.

4:06PM X16.00009 Fragile Magnetic Ground State in Half-Doped Manganite $\text{LaSr}_2\text{Mn}_2\text{O}_7$: Orbital Instability, J.-S. LEE, C.-C. KAO, SSRL/SLAC, C.S. NELSON, BNL, S.B. KIM, Y.J. CHOI, S.-W. CHEONG, Rutgers Univ., S. SMADICI, P. ABBAMONTE, UIUC, H. JANG, K.-T. KO, J.-H. PARK, POSTECH — Recently, a careful doping control study, however, reported that the $\text{La}_{2-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$ material has an exotic phase diagram very near the half doping with extremely narrow antiferromagnetic phase boundaries at $x \approx 0.5 \pm 0.005$ — the CE-type within the boundaries but the A-type outside.¹ To understand a complexity on this material's phase diagram, we investigated the orbital and antiferromagnetic ordering behaviors of the half-doped bilayer manganite $\text{La}_{2-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$ ($x \approx 0.5$) by using Mn $L_{2,3}$ -edge resonant soft x-ray scattering. We confirmed the predicted CE-type antiferromagnetic order for the true half-doped ($x = 0.5$) case. Moreover, we found that such a narrow phase boundary is due to the close competition of the two antiferromagnetic ordering phases via 3d Mn e_g orbital instability. Our study reveals the spin and orbital orders of electrons in the sample as well as information about their ground states.²

¹Q. Li *et al.*, Phys. Rev. Lett. 98, 167201 (2007).

²J.-S. Lee *et al.*, Phys. Rev. Lett. 107, 037206 (2011).

4:18PM X16.00010 Bilayer manganites reveal polarons in the midst of a metallic breakdown¹, F.

MASSEE, S. DE JONG, Y. HUANG, W. K. SIU, I. SANTOSO, A. MANS, Van der Waals-Zeeman Institute, University of Amsterdam, 1018XE Amsterdam, The Netherlands, A. T. BOOTHROYD, D. PRABHAKARAN, Clarendon Laboratory, Oxford University, OX1 3PU Oxford, UK, R. FOLLATH, A. VARYKHALOV, BESSY GmbH, Albert-Einstein-Strasse 15, 12489 Berlin, Germany, L. PATTHEY, M. SHI, Paul Scherrer Institute, Swiss Light Source, CH-5232 Villigen, Switzerland, J.B. GOEDKOOP, M.S. GOLDEN, Van der Waals-Zeeman Institute, University of Amsterdam, 1018XE Amsterdam, The Netherlands — Just what tips the balance between the wealth of competing phases and textures in spin, charge and orbital degrees of freedom in the CMR manganites such as $\text{La}_{2-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$ (LSMO)? Combining ARPES and STM/S measurements on bilayered LSMO ($0.30 \leq x < 0.5$), we arrive at a compelling explanation for the seemingly contradictory data on the electronic structure of bilayered LSMO that has appeared in the literature. We show that the true signature of bilayered ($N=2$) LSMO is that of a gapped non-metal on the verge of a metallic breakdown. All the former confusion stems from the intrinsic presence of stacking faults leading to either more gapped single layer ($N=1$) LSMO or sharply peaked, $N>2$ slabs displaying true metallic double-exchange.

¹This work is part of the research program of the Foundation for Fundamental Research on Matter (FOM), which is part of the Netherlands Organisation for Scientific Research (NWO).

4:30PM X16.00011 The intrinsic electronic structure of bilayer manganites from Angle Resolved Photoemission, S.

SANNE DE JONG, SLAC National Accelerator Laboratory/ LCLS, R. KUKREJA, M.A. HOSSAIN, SLAC National Accelerator Laboratory/ SINES, M.S. GOLDEN, E. VAN HEUMEN, F. MASSEE, Y. HUANG, University of Amsterdam, WZI, A.T. BOOTHROYD, P. PAB-HAKARAN, University of Oxford, Dept. Phys., A. WALTER, A. BOSTWICK, E. ROTENBERG, ALS, Lawrence Berkeley National Laboratory, H.A. DURR, SLAC National Accelerator Laboratory/ PULSE, SINES — The Colossal MagnetoResistant (CMR) manganites are one of the most studied condensed matter physics systems since decades. Yet, the mechanism behind the CMR effect and their electronic structure are still under hot debate. Recent angle resolved photoemission (ARPES) studies on the bilayer manganite $\text{La}_{(2-2x)}\text{Sr}_{(1+2x)}\text{Mn}_2\text{O}_7$, LSMO327, reported contradictory results [1]. Here we present an ARPES study unveiling the intrinsic k - and temperature dependent electronic structure of LSMO327, while carefully steering away from the recently reported sample inhomogeneities [2] that have caused all the confusion.

[1] N. Mannella, Nature (2005); S. Sun Nature Phys. (2007); S. de Jong, PRB (2007)

[2] F. Massee, Nature Phys(2011)

4:42PM X16.00012 Unconventional response of acoustic phonons to the onset of charge order in a bilayer manganite, S.

ROSENKRANZ, Argonne National Laboratory, F. WEBER, Karlsruhe Institute of Technology, J.P. CASTELLAN, R. OSBORN, H. ZHENG, J.F. MITCHELL, Argonne National Laboratory, S. CHI, J.W. LYNN, NIST Center for Neutron Research, D. REZNIK, University of Colorado, Boulder — The acoustic phonons in the 50% doped bilayer manganite $\text{LaSr}_2\text{Mn}_2\text{O}_7$ exhibiting CE type charge order were investigated using inelastic neutron scattering. At the onset of charge ordering, we observe an abrupt increase of the energies and a decrease of the linewidths of the transverse mode along (1,1,0), which crosses the CE ordering wavevector. This effect is however not localized to the CE ordering wavevector, but is observed over an extended range of momentum transfers for which the phonon energy is lower than 15 meV. These observations indicate a reduced electron-phonon coupling due to a partial removal of the Fermi surface and provide direct evidence for a link between electron-phonon coupling and charge order in manganites. However, the observed response of the phonons is not consistent with a standard CDW mechanism, clearly showing that the transition is unconventional. Work supported by US DOE BES-DMS DE-AC02-06CH11357.

4:54PM X16.00013 Magnetoelastic Spin Flip in $\text{La}_{1.4}\text{Sr}_{1.6}\text{Mn}_2\text{O}_7$, K.-T. KO, H. JANG, J.-H. PARK, Dept. Physics,

Pohang University of Science and Technology, Korea, B.-G. PARK, J.-Y. KIM, Pohang Accelerator Laboratory, SUNG BAEK KIM, The College of General Education, Konyang University, Korea, S.-W. CHEONG, Dept. Physics and Astronomy, Rutgers University, USA — The magnetoelastic coupling in a bilayer manganite was investigated by using x-ray absorption spectroscopy (XAS) and resonant soft x-ray scattering (RSXS) at Mn $L_{2,3}$ -edge. Huge occupation reversal of e_g level from $d_{3z^2-r^2}$ to $d_{x^2-y^2}$ was observed at the temperature and magnetic field induced phase transition in $\text{La}_{1.4}\text{Sr}_{1.6}\text{Mn}_2\text{O}_7$. The CI model calculation indicated that the direction of magnetocrystalline anisotropy is affected by the configuration of e_g level, and the sharp spin flip transition was expected. The field dependent RSXS measurements demonstrated a strong magnetoelastic coupling in $\text{La}_{1.4}\text{Sr}_{1.6}\text{Mn}_2\text{O}_7$, where the AFM spin axis was changed from out-of-plane to in-plane as a result of the field induced change of e_g orbital occupation. Finally, we discuss the spin-orbital-lattice coupling in bilayer manganites.

Thursday, March 1, 2012 2:30PM - 5:30PM –

Session X17 DMP: Focus Session: Nanostructures and Metamaterials, Growth, Structure, and Characterization – Improved Materials and Applications II 252A

2:30PM X17.00001 Low-loss multilayered metamaterial exhibiting a negative index of refraction at visible wavelengths¹, CARLOS GARCIA-MECA, Universidad Politecnica de Valencia. Nanophotonics Technology Center. — Over the

last decade, metamaterials have attracted a great interest thanks to their potential to expand the range of electromagnetic properties found in natural materials. In particular, the possibility of achieving negative refractive index media (NIM) enables us to implement superlenses and optical storing devices. Since the first experimental demonstration at microwave frequencies, much effort has been put in extending negative refraction to the visible spectrum, where we can take full advantage of NIM properties. For instance, the superior imaging ability of NIM would be essential for visible microscopy. The desired features for NIM are low loss and isotropy. This last property includes polarization independence and negative-index behavior in all spatial directions. None of these features have been attained in previous experiments. Thus, the current challenge is to improve such aspects in order to make NIM suitable for practical applications. In this work, we experimentally demonstrate a low-loss multilayer metamaterial exhibiting a double-negative index in the visible spectrum, while presenting polarization independence at normal incidence. This has been achieved by exploiting the properties of a second-order magnetic resonance of the so-called fishnet structure, in contrast to previous works that used first-order magnetic resonances, both related to gap surface plasmon polariton (SPP) modes. The low-loss nature of the employed magnetic resonance, together with the effect of the interacting adjacent layers, results in a figure of merit as high as 3.34. A wide spectral range of negative index is achieved, covering the wavelength region between 620 and 806 nm with only two different designs. The fabricated metamaterials are the first experimental multilayer NIM in the visible spectrum, which entails an important step towards homogeneous NIM in this range. Finally, we found that the SPP modes determining the permeability resonance display weak angular dispersion.

¹Financial support by the Spanish Ministerio de Ciencia e Innovacion (contract CSD2008-00066 and FPU grant) is gratefully acknowledged.

3:06PM X17.00002 Photonic-Plasmonic Coupling and Near Field Engineering in Nanoparticle Necklaces, ALYSSA PASQUALE, Boston University Electrical and Computer Engineering Department, BJÖRN REINHARD, Boston University Chemistry Department, LUCA DAL NEGRO, Boston University Electrical and Computer Engineering Department — Particle clusters with different degrees of rotational symmetry consisting of circular loops of gold nanoparticles, dubbed nanoplasmonic necklaces, are proposed as a novel, reproducible platform for elastic and inelastic optical sensors with polarization insensitive behavior. Engineering of the necklaces allows for full control of the plasmonic hot-spot locations and near-field strength by coupling photonic resonances to the circular resonator structure. The polarization insensitivity of necklaces guarantees that the plasmonic hot-spots remain excited within the necklaces irrespective of the incident polarization of the excitation field, which is a significant advantage compared to hot-spots in dimer configurations. Near-fields can be further enhanced using radiative coupling in concentric necklaces having integer multiple diameters. Engineering design rules are determined for hot-spot formation, polarization insensitivity, and intensity distribution in necklaces using 3-dimensional Finite-Difference Time-Domain simulations. Plasmonic necklaces of different rotational axes were fabricated using electron-beam lithography and electron-beam deposition of gold films. Surface enhanced Raman scattering measurements were used to experimentally validate our near-field calculations.

3:18PM X17.00003 Probing Thermomechanics at the Nanoscale: Impulsively Excited Pseudo-surface Acoustic Waves in Hypersonic Phononic Crystals, D. NARDI, Q. LI, K. HOOGEBOOM-POT, M. MURNANE, H. KAPTEYN, JILA - University of Colorado at Boulder, USA, M. SIEMENS, Department of Physics and Astronomy - University of Denver, USA, M. TRAVAGLIATI, Center for Nanotechnology Innovation @NEST - IIT, Pisa, Italy, F. PARMIGIANI, Dipartimento di Fisica - Università degli Studi di Trieste, Italy, G. FERRINI, F. BANFI, Dipartimento di Matematica e Fisica - Università Cattolica, Brescia, Italy — Hypersonic-frequency surface acoustic waves can be generated by ultrafast laser excitation of nanoscale patterned surfaces and are of great interest because of their high sensitivity to the mechanical properties of the material in which they propagate. By modeling nanoscale thermomechanics from first principles, we can calculate a composite system's initial heat-driven response and follow its evolution in time. A spectral decomposition of the response on the calculated eigenmodes of the system allows evaluation of impulsively excited pseudosurface acoustic wave frequencies and lifetimes, expanding our understanding of surface waves scattering in mesoscale metamaterials, while providing crucial information about non-destructive photoacoustic characterization and imaging of nanostructures for nanoelectronics, nanomedicine and photovoltaic applications. The model is successfully benchmarked against time-resolved optical diffraction measurements performed on 1D and 2D surface phononic crystals, probed using extreme ultraviolet and near-infrared light. Reference: D. Nardi et al., Nano Lett. 11, 4126 (2011).

3:30PM X17.00004 Plasmonic nanotips for spectroscopy with nanometer-scale resolution, JOHANNES FEIST, ITAMP, Harvard-Smithsonian Center for Astrophysics, SEMION K. SAIKIN, Department of Chemistry and Chemical Biology, Harvard University, M.T. HOMER REID, Research Laboratory of Electronics, Massachusetts Institute of Technology, ALÁN ASPURU-GUZIK, Department of Chemistry and Chemical Biology, Harvard University, MIKHAIL D. LUKIN, Department of Physics, Harvard University — We theoretically investigate the use of metallic nanotips, i.e. nanowires with a sharp tip, as tools for spectroscopic applications such as surface-enhanced Raman scattering (SERS). Nanotips can provide strong coupling between guided plasmon modes and single emitters such as atoms or molecules. At the same time, the spatial localization of the plasmon response can potentially provide nanometer-scale spatial resolution in a scanning-tip setup. In particular, we will focus on the possibilities of transporting the electromagnetic field to the target through the surface plasmon mode on the wire, and on coupling the emitted radiation into the same mode. We compare the performance of such an approach with more conventional SERS setups, where localized surface plasmons are used to enhance the local field of an incoming laser beam and the emitted free-space radiation. Finally, we will discuss whether single-molecule sensitivity can be reached.

3:42PM X17.00005 Structural and Optical Properties of Metals in Photonic Semiconductor Devices, MENG-MU SHIH, University of Florida — Metals can play important roles in semiconductor photonics if properly incorporated and designed. The mode-coupling coefficient of the periodic waveguide in the device is the key parameter for analyzing optoelectronic performance. This work constructs a modified model to show how the metal gratings on the semiconductor surfaces and how the metal compositions inside the semiconductors can affect the coupling coefficients. Metal gratings with various materials and nano-structures can affect optical interactions at corrugated metal-semiconductor interfaces. Optical effects such as wavelength and wave polarization can affect the optical properties of metals and semiconductors. In addition, metal compositions in semiconductor compounds can change the optical properties of semiconductors. Semiconductors with different optical and structural properties can generate specific wavelengths. Consequently, the above factors related to optical properties and interactions of metals can affect the coupling coefficients. Computational results with physical interpretations provide insights into photonic devices for more applications.

3:54PM X17.00006 Cavity Resonances in Plasmonic Patch Nanoantennas, AYAN CHAKRABARTY, FENG WANG, FRED MINKOWSKI, QI-HUO WEI, Kent State University — Plasmonic nanoantennas allow for confining and detecting photons at very small length scales. This work presents our recent experimental and theoretical studies of two dimensional periodic arrays of elliptical metal nano-patches on a silver film with a dielectric gap layer. Simulation and theoretical results shows that various cavity modes can be excited with tilted or normal incident light, and that the azimuthal symmetry breaking makes the nanoantennas polarization sensitive due to different resonant frequencies of the even and odd cavity modes. Particularly, it is shown that the cavity modes can be well described by a product of Mathieu functions, providing good agreements with both simulations and experiments. The effects of coupling between the cavity modes and the propagating plasmons will be discussed.

4:06PM X17.00007 Efficient calculation for waveguides and for photonic crystal band structures using improved finite elements in 2D¹, C.R. BOUCHER, C.I. AHENG, L.R. RAM-MOHAN, WPI — We employ scalar, fifth-order Hermite interpolation polynomials to solve Maxwell's equations in two dimensions in the finite element method. We analyze homogeneous conducting waveguides, inhomogeneous waveguides, and photonic crystals. The Hermite interpolation functions provide greater accuracy than vector finite elements of equal polynomial order, while bypassing the issue of spurious modes observed when using Lagrange polynomials. The scalar Hermite elements offer a level of flexibility which is not seen with vector finite elements, as in multiphysics problems such as coupled Schrödinger-Maxwell problems. The use of Hermite elements is an attractive alternative to plane-wave methods for modeling photonic crystals, leading to sparse matrices due to local connectivity of the finite elements, greater flexibility in modeling, and lower computational costs.

¹This work has been supported by Quantum Semiconductor Algorithms, Inc., and by AFRL/DARPA under grant FA8650-10-1-7046. 1

4:18PM X17.00008 Diffusion of a Plasmon-Exciton Polaron¹, CHARLES CHERQUI, DAVID DUNLAP, Department of Physics and Astronomy, University of New Mexico, ANDREI PIYATINSKI, Center for Nonlinear Studies, Los Alamos National Lab — We consider the motion of an exciton constrained to a quasi-one-dimensional geometry in the vicinity of a metal interface. For weak coupling, the metal causes damping of the center of mass motion, leading to a decrease in the exciton diffusion constant. This can be modeled as non-contact dielectric friction between an oscillating dipole and a substrate, where the frictional force is related to the response of the metal through the fluctuation dissipation theorem [1]. When the exciton frequency is in the neighborhood of the plasma resonance, the interaction can no longer be described by linear response theory, for the exciton and plasmon form a quasiparticle, an exciton-plasmon polaron. We calculate the transmission and reflection coefficients for the exciton-plasmon polaron in the neighborhood of a metal interface, as well as the diffusion rate and radiative lifetime versus coupling strength.

[1] Seppe Kuehn, John A. Marohn, and Roger F. Loring, 110(30) J. Phys. Chem. B, (2006) 1425

¹Work supported by the Department of Energy and the Center for Nanointegrated Technologies

4:30PM X17.00009 Coherent interband transport in binary zigzag optical waveguide arrays¹, KIN CHUNG AU YEUNG, NAI JING DENG, CHEUNG WAI CHAU, SAI KIT YUNG, KIN WAH YU, The Chinese University of Hong Kong — We have studied the optical oscillation and Zener tunneling of light waves in binary zigzag optical waveguide arrays in which the evanescent coupling in the array is included up to the second order. By tuning the ratio of the first order and second order coupling strengths, there is a miniband-minigap structure in the dispersion diagram. Moreover, by adding a gradient in the propagation constant transverse to propagation, Bloch-Zener oscillation (BZO) and Zener tunneling between two bands can be realized. The occurrence of BZO and Zener tunneling is simulated by the field-evolution analysis using an input Gaussian beam. Through a visual band picture, the simulation results confirm the band structure of the waveguide arrays. A rate equation is proposed to understand the coherent transport behaviors between the two minibands across the gap.

¹Supported by the General Research Fund of the HKSAR Government

4:42PM X17.00010 Tunable rainbow trapped in a self-similar liquid crystal waveguide, QING HU, SI-HUI WANG, DI-HU XU, YU ZHOU, RU-WEN PENG, MU WANG, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China — We have investigated the optical propagation through a self-similar dielectric waveguide, where a hollow core is surrounded by a coaxial Thue-Morse multilayer. It is found that due to the self-similar furcation feature in the photonic band structure, the transmission multibands are achieved. And different frequency ranges of the transmission modes can be selectively guided and spatially confined along the waveguide. Consequently, a rainbow can be trapped in the waveguide. Then by infiltrating liquid crystal into the cladding layers, the transmission modes and rainbow trapping can be tuned by altering the temperature. And transverse electric (TE) and transverse magnetic (TM) polarizations present different propagating features. The attenuation and energy density distributions of different modes in the waveguide are also discussed. The finding can be applied to designing miniaturized compact photonic devices, such as a spectroscopy on a chip, color-sorters on a chip, and photon sorters for spectral imaging. Reference: Qing Hu, Jin-Zhu Zhao, Ru-Wen Peng, Feng Gao, Rui-Li Zhang, and Mu Wang, Appl. Phys. Lett. (2010) 96, 161101; and Qing Hu, Ru-Wen Peng, Si-Hui Wang, and Mu Wang, manuscript prepared(2011).

4:54PM X17.00011 A New Strategy for Designing Broadband Epsilon-Near-Zero Metamaterials¹, HON PING LEE, KA SHING HUI, LEI SUN, KIN WAH YU, The Chinese University of Hong Kong — We have developed a new strategy for designing metamaterials in multi-layered film with permittivity being closed to zero over a broad frequency range, which is as known as broadband epsilon-near-zero (ENZ) materials. Milton representation, Bergman-Milton representation and electromagnetic representation of the effective permittivity (ϵ_{eff}) are used, and the strategy consist of the following 3 parts: choosing the operation frequency range, properly placing the poles and zeros into the range, and solving the inverse problem by equating different representations of ϵ_{eff} . Demonstration of the strategy is carried out by zeroth and first order design with several examples. The distribution of electric field inside the designed materials is investigated to reveal the physical principles of the broadband ENZ phenomenon. The study would be further extended to other geometries (e.g. multi-shell cylinder) through conformal transformation. The results obtained are useful for designing ENZ metamaterials.

¹Work supported by the General Research Fund of Hong Kong SAR Government

5:06PM X17.00012 Effective permittivity of ensemble-averaged waves in dense random plasmonic composites¹, SATVIK WANI, Department of Biomedical and Chemical Engineering, Syracuse University, Syracuse, NY 13244, USA, ASHOK SANGANI², National Science Foundation, Arlington, VA 22230, USA, RADHAKRISHNA SURESHKUMAR, Department of Biomedical and Chemical Engineering and Department of Physics, Syracuse University, Syracuse, NY 13244, USA — Random composites of metallic nanospheres (Ag, Au, Cu, etc.) in transparent media are highly opaque due to absorption resulting from plasmon resonance. A new technique for calculating the effective properties of such dense composites is described. The underlying physical motif is the separation of the space surrounding any inclusion into two regions, one immediately surrounding the particle with the properties of the matrix (the size of this region depends on the static structure factor) and an effective medium. Self consistent closure relations are found for the conditionally averaged fields by solving the vector Helmholtz equations for a layered sphere in an infinite matrix by utilizing a multipole expansion technique. For finitely large ϕ , the effective permittivity is given by $\epsilon_{eff}/\epsilon_m = 1 + 3\beta\phi + \frac{3}{4}(\beta+4)\beta^2\phi^2 + O(\phi^3)$ where ϵ_m is the permittivity of the medium and β is the particle polarizability per unit volume. For denser systems, the particle and effective medium fields interfere to give rise to a Fano-like line shape for $Im(\epsilon_{eff})$. The resonance conditions result in a ϕ dependent red-shift of the resonance peak. Effects of polydispersity and multiple particle species on ϵ_{eff} will be discussed.

¹NSF Grant No. CMMI 0757589

²On leave from Syracuse University

5:18PM X17.00013 Microfabrication of highly absorbent THz metafilms tuned for specific frequencies¹, DRAGOSLAV GRBOVIC, FABIO ALVES, BRIAN KEARNEY, GAMANI KARUNASIRI, Naval Postgraduate School — THz imaging has gained increased attention in recent years. The main motivation is the property of THz radiation to penetrate through most non-metalic materials and fabrics, making it attractive for medical and security applications. In addition, the radiation is non-ionizing and therefore does not present a risk for human health. However, THz imaging requires external illumination, often by quantum cascade lasers (QCLs). Metafilm absorbers with nearly 100% absorption, at frequencies matched to appropriate QCLs, have been designed and fabricated using a periodic array of aluminum (Al) squares and an Al ground plane, separated by a thin SiO₂ dielectric film. All metafilms are below 2 μ m and are suitable for integration with microbolometers or bimaterial sensors for THz imaging. The THz spectral characteristics of structures were probed using FTIR spectrometer. Films with different dielectric layer thicknesses exhibited resonant absorption at close to 100% at respective frequencies. The measured THz reflection, from thin film of both broad-band and resonant metamaterial structures, exhibit excellent agreement with their respective finite element models.

¹Supported by ONR and NRO

Thursday, March 1, 2012 2:30PM - 5:18PM –

Session X18 DMP DCMP: Growth and Properties of Nanoparticles and Nanowires 252B

2:30PM X18.00001 Electronic structures and adsorption configurations of gold nanoclusters on cerium oxide defect surfaces, LU WANG, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68132, NEIL LAWRENCE, JOSEPH R. BREWER, JAMES WELLS-KINGSBURY, MARCELLA IHRIG, GONGHUA WANG, CHIN LI CHEUNG, Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588, YUN-LIANG SOO, Department of Physics, National Tsing Hua University, Taiwan — Fluorite-structured cerium oxide (or ceria, CeO_{2-x} , $0 \leq x \leq 0.5$) has been shown to be an important material in catalysis, yet few study has investigated the effect of non-dopant introduced oxygen vacancy defect (OVD). In addition, we found experimentally that when doped with Au nanoclusters, the catalytic ability of ceria enhanced. In this work, we modeled and optimized an (111) fluorite-structured slab model of defective ceria with a chemical formula corresponding to $\text{CeO}_{1.5}$. The optimized surface structure of this model was found to contain both surface and sub-surface OVDs, similar to those observed in our HRTEM data for low pressure activated nanoceria. Significantly, the model captures comparable reduction in the average Ce-O bond distance and also atomic coordination numbers observed in our EXAFS data. To explore the roles of Au nanoclusters, we adsorbed flat clusters of 3, 4, 9, 10, and 19 Au atoms on ceria slabs, optimized their configurations, and computed the corresponding electronic structures applying first-principle approach. Consequently, we present the density of states results to elucidate the experimentally observed optical property change and $s-d$ hybridization.

2:42PM X18.00002 The Kirkendall Effect in Copper Nanocrystals, MARK STOYKOVICH, KATHERINE RICE, Department of Chemical and Biological Engineering, University of Colorado - Boulder, DEPARTMENT OF CHEMICAL AND BIOLOGICAL ENGINEERING, UNIVERSITY OF COLORADO - BOULDER TEAM — The study of copper nanocrystals, unlike nanocrystals of other noble metals such as gold and silver, has been limited due to challenges in the synthesis of monodisperse copper nanoparticles and their reactivity at ambient conditions. Copper is a material of broad interest, however, because of its unique optical and catalytic properties, as well as its non-toxic nature and relative abundance. Copper nanocrystals in the process of being oxidized are subject to the Kirkendall effect, which describes independent diffusion rates in a binary system (Cu and oxygen in this case) and that causes the formation of voids at the core of spherical nanocrystals. Previous studies have attributed the Kirkendall effect in Cu/Cu₂O nanocrystals to interactions between the organic passivation layer and the solvent. Here we will present our results on the kinetics of oxidation of Cu nanocrystals in solvent-less conditions as a function of temperature and show that void formation occurs at a relatively narrow range of temperatures. In-situ UV-vis spectroscopy, x-ray diffraction, and electron microscopy have been used to monitor the oxidation process in Cu nanocrystals and a model has been developed to describe hollow particle formation in the Cu/Cu₂O system.

2:54PM X18.00003 Systematic Study of Supported Ni, Pd, Pt Metal Nanocrystals for Catalytic Energy Conversion, VICKY DOAN-NGUYEN, University of Pennsylvania, MATTEO CARGNELLO, University of Trieste, THOMAS R. GORDON, KEVIN BAKHMUTSKY, University of Pennsylvania, PAOLO FORNASIERO, University of Trieste, RAYMOND GORTE, CHRISTOPHER B. MURRAY, University of Pennsylvania — Ni, Pd, and Pt nanocrystals ranging from 4-12 nm have been synthesized with great control in size and shape using a high-temperature chemical synthetic method for gas-phase catalytic testing. The tunability in size allows for controlled catalytic study of model reactions such as CO oxidation, CO hydrogenation and methane oxidation. The monodispersity of the particles allow for a systematic correlation between size and catalytic activity. There is consistent size dependence of CO oxidation for each of the metal systems on CeO₂ support as indicated by the lower temperatures needed for full conversion. Our calculated activation energy using the Arrhenius equation for each size and material correlated with surface-area-to-volume ratio. Consistent with the light-off studies, the smallest particles were the most catalytically active under differential conditions. The same trend was observed for CO hydrogenation amongst each system. This trend was inverted for the oxidation of methane. This current study aims to elucidate the size dependence of catalytic activity in model systems with supported uniform nanocrystals.

3:06PM X18.00004 Ab Initio Investigation of the Structures of Fe-Doped Carbon Clusters, CHRISTELLA LOVATO, CLIFTON BROWNRIGG, AJIT HIRA, Northern New Mexico College — We continue our interest in the theoretical study of carbon clusters to examine the effects of the doping of small carbon clusters (C_n , $n = 2 - 15$) with iron atoms. This work applies the hybrid ab initio methods of quantum chemistry to derive the different Fe_mC_n ($m = 1-3$) geometries. Of particular interest are linear, fan, and cyclic geometries. Electronic energies, rotational constants, dipole moments, and vibrational frequencies for these geometries are calculated. Exploration of the singlet, triplet, quintet, and septet potential energy surfaces is performed. The type of bonding in terms of competition between sp^2 and sp^3 hybridization is examined, with a view to addressing the possibility of the stabilization of the doped carbon nano-particles in a diamond type structure. The potential for the existence of new pathways to the fabrication of nanotubes is explored.

3:18PM X18.00005 Electrical Detection of Mechanical Resonance of ZnO Nanowhiskers, DEEPIKA SAINI, DOYL DICKEL¹, RAMAKRISHNA PODILA, HERBERT BEHLOW, MALCOLM SKOVE, APPARAO RAO, Clemson University — Here, we present the fundamental mechanism for the observation of electrically actuated resonances in semi-conducting ZnO nanowhiskers (NWs). Previous studies have claimed that various mechanisms including charge induction lead to a mechanical resonance in NWs. Many of such studies employ an electron beam to visualize the resonance of NWs. However, we find that the use of an electron beam changes the electrical character of the NWs making it difficult to understand fundamental actuation mechanism. In this article, we developed a novel, fully electrical harmonic detection of resonance (HDR) method that enables us to probe mechanical resonances of NWs even in the absence of an electron beam. In contrast to the traditional optical detection scheme, the HDR method allows us to successfully decouple the effects of the electron probe beam from the actual driving force. Interestingly, we find that the observed mechanical resonance of ZnO NWs is dominated by their interactions with the electron probe beam. Importantly, ZnO NWs exhibit strong (weak) mechanical resonance only in presence (absence) of the electron probe beam suggesting that the observed behavior originates from dynamically induced (static) charges.

¹First and second author contributed equally

3:30PM X18.00006 Direct growth of vertically aligned long ZnO nanowires on FTO substrates and their application for dye sensitized solar cells, LIYOU LU, JIAJUN CHEN, WENYONG WANG, Department of Physics and Astronomy, University of Wyoming — In this research we report a direct growth of vertically aligned ZnO nanowires on fluorine-doped-tin-oxide (FTO) coated substrates for dye sensitized solar cell (DSSC) applications. ZnO nanowires with length of more than 30 μm were synthesized using a fine-tuned chemical vapor deposition method at temperatures as low as 550 °C. The nanowires grew along the [0001] direction and exhibited a needle-like shape with a wurtzite single crystal structure. Compared to the ZnO nanowires fabricated by solution based methods, the nanowires synthesized in this study have much longer length, thus could increase the amount of dye loading and improve DSSC performance. Furthermore, since the nanowires were directly synthesized on FTO substrates, DSSCs could be fabricated using the as-grown nanowires without the usual wire transfer processing that caused nanowire breaking and created additional transport barriers and recombination possibilities for photo-generated carriers. DSSCs fabricated in this study showed attractive performance with short-circuit current density of 5.1 mA/cm^2 and power conversion efficiency of 1.66%. Dependence of the DSSC performance on nanowire length and annealing processing was also examined in this research.

3:42PM X18.00007 Competing gas phase reactions during vapor transport deposition of ZnO nanowires, ERIC DRISCOLL, Lock Haven University, KEVIN RANGE, Lock Haven University, Department of Chemistry, MARIAN TZOLOV, Lock Haven University, Department of Physics — We present results illuminating some of the major chemical processes in the vapor deposition of ZnO nanowires. The analysis of our deposition experiments indicates that carbon dioxide is a major oxidizing agent rather than carbon monoxide as previously thought. Additionally, we present evidence that carbon monoxide will etch zinc oxide at high temperatures. Zinc oxide nanowires have been prepared by using chemical vapor deposition on silicon (100) substrates with a 10-15nm layer of gold as a catalyst. Zinc oxide and graphite powders were heated to approximately 1000°C in a tube furnace in a flow of argon. We have delivered oxygen gas specifically in the growth zone to facilitate the formation of high aspect ratio nanowire growth. Thermodynamics calculations were used to justify the growth and etching processes. Imaging of samples was performed with scanning electron microscopy. Chemical composition was determined by energy dispersive x-ray spectroscopy. Photoluminescence spectroscopy was used to characterize the emission properties of the zinc oxide samples.

3:54PM X18.00008 Study on Pure Phase Formation of Lead Oxide Nanowires by Oxidation of Lead Nanowires, KUO HAI, XIAOGANG WANG, Hunan Normal University, DEPARTMENT OF PHYS., HUNAN NORMAL UNIVERSITY TEAM — Lead-oxide nanowires were synthesized by oxidizing lead metal nanowires. The phase structures, sizes and morphologies of the nanowires were investigated by atomic force microscopy and x-ray diffraction, and the band gap of the nanowires was determined by UV-Vis-NIR reflectance diffusion spectrums. The thermodynamic environment for the pure phase formation has been studied. The first-principle computation has been done to help understand the phase formation. Our results reveal that the pure phase formation strongly relies on both the process temperature and the oxygen flow/oxygen partial pressure, and the pure phase γ -PbO nanowires can be obtained only in a narrow, low temperature range under a low oxygen flow.

4:06PM X18.00009 Formation of metallic gold chain on patterned hydrogen terminated Si(001)-2×1 surface: Density functional study, BIKASH GUPTA, PURUSOTTAM JENA, Department of Physics, Virginia Commonwealth University, Richmond, VA 23284 — Metal adsorption on silicon surface for the formation of linear metallic chain is one of the important research areas for the advancement of nanotechnology. Due to the presence of dangling bonds all over the surface of bare Si(001), metals when deposited, generally do not tend to form stable wire structures. However, patterned hydrogen terminated Si-surface may be a good choice for the formation of atomic chain structures of metals. Since patterned hydrogen terminated Si(001):2×1 surface is very stable, we consider patterning it by removing desired hydrogen atoms and adsorbing gold atoms. We have examined the structure, energetic and electrical properties of such gold adsorbed surface by varying gold coverage. We have found that linear gold chain structures may be formed by controlling gold coverage. Some of these gold chain structures are metallic in nature. We hope that our results will motivate synthesis of gold chains on patterned hydrogen terminated Si(001): 2×1 surface.

4:18PM X18.00010 Catalytic role of Au nanoparticle in GaAs nanowire growth¹, PETER KRATZER, SUNG SAKONG, VOLKER PANKOKE, University Duisburg-Essen, Germany — The energetics of Ga, As and GaAs species on the Au(111) surface (employed as a model for Au nanoparticles) is investigated by means of density-functional calculations. Apart from formation of the compound Au₇Ga₂, Ga is found to form a surface alloy with Au, with comparable $\Delta H \sim 0.5$ eV for both processes. Dissociative adsorption of As₂ is found to be exothermic by more than 2 eV on both clean Au(111) and AuGa surface alloys. The As-Ga species formed by reaction of As with the surface alloy is sufficiently stable to cover the surface of an Au particle *in vacuo* in contact with a GaAs substrate. Concerning the Au-catalysed growth of GaAs nanowires, we conclude that impingement of As₂ or As₄ molecules on the Au particle suffices as supply of arsenic to the growth zone. We identify a regime of temperatures and As₂ partial pressures suitable for Au-catalysed nanowire growth in molecular beam epitaxy.

¹supported by Deutsche Forschungsgemeinschaft

4:30PM X18.00011 Engineering Enhanced Optical Properties of Near-IR Upconverting Nanoparticles, DANIEL GARGAS, ALEXIS OSTROWSKI, EMORY CHAN, DELIA MILLIRON, BRUCE COHEN, P. JAMES SCHUCK, The Molecular Foundry, Lawrence Berkeley Laboratory — Due to their unique properties in converting low energy light into higher energy electronic transitions, upconverting nanoparticles (UCNPs) have garnered considerable interest in bio-imaging, photovoltaic, and opto-electronic applications. In particular, lanthanide-doped UCNPs have demonstrated a host of functionalities due to their nanoscale dimensions, wide range in transition-metal doped compounds, and high photostability in both aqueous and ambient environments.¹ In addition, their mixed electric and magnetic dipole transitions make them ideal materials for study of plasmon-enhanced properties with metal nanostructures in which tunable surface properties can mediate energy transfer processes. Here we report on the luminescence properties of Er³⁺, Yb³⁺-doped NaYF₄ UCNPs with diameters ranging from 5 – 50 nm in both core and core-shell architectures. Optical characterization of the luminescence lifetime and spectral emission from both UCNP films and single particles reveal a strong dependence on particle size and surface functionalization. Furthermore, by utilizing the large shift (anti-stokes) in absorption energy versus transition energy, we investigate the interaction of energy transfer across metal-semiconductor nano-interfaces whereby the intrinsic luminescence lifetimes are probed for Purcell enhancement and emission rate modification.

¹P.J. Schuck, et al *Proc. Nat. Acad. Sci.* **106**, 10917, 2009

4:42PM X18.00012 Tuning the parameters to establish Quenching and enhancement regimes in hybrid Gold nanoparticles and CdSe Quantum dots monolayer¹, LAXMINARAYAN TRIPATHI, PRAVEENA M., J.K. BASU, Department of Physics, Indian Institute of science, Bangalore, India — The multi-component nanomaterials combine the individual properties and give rise to emergent phenomenon. Optical excitations in such hybrid nonmaterial's (for example Exciton in semiconductor quantum dots and Plasmon in Metal nanomaterials) undergo strong weak electromagnetic coupling. Such exciton-plasmon interactions allow design of absorption and emission properties, control of nanoscale energy-transfer processes, and creation of new excitations in the strong coupling regime. This Exciton plasmon interaction in hybrid nanomaterial can lead to both enhancement in the emission as well as quenching. In this work we prepared close-packed hybrid monolayer of thiol capped CdSe and gold nanoparticles. They exhibit both the Quenching and enhancements the in PL emission. The systematic variance of PL from such hybrid nanomaterials monolayer is studied by tuning the Number ratio of Gold per Quantum dots, the surface density of QDs and the spectral overlap of emission spectrum of QD and absorption spectrum of Gold nanoparticles. Role of Localized surface Plasmon which not only leads to quenching but strong enhancements as well, is explored.

¹Indian Institute of science, Bangalore, India

4:18PM X19.00004 Electronic and structural correlations at 2DEG oxide heterointerfaces¹, M.S. RZCHOWSKI, Physics Dept., University of Wisconsin-Madison — The formation of a two-dimensional electron gas (2DEG) at complex oxide interfaces is directly influenced by the rich electronic and structural characteristics of the bulk oxides, as well as new phenomena arising at the interface. We investigated how local correlations control oxide 2DEGs by inserting a single atomic layer of a rare-earth oxide (RO) [(R is lanthanum (La), praseodymium (Pr), neodymium (Nd), samarium (Sm), or yttrium (Y))] into an epitaxial SrTiO₃ matrix using pulsed-laser deposition with atomic layer control [1]. We find that structures with La, Pr, and Nd ions result in conducting 2DEGs at the inserted layer, whereas the structures with Sm or Y ions are insulating. Our local spectroscopic results, and our theoretical results, indicate that the interfacial conductivity is dependent on electronic and structural correlations that decay spatially into the SrTiO₃ matrix and are determined by the local rare-earth ion. We also find that at least the structural correlations play a role in the properties of the 2DEG at LaAlO₃/SrTiO₃ interfaces. We used different lattice constant single-crystal substrates to produce LaAlO₃/SrTiO₃ interfaces with controlled levels of biaxial epitaxial strain [2], finding that tensile-strained SrTiO₃ destroys the conducting 2DEG, while compressively strained SrTiO₃ retains the 2DEG, but with reduced carrier concentration. In addition, the critical LaAlO₃ overlayer thickness for 2DEG formation increases with SrTiO₃ compressive strain. Our first-principles calculations suggest that a strain-induced electric polarization in the SrTiO₃ layer, stabilized by the LaAlO₃ overlayer, is responsible for this behavior. This work was done in collaboration with H.W. Jang, C.W. Bark, D.A. Felker, T. Hernandez, Y. Wang, M.K. Niranjan, C.T. Nelson, Y. Zhang, D. Su, C.M. Folkman, S.H. Baek, S. Lee, K. Janicka, H. Zhou, Y. Zhu, X.Q. Pan, D.D. Fong, E.Y. Tsymlal, C. B. Eom. This work was supported by the National Science Foundation through grant DMR-0906443.

[1] H.W. Wang et al., *Science* **331**, 886 (2011).

[2] C.W. Bark et al., *P. Natl Acad Sci USA* **108**, 4720 (2011).

¹This work was supported by the National Science Foundation through grant DMR-0906443

4:54PM X19.00005 Electronic structure and two-dimensional electron gas at the surface of SrTiO₃¹, ANDRES FELIPE SANTANDER-SYRO, CSNSM, Universite Paris-Sud, Bat. 108, 91405 Orsay, France — Similar to silicon that is the basis of conventional electronics, strontium titanate (SrTiO₃) is the bedrock of the emerging field of oxide electronics. SrTiO₃ is the preferred template to create exotic two-dimensional (2D) phases of electron matter at oxide interfaces, exhibiting metal-insulator transitions, superconductivity, large magnetoresistance, or coexistence of superconductivity and ferromagnetism. However, the physical nature of the electronic structure underlying these 2D electron gases (2DEGs) remains elusive, although its determination is crucial to understand their remarkable properties. In this talk, we present our angle-resolved photoemission spectroscopy (ARPES) results showing that there is a highly metallic universal 2DEG at the vacuum-cleaved surface of SrTiO₃, independent of bulk carrier densities over more than seven decades, including the undoped insulating material [A. F. Santander-Syro *et al.* *Nature* **469**, 189-193 (2011)]. Our data unveil a remarkable electronic structure consisting on multiple subbands of heavy and light electrons. We find that the 2DEG is confined within a region of ~5 unit cells and has a sheet carrier density of ~0.33 electrons per a^2 (a is the cubic lattice parameter). The similarity of this 2DEG with those reported in SrTiO₃-based heterostructures and field-effect transistors suggests that different forms of electron confinement at the surface of SrTiO₃ lead to essentially the same 2DEG. Our discovery provides thus a model system for the study of the electronic structure of 2DEGs in SrTiO₃-based devices and a novel route to generate 2DEGs at surfaces of other functional oxides.

¹This project was supported by the ANR "Oxitronics."

Thursday, March 1, 2012 2:30PM - 5:30PM – Session X20 FIAP: Invited Session: Physics of Color Reflective Displays 253C

2:30PM X20.00001 Bio-Inspired Adaptive Coloration – Knowledge Gained by Comparison of Nature and Man-Made Technologies, JASON HEIKENFELD, University of Cincinnati — Adaptive coloration, achieved through the use of pigments and reflective surfaces, is used by biological organisms to resemble natural surfaces and/or vividly communicate information. The key to this approach is that light incident on the organism is manipulated to perform the adaptive coloration (i.e., no light is created in the process). Only recently have man-made display technologies (E-paper) attempted to achieve similar adaptive reflective properties. For biological organisms, as well as display technologies, the following features must be controlled simultaneously while minimizing optical losses: pattern, texture, multiple colors, diffuseness, reflectance, and polarization. Many e-Paper technologies have attempted to duplicate optical effects that are utilized in nature. However, to date, they fail in comparison to the optical performance of biological systems. Thus, engineers working on adaptive reflective surfaces may benefit by examining equivalent biological systems in greater detail than previously achieved. On the other hand, intense research and development into adaptive reflective surfaces has given us a mature understanding of the optics of man-made surfaces, and the advanced measurement standards required for scientific involvement. Although this framework currently exists, it is underutilized for the analysis of biological coloration. To advance the field of adaptive coloration, the gap between biology and engineering must be bridged by developing a consistent framework of scientific metrics important to the performance of all platforms of adaptive reflective surfaces. In this presentation, the optics of adaptive coloration are presented in detail. Biological and technological methods are compared based on the construction, physics, and optical performance of each type of adaptive coloration. These comparisons are discussed at the system (organism), device (organ), and pixel/materials (cellular) levels. The main outcomes of this investigation are: display engineers gain insight from techniques perfected in nature; biologists benefit from an understanding of the types of characterization and metrics that could be extracted from biological organisms; and all scientists gain a clearer picture of the long-term prospects for adaptive reflective technologies.

3:06PM X20.00002 Hewlett-Packard's Approaches to Full Color Reflective Displays, GARY GIBSON, Hewlett-Packard Laboratories, Hewlett-Packard — Reflective displays are desirable in applications requiring low power or daylight readability. However, commercial reflective displays are currently either monochrome or capable of only dim color gamuts. Low cost, high-quality color technology would be rapidly adopted in existing reflective display markets and would enable new solutions in areas such as retail pricing and outdoor digital signage. Technical breakthroughs are required to enable bright color gamuts at reasonable cost. Pixel architectures that rely on pure reflection from a single layer of side-by-side primary-color sub-pixels use only a fraction of the display area to reflect incident light of a given color and are, therefore, unacceptably dark. Reflective devices employing stacked color primaries offer the possibility of a somewhat brighter color gamut but can be more complex to manufacture. In this talk, we describe HP's successes in addressing these fundamental challenges and creating both high performance stacked-primary reflective color displays as well as inexpensive single layer prototypes that provide good color. Our stacked displays utilize a combination of careful light management techniques, proprietary high-contrast electro-optic shutters, and highly transparent active-matrix TFT arrays based on transparent metal oxides. They also offer the possibility of relatively low cost manufacturing through roll-to-roll processing on plastic webs. To create even lower cost color displays with acceptable brightness, we have developed means for utilizing photoluminescence to make more efficient use of ambient light in a single layer device. Existing reflective displays create a desired color by reflecting a portion of the incident spectrum while absorbing undesired wavelengths. We have developed methods for converting the otherwise-wasted absorbed light to desired wavelengths via tailored photoluminescent composites. Here we describe a single active layer prototype display that utilizes these materials along with an innovative optical out-coupling scheme. Further benefits of our approach include means for highly power-efficient back-lighting under low ambient light conditions and the possibility of video rate operation.

3:42PM X20.00003 Opalux Photonic Ink: Full-color, bistable, reflective displays, ANDRE ARSENAULT, Opalux Inc. — No abstract available.

4:18PM X20.00004 Cholesteric Liquid Crystal Based Reflex Color Reflective Displays, ASAD KHAN, Kent Displays, Inc. — Bistable color cholesteric liquid crystal displays are unique LCDs that exhibit high reflectivity, good contrast, extremely low power operation, and are amenable to versatile roll-to-roll manufacturing. The display technology, now branded as Reflex™ has been in commercialized products since 1996. It has been the subject of extensive research and development globally by a variety of parties in both academic and industrial settings. Today, the display technology is in volume production for applications such as dedicated eWriters (Boogie Board™), full color electronic skins (eSkin), and displays for smart cards. The flexibility comes from polymerization induced phase separation using unique materials unparalleled in any other display technology. The blend of monomers, polymers, cross linkers, and other components along with nematic liquid crystals and chiral dopants is created and processed in such ways so as to enable highly efficient manufacturable displays using ultra thin plastic substrates – often as thin as 50μm. Other significant aspects include full color by stacking or spatial separation, night vision capability, ultra high resolution, as well as active matrix capabilities. Of particular note is the stacking approach of Reflex based displays to show full color. This approach for reflective color displays is unique to this technology. Owing to high transparency in wavelength bands outside the selective reflection band, three primary color layers can be stacked on top of each other and reflect without interfering with other layers. This highly surprising architecture enables the highest reflectivity of any other reflective electronic color display technology. The optics, architecture, electro-topics, and process techniques will be discussed. This presentation will focus on the physics of the core technology and color, it's evolution from rigid glass based displays to flexible displays, development of products from the paradigm shifting concepts to consumer products and related markets. This is a development that spans a wide space of highly technical development and fundamental science to products and commercialization to enable the entry of the technology into consumer markets.

4:54PM X20.00005 Mirasol displays: the revolution in display technology, BRIAN GALLY, Qualcomm —
No abstract available.

Thursday, March 1, 2012 2:30PM - 5:18PM –

Session X21 DCMP: Fluctuation Phenomena (noise, nonequilibrium effects, localization effects)

254A

2:30PM X21.00001 Fluctuoscopia of Disordered Two-Dimensional Superconductors¹, ANDREAS GLATZ, Argonne National Laboratory, ANDREY VARLAMOV, University of Rome, Tor Vergata, VALERII VINOKUR, Argonne National Laboratory — In this talk I will present our results for the fluctuation conductivity (FC) in disordered two-dimensional superconductors placed in a perpendicular magnetic field. In our works [1,2] we finally derived the complete solution in the temperature-magnetic field phase diagram. The obtained expressions allow both to perform straightforward (numerical) calculation of the FC surface $\delta\sigma(T, H)$ and to get all 27 asymptotic expressions in the seven qualitatively different domains of the phase diagram. This surface becomes in particular non-trivial at low temperatures, where it is trough-shaped and close to the quantum phase transition non-monotonic, in agreement with experimental findings. I will show our main results and demonstrate how these can be used as a high precision tool (fluctuoscope) to determine the critical temperature, critical magnetic field, and dephasing time from experimental data in superconducting films.

[1] A. Glatz, A. A. Varlamov, and V. M. Vinokur, EuroPhys. Lett. **94**, 47005 (2011).

[2] A. Glatz, A. A. Varlamov, and V. M. Vinokur, Phys. Rev. B **84**, 104510 (2011).

¹Work supported by the U.S. DOE, Office of Science, under Contract No. DE-AC02-06CH11357.

2:42PM X21.00002 Majorana modes in a superconducting wire with quasiperiodic and, WADE DEGOTTARDI, University of Illinois at Urbana-Champaign, MANISHA THAKURATHI, DIPTIMAN SEN, Centre for High Energy Physics, Indian Institute of Science, SMITHA VISHVESHWARA, University of Illinois at Urbana-Champaign — We present a systematic study of the role quasiperiodic and disordered potentials play in the topology of 1D *p*-wave superconducting systems based on a lattice model which we analyze using a transfer matrix approach. We employ a similarity transformation to demonstrate that the existence of Majorana modes is intimately connected to the band structure of the corresponding normal state system (i.e one which, though otherwise identical, lacks superconducting order). We illustrate this correspondence using the case of an electron moving in a quasiperiodic potential. The Hamiltonian of this system is the so-called “almost Mathieu operator” whose bulk spectrum (for a certain choice of parameters) is described by a fractal known as Hofstadter's butterfly. Specifically, we prove that states belonging to this spectrum host end Majoranas for arbitrarily weak superconductivity and that increasing the magnitude of the superconducting gap causes these topologically non-trivial regions of the phase diagram to expand and fill in the butterfly. We show that similar considerations give us excellent theoretical control over the topological phase diagram of systems with disordered potentials.

2:54PM X21.00003 A Preformed Pair Approach to Diamagnetism in the Cuprates, VIVEK MISHRA, DAN WULIN, K. LEVIN, James Franck Institute, University of Chicago — Enhanced diamagnetism extending beyond the critical regime is associated with the pseudogap. It has been one of the key experiments supporting the precursor superconductivity scenario for this normal state gap. In this talk we demonstrate how non-condensed pairs (rather than normal state vortices) yield a large low field diamagnetic signal. Our work is based on a 3d BCS-BEC crossover scenario where the diamagnetic susceptibility calculation is well controlled and built on a sum-rule compatible correlation function approach. We demonstrate reasonable semi-quantitative agreement with experiment, with no adjusted parameters.

3:06PM X21.00004 Transport theory of superconductors in paramagnetic limit, MAXIM KHODAS, University of Iowa, ALEX LEVCHENKO, Michigan State University, GIANLUIGI CATELANI, Yale University — We report on the study of the quantum phase transition from metastable normal to superconductive state in thin films driven by in-plane magnetic field. In this system resistivity exhibits hysteresis at low temperature when the strong Zeeman field is gradually turned off and on. Quantum fluctuations smear the transition from the metastable normal state to paramagnetically limited superconductivity. The typical energy scale for fluctuations is $\bar{\Omega} = \sqrt{E_z^2 - \Delta^2}$, where E_z is the Zeeman energy and Δ is zero temperature gap. At the onset of the transition $\bar{\Omega} \rightarrow 0$ quantum fluctuations cause non-analytic corrections to the conductivity. The most singular corrections are presented. The result is strongly sensitive to the strength of the spin-orbit scattering. We argue that our theory qualitatively agrees with experimental findings provided the spin-orbit scattering is taken into account.

3:18PM X21.00005 Proliferation of mesoscopic effects in transport of superconductors, MENGJING ZHANG, ALEX LEVCHENKO, Michigan State University — Universality of conductance fluctuations is the hallmark of mesoscopic physics. This phenomenon emerges from the quantum coherence of electron trajectories and is sensitive to changes in external magnetic field or gate voltage. There exists compelling physical evidence, ranging from the experiments in sub-micron scale superconducting rings to granular films driven across superconductor-insulator transition, that the role of mesoscopic fluctuations proliferate in the presence of superconducting correlations. We thus study theoretically the fate of universality of mesoscopic fluctuations in superconductors focusing on the kinetic characteristics such as conductance, thermopower, NMR relaxation rate, spin susceptibility etc.

3:30PM X21.00006 Superconducting fluctuation regime in the cuprates revealed by torque magnetometry¹, GUICHUAN YU, University of Minnesota — The extent of the superconducting fluctuation regime in the normal state of the cuprate superconductors has remained unclear. For the single-CuO₂-layer compounds La_{2-x}Sr_xCuO₄ (LSCO) and Bi₂(Sr,La)₂CuO_{6+δ} (Bi2201), one class of experiments indicates characteristic temperatures as high as 2-3 times T_c at optimal doping, whereas a second class reveals superconducting fluctuations in a relatively narrow temperature range above T_c . Here we report a systematic torque magnetometry study of the superconducting fluctuation regime in three single-layer compounds, LSCO, Bi2201 and HgBa₂CuO_{4+δ}. We find in all three cases that the regime of fluctuating diamagnetism is narrow and closely tracks the doping dependence of T_c , consistent with the second class of experiments [1]. The seemingly controversial results can be understood if short-range phase correlations develop only in the vicinity of T_c , whereas local pair formation appears at a relatively high temperature that is universal among all single-layer cuprates.

[1] G. Yu, D.-D. Xia, N. Barišić, R.-H. He, N. Kaneko, Yangmu Li, Yuan Li, T. Sasagawa, A. Shekhter, X. Zhao and M. Greven, unpublished

¹This work has been supported by the NSF and DOE BES

3:42PM X21.00007 The potential for persistent current measurements in mesoscopic rings of underdoped cuprates, THOMAS LIPPMAN, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA, ILYA SOCHNIKOV, Geballe Laboratory for Advanced Materials, Stanford University, Stanford, California 94305-4045, USA, KATHRYN MOLER, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA — Dimensionality, disorder, order parameter symmetry, competing phases, quantum critical points, thermal phase fluctuations, and quantum phase fluctuations all play a role in the physics of the underdoped cuprates. Measurements of the persistent current in mesoscopic rings near phase transitions can provide valuable information about underlying coherent states. We evaluate the prospects for such measurements in the underdoped cuprates, considering both likely signatures of various theoretical scenarios and experimental feasibility in terms of fabrication and signal levels.

3:54PM X21.00008 Cantilever torque magnetometry study of multiply connected BSCCO arrays near T_c ¹, GRIGORIY POLSHYN, RAFFI BUDAKIAN, University of Illinois at Urbana-Champaign — The goal of this work is to study the superconducting coherence length in the fluctuation regime in cuprate superconductors. In this work we present cantilever torque magnetometry measurements of micron-size BSCCO flakes patterned with arrays of nanometer scale rings or holes. Using ultrasensitive dynamic torque magnetometry, oscillations in magnetization are observed near T_c as a function of the applied magnetic flux threading the array. Special effort was made to detect the oscillations in magnetization at temperatures above T_c , where the Nernst effect and magnetization measurements suggest the possibility of pairing. To constrain the magnitude of the coherence length in the fluctuation regime, we will present the dependence of the amplitude of the $h/2e$ period oscillations as a function of temperature and hole size.

¹This work was supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. DOE, Office of Science, under Award No. DE-AC0298CH1088.

4:06PM X21.00009 Properties of ultrathin Bi₂Sr₂CaCu₂O_{8+x} films grown by pulsed laser deposition, MICHAEL HINTON, JIE YONG, STANLEY STEERS, ADAM AHMED, JOHN DRASKOVIC, TOM LEMBERGER, Ohio State University — Thermal and quantum fluctuations in superconductors are expected to grow as film thickness decreases. Such behavior has been observed in YBa₂Cu₃O_{7-δ} (YBCO) films as thickness is reduced to two unit cells. In particular, a Kosterlitz-Thouless like drop in superfluid density appears and shows that 2D fluctuations are correlated through the YBCO film thickness. Since Bi₂Sr₂CaCu₂O_{8+x} (Bi-2212) plays such a prominent role in important ARPES and Scanning Probe measurements of the superconducting gap, it is important to see how this compound behaves in reduced dimensions. To that end, we are working to grow films of Bi-2212 as thin as possible, by pulsed laser deposition in on-axis and off-axis geometries. One goal is to look for the KT transition in the superfluid density, to see whether 2D fluctuations are correlated layer-to-layer even in this highly anisotropic compound, and complement the cuprate picture dominated by the wealth of YBCO data. This requires films to be quite homogeneous. To effectively improve homogeneity, we focus the ac magnetic field of our two-coil measurement system by masking the film of interest with a thick superconducting film with a hole etched through it. Thus, the film area probed is greatly reduced and transition widths are narrowed.

4:18PM X21.00010 Ghost critical field and weak localization phenomena in superconducting Tantalum Nitride films, NICHOLAS BREZNAY, AHARON KAPITULNIK, Stanford University — We study the appearance of superconducting fluctuations and weak localization effects in disordered conducting thin films using magnetotransport measurements. At temperatures above T_c , we observe a positive magnetoresistance that is 4 orders of magnitude larger than the predicted classical effect. Well above T_c this behavior is consistent with the magnetic field dependence of localization quantum corrections to the conductivity in the presence of strong spin-orbit scattering. Close to T_c the observed magnetoresistance is well described by theories that describe both localization and superconducting fluctuations effects. This analysis allows for careful study of the so-called ghost critical field and inelastic scattering rates close to T_c .

4:30PM X21.00011 Coexistence of superconducting gap and pseudogap above and below T_c in cuprates, JEFFERY TALLON, JAMES STOREY, MacDiarmid Institute, Industrial Research, JOHN LORAM, Cavendish Lab., Cambridge University — We develop a new method to calculate the full T -dependent superconducting (SC) gap from thermodynamic measurements and apply to the cuprates. We find that the SC gap persists high above T_c due to strong SC fluctuations and coexists there with the pseudogap. This allows the (disputed) phase diagram to be mapped more accurately than previously. We apply the results below T_c to understand the doping and temperature evolution of critical currents in practical conductors.

4:42PM X21.00012 On-chip detection of photon-assisted shot noise and photocurrent of quantum point contact, Y. JOMPOL, P. ROULLEAU, F. PORTIER, P. ROCHE, D.C. GLATTLI, SPEC, CEA/Saclay, France, I. FARRER, D.A. RITCHIE, Cavendish Laboratory, University of Cambridge, England — We present the first experimental realization of on-chip shot noise detection in capacitively-coupled quantum point contacts (QPCs). The detection is based on the photon-assisted effects. A dc voltage biased QPC: the emitter generates broad frequency current shot noise, inducing voltage fluctuations on the second QPC: the detector. This yields photon induced electron-hole pairs whose partitioning between left and right contact causes a current noise called photon-assisted shot noise (PASN). Alternatively, the electron-hole pairs may also generate a photon-assisted current for energy-dependent transmission. Both the photocurrent and PASN are proportional to the product $D(1-D)$, where D is the transmission of a QPC. Our sample is realized using a set of quantum point contacts positioned onto two separate mesas of a two-dimensional electron gas. The QPC emitter is DC biased and emits high-frequency shot noise that is converted into voltage fluctuations at the QPC detector via an interdigital capacitor, C . Two additional QPCs next to the emitter and the detector serve as tunable quantum resistors and are used to control impedance of the circuit. We show that by varying both the emitter and detector transmissions, D^E , D^D , the measured current at the QPC detector is proportional to $D^D(1-D^D) D^E(1-D^E)$ for a given V_{ds} , which is in good agreement with the theoretical prediction. This new way of detection should find fundamental applications in electronic quantum physics.

4:54PM X21.00013 Direct access to quantum non-Gaussian noise through cross-correlation measurements, IURI CHERNII, EUGENE SUKHORUKOV, University of Geneva — Detection of quantum non-Gaussian fluctuations is often difficult since they are dominated by the classical Gaussian noise, and requires the use of high frequency amplifiers. In our work we investigate the possibility to employ the cross-correlation technique in order to overcome these difficulties. We propose to measure the cross-correlator of outputs of a pair of two-level detectors, coupled to the source of fluctuations via an electric circuit. In the weak coupling regime, the noise induces rare stochastic transitions in the detectors, that allows one to perform the long time measurement. The transition rates can be derived from the evolution of the density matrix, calculated to the fourth order in level mixing of the two-level detectors. We express the cross-correlator in terms of these rates, and demonstrate that there is a range of parameters, where the main contribution to the cross-correlator is proportional to the intensity of the quantum non-Gaussian noise.

5:06PM X21.00014 Interferometric and Noise Signatures of Majorana Fermion Edge States in Transport Experiments, WOLFGANG BELZIG, University of Konstanz, GREGORY STRUEBLI, University of Basel, MAHN-SOO CHOI, Korea University, CHRISTOPH BRUDER, University of Basel — Domain walls between superconducting and magnetic regions placed on top of a topological insulator support transport channels for Majorana fermions. We propose to study noise correlations in a Hanbury Brown-Twiss type interferometer and find three signatures of the Majorana nature of the channels. First, the average charge current in the outgoing leads vanishes. Furthermore, we predict an anomalously large shot noise in the output ports for a vanishing average current signal. Adding a quantum point contact to the setup, we find a surprising absence of partition noise which can be traced back to the Majorana nature of the carriers.

Thursday, March 1, 2012 2:30PM - 5:18PM –
Session X22 DMP DCOMP: Focus Session: Fe-based Superconductors - Exchange Coupling Theory 254B

2:30PM X22.00001 Strong Versus Weak Coupling Pairing in Iron-Based Superconductors¹, B. ANDREI BERNEVIG, Princeton University — We use the functional renormalization group as well as strong-coupling methods to analyze the phase diagram of several of the iron-based superconductors. As in the previous studies by F. Wang, D.H. Lee et. al., we observe a nodeless sign-changing order parameter to be favored over a sizable part of the parameter space, but the physics quickly develops peculiarities depending on the doping, shape, size and orbital content of the Fermi surfaces in the different superconducting compounds. Using several new one-body models available in the literature (due to Kuroki, Graser and Raghu), we analyze the orbital content of the superconducting gap, which should be observable in spin-polarized ARPES experiments. We find that the effective theory of the iron-based superconductors is a $J_1 - J_2$ model in orbital space with $J_2 > |J_1|$ and antiferromagnetic, and analyze the behavior of the physical properties such as superconducting gap for systems ranging from electron overdoped $(K, Cs)Fe_{2-x}Se_x$ to hole-doped $K_xBa_{1-x}Fe_2As_2$.

¹NFS, Packard

3:06PM X22.00002 Hund's metal physics in iron-based superconductors, GABRIEL KOTLIAR, ZHIPING YIN, KRISTJAN HAULE, Department of Physics and Astronomy, Rutgers University — The role of Hubbard U and Hund's J in a material depends on the energy scale of the crystal field splitting. In transition metal oxides, the crystal field splitting is usually considerably larger than Hund's J thus Hubbard U plays the dominating role. However, the crystal field splitting in iron-based superconductors is substantially smaller and the physics in this family is governed primarily by Hund's rule. In this talk, we will show that the combination of density functional theory and dynamic mean field theory properly incorporates the Hund's physics as well as realistic band structure thereby is well suited to capture and predict a wide range of physical properties and their trends in iron pnictides and chalcogenides, such as optical conductivity, x-ray spectroscopy, Fermi surface, magnetic ordering and moments, spin excitations, effective masses and so on. We will demonstrate two important mechanisms operating in this family, namely, Hund's blocking and Kinetic frustration. The importance of electronic correlation caused by the Hund's physics and its relation to various experimental observations will also be discussed.

3:18PM X22.00003 Consistent theory of magnetism and superconductivity in iron pnictides, MICHAEL KATSNELSON, Radboud University Nijmegen, Netherlands, VLADIMIR ANTROPOV, LIQIN KE, Ames Laboratory, USA, MARK VAN SCHILF-GAARDE, Kings College, London, UK — We show that iron pnictide systems possess unusual quantum spin fluctuations which strongly affect their magnetic properties and may be relevant in the mechanism of superconductivity. These fluctuations represent highly non-linear anharmonic excitations and have both transversal and longitudinal components which may contribute differently to the observed properties. From the point of view of magnetism, these fluctuations are responsible for the stability of the observed magnetic ground states, and thus determine the spin-wave spectra. The anharmonic character of the excitations under consideration provides a strong coupling with electron degrees of freedom which may be relevant for the appearance of high-temperature superconductivity. We discuss a mechanism of superconductivity related to spin fluctuation which uses the same pool of fluctuations to explain the Cooper pairing. Theory predicts some correlations between superconductivity temperature and magnetic characteristics and they seem to be in agreement with the available experimental data for pnictides and selenides. We discuss also other materials where one can expect a similar behavior.

3:30PM X22.00004 Giant spin zero-point fluctuations in iron superconductors, VLADIMIR ANTROPOV, Ames Laboratory, USA, PAWEŁ BUCZEK, FRANK ESSENBERGER, ARTHUR ERNST, LEONID SANDRATSKII, E.K.U. GROSS, MPI Halle, Germany — We analyze the strength of quantum spin fluctuations in novel iron superconductors. By using linear response calculations and the density functional approach, we show that many of these materials can be classified as highly responsive magnetic materials with very strong non-linear quantum spin fluctuations. Furthermore, by using the newly developed theory of magnetic instabilities in systems with strong spin zero-point motion, we show that the inclusion of fluctuations dramatically improves an agreement with the experiment for systems such as $CaFe_2As_2$, $LiFeAs$ and $FeSe$, while for $FeTe$, the results are less affected by fluctuations. We demonstrate how spin fluctuations influence the criteria of local magnetic moment and long range magnetic order existence. In addition to iron superconductors, several other groups of materials with possible giant quantum spin fluctuations are identified.

3:42PM X22.00005 Spectral and magnetic properties of the iron-based superconductors: The role of electronic correlation, ALESSANDRO TOSCHI, Vienna University of Technology, P. HANSMANN, Centre de Physique Theorique, Ecole Polytechnique, R. ARITA, Department of Applied Physics, University of Tokyo, S. SAKAI, Centre de Physique Theorique, Ecole Polytechnique, G. SANGIOVANNI, K. HELD, Vienna University of Technology — Electronic correlation plays a subtle role in Fe-based superconductors. In fact, due to the presence of several moderately correlated bands close to the Fermi level, one observes the formation of localized magnetic moments driven by the Hund's exchange interactions, which takes place, however, in a mainly metallic background ("Hund's metal" [1]). This physical scenario provides the key to understand [2,3] the discrepancies observed between experimental estimates of the magnetic moments in the magnetically ordered phase and those obtained via standard LSDA calculations. The magnitude of the discrepancy observed in different compounds would be hence related to the efficacy of the metallic screening, which is decreasing when going from the 1111 (e.g., $LaFeAsO$) to the 122 class, and eventually to the 11 materials (like $FeTe$). Also important to be considered for the interpretation of the ARPES experiments and of the symmetry of the superconducting pairing within the Hund's exchange scenario is the interplay between the electronic correlations and the details of the band-structure of the specific compound considered.

[1] K. Haule and G. Kotliar, NJP 11 025021 (2009). [2] P. Hansmann, et al., PRL 104, 197002 (2010). [3] A. Toschi, et al. in preparation

3:54PM X22.00006 *Ab initio* Evidence of Strong Correlation Associated with Mott Proximity in Iron-Based Superconductor, TAKAHIRO MISAWA, KAZUMA NAKAMURA, MASATOSHI IMADA, Dept. of Applied Physics, Univ. of Tokyo — Recently discovered iron-based superconductors have attracted much interest because of their high superconducting critical temperatures (T_c). Although it is believed that electron correlations play key roles in the unconventional high- T_c superconductivity, their roles are not fully understood yet. To clarify electron correlation effects from a microscopic point of view, we study the *ab initio* low-energy effective models for iron-based superconductors by using multi-variable variational Monte Carlo (mVMC) method. From the *ab initio* calculations, we show that the iron-based superconductors found around d^6 configuration (namely, five Fe $3d$ orbitals filled by 6 electrons on average) are under the umbrella of an unexpectedly large-scale dome of correlated-electron matter centered at the Mott insulator at d^5 (namely, half filling). This proximity of the large-dome of strong electron correlations yields a variety with bad insulating (or incoherent metallic) states, quantum criticality of antiferromagnetism, orbital fluctuations and differentiations arising from interplay between the Hund's rule coupling and Mott physics.

4:06PM X22.00007 Two-orbital quantum spin model of magnetism in the iron pnictides¹, CHEN LIU, Boston University, DAO-XIN YAO, Sun Yat-Sen University, ANDERS SANDVIK, Boston University — We study a two-orbital spin model to describe $(\pi, 0)$ stripe antiferromagnetism in the iron pnictides. The “double-spin” model has an on-site Hund's coupling and inter-site interactions extending to second neighbors on the square lattice. Using a variational method based on a cluster decomposition, we optimize wave functions with up to 8 cluster sites (up to 2^{16} variational parameters). We focus on the anomalously small ordered moments in the stripe state of the pnictides. To account for it, and large variations among different compounds, we show that the second-neighbor cross-orbital exchange constant should be ferromagnetic, which leads to “partially hidden” stripe order. In a different parameter region, we confirm a canted state previously found in spin-wave theory.

¹NSF DMR-1104708

4:18PM X22.00008 Spin waves of 2D J_1 - J_2 model and single hole dynamics via nearest neighbor hole hopping, SATYAKI KAR, University of North Florida — We study the two dimensional J_1 - J_2 model using the spin wave approximation and find the spin wave modes at different values of parameter $\lambda = J_2/J_1$. Competing antiferromagnetic (π, π) and $(\pi, 0)$ (or, $(0, \pi)$) orders preferred by the J_1 and J_2 terms respectively creates frustration in such a system and the spin wave excitations about different vacuum states are observed for different values of λ . We investigate the stability of different zero spin deviation states as λ is varied from 0 to 1.5. We discuss the band folding of the super-lattice structure that appears with the emergence of the J_2 term and study the different spin wave modes that the system inherits. Dynamics of a foreign hole put in such a system is studied using a t - J_1 - J_2 model and the hole spectra obtained by solving the Dyson's equation self-consistently within the non-crossing approximation are compared with the ARPES spectra from the newly discovered FeAs superconducting compounds.

4:30PM X22.00009 An unified minimum effective model of magnetism in iron-based superconductors, JIANGPING HU, Department of Physics, Purdue University, West Lafayette, Indiana 47907, USA, BAO XU, WUMING LIU, NINGNING HAO, YUPENG WANG, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, P. O. Box 603, Beijing 100190, China — Since 2008, many new families of iron-based high temperature (high- T_c) superconductors have been discovered. Unlike all parent compounds of cuprates that share a common antiferromagnetically (AF) ordered ground state, those of iron-based superconductors exhibit many different AF ordered ground states, including collinear-AF (CAF) state in ferropnictides, bicollinear-AF (BCAF) state in 11-ferrochalcogenide FeTe, and block-AF vacancy (BAFv) order state in 122-ferrochalcogenide $K0.8Fe1.6Se2$. While the universal presence of antiferromagnetism suggests that superconductivity is strongly interrelated with magnetism, the diversity of the AF ordered states obscures their interplay. Here we show that all magnetic phases can be unified within an effective magnetic model. This model captures three incommensurate magnetic phases as well, two of which have been observed experimentally. The model characterizes the nature of phase transitions between the different magnetic phases and explains a variety of magnetic properties, such as spin-wave spectra and electronic nematism. Most importantly, by unifying the understanding of magnetism, we cast new insight on the key ingredients of magnetic interactions which are critical to the occurrence of superconductivity.

4:42PM X22.00010 Spin dynamics of the J_1 - J_2 Model with Biquadratic Spin Interactions for the Paramagnetic Phase of the Iron Pnictides, ZHENTAO WANG, RONG YU, Rice University, PALLAB GOSWAMI, Florida State University, ANDRIY NEVIDOMSKYY, QIMIAO SI, Rice University, ELIHU ABRAHAMS, UCLA — The parent compounds of the iron pnictides are bad metals, and are hence interpreted as being located at the boundary of localization and itinerancy. As such, the effective exchange interactions will naturally include more than two spin components. Here we study the $J_1 - J_2$ antiferromagnetic Heisenberg model with a biquadratic spin-spin coupling $-\kappa(\vec{S}_i \cdot \vec{S}_j)^2$ to explore the spin excitations in the paramagnetic phase of the iron pnictides which has a $(\pi, 0)$ collinear antiferromagnetic ground state. By using the modified spin wave theory and Schwinger Boson mean field theory, we determine the spin dynamics at finite temperatures. We show that a moderate biquadratic coupling κ can induce sizable anisotropy in the spin excitation spectrum. The calculated dynamical structure factor $S(\vec{q}, \omega)$ shows anisotropic elliptic features near $(\pi, 0)$, which expand with increasing frequency (ω), in a way that agrees with recent experiment on $BaFe_2As_2$ above its Neel transition temperature (L. W. Harriger *et.al.*, PRB **84**, 054544, 2011).

4:54PM X22.00011 Dimensional crossover in the quasi-two-dimensional Ising-O(3) model, NAOIKI KAWASHIMA, Institute for Solid State Physics, University of Tokyo, YOSHITOMO KAMIYA, CRISTIAN BATISTA, Theoretical Division, Los Alamos National Laboratory — We present results of our Monte Carlo simulation of the Ising-O(3) model on the two-dimensional (2D) and quasi-2D lattices. This model is an effective classical model for the stacked square-lattice J_1 - J_2 Heisenberg model where the nearest neighbor (J_1) and next-nearest neighbor (J_2) couplings are frustrated and we assume that J_2 is dominant. We find an Ising ordered phase where the O(3) spins remain disordered in a moderate quasi-2D region. There is a single first order transition for a sufficiently large 3D coupling in agreement with a renormalization group treatment. The subtle region where the single transition splits into two transitions is also discussed and compared against recent measurements of two very close transitions in $BaFe_2As_2$. Our results can provide a qualitative explanation on the experiments on ferropnictides, namely observed sequence and orders of the structural and magnetic transitions, in terms of the ratio between the inter-layer and intra-layer coupling.

5:06PM X22.00012 Are Spinwaves Glue for Cooper Pairs in Iron-Pnictide High- T_c Superconductors?¹, JOSE RODRIGUEZ, California State University at Los Angeles — We study the 2-orbital t-J model over the square lattice via Schwinger-boson-slave-fermion mean-field theory and by exact numerical diagonalization of two holes over a 4×4 grid. The two orbitals in question are the degenerate $d_{\pm} = 3d_{(x \pm iy)z}$ ones, which maximize the Hund's Rule coupling. The mean-field theory predicts the existence of a quantum critical point (QCP) that separates a commensurate spin-density-wave (cSDW) metal at strong Hund's Rule coupling from a hidden half metal at weak Hund's Rule coupling. Holes in the hidden half metal hop through a $\backslash_{d+} \backslash_{d-}$ spin background without much hopping across orbitals. Mean-field theory further predicts a critical spin-wave spectrum that shows hidden low-energy excitations at zero momentum, and that shows observable low-energy excitations at cSDW momenta. We find that the virtual exchange of such spin-waves by mobile holes can be attractive, and that it can result in the formation of hole pairs. We seek to corroborate this by exact diagonalization of two holes in the 2-orbital t-J model.

¹Research supported in part by the AFOSR under grant FA9550-09-1-0660.

Thursday, March 1, 2012 2:30PM - 5:30PM – Session X23 GMAG: Magnetic Field Effects: Experimental II 255

2:30PM X23.00001 Investigating the field evolution of four-fold anisotropy in the basal plane of $\text{TmNi}_2\text{B}_2\text{C}$ ¹, P. DAS, C. RASTOVSKI, K. SCHLESINGER, M.R. ESKILDSEN, University of Notre Dame, IN, USA, J.M. DENSMORE, Lawrence Livermore National Laboratory, CA, USA, S.L. BUD'KO, P.C. CANFIELD, Ames Laboratory and Iowa State University, IA, USA — The superconductor $\text{TmNi}_2\text{B}_2\text{C}$ possesses a significant 4-fold in-plane anisotropy originating from the Fermi surface and possibly also from the superconducting pairing. However, unlike other members of the borocarbide superconductors, the anisotropy appears to decrease with increasing field, attributed to strong Pauli paramagnetic effects (PPE) and a vortex core expansion close to H_{c2} . We have investigated the field evolution of the four-fold anisotropy by small-angle neutron scattering (SANS) of the vortex lattice (VL), measuring several higher order Bragg peaks which allow a real space reconstruction of the VL field modulation. The measurements are possible due to the PPE which lead to a large field modulation (e.g. $\sim 65\%$ of the applied field at 0.2 T). Our results present the first *direct* demonstration of the decreasing anisotropy and furthermore, allows this to be measured quantitatively. This provides an explanation for the reentrant square VL phase observed in $\text{TmNi}_2\text{B}_2\text{C}$.

¹Supported by NSF award no. DMR-0804887 (Notre Dame) and DOE BES contract No. DE-AC02-07CH11358 (Ames). LLNL is operated by Lawrence Livermore National Security, LLC, for the U.S. DOE, National Nuclear Security Admin. under Contract DE-AC52-07NA27344.

2:42PM X23.00002 Vortex Lattice Anisotropy in Sr_2RuO_4 with $H \parallel a^1$, M.R. ESKILDSEN, C. RASTOVSKI, University of Notre Dame, IN, USA, C.D. DEWHURST, Institut Laue-Langevin, France, W.J. GANNON, Northwestern University, IL, USA, D.C. PEETS, H. TAKATSU, Y. MAENO, Kyoto University, Japan — We have studied the vortex lattice (VL) in superconducting Sr_2RuO_4 using spin-polarized small-angle neutron scattering (SP-SANS) and with magnetic fields (H) close to, but not perfectly aligned with, the crystalline basal plane. In this configuration the VL possesses a large transverse field component, due to the large anisotropy of Sr_2RuO_4 , which greatly increases the spin-flip SANS scattered intensity. Bragg reflections indicative of a highly distorted hexagonal VL were observed, and an analysis of the magnitude of the scattering vector yielded an anisotropy of 50–60, roughly two times the H_{c2} anisotropy. We discuss implications of this result in relation to theoretical predictions of Pauli paramagnetic effects in Sr_2RuO_4 with $H \perp c$ [K. Machida and M. Ichioka, Phys. Rev. B **77**, 184515 (2008)].

¹This work was supported by the Department of Energy, Basic Energy Sciences under Award No. DE-FG02-10ER46783.

2:54PM X23.00003 Influence of intrinsic superconducting parameters on the vortex dynamics and critical currents of different superconductor materials¹, N. HABERKORN, JEEHOON KIM, I. USOV, B. MAIOROV, M. WEIGAND, L. CIVALE, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — Vortex physics became a major field in condensed matter and statistical physics since the discovery of the oxide high temperature superconductors (HTS). Although the rich HTS vortex phenomenology arises from the large influence of thermal fluctuations, there is no hard boundary between HTS and conventional low temperature superconductors. The discovery of the iron-based superconductors provided a chance to study vortex matter in a new family of materials with broad ranges of superconductor transition temperature and crystalline anisotropy, where the small coherence length in some of them results in large fluctuation effects similar to those found in the oxide HTS. In this presentation, we will discuss the vortex dynamics of iron arsenide and oxide HTS by performing magnetization measurements of the critical current density (J_c) and flux creep rate (S). We will analyze the different creep regimes and crossovers that appear in the different samples and their relations to intrinsic superconducting parameters.

¹This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.

3:06PM X23.00004 Electrostatic manipulation of magnetic flux quanta at the nanoscale, ARNAUD CRASSOUS, ROZENN BERNARD, STEPHANE FUSIL, KARIM BOUZEHOUE, JAVIER BRIATICO, MANUEL BIBES, AGNES BARTHELEMY, JAVIER VILLEGAS, Unite Mixte de Physique CNRS/THALES — The electrostatic tuning of physical properties in materials offers significant potential in a large variety of systems. For example, the application of an electric field allows depressing or enhancing superconductivity in certain oxides. Using heterostructures that combine a large-polarization ferroelectric (BiFeO_3) and a high-temperature superconductor ($\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$), we demonstrate here the nanoscale modulation of the superconducting condensate via ferroelectric field effects [1]. The ability to design the ferroelectric domain structure at will enables us to create nanoscale “patterns” of normal regions within the superconductor, in a reversible and modifiable way. This produces an energy landscape for magnetic flux quanta and, in turn, couples the local polarization in the ferroelectric to the local magnetic induction in the superconductor. This new form of magnetoelectric coupling allows the electrostatic manipulation of magnetic flux quanta.

[1] A. Crassous et al., Phys. Rev. Lett. in press (2011)

3:18PM X23.00005 Strong periodic flux pinning in oxygen-ion-irradiated high- T_c superconductors¹, JAVIER VILLEGAS, I. SWIECICKI, J. BRIATICO, R. BERNARD, A. CRASSOUS, Unite Mixte de Physique CNRS/Thales, France, T. WOLF, N. BERGEAL, J. LESUEUR, LPEM, CNRS-ESPCI, France, C. ULYSSE, G. FAINI, CNRS, Phynano Team, LPN, France, X. HALLET, L. PIRAUX, Universite Catholique de Louvain, Belgium — We used oxygen ion irradiation to transfer into high- T_c superconducting thin films the nanoscale pattern of different types of masks (alumina [1] and [2] PMMA templates with ordered arrays of holes). This causes a nanoscale spatial modulation of superconductivity, and strongly affects the magneto-transport in the mixed-state. By tuning the irradiation dose and the array parameters, it is possible to engineer vortex energy landscapes sufficiently strong to govern flux dynamics. This is evidenced by a periodic series of strong magneto-resistance oscillations, the well-known fingerprint of periodic flux pinning. Interestingly, this irradiation technique allows tuning the *geometry* and the *strength* of the pinning potential wells at the nanoscale. This allows the observation of unusually strong matching effects at relatively high fields (up to several kOe). We show that the amplitude of the magneto-resistance oscillations is intimately connected with vortex channeling effects. [1] J.E. Villegas et al. Nanotechnology **22** 075302 (2011). [2] I. Swiecicki et al. submitted

¹Work supported by French ANR via ”SUPERHYBRIDS-II”

3:30PM X23.00006 Single vortex manipulation in superconducting $\text{NdFeAsO}_{1-x}\text{F}_x$, MAGDALENA HUEFNER, JEEHOON KIM, Harvard University, MATT TILLMAN, PAUL CANFIELD, Ames Laboratory and Iowa State University, JENNIFER HOFFMAN, Harvard University — Vortex pinning challenges have severely hampered attempts to incorporate cuprate high T_c superconductors into technology. Understanding and improving the pinning of quantized magnetic vortices in high T_c superconductors remains an important challenge. We use a homebuilt low temperature magnetic force microscope to image and manipulate individual vortices in single crystal $\text{NdFeAsO}_{1-x}\text{F}_x$ ($T_c=50\text{K}$). By exerting a large force on a single vortex we can deliberately depin it from its original position and permanently move it to a different, predetermined position. We can also drag the top of a single vortex for a short distance without permanently depinning its full length. By dragging individual vortices along different directions, we observe a 4-fold anisotropy of the dragging distance, with the easy-drag direction along the Fe-Fe axis. Our results shed light on the questions of anisotropy and pinning mechanisms in iron pnictides.

3:42PM X23.00007 Anisotropy and Vortex Pinning of Heavy Ion irradiated $\text{SmFeAsO}_{0.8}\text{F}_{0.15}$ and $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ Crystals¹, WAI-KWONG KWOK, LEI FANG, CARLOS CHAPARRO, YING JIA, ULRICH WELP, ALEXEI KOSHELEV, SHAOFEI XU, Argonne National Laboratory, GEORGE CRABTREE, Argonne National Laboratory and University of Illinois at Chicago, JANUSZ KARPINSKI, ETH, Zurich — We report specific heat and magnetization measurements on $\text{SmFeAsO}_{0.8}\text{F}_{0.15}$ and $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ single crystals irradiated with high energy heavy ions of 1.4 GeV Pb to dose matching fields up to 4 Tesla. We find a nearly one half reduction in the superconducting anisotropy and doubling of the irreversibility field in $\text{SmFeAsO}_{0.8}\text{F}_{0.15}$ after irradiation and virtually no change in the zero-field superconducting transition temperature. In both $\text{SmFeAsO}_{0.8}\text{F}_{0.15}$ and $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ crystals, we find a substantial increase in the critical current determined from SQUID and micro-Hall probe magnetization measurements. Pinning force analysis on proton and heavy ion irradiated pristine overdoped $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ crystals indicates presence of induced ΔT_c -type pinning defects in these samples.

¹Work supported by the US DoE-BES funded Energy Frontier Research Center (LF, CC, YJ, GWC), and by Department of Energy, Office of Science, Office of Basic Energy Sciences (WKK, UW, AEK, SFZ), under Contract No. DE-AC02-06CH11357

3:54PM X23.00008 High Dose Heavy-Ion Irradiation Effects on the Multiband Superconductor $(\text{Ba}_{0.6}\text{K}_{0.4})\text{Fe}_2\text{As}_2$ ¹, LEI FANG, CARLOS CHAPARRO, GOUTAM SHEET, YING JIA, SHAO-FEI ZHU, Argonne National Laboratory, HE-FEI HU, JIAN-MIN ZUO, University of Illinois at Urbana-Champaign, HAI-HU WEN, Nanjing University, China, ULRICH WELP, ALEXEI KOSHELEV, GEORGE CRABTREE, WAI-KWONG KWOK, Argonne National Laboratory — Optimal doped crystals of $(\text{Ba}_{0.6}\text{K}_{0.4})\text{Fe}_2\text{As}_2$ were irradiated with 1.4 GeV Pb ions to dose-matching fields ranging from 4 Tesla to 21 Tesla. Plan-view transmission electron microscopy shows creation of defects with diameters of $2 \sim 5$ nm. Post-irradiation characterization shows that the superconducting anisotropy is reduced to near unity, probably due to the increase in intra-band scattering. In addition, the critical current density J_C determined from magnetization measurements shows systematic enhancement up to ~ 5 MA/cm² at T=5K. We show that the decay of the critical current with magnetic field can be greatly mitigated with dense defects with approximately 20nm spacing produced by a dose matching field irradiation of 21T. Remarkably, the superconducting transition temperature remain unchanged for all matching field irradiation, suggesting that inter-band scattering due to non-magnetic impurity does not play a dominant role in pair-breaking.

¹ Work supported by the US DOE-BES funded Energy Frontier Research Center (LF, CC, YJ, GWC), and by Department of Energy, Office of Science, Office of Basic Energy Sciences (WKK, UW, AEK, SFZ), under Contract No. DE-AC02-06CH11357

4:06PM X23.00009 Angular dependence of magneto-transport properties in $\text{Ba}_{1-x}\text{K}_x(\text{FeAs})_2$ and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ single crystals, GOUTAM SHEET, ULRICH WELP, YING JIA, WAI-KWONG KWOK, Materials Science Division, Argonne National Laboratory, Argonne, USA, E.C. BLOMBERG, M.A. TANATAR, N. NI, S.L. BUD'KO, P.C. CANFIELD, R. PROZOROV, Iowa State University, Ames, Iowa, USA, H.H. WEN, University of Nanjing, Nanjing, China — We find unexpectedly sharp minima in the angular dependence of the flux-flow resistance of a series of $\text{Ba}_{1-x}\text{K}_x(\text{FeAs})_2$ and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ crystals when the magnetic field is applied parallel to the FeAs-planes. These minima are too sharp to be accounted for by effective mass anisotropy. Furthermore, since the c-axis coherence length is substantially larger than the FeAs layer spacing, intrinsic pinning mechanisms are ruled out. However, high-resolution cross-sectional SEM reveal the presence of plate-like inclusions of 50 - 100 nm thickness, which in a natural way can account for the enhanced pinning for $H \parallel ab$. On crystals that have been irradiated with heavy ions along the c-axis we observe additional resistance minima for $H \parallel c$, indicating the correlated nature of the irradiation induced defects.

4:18PM X23.00010 Combination of strong natural and artificial pinning centers in Co-doped BaFe_2As_2 films¹, BORIS MAIOROV, Los Alamos National Laboratory, NM 87545, T. KATASE, Tokyo Institute of Technology, Yokohama, Japan, M. WEIGAND, I. USOV, N. HABERKORN, Los Alamos National Laboratory, NM 87545, H. HIRAMATSU, H. HOSONO, Tokyo Institute of Technology, Yokohama, Japan, L. CIVALE, Los Alamos National Laboratory, NM 87545 — Studying the angular dependence of the critical current density (J_c) as a function of temperature in superconductors with complex pinning landscapes is very important from technical and fundamental points of view. The low anisotropy found in the $\text{BaFe}_2\text{As}_2(\text{Ba122})$ family together with strong naturally grown pinning make Ba122 films very attractive. We present results on Ba122 superconducting films with naturally grown correlated defects with the addition of different amounts of random defects produced by consecutive irradiations with 3MeV protons. We analyze the changes of J_c , H_{irr} and H_{c2} as a function of field, angle and temperature. Irradiations produce a small decrease in critical temperature (T_c) of 0.5 K per 1×10^{16} cm⁻² dose. After the irradiation, the pinning near the c-axis remains almost unchanged (except for the effects from the decrease of T_c). On the other hand, an increase of J_c is observed for other field orientations indicating and stronger random pinning contribution, particularly at high fields.

¹Work at Los Alamos was supported by the US Department of Energy (Division of Materials Sciences and Engineering)

4:30PM X23.00011 Highly Mobile In-plane Vortex Arrangement in $\text{SmFeAs}(\text{O},\text{F})$ ¹, PHILIP MOLL, Laboratory for Solid State Physics, ETH Zurich, Switzerland, LUIS BALICAS, National High Magnetic Field Laboratory, Tallahassee, FL, USA, JANUSZ KARPINSKI, NIKOLAI D. ZHIGADLO, BERTRAM BATLOGG, Laboratory for Solid State Physics, ETH Zurich, Switzerland — We observed a strong enhancement of flux flow dissipation for current flowing along the inter-planar direction in single crystals of the iron pnictide high- T_c superconductor $\text{SmFeAs}(\text{O},\text{F})$ ($T_c \sim 50\text{K}$) in high magnetic fields precisely aligned with the FeAs planes. The dissipation reaches significant fractions of the resistance in the normal state at all temperatures and fields, far below $H_{c2} \parallel ab$, estimated to be well above 100T at low temperatures. Even slightest field misalignments from the FeAs planes ($< 0.1^\circ$) restore the dissipation free state characterized by very high critical current densities ($\sim 10^6 \text{ A/cm}^2$) at low temperatures. We attribute this feature to vortices arranging themselves between the FeAs layers, accompanied by a reduced effectiveness of pinning. The qualitative features are reminiscent of the well-known lock-in effect in the cuprates, yet there are clear differences evident: The angular range of enhanced dissipation is reduced upon cooling in $\text{SmFeAs}(\text{O},\text{F})$, whereas in the cuprates it significantly broadens as H_{c1} increases at lower temperatures. Furthermore, the lock-in effect is most pronounced in strongly anisotropic materials, while $\text{SmFeAs}(\text{O},\text{F})$ is moderately anisotropic ($\gamma \sim 6-8$), becoming more isotropic at low temperature.

¹This work was supported by the NHMFL User Collaboration Grant

4:42PM X23.00012 Meissner holes in iron-based superconductors¹, TSUYOSHI TAMEGAI, SHYAM MOHAN, YUJI TSUCHIYA, YASUYUKI NAKAJIMA, Department of Applied Physics, The University of Tokyo — Magnetic flux penetrates into a superconductor in the form of quantized vortices. This process is usually described by the Bean model, and the flux front forms a regular pattern reflecting the shape of the sample. However, a novel form of flux penetration accompanying wiggling fronts between vortices and antivortices has been observed in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ upon remagnetization [1]. Such a phenomenon is ascribed to the presence of special arrangements of vortices at the front accompanying flux free regions and excess current around it. The flux free region is called as 'Meissner hole'. We have performed extensive magneto-optical imagings of iron-based superconductor single crystals and found similar anomalous features for the first time in superconductors other than 123-type cuprates [2]. Implications of this finding will be discussed with possible origins of the anomalous vortex arrangements. [1] V. K. Vlasko-Vlasov *et al.*, Phys. Rev. B **56**, 5622 (1997). [2] S. Mohan, Y. Tsuchiya, Y. Nakajima, and T. Tamegai, Phys. Rev. B **84**, 18050X (2011).

¹This work is partly supported by JST, Transformative Research-Project on Iron Pnictides (TRIP)

4:54PM X23.00013 Thermo-magnetic stability of NbN films with controlled nano-granularity, VITALIY YURCHENKO, University of Oslo, KONSTANTIN ILIN, Karlsruhe Institute of Technology, PAVLO MIKHEENKO, University of Oslo, M. SIEGEL, Karlsruhe Institute of Technology, YURI GALPERIN, TOM HENNING JOHANSEN, University of Oslo, UNIVERSITY OF OSLO TEAM, KARLSRUHE INSTITUTE OF TECHNOLOGY TEAM — The critical state in superconductors (SC) is metastable and can be destructed either by flux creep or by abrupt massive flux avalanches. The avalanches are associated with thermo-magnetic instability (TMI) of superconductors, which appears when the heat generated by the moving vortices is greater than the heat released into an environment. In that sense NbN films are known to be unstable, i.e. even the smallest increase of the external field may trigger a massive flux avalanche. Most theories developed to formulate the criteria of TMI operate in terms of intrinsic parameters of SC, such as heat capacity, critical current etc., and disregard the origins and the nature of the triggering mechanisms of the avalanches. We will present the most recent results of magneto-optical visualizations of flux dynamics in a series of NbN films with nano-scale disorder (ND) introduced in a well controlled fashion. We will demonstrate that not only do ND stipulate increase of the critical current but also promote correlated motion of large vortex bundles - micro jumps, which in turn trigger the macro avalanches.

5:06PM X23.00014 Quasi-1D intermittent flux dynamics in superconducting films, TOM H. JOHANSEN, ATLE J. QVILLER, VITALIY V. YURCHENKO, JORN I. VESTGARDEN, Dept. of Physics, University of Oslo, Norway, PETER B. MOZHAEV, JORN B. HANSEN, Dept. of Physics, Technical University of Denmark, Lyngby, Denmark, YURI M. GALPERIN, Dept. of Physics, University of Oslo, Norway — The stability of pinned vortex systems is constantly challenged in superconductors. In this work, magneto-optical imaging was used to reveal a new type of intermittent flux behavior in films of $\text{YBa}_2\text{Cu}_3\text{O}_x$. Films were grown on tilted NdGaO_3 substrates, where the terrace structure creates a high density of planar defects. The flux penetration along the terrace steps consists of numerous 1-dimensional avalanches, some starting at the film edge, some fully internal. In spite the vivid dynamics the flux front advances in accordance with the critical state model. Analysing more than 10000 avalanche events, we find a power-law size distribution and finite-size-scaling with the depth of the flux front as crossover length. The intermittent behaviour shows no threshold value in the applied field. These new characteristics largely contrast those of the thermo-magnetic avalanches observed in many superconducting films, and suggest that a different mechanism is responsible for the 1-dimensional avalanches.

5:18PM X23.00015 Investigation of the magnetic field angle dependence of resistance, irreversibility field, upper critical field and critical current density in DC sputtered Bi-2223 thin film¹, MURAT ERDEM, MUSTAFA AKDOGAN, GURCAN YILDIRIM, SEVGİ POLAT ALTINTAS, AHMET VARILCI, CABIR TERZIOGLU, Abant İzzet Baysal University — We measured resistivity and transport critical current density as a function of DC magnetic field and the angle between the surface of the film and the magnetic field on ex-situ annealed, c-axis oriented Bi-2223 thin films fabricated by DC sputtering method. Irreversibility field and upper critical field were determined from the resistivity vs. the applied magnetic field graph. It is observed that the superconducting properties of the films strongly depend on the direction and strength of the field. Penetration depths and coherence lengths were also determined from the irreversibility field and upper critical field versus temperature graphs, respectively. The anisotropic J_c behavior of the film is found to be intrinsic. We provided a theoretical analysis of the obtained results in the framework of intrinsic pinning theory of superconductors. Microstructural properties of the produced films were investigated by XRD and SEM measurements. XRD patterns indicate that the films are c-axis oriented based on the prominent (00l) peaks. SEM images show needle-like grain structures dominate the surface morphology of the films.

¹Supported partly by TUBITAK (Project nos. 108M201 and 104T323) and the Turkish State Planning Organization (Project no. 2004K120200).

Thursday, March 1, 2012 2:30PM - 5:30PM – Session X24 DCOMP: Electronic Structure: Quantum Monte Carlo 256

2:30PM X24.00001 The Homogeneous Electron Gas: Beyond Fixed Nodes, JAMES SHEPHERD, GEORGE BOOTH, ANDREAS GRUNEIS, ALI ALAVI, The University Chemical Laboratory, University of Cambridge — The ground state energy of the homogeneous electron gas (HEG) still presents a significant challenge to Quantum Chemical methods, in spite of being a model Hamiltonian that has been studied for many decades and is often regarded as the archetypal system in solid state physics and in Fermi liquid theory. To date the only truly successful methods to yield accurate ground state energies at a range of densities have been quantum Monte Carlo techniques, in particular Diffusion Monte Carlo (DMC). Attempts to go beyond the fixed-node approximation have been met with some success, however elimination of this error all-together has not been achieved. Full Configuration Interaction (FCI) would provide an exact solution to this problem in the limit of an infinite basis set, which can be approached in a systematically improvable way. However, this is prohibitively expensive, scaling exponentially in the electron number and the size of the underlying one-electron basis with very large pre-factors. We present the application of a new method, FCI Quantum Monte Carlo, which stochastically samples the exact wavefunction producing FCI accuracy at a greatly improved computational cost, to the high-density HEG.

2:42PM X24.00002 Simulation of the Warm-Dense Homogeneous Electron Gas¹, ETHAN BROWN, DAVID CEPERLEY, University of Illinois at Urbana-Champaign, JONATHAN DUBOIS, Lawrence Livermore National Laboratory — Warm-dense matter (WDM), where both the Coulomb coupling parameter ($\Gamma \equiv q^2/(r_s k_B T)$) and the electron degeneracy parameter ($\Theta \equiv k_B T/\epsilon_F$) are approximately unity, exists in systems as disparate as planetary interiors and along the pathway to inertial confinement fusion. Attempts to characterize this regime through the use of Density Functional Theory (DFT) require an accurate equation of state. Here we present results for a first-principles simulation of the homogeneous electron gas (HEG) in the warm-dense regime through Restricted Path Integral Monte Carlo (RPIMC). These results could be used as a benchmark for improved functionals, as well as input for orbital-free DFT formulations.

¹DOE DE-F652-06NA26170

2:54PM X24.00003 Improved Full Configuration Interaction Monte Carlo for the Hubbard Model¹, HITESH CHANGLANI, ADAM HOLMES, FRANK PETRUZIELO, GARNET CHAN, C.L. HENLEY, C.J. UMRIGAR, Cornell University — We consider the recently proposed full configuration interaction quantum Monte Carlo (FCI-QMC) method and its “initiator” extension, both of which promise to ameliorate the sign problem by utilizing the cancellation of positive and negative walkers in the Hilbert space of Slater determinants. While the method has been primarily used for quantum chemistry by A.Alavi and his co-workers [1,2], its application to lattice models in solid state physics has not been tested. We propose an improvement in the form of choosing a basis to make the wavefunction more localized in Fock space, which potentially also reduces the sign problem. We perform calculations on the 4x4 and 8x8 Hubbard models in real and momentum space and in a basis motivated by the reduced density matrix of a 2x2 real space patch obtained from the exact diagonalization of a larger system in which it is embedded. We discuss our results for a range of fillings and U/t and compare them with previous Auxiliary Field QMC and Fixed Node Green's Function Monte Carlo calculations.

[1] George Booth, Alex Thom, Ali Alavi, J Chem Phys, 131, 050106, (2009)

[2] D Cleland, GH Booth, Ali Alavi, J Chem Phys 132, 041103, (2010)

¹We acknowledge support from NSF CHE-1112097 DOE DE-FG02-07ER46365

3:06PM X24.00004 Semi-stochastic full configuration interaction quantum Monte Carlo¹, ADAM HOLMES, FRANK PETRUZIELO, MIHIR KHADILKAR, HITESH CHANGLANI, Laboratory of Atomic and Solid State Physics, Cornell University, M.P. NIGHTINGALE, Department of Physics, University of Rhode Island, C.J. UMRIGAR, Laboratory of Atomic and Solid State Physics, Cornell University — In the recently proposed full configuration interaction quantum Monte Carlo (FCIQMC) [1,2], the ground state is projected out stochastically, using a population of walkers each of which represents a basis state in the Hilbert space spanned by Slater determinants. The infamous fermion sign problem manifests itself in the fact that walkers of either sign can be spawned on a given determinant. We propose an improvement on this method in the form of a hybrid stochastic/deterministic technique, which we expect will improve the efficiency of the algorithm by ameliorating the sign problem. We test the method on atoms and molecules, e.g., carbon, carbon dimer, N₂ molecule, and stretched N₂.

[1] Fermion Monte Carlo without fixed nodes: a Game of Life, death and annihilation in Slater Determinant space. George Booth, Alex Thom, Ali Alavi. J Chem Phys 131, 050106, (2009).

[2] Survival of the fittest: Accelerating convergence in full configuration-interaction quantum Monte Carlo. Deidre Cleland, George Booth, and Ali Alavi. J Chem Phys 132, 041103 (2010).

¹NSF CHE-1112097, DOE DE-FG02-07ER46365

3:18PM X24.00005 Excited state calculations in solids by auxiliary-field quantum Monte Carlo¹, FENGJIE MA, SHIWEI ZHANG, HENRY KRAKAUER, Dept. of Physics, College of William & Mary — We have studied electronic excitations in solid systems using the phaseless auxiliary-field quantum Monte Carlo (AFQMC) method.² Trial wave functions for excited states are simply constructed from the corresponding density functional theory (DFT) ground state orbitals by promoting electrons to conduction bands. The post-processing finite size (FS) correction method³ is applied to remove the many-body FS effects. By fitting the calculated excitation energies at various crystal momentum values, a many-body electronic band structure is obtained. Our results for prototypical semiconductors such as silicon are compared to those from the GW approximation⁴ and diffusion Monte Carlo calculations.⁵

¹Supported by DOE, NSF, ONR.

²S. Zhang and H. Krakauer, Phys. Rev. Lett. **90**, 136401 (2003); W. Purwanto, S. Zhang, and H. Krakauer, J. Chem. Phys. **130**, 094107 (2009).

³F. Ma, S. Zhang, and H. Krakauer, Phys. Rev. B **84**, 155130 (2011); H. Kwee, S. Zhang, and H. Krakauer, Phys. Rev. Lett. **100**, 126404 (2008).

⁴M. Rohlfing, P. Krüger, and J. Pollmann, Phys. Rev B. **48**, 17791 (1993).

⁵A. J. Williamson, R. Q. Hood, R. J. Needs, and G. Rajagopal, Phys. Rev. B **57**, 12140 (1998).

3:30PM X24.00006 Frozen core method in auxiliary-field quantum Monte Carlo¹, WIRAWAN PURWANTO, SHIWEI ZHANG, HENRY KRAKAUER, Department of Physics, College of William and Mary, Williamsburg, VA — We present the implementation of the frozen-core approach in the phaseless auxiliary-field quantum Monte Carlo method (AFQMC). Since AFQMC random walks take place in a many-electron Hilbert space spanned by a chosen one-particle basis, this approach can be achieved without introducing additional approximations, such as pseudopotentials. In parallel to many-body quantum chemistry methods, tightly-bound inner electrons occupy frozen canonical orbitals, which are determined from a lower level of theory, e.g. Hartree-Fock or CASSCF. This provides significant computational savings over fully correlated all-electron treatments, while retaining excellent transferability and accuracy. Results for several systems will be presented. This includes the notoriously difficult Cr₂ molecule, where comparisons can be made with near-exact results in small basis sets, as well as an initial implementation in periodic systems.

¹Supported by DOE, ONR, and NSF. Calculations were performed at OLCF Jaguar and CPD.

3:42PM X24.00007 Tests on novel pseudo-potentials generated from diffusion Monte Carlo data.¹, FERNANDO REBOREDO, Oak Ridge National Laboratory, RANDOLPH HOOD, Lawrence Livermore National Laboratory, MICHAL BAJDICH, Lawrence Berkeley National Laboratory — Since Dmitri Mendeleev developed a table in 1869 to illustrate recurring (“periodic”) trends of the elements, it has been understood that most chemical and physical properties can be described by taking into account the outer most electrons of the atoms. These valence electrons are mainly responsible for the chemical bond. In many ab-initio approaches only valence electrons are taken into account and a pseudopotential is used to mimic the response of the core electrons. Typically an all-electron calculation is used to generate a pseudopotential that is used either within density functional theory or quantum chemistry approaches. In this talk we explain and demonstrate a new method to generate pseudopotentials directly from all-electron many-body diffusion Monte Carlo (DMC) calculations and discuss the results of the transferability of these pseudopotentials. The advantages of incorporating the exchange and correlation directly from DMC into the pseudopotential are also discussed.

¹Research supported by the Materials Sciences and Engineering (MSE) Division of the Office of Science U.S. DOE

3:54PM X24.00008 A diffusion Monte Carlo study of sign problems from non-local pseudopotentials, NORM TUBMAN, University of Illinois at Urbana-Champaign, MIGUEL MORALES-SILVA, JONATHAN DUBOIS, RANDOLPH HOOD, Lawrence Livermore National Lab — Difficulties can arise in simulating various Hamiltonian operators efficiently in diffusion Monte Carlo (DMC) such as those associated with non-local pseudopotentials which require the introduction of an approximate form. The locality approximation and T-moves are two widely used techniques in fixed-node diffusion Monte Carlo (FN-DMC) that provide a tractable approach for treating non-local pseudopotentials, however their use introduces an uncontrolled approximation. Exact treatment of the non-local pseudopotentials in FN-DMC introduces a sign problem with the associated Green's function matrix elements which take on both positive and negative values. Here we present an analysis of the nature of the sign problem that non-local operators introduce into the Green's function. We then consider the feasibility of running DMC simulations in which the non-local pseudopotentials are treated exactly and demonstrate the algorithm on a few molecular systems.

4:06PM X24.00009 Variational and diffusion quantum Monte Carlo methods for spin-orbit interactions in heavy element systems¹, LUBOS MITAS, RENE DERIAN, SHI GUO, North Carolina State University — In most electronic structure quantum Monte Carlo calculations spins of individual electrons have fixed values which are determined by the spin and spatial symmetries of the desired eigenstate. However, for heavy atoms the spin-orbit interaction becomes important and its influence on electronic structure becomes comparable to the electron exchange, correlations or other many-body effects. In such cases the simplest antisymmetric wave function based on one-particle states is a determinant of spinors, while the simplest pairing wave function is a pfaffian. We will present calculations using variational and diffusion Monte Carlo for heavy atoms systems with spin-orbit operators. We eliminate the atomic cores by effective core potentials (pseudopotentials) which are formulated so as to include also effective spin-orbit operators. We test both discrete spin sampling as well as continuous spin representation in the variational and diffusion Monte Carlo methods. Corresponding generalizations of the fixed-node/fixed-phase methods will be discussed as well.

¹Supported by DOE, NSF and ARO

4:18PM X24.00010 Progress in exact treatment of fermions at finite temperature¹, JONATHAN L. DUBOIS, BERNI J. ALDER, Lawrence Livermore National Lab — We will discuss some key features of the structure of permutation space for interacting Fermi systems. Exploiting these features, we will then demonstrate improved efficiency in the exact path integral Monte Carlo treatment of liquid ³He by using importance sampling to deemphasize the contribution of long permutation cycles to the partition function. Finally, a route to a polynomial scaling algorithm for homogeneous Fermi systems will be presented.

¹This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

4:30PM X24.00011 An energy density estimator for quantum Monte Carlo calculations, JARON KROGEL, University of Illinois at Urbana-Champaign, JEONGNIM KIM, University of Illinois at Urbana-Champaign; Oak Ridge National Laboratory, DAVID CEPERLEY, University of Illinois at Urbana-Champaign — We establish a physically meaningful representation of a quantum energy density for use in quantum Monte Carlo calculations. The energy density operator, defined in terms of Hamiltonian components and density operators, returns the correct Hamiltonian when integrated over a volume containing a cluster of particles. This property is demonstrated for a Helium-Neon "gas," showing that atomic energies obtained from the energy density correspond to eigenvalues of isolated systems. The formation energies of defects or interfaces are typically calculated as total energy differences. Using a model of delta doped Silicon (where dopant atoms form a thin plane) we show how interfacial energies can be calculated more efficiently with the energy density, since the region of interest is small. We also demonstrate how the energy density correctly transitions to the bulk limit away from the interface where the correct energy is obtainable from a separate total energy calculation.

4:42PM X24.00012 Metal-Insulator Transition in Low Density Atomic Hydrogen¹, JEREMY MCMINIS, University of Illinois, JEONGNIM KIM, Oak Ridge National Lab, DAVID CEPERLEY, University of Illinois — At low density BCC hydrogen undergoes a metal-insulator transition. We compute the zero temperature equation of state for the paramagnetic and anti-ferromagnetic phases using diffusion Quantum Monte Carlo. We predict the phase transition density, investigate the shape of the anti-ferromagnetic curve, and compare to previous results

¹The work supported by the National Science Foundation under No. 0904572 and EFRC - Center for Defect Physics sponsored by the US DOE, Office of Basic Energy Sciences.

4:54PM X24.00013 Quantum Monte Carlo of ThO₂¹, SHUMING HU, LUBOS MITAS, Physics Department, North Carolina State University — Thorium dioxide solid is a unique optical and heat-resistant actinide material with large gap and cohesion. It is a diamagnet, unlike a number of other similar actinide oxides. We investigate the electronic structure of ThO₂ using Density Functional Theory (DFT) and quantum Monte Carlo (QMC) methods. We adopt Stuttgart RLC and RSC effective core potentials (pseudopotentials) for the Th atom. In the DFT calculations, some of the properties are verified in all-electron calculations using the FLAPW techniques. Using the fixed-node diffusion Monte Carlo we calculate the ground state and several excited states from which we estimate the cohesion and the band gap. Simulation cells of several sizes are used to estimate/reduce the finite size effects. We compare the QMC results with recent DFT calculations with several types of functionals which include hybrids such as PBE0 and HSE. Insights from QMC calculations give us understanding of the correlations beyond the DFT approaches and pave the way for accurate electronic structure calculations of other actinide materials.

¹Supported by DOE and NSF

5:06PM X24.00014 Quantum Monte Carlo for the Spectroscopy of Core Excited States, DMITRY ZUBAREV, UC Berkeley — X-ray absorption spectroscopy is a powerful experimental tool that is capable of delivering valuable information about very delicate aspects of electronic structure and reveals details of the local chemical environment in many systems of fundamental and applied importance. The rigorous interpretation of core-level spectra requires very accurate quantum chemical simulations. The trade-off between feasibility of treatment of large systems and consistency in description of electron correlation tremendously hinders the generation of accurate theoretical results for many experimental studies. We show that the fixed-node diffusion Monte Carlo (FN-DMC) approach can be used straightforwardly for the accurate simulation of core-level spectra. Basic methodological aspects are addressed, including the strategy for the construction of adequate trial wave functions. Examples of FN-DMC calculations of core-level spectra of water and pyrrole are presented. The possibility of the simulation of X-ray absorption spectra of solvent-solute systems is discussed.

5:18PM X24.00015 Density Functional Monte Carlo: an efficient way to calculate the ground state density profile of nanostructures, FONS BROSENS, KATRIJN PUTTENEERS, University of Antwerpen — We present a method in which the Hohenberg-Kohn theorems are implemented directly by simulating the density profile using Bernoulli walkers and conserving the total number of particles during the Monte Carlo process. This leads to a much faster algorithm than, e.g., by solving the Kohn-Sham equations. The method is explained in detail and results are shown for a nanoshell which contains several millions of conduction electrons.

Thursday, March 1, 2012 2:30PM - 5:30PM –

Session X25 DCOMP: Focus Session: Modeling of Rare Events: Methods and Applications II

257A

2:30PM X25.00001 Accelerated Molecular Dynamics of Rare Events with the Bond-Boost Method¹, KRISTEN FICHTHORN, Penn State University — A continuing challenge in materials simulation is to conduct long time and large length simulations of structural evolution, while accurately retaining atomic detail. For many materials, dynamical evolution occurs through a series of “rare events,” in which the system spends a long-time period in one free-energy minimum before escaping and moving on to another. To address the rare-event problem for materials evolution, we developed the bond-boost method, which is a variant of hyperdynamics. We will introduce the bond-boost method and demonstrate several applications of it to thin-film growth and surface kinetics. A significant problem that plagues rare-event simulations is the “small barrier problem” and we will discuss how this problem can be addressed within the bond-boost method. We will also discuss our recent efforts to combine this method with kinetic Monte Carlo simulations.

¹Supported by NSF DMR-1006452

3:06PM X25.00002 Generalizations of the string method, ERIC VANDEN-EIJNDEN, Courant Institute, NYU — Generalizations of the string method will be presented that permit to identify the saddle points by which the process escapes the basin of attraction of a minimum of the potential due to thermal noise, or to map out the volume of this basin. These methods will be illustrated via examples such as thermal reorganization of Lennard-Jones clusters and packings of soft-spheres.

3:42PM X25.00003 String method for the computation of minimum energy paths and saddle points, WEIQING REN, National University of Singapore and IHPC — Many problems arising from applied sciences can be abstractly formulated as a system that navigates over a complex energy landscape of high or infinite dimensions. The system is confined in metastable states for long times before making important transitions from one metastable state to another. For gradient systems driven by small noise, the transitions follow the minimum energy path, i.e. the heteroclinic orbit connecting the metastable states. I will talk about the zero-temperature string method for computing the minimum energy paths and the saddle points.

3:54PM X25.00004 Rare events in viscoelastic escape dynamics and subdiffusive transport¹, IGOR GOYCHUK, University of Augsburg — Anomalously slow relaxation, escape and transport processes become increasingly important in many research domains. This talk is focused on a profound question: Does anomalously slow subdiffusive dynamics imply rare events with a divergent mean time separating such events in multistable potentials? The answer depends on the underlying physical mechanism. It is shown that the subdiffusive dynamics originated due to the medium's viscoelasticity and described by a power law memory kernel within the non-Markovian generalized Langevin equation (GLE) approach does not imply such anomalously rare events [1]. Based on a Markovian multidimensional embedding of the GLE dynamics it is shown that the kinetics of subdiffusive Kramers escape is asymptotically stretched exponential for intermediate barriers. It is characterized by a finite mean escape time, and all the higher moments are also finite. Moreover, it approaches normal exponential kinetics for very high barriers which coexists with anomalously slow subdiffusion and transport in washboard potentials [1]. Rare escape events for such subdiffusive dynamics are not presenting the transport limiting step.

[1] I. Goychuk, Phys. Rev. E 80, 046125 (2009); Adv. Chem. Phys. 150 (2012, in press).

¹Supported by the DFG, grant GO 2052/1-1.

4:06PM X25.00005 Non-axisymmetric Deformations of Monovalent Metallic Nanowires: A Stochastic Field Theory Approach, LAN GONG, DANIEL STEIN, New York University, JEROME BUERKI COLLABORATION, CHARLES STAFFORD COLLABORATION — A stochastic Ginzburg-Landau field theory is used to describe the noise-induced transition of monovalent metallic nanowires. Here the transition consists of the nanowire changing from one locally stable radius to another (and thereby changing its conductance as well). The lifetime of a specific wire configuration is obtained from the Kramers rate formula in the limit of weak noise. We found a “phase transition” in the saddle state under general conditions, and have constructed a phase diagram of the activated transition. To study the transition process further, we employed a numerical approach called the string method in order to obtain in detail the complete transition path, crucial to solving the dynamics of wire deformation and transition under noise. We also discuss several interesting applications to lifetime calculations for real nanowires.

4:18PM X25.00006 Study of Evaporation Rate of Water in Hydrophobic Confinement using Forward Flux Sampling, SUMIT SHARMA, PABLO G. DEBENEDETTI, Princeton University — Drying of hydrophobic cavities is of interest in understanding biological self assembly, protein stability and opening and closing of ion channels. Liquid-to-vapor transition of water in confinement is associated with large kinetic barriers which preclude its study using conventional simulation techniques. Using forward flux sampling to study the kinetics of the transition between two hydrophobic surfaces, we show that a) the free energy barriers to evaporation scale linearly with the distance between the two surfaces, d; b) the evaporation rates increase as the lateral size of the surfaces, L increases, and c) the transition state to evaporation for sufficiently large L is a cylindrical vapor cavity connecting the two hydrophobic surfaces. Finally, we decouple the effects of confinement geometry and surface chemistry on the evaporation rates.

4:30PM X25.00007 Reaching extended length-scales with accelerated dynamics¹, BRADLEY HUBARTT, YUNSHI SHIM, JACQUES AMAR, University of Toledo — While temperature-accelerated dynamics (TAD) has been quite successful in extending the time-scales for non-equilibrium simulations of small systems, the computational time increases rapidly with system size. One possible solution to this problem, which we refer to as parTAD¹ is to use spatial decomposition combined with our previously developed semi-rigorous synchronous sublattice algorithm². However, while such an approach leads to significantly better scaling as a function of system-size, it also artificially limits the size of activated events and is not completely rigorous. Here we discuss progress we have made in developing an alternative approach in which localized saddle-point searches are combined with parallel GPU-based molecular dynamics in order to improve the scaling behavior. By using this method, along with the use of an adaptive method to determine the optimal high-temperature³, we have been able to significantly increase the range of time- and length-scales over which accelerated dynamics simulations may be carried out. [1] Y. Shim et al, Phys. Rev. B **76**, 205439 (2007); *ibid*, Phys. Rev. Lett. **101**, 116101 (2008). [2] Y. Shim and J.G. Amar, Phys. Rev. B **71**, 125432 (2005). [3] Y. Shim and J.G. Amar, J. Chem. Phys. **134**, 054127 (2011).

¹Supported by NSF-DMR 0907399

4:42PM X25.00008 A computational atomistic study of the relaxation of ion-bombarded c-Si on experimental time-scales: an application of the kinetic Activation Relaxation Technique, LAURENT KARIM BÉLAND, NORMAND MOUSSEAU, Dept. de physique and RQMP, Université de Montréal, Canada — The kinetic activation relaxation technique (kinetic ART) method, an off-lattice, self-learning kinetic Monte Carlo (KMC) algorithm with on-the-fly event search,¹ is used to study the relaxation of c-Si after Si⁻ bombardment at 3 keV. We describe the evolution of the damaged areas at room-temperature and above for periods of the order of seconds, treating long-range elastic deformations exactly. We assess the stability of the nanoscale structures formed by the damage cascade and the mechanisms that govern post-implantation annealing.

¹L. K. Béland, P. Brommer, F. El-Mellouhi, J.-F. Joly and N. Mousseau, Phys. Rev. E **84**, 046704 (2011).

4:54PM X25.00009 Dislocation Cross-slip Mechanisms in Aluminum, YANG XIANG, Hong Kong University of Science and Technology, CONGMING JIN, Zhejiang Sci-Tech University, China, GANG LU, California State University Northridge — We have systematically studied dislocation cross-slip in Al at zero temperature by atomistic simulations, focusing on the dependence of the transition paths and energy barriers on dislocation length and position. We find that for a short dislocation segment, the cross-slip follows the uniform Fleischer (FL) mechanism. For a longer dislocation segment, we have identified two different cross-slip mechanisms depending on the initial and final positions of the dislocation. If the initial and final positions are symmetric relative to the intersection of the primary and cross-slip planes, the dislocation cross-slips via the Friedel-Escaig (FE) mechanism. However, when the initial and final positions are asymmetric, the dislocation cross-slips via a combination of the FL and FE mechanisms. The leading partial folds over to the cross-slip plane first, forming a stair-rod dislocation at the intersection with which the trailing partial then merges via the FL mechanism. Afterwards, constrictions appear asymmetrically and move away from each other to complete the cross-slip via the FE mechanism.

5:06PM X25.00010 The Effects of Hydrogen on the Potential-Energy Surface of Amorphous Silicon, JEAN-FRANCOIS JOLY, NORMAND MOUSSEAU, Université de Montréal — Hydrogenated amorphous silicon (a-Si:H) is an important semiconducting material used in many applications from solar cells to transistors. In 2010, Houssem et al. [1], using the open-ended saddle-point search method, ART nouveau, studied the characteristics of the potential energy landscape of a-Si as a function of relaxation. Here, we extend this study and follow the impact of hydrogen doping on the same a-Si models as a function of doping level. Hydrogen atoms are first attached to dangling bonds, then are positioned to relieve strained bonds of fivefold coordinated silicon atoms. Once these sites are saturated, further doping is achieved with a Monte-Carlo bond switching method that preserves coordination and reduces stress [2]. Bonded interactions are described with a modified Stillinger-Weber potential and non-bonded Si-H and H-H interactions with an adapted Slater-Buckingham potential. Large series of ART nouveau searches are initiated on each model, resulting in an extended catalogue of events that characterize the evolution of potential energy surface as a function of H-doping.

[1] Houssem et al., Phys Rev. Lett., 105, 045503 (2010)

[2] Mousseau et al., Phys Rev. B, 41, 3702 (1990)

5:18PM X25.00011 Order-order Nucleation in Copolymers: A String Method Approach¹, XIUYUAN CHENG, PACM, Princeton University, WEINAN E, PACM, Princeton University; SMS, Peking University, PINGWEN ZHANG, SMS, Peking University, ANCHANG SHI, Department of Physics and Astronomy, McMaster University, Canada, CHU WANG, SMS, Peking University — The mechanism of nucleation in order-order phase transitions of block copolymers is an interesting problem presenting both theoretical and numerical challenges. In this talk we will introduce our recent work of applying the string method to the order-order nucleation in diblock copolymer. We use the self-consistent field model, and search for the saddle point of the free energy functional by solving a variational problem. We will also talk about a study of the epitaxial relation between ordered phases (work by Wang Chu et al.), which verifies one of the assumptions taken by the numerical method beforehand.

¹NNSF of China (50930003), NSERC of Canada, computational facilities by SHARCNET: www.sharcnet.ca

Thursday, March 1, 2012 2:30PM - 4:54PM – Session X26 DCOMP: Focus Session: Non-Adiabatic Dynamics in Irradiated Materials 257B

2:30PM X26.00001 First-principles calculation of electronic stopping power in metals and insulators via time-dependent DFT simulations, JORGE KOHANOFF¹, Atomistic Simulation Centre, Queens University Belfast, Belfast BT7 1NN, Northern Ireland, United Kingdom — Projectiles interacting with solid or liquid targets are subject to two main inelastic collision channels: electronic and nuclear. The end result is a slowing down – or stopping – of the projectile due to energy deposition onto electronic excitations or motion of the target nuclei. At high projectile velocities, cross sections for nuclear stopping are exceedingly small, thus leaving electronic stopping as the only relevant channel. At low velocities nuclear stopping becomes predominant. In metals, it coexists with electronic stopping, but in insulators the existence of an energy gap for electronic excitations translates into a velocity threshold for electronic stopping. In this presentation I will introduce a recently developed computational methodology designed to study electronic stopping at the first-principles level, by means of time-dependent density-functional (TDDFT) simulations. I will then discuss the results for a variety of systems, starting from the first application to the ionic crystal LiF, moving to metallic systems like Al and Au, and then to the insulating water ice. In all cases I will compare to available experimental data to emphasize the astonishing accuracy of TDDFT results. I will also discuss how these simulations provide further insight into open questions such as the difference in stopping between H and He projectiles, and I will focus on the interplay between electronic excitations and non-adiabatic forces on the nuclei. Finally, I will touch on computational methods to simulate the combined dynamics of nuclei and electrons.

¹Work done in collaboration with E. Artacho (University of Cambridge, UK), D. Sánchez-Portal (Donostia International Physics Center, Spain), A. Caro (Los Alamos National Laboratory, USA), and A. Correa (Lawrence Livermore National Laboratory, USA)

3:06PM X26.00002 Nonadiabatic Molecular Dynamics with Trajectories , IVANO TAVERNELLI, École

Polytechnique Fédérale de Lausanne (EPFL) — In the mixed quantum-classical description of molecular systems, only the quantum character of the electronic degrees of freedom is considered while the nuclear motion is treated at a classical level. In the adiabatic case, this picture corresponds to the Born-Oppenheimer limit where the nuclei move as point charges on the potential energy surface (PES) associated with a given electronic state. Despite the success of this approximation, many physical and chemical processes do not fall in the regime where nuclei and electrons can be considered decoupled. In particular, most photoreactions pass through regions of the PES in which electron-nuclear quantum interference effects are sizeable and often crucial for a correct description of the phenomena. Recently, we have developed a trajectory-based nonadiabatic molecular dynamics scheme that describes the nuclear wavepacket as an ensemble of particles following classical trajectories on PESs derived from time-dependent density functional theory (TDDFT) [1]. The method is based on Tully's fewest switches trajectories surface hopping (TSH) where the nonadiabatic coupling elements between the different potential energy surfaces are computed *on-the-fly* as functionals of the ground state electron density or, equivalently, of the corresponding Kohn-Sham orbitals [2]. Here, we present the theoretical fundamentals of our approach together with an extension that allows for the direct coupling of the dynamics to an external electromagnetic field [3] as well as to the external potential generated by the environment (solvent effects) [4]. The method is applied to the study of the photodissociation dynamics of simple molecules in gas phase and to the description of the fast excited state dynamics of molecules in solution (in particular Ruthenium (II) tris(bipyridine) in water).

[1] E. Tapavicza, I. Tavernelli, U. Rothlisberger, *Phys. Rev. Lett.*, **98**, (2007) 023001.

[2] Tavernelli I.; Tapavicza E.; Rothlisberger U., *J. Chem. Phys.*, **130**, (2009) 124107; Tavernelli I., Curchod B.F.E., Rothlisberger U., *J. Chem. Phys.*, **131**, (2009) 196101; Tavernelli I., Curchod B.F.E., Laktionov A., Rothlisberger U., *J. Chem. Phys.*, **133**, (2010) 194104.

[3] Tavernelli I., Curchod B.F.E., Rothlisberger U., *Phys. Rev. A*, **81**, (2010) 052508.

[4] Tavernelli I., Curchod B.F.E., Rothlisberger U., *Phys. Chem.*, accepted 2011.

3:42PM X26.00003 Advances on Time-dependent DFT Simulations of Electronic Stopping¹ ,

ALFREDO CORREA, ANDRE SCHLEIFE, Lawrence Livermore National Laboratory, YOSUKE KANAI, University of North Carolina at Chapel Hill, JORGE KOHANOFF, Queen's University, Belfast, ALFREDO J. CARO, Los Alamos National Laboratory — Radiation damage of reactor materials is a topic of interest and continuous research in the nuclear industry. A single nuclear decay event (e.g. alpha) produces a cascade of collisions involving the displacement of thousands of atoms in a crystalline material. While atomistic-scale simulations would be the ideal tool to understand these processes, the fact that they currently work on the assumption that electrons respond adiabatically to the atomic motion does not provide valid answers, for example to the stopping power problem. An alternative approach to attacking this problem is a method which explicitly takes into account electron non-adiabatic dynamics. We will present results obtained by time-depending DFT on the electronic stopping power of channeling protons in prototypical metals and insulators obtained by recent implementations of non-adiabatic electron dynamics methods.

¹Prepared by LLNL under Contract DE-AC52-07NA27344

3:54PM X26.00004 Electronic stopping of slow H and He atoms in gold from first principles

, M. AHSAN ZEB, Cavendish Lab, Cambridge, UK, JORGE KOHANOFF, Physics, Queens U, Belfast, UK, DANIEL SANCHEZ-PORTAL, CFM-CSIC, San Sebastian, Spain, ANDRES ARNAU, J.I. JUARISTI, CFM-UPV, San Sebastian, Spain, EMILIO ARTACHO, Nanogune & Ikerbasque, San Sebastian, Spain, and Cavendish Lab, Cambridge, UK — In spite of a long history, the quantitative understanding of non-adiabatic processes in condensed matter and our ability to perform predictive theoretical simulations of processes coupling many adiabatic energy surfaces is very much behind what accomplished for adiabatic situations, for which first-principles calculations provide predictions of varied properties within a few percent accuracy. We will present here high-accuracy results for the electronic stopping power of H and He moving through gold, using time-evolving density-functional theory, thereby conveying usual first-principles accuracies to strongly coupled, continuum non-adiabatic processes in condensed matter. The two key unexplained features of what observed experimentally have been reproduced and understood: (i) The non-linear behavior of stopping power versus velocity is a gradual crossover as excitations tail into the *d*-electron spectrum; and (ii) the higher stopping for He than for H at low velocities is explained by the substantial involvement of the *d* electrons in the screening of the projectile even at the lowest velocities where the energy loss is generated by *s*-like electron-hole pair formation only.

4:06PM X26.00005 Golden Rule of Radiation Hardness: a Study of Strain Effect on Controlled Radiation Damage¹ ,

QING PENG, WEI JI, SUVRANU DE, Rensselaer Polytechnic Institute — Stain is widely presented in microstructures. Strain effect to radiation hardness is critical in understanding and engineering nano-materials. Here we studied the strain effect on the controlled radiation damage in monolayer hexagonal boron nitride (h-BN) through *ab initio* density functional theory calculations. We observed a general behavior of reduction in the radiation hardness by the strain, for both B-vacancy and N-vacancy configurations, in both compressive and tensile strain states, at the directions of zigzag, armchair and bi-axial. We proposed a golden rule of the radiation hardness states that any effort adding energy to the system will reduce the radiation hardness. Such golden rule of radiation hardness could be widely applied to material design and engineering for those devices working in irradiation-enrich environments, for example, electronic and optoelectronic devices in outer space.

¹The authors would like to acknowledge the generous financial support from the Defense Threat Reduction Agency (DTRA) Grant # BRBAA08-C-2-0130, and the U.S. Nuclear Regulatory Commission Faculty Development Program under contract # NRC-38-08-950.

4:18PM X26.00006 First-principles simulation of laser irradiation of graphene and graphane¹ ,

KALMAN VARGA, SERGIY BUBIN, Vanderbilt University — In the framework of real-time real-space time-dependent density functional theory complemented with classical molecular dynamics for ions, we have studied the behavior of graphene and graphane fragments irradiated with strong laser pulses. In particular, we have investigated how the response of graphene and graphane changes when laser pulses of different frequency (near IR, visible, and UV) are shot. Damage thresholds have been established and compared with existing experimental data.

¹supported by NSF through grant CMMI-0927345

4:30PM X26.00007 Electron-Phonon Coupling in a CdSe Nanowire¹ ,

CHRISTOPHER BARRETT, Department of Materials Science & Engineering, UC Berkeley, LIN-WANG WANG, Materials Sciences Division, Lawrence Berkeley National Laboratory — It is important to calculate the coupling between phonons and electrons in realistic nanostructures, e.g. to understand carrier cooling and dynamics in a nanowire. In this talk, we will present results of phonon spectrum calculations using a customized valence force field (VFF) method. This customized VFF method is developed to be fittable to the results of any *ab-initio* calculations, with density functional theory (DFT) results being used in this work. By fitting many different DFT calculations on different motifs and their perturbations, we have obtained in the custom VFF a very efficient method that closely reproduces DFT phonons for CdSe nanowires with (10-10) surfaces having Cd-Se dimerization. We have also combined the results of these phonon spectrum calculations with electronic structure calculations to obtain the electron-phonon coupling. We will present this result and show how the electron-phonon coupling affects the carrier dynamics in the nanowire.

¹This work is supported by U.S. Department of Energy BES, Office of Science, under Contract No. DE-AC02-05CH11231.

4:42PM X26.00008 Deviational formulations for efficient simulation of multiscale phonon transport , JEAN-PHILIPPE PERAUD, NICOLAS HADJICONSTANTINO, Mechanical Engineering, MIT — We show that by simulating only the deviation from equilibrium, considerable computational savings can be realized in Monte Carlo solutions of the Boltzmann equation describing phonon transport at small scales. The computational savings manifest themselves in the form of significantly smaller statistical uncertainty compared to standard Monte Carlo solution methods in the limit of small deviation from equilibrium (e.g. small temperature differences). Additional computational savings are realized in multiscale problems where the degree of deviation from equilibrium varies considerably over the simulation domain. By developing rigorous evolution equations for the deviation from equilibrium from the governing kinetic equation, the resulting algorithm seamlessly bridges the near- and far-equilibrium regions without introducing any approximation. We also show that considering an energy-based Boltzmann equation lends itself naturally to algorithms that conserve energy exactly, thus improving the simulation fidelity. Application of the proposed methods to practical problems of current interest, such as a transient thermoreflectance experiment used to extract information about the mean free path of heat carriers in various materials, will be presented and discussed.

Thursday, March 1, 2012 2:30PM - 5:30PM –
Session X27 DMP DCMP: Invited Session: Physics for Everyone: Innovative Materials for Energy 258AB

2:30PM X27.00001 Materials research needs for energy , ARUN MAJUMDAR, Advanced Research Projects Agency - Energy — No abstract available.

3:06PM X27.00002 Water Splitting with Materials and Sunlight , TOM JARVI, Sun Catalytix Corporation — Sun Catalytix has been developing technology for energy storage and the generation of renewable fuels in an ARPA-E sponsored program. The program has focused on the development and deployment of low-cost earth-abundant catalytic materials coupled to light-absorbing semiconductor systems to capture and convert solar energy into chemical species. This talk will focus on recent work done to couple cobalt-based water-oxidation and nickel-based hydrogen evolution catalysts with silicon-based solar cells. The results demonstrate direct wireless coupling of solar collection with catalytic materials and operate in relatively benign conditions at reasonable conversion efficiency. These results suggest development pathways for solar hydrogen generation using catalyzed particulate solar absorbing materials. Such pathways will be discussed as they may offer relevant means to generate solar-derived hydrogen as a cost-effective fuel for the future.

3:42PM X27.00003 Advanced materials manufacturing for solar energy , FRANK VAN MIERLO, 1366 Technologies Inc. — The US has a robust technical roadmap to get to a \$1/W total installed cost with several potential winners in the race. We dominate in the new technology arena and there is a good chance that tomorrow's winning technology will be from the current crop of contenders. One potential breakthrough is Direct WaferTM a new manufacturing technique to make silicon wafers at a fraction of the traditional cost. Current wafer manufacturing is a multi-step, energy- and capital-intensive process that wastes half of the valuable silicon feedstock. 1366's Direct Wafer technology forms a standard, 156mm multi-crystalline wafer directly from molten silicon in a semi-continuous, efficient, high-throughput process that eliminates silicon waste. Direct WaferTM cuts the amount of consumables by a factor of four and requires only half the capital per GigaWatt production capacity thus enabling solar to compete successfully with coal generated electricity.

4:18PM X27.00004 Genetically Engineered Materials for Biofuels Production , MICHAEL RAAB, Agrivida, Inc. — Agrivida, Inc., is an agricultural biotechnology company developing industrial crop feedstocks for the fuel and chemical industries. Agrivida's crops have improved processing traits that enable efficient, low cost conversion of the crops' cellulosic components into fermentable sugars. Currently, pretreatment and enzymatic conversion of the major cell wall components, cellulose and hemicellulose, into fermentable sugars is the most expensive processing step that prevents widespread adoption of biomass in biofuels processes. To lower production costs we are consolidating pretreatment and enzyme production within the crop. In this strategy, transgenic plants express engineered cell wall degrading enzymes in an inactive form, which can be reactivated after harvest. We have engineered protein elements that disrupt enzyme activity during normal plant growth. Upon exposure to specific processing conditions, the engineered enzymes are converted into their active forms. This mechanism significantly lowers pretreatment costs and enzyme loadings (>75% reduction) below those currently available to the industry.

4:54PM X27.00005 Innovative oxide materials for electrochemical energy conversion , ERIC D. WACHSMAN, University of Maryland — Research in functional materials has progressed from those materials exhibiting structural to electronic functionality. The study of ion conducting ceramics ushers in a new era of "chemically functional materials." This chemical functionality arises out of the defect equilibria of these materials, and results in the ability to transport chemical species and actively participate in chemical reactions at their surface. Moreover, this chemical functionality provides a promise for the future whereby the harnessing of our natural hydrocarbon energy resources can shift from inefficient and polluting combustion - mechanical methods to direct electrochemical conversion. The unique properties of these materials and their applications will be described. The focus will be on the application of ion conducting ceramics to energy conversion and storage, chemical sensors, chemical separation and conversion, and life support systems. Results presented will include development of record high power density (3 kW/kg) solid oxide fuel cells, NO_x/CO species selective solid-state sensors, high yield membrane reactors, and regenerative life support systems that reduce CO₂ to O₂ and solid C.

Thursday, March 1, 2012 2:30PM - 5:30PM –
Session X29 GQI: Focus Session: Semiconductor Qubits - Managing or Eliminating Nuclei 259A

2:30PM X29.00001 Ultrafast optical coherent control of individual electron and hole spins in a semiconductor quantum dot, KRISTIAAN DE GREVE, E.L. Ginzton Laboratory, Stanford University — We report on the complete optical coherent control of individual electron and hole spin qubits in InAs quantum dots. With a magnetic field in Voigt geometry, broadband, detuned optical pulses couple the spin-split ground states, resulting in Rabi flopping. In combination with the Larmor precession around the external magnetic field, this allows an arbitrary single-qubit operation to be realized in less than 20 picoseconds [1,2]. Slow fluctuations in the spin's environment lead to shot-to-shot variations in the Larmor precession frequency. In a time-ensemble measurement, these would prevent a measurement of the true decoherence of the qubit, and instead give rise to ensemble dephasing. This effect was overcome by implementing a spin echo measurement scheme for both electron and hole spins, where an optical π -pulse refocuses the spin coherence and filters out the slow variations in Larmor precession frequency. We measured coherence times up to 3 microseconds [2,3]. Finally, our optical pulse manipulation scheme allows us to probe the hyperfine interaction between the single spin and the nuclei in the quantum dot. Interesting non-Markovian dynamics could be observed in the free-induction decay of a single electron spin, whereas the complete absence of such effects illustrates the reduction of the hyperfine interaction for hole spin qubits. We measured and modeled these effects, and explain the non-Markovian electron spin dynamics as involving a feedback effect resulting from both the strong Overhauser shift of the electron spin and spin dependent nuclear relaxation [2,4].

- [1] D. Press, T. D. Ladd, B. Zhang and Y. Yamamoto, *Nature* **456**, 218 (2008)
- [2] K. De Greve, P. McMahon, D. Press *et al.*, *Nat. Phys.* **7**, 872 (2011)
- [3] D. Press, K. De Greve, P. McMahon *et al.*, *Nat. Phot.* **4**, 367 (2010)
- [4] T. D. Ladd, D. Press, K. De Greve *et al.*, *Phys. Rev. Lett.* **105**, 107401 (2010)

3:06PM X29.00002 Ultrafast optical control of interacting hole spins in coupled quantum dots, SAMUEL CARTER, Naval Research Laboratory, Washington, DC 20375, ALEX GREILICH, Naval Research Laboratory, Washington, DC 20375; University of Maryland, College Park, Maryland 20742, DANNY KIM, Naval Research Laboratory, Washington, DC 20375; University of Michigan, Ann Arbor, Michigan 48109, ALLAN BRACKER, DANIEL GAMMON, Naval Research Laboratory, Washington, DC 20375 — Recently, hole spins in quantum dots (QDs) have shown great promise as quantum bits due to a reduced hyperfine interaction with nuclear spins, the primary source of decoherence for electron spins. We have developed a system of two vertically stacked InAs QDs that can be charged with a number of holes. In this way, an isolated hole in one QD or two interacting holes in separate dots can be studied. We demonstrate ultrafast optical control of both systems and find a number of differences compared to electron spins. Complete control of the single hole qubit is obtained through optical initialization and single qubit rotations. These control measurements give a hole spin T_2^* of 20ns, an order of magnitude longer than electrons in similar QDs. Spin echo experiments extend the coherence time but are complicated by oscillations in the echo amplitude. For the case of two hole spins, we can observe and tune the coherent exchange interaction that acts as a two qubit gate. We also initialize and perform gates on an entangled spin state, taking a significant step toward a scalable platform for quantum information processing. [1] "Optical control of one and two hole spins in interacting quantum dots," A. Grelich, S. G. Carter, D. Kim, A. S. Bracker and D. Gammon. *Nature Photon.* **5**, 702 (2011).

3:18PM X29.00003 Electrical control of single hole spins in InSb nanowire quantum dots, VLAD PRIBIAG, STEVAN NADJ-PERGE, JOHAN VAN DEN BERG, SERGEY FROLOV, TU Delft, SEBASTIEN PLISSARD, TU Eindhoven, ERIK BAKKERS, LEO KOUWENHOVEN, TU Delft — The spin-orbit interaction provides an efficient handle for all-electric control of individual spins in quantum dots. Recently, III-V semiconductor nanowires, which have a strong spin-orbit coupling, have emerged as a promising platform for spin-based qubits. Previous work has been focused on the electrical control of electron spins in InAs nanowires. In contrast, spin-dependent quantum transport with holes has so far remained largely unexplored. Here, we demonstrate gate tuning from the few-electron double dot to the few-hole double-dot regimes in InSb nanowires and observe Pauli spin-blockade for both electrons and holes. We use electric-dipole spin resonance (EDSR) to determine the effective g-factors of the two types of carriers. EDSR control over the hole spins is promising for driving coherent rotations of hole-spin qubits. These hole qubits are expected to be less sensitive to hyperfine-mediated decoherence effects than electron-spin qubits as a result of the p-wave symmetry of the hole wavefunction.

3:30PM X29.00004 Theory of heavy-hole spin-echo decay, XIAOYA JUDY WANG, WILLIAM COISH, McGill University — Heavy-hole spin states have emerged as a robust new candidate for realizing a qubit. Nevertheless, the coupling of the hole spin to nuclei in the surrounding medium likely limits hole-spin coherence and has, until very recently, been overlooked. We describe the real-time spin decoherence of a heavy-hole in a semiconductor quantum dot, subject to spin echo pulses. We obtain an analytical expression which we compute numerically for an experimentally realistic number ($\sim 10^4$) of nuclear spins. Including the (previously neglected) nuclear Zeeman term in the Hamiltonian, we observe novel effects uniquely characterizing the decoherence mechanisms under study. In particular, we find a nontrivial dependence of the decay on the applied magnetic field, as well as novel predictions for motional narrowing and envelope modulation, which could significantly extend the hole-spin memory time in near-future experiments.

3:42PM X29.00005 High Quality Two-Dimensional Electron Gases (2DEGs) in Isotopically-Enriched Strained Silicon, JIUN-YUN LI, CHIAO-TI HUANG, Department of Electrical Engineering and Princeton Institute for the Science and Technology of Materials (PRISM), Princeton University, LEONID ROKHINSON, Department of Physics, Purdue University, JAMES OHLHAUSEN, MALCOLM CARROLL, Sandia National Laboratories, JAMES STURM, Department of Electrical Engineering and Princeton Institute for the Science and Technology of Materials (PRISM), Princeton University — Silicon quantum dots (QDs) formed in a Si/SiGe two-dimensional electron gas (2DEG) are a promising candidate for quantum computation. To capture a single electron in a QD, the dot must be very small, which requires a short distance from the surface to Si 2DEG layer for fine gating. Here we demonstrate a high quality modulation-doped Si 2DEG grown by chemical vapor deposition (CVD), with a distance of 65 nm from the surface to 2DEG layer. The electron mobility at 0.3K of 504,000 $\text{cm}^2/\text{V-s}$ (density $4.3 \times 10^{11} \text{ cm}^{-2}$) is the highest yet reported by CVD for ungated Si 2DEGs. Further, a Si 2DEG layer consists of isotopically-enriched ^{28}Si to minimize spin decoherence due to ^{29}Si . SIMS results show that in the Si 2DEG layer, ^{28}Si is enriched from natural abundance of 92.2% to 99.8% with ^{29}Si reduced from 4.7% to an upper limit of $\sim 0.24\%$ and ^{30}Si reduced from 3.1% to $\sim 63\text{ppm}$. Finally, effective Schottky gating requires a sharp turn-off slope in phosphorus from the doped layer to the surface for low electric fields near the surface. We have achieved ultra-sharp turn-off slope of $\sim 16 \text{ nm/dec}$, and demonstrate Schottky gating to fully deplete the 2DEG with extremely low leakage current.

3:54PM X29.00006 Implanted bismuth donors in 28-Si: Process development and electron spin resonance measurements, C.D. WEIS, C.C. LO, Lawrence Berkeley National Laboratory, V. LANG, R.E. GEORGE, University of Oxford, A.M. TYRYSHKIN, Princeton University, J. BOKOR, University of California at Berkeley, S.A. LYON, Princeton University, J.J.L. MORTON, University of Oxford, T. SCHENKEL, Lawrence Berkeley National Laboratory — Spins of donor atoms in silicon are excellent qubit candidates. Isotope engineered substrates provide a nuclear spin free host environment, resulting in long spin coherence times [1,2]. The capability of swapping quantum information between electron and nuclear spins can enable quantum communication and gate operation via the electron spin and quantum memory via the nuclear spin [2]. Spin properties of donor qubit candidates in silicon have been studied mostly for phosphorous and antimony [1-3]. Bismuth donors in silicon exhibit a zero field splitting of 7.4 GHz and have attracted attention as potential nuclear spin memory and spin qubit candidates [4,5] that could be coupled to superconducting resonators [4,6]. We report on progress in the formation of bismuth doped 28-Si epi layers by ion implantation, electrical dopant activation and their study via pulsed electron spin resonance measurements showing narrow linewidths and good coherence times.

- [1] A. M. Tyryshkin, et al. arXiv: 1105.3772 [2] J. J. L. Morton, et al. *Nature* (2008) [3] T. Schenkel, et al. *APL* 2006; F. R. Bradbury, et al. *PRL* (2006)
- [4] R. E. George, et al. *PRL* (2010) [5] G. W. Morley, et al. *Nat Mat* (2010) [6] M. Hatridge, et al. *PRB* (2011), R. Vijay, et al. *APL* (2010) This work was supported by NSA (100000080295) and DOE (DE-AC02-05CH11231).

4:06PM X29.00007 Isotopic enrichment and growth of material for quantum coherent devices

, KEVIN DWYER, NIST, University of Maryland, JOSHUA POMEROY, NIST — We demonstrate isotopic enrichment and growth of highly pure materials in support of quantum coherent devices. Efforts to produce devices capable of quantum computation rely on long coherence times of the electron or nuclear spin being used. Impurities with nuclear spin are a major cause of decoherence in such systems, and their elimination is essential towards longer T_2 realization. The produced material must be isotopically enriched as well as chemically pure and defect free, and we present an alternative method for achieving these goals. Unenriched material is ionized and filtered using a mass selecting magnet and then epitaxially deposited. As an initial check on enrichment, ^{22}Ne is implanted into Si demonstrating an isotopic selectivity over 1800:1 which extrapolates to a ^{28}Si enrichment better than 99.994%. In progression towards Si deposition from a silane precursor, methane is used as an analog to grow enriched ^{13}C on semiconductor grade silicon. Analysis of this material by SIMS and ESR as a check on estimated levels of isotopic and chemical purity is presented.

4:18PM X29.00008 Realization of a double quantum dot in an isotopically purified ^{28}Si 2DES

, ANDREAS WILD, JUERGEN SAILER, GERHARD ABSTREITER, Walter Schottky Institut, Technische Universitaet Muenchen, Germany, J.W. AGER, E.E. HALLER, Department of Materials Science and Engineering, University of California at Berkeley, USA, STEFAN LUDWIG, Fakultät für Physik, Ludwig-Maximilians Universitaet Muenchen, Germany, JOHANNES KIERIG, DOMINIQUE BOUGEARD, Institut für Experimentelle und Angewandte Physik, Universitaet Regensburg, Germany — The Si/SiGe material system shows great promise for the realization of electron spin qubits due to the weak hyperfine interaction in natural silicon [2]. The electron spin coherence time is expected to further increase for spins embedded in a nuclear spin-refined ^{28}Si host crystal. In this contribution, we report on the realization and characterization of a 2DES in a MBE grown hybrid ^{28}Si /SiGe heterostructure with a record mobility of $5.5 \cdot 10^4 \text{ cm}^2/\text{Vs}$ at an electron density of $3 \cdot 10^{11}/\text{cm}^2$ in which the electron-nuclear spin overlap is greatly suppressed [1]. Based on this heterostructure, we present the first double quantum dot device in isotopically purified silicon. Our device can be operated down to the few electron regime and by using an additional global topgate above the quantum dot gates, the overall charge noise performance can be optimized significantly. This recent progress is fundamental for further experiments towards e.g. measurements of spin relaxation times in ^{28}Si .

[1] J. Sailer et al., Phys. status solidi RRL 3, 61 (2009)

[2] A. Wild et al., New J. Phys. 12, 113019 (2010)

4:30PM X29.00009 Deterministic preparation of Dicke states of donor nuclear spins in silicon¹

, YU LUO, HONGYI YU, WANG YAO, Department of Physics and Center of Theoretical and Computational Physics, The University of Hong Kong, Hong Kong, China — We present a scheme to deterministically prepare various symmetric and asymmetric Dicke states for donor nuclear spins in silicon. The state preparation is realized by cooperative pumping of nuclear spins by coupled donor electrons, and the required controls are in situ to the prototype Kane's architecture for quantum computation. This scheme only requires a sub-gigahertz donor exchange coupling which can be achieved without atomically precise donor placement, hence it could be a practical way to prepare multipartite entanglement of spins in silicon with current technology. All desired Dicke states appear as the steady state under various pumping scenarios and therefore the preparation is robust and does not require accurate temporal controls. Numerical simulations with realistic parameters show that Dicke states of 10 - 20 qubits can be prepared with high fidelity in the presence of decoherence and undesired dynamics.

¹The work was supported by the Research Grant Council of Hong Kong under Grant No. HKU 706711P.

4:42PM X29.00010 Optical Patterning of Nuclear Polarization in Gallium Arsenide , JONATHAN

KING, University of California, Berkeley, YUNPU LI, CARLOS MERILES, City College of New York, JEFFREY REIMER, University of California, Berkeley — Large enhancements of nuclear spin polarization can quench weak electron-nuclear fluctuations, mitigate electron spin decoherence, and provide control of electron spins in devices for quantum information processing. Such enhancements might include spatially patterned regions of polarized nuclei so as to prepare a spatially-dependent effective Zeeman field acting on electron spins as well as coherently manipulate the spin state of drifting electrons. By exploiting two competing mechanisms for optical nuclear polarization in semi-insulating GaAs, we use high field stray-field NMR imaging to demonstrate all-optical creation of three-dimensional patterns of positive and negative nuclear polarization without the need for ferromagnets or lithographic patterning techniques. These patterns may be controlled on the micron length scale.

4:54PM X29.00011 Integrating MREV and XXYX Pulse Sequences to Decouple Dipolar Interactions in ESR Experiments , ALEXEI TYRYSKHIN, STEPHEN LYON, Princeton University — Dynamical decoupling (DD) techniques

employ a series of strong refocusing pulses to combat decoherence in quantum systems. A great number of the new improved DD sequences have been designed recently aiming to decouple from a specific kind of decohering noise, arising in the direction of an externally applied quantizing field. MREV-type pulse sequences have long been used in NMR community to decouple spins from another source of decoherence - the dipolar interactions between like spins. Here, we report on our experience while using MREV sequences in ESR experiments on donors in silicon. We find MREV sequences to be very sensitive to even small instrumental errors in the applied pulses. The errors accumulate upon repeating the MREV pulse sequence, destroying the coherence instead of protecting it. A possible solution to this pulse error problem is found by integrating an MREV pulse sequence with a self-correcting XXYX sequence. The new MREV-XXYX sequence appears to satisfy all the requirements of a "good" DD sequence: (1) providing a protection to an arbitrary coherent state with good fidelity (at least 95% after more than 17,000 pulses), (2) decoupling from dipolar interactions of like spins, and (3) cancelling the phase noise arising from fluctuations in the magnetic field.

5:06PM X29.00012 Master equation approach to the central spin decoherence problem¹ , EDWIN

BARNES, Condensed Matter Theory Center, Dept. of Physics, University of Maryland, LUKASZ CYWINSKI, Institute of Physics, Polish Academy of Sciences, SANKAR DAS SARMA, Condensed Matter Theory Center, Dept. of Physics, University of Maryland — The electron-nuclear hyperfine interaction is the leading source of decoherence for electron spin qubits in III-V semiconductor quantum dots. For sufficiently low external B-field, the dynamics is purely hyperfine-induced. Generalized master equations embody an attractive approach to this problem due to strong analytical control, but so far they have only been applied in the case of high magnetic fields where a standard perturbative treatment is reliable. In the low field regime where pure hyperfine effects are measurable, this standard treatment breaks down. We show how to overcome this problem by first arguing that the detailed shape of the electron wavefunction is irrelevant for the electron spin decoherence at low B-fields. We then employ a powerful technique involving so-called correlated projection operators to vastly improve the convergence of the perturbative master equation approach by taking advantage of the symmetries that arise when the electron wavefunction is coarse-grained. This brings the low B-field regime into the scope of the master equation description, paving the way for the development of a well-controlled theory of pure hyperfine decoherence that is relevant for current experiments. [E. Barnes, L. Cywinski, S. Das Sarma, Phys. Rev. B 84, 155315 (2011)]

¹Work supported by LPS-CMTC, CNAM, and IARPA

5:18PM X29.00013 Two-electron-spin dephasing due to hyperfine interaction in a GaAs double dot, JO-TZU HUNG, Department of Physics, University at Buffalo, SUNY, LUKASZ CYWINSKI, Institute of Physics, Polish Academy of Sciences, XUEDONG HU, Department of Physics, University at Buffalo, SUNY, SANKAR DAS SARMA, Department of Physics, University of Maryland — We study hyperfine interaction induced pure dephasing of two electron spin states in a GaAs double quantum dot. We construct the effective pure dephasing Hamiltonian for the two electron spins, and apply the ring-diagram theory [1] to calculate the decoherence function of the double dot two-spin system. With a finite exchange coupling, singlet and triplet states are the electron spin eigenstates, and we focus on the dephasing between the singlet state S and the unpolarized triplet state T_0 . We find that the effective Overhauser fields for these two states are suppressed because of their state symmetries, leading to weaker effective coupling between the nuclear spins. On the other hand, the weaker Overhauser field also allows more nuclear spins to flip-flop with each other. We show that these competing effects lead to interesting two-spin decoherence dynamics. We calculate the coherence decay as functions of the external field, the exchange splitting, and the quantum dot size, and compare our results with those for a single spin and for two uncorrelated spins. [1] L. Cywinski, W. Witzel, and S. Das Sarma, Phys. Rev. B 79, 245314 (2009).

Thursday, March 1, 2012 2:30PM - 5:18PM –
Session X30 GQI: Focus Session: Quantum Information for Quantum Foundations - Foundational Experiments and Experimental Proposals 259B

2:30PM X30.00001 Experimental violation of the Leggett-Garg inequality under decoherence¹, JIN-SHI XU, CHUAN-FENG LI, XU-BO ZOU, GUANG-CAN GUO, University of Science and Technology of China — Despite the great success of quantum mechanics, questions regarding its application still exist and the boundary between quantum and classical mechanics remains unclear. Based on the philosophical assumptions of macrorealism and noninvasive measurability, Leggett and Garg devised a series of inequalities (LG inequalities) involving a single system with a set of measurements at different times. Introduced as the Bell inequalities in time, the violation of LG inequalities excludes the hidden-variable description based on the above two assumptions. Here, we experimentally investigate the single photon LG inequalities in a dephasing environment simulated by birefringent media. By implementing an optical Controlled-Not gate on a single photon, the LG inequalities are shown to be maximally violated in a coherent evolution process. This disproves its classical realistic description with the two assumptions of the LG inequalities. With the increase of birefringent media, the violation of LG inequalities becomes weaker and is shown to be not violated anymore at some time. The ability to violate the LG inequalities can be used to set the boundary of the classical realistic description.

¹This work was supported by the National Basic Research Program of China (Grants No. 2011CB9212000), National Natural Science Foundation of China (Grant Nos. 60921091, 10874162, 11004185), China Postdoctoral Science Foundation (Grant No. 20100470836)

2:42PM X30.00002 A condition for macroscopic realism beyond the Leggett-Garg inequalities, JOHANNES KOFLER, Max Planck Institute of Quantum Optics — In 1985, Leggett and Garg have put forward the concept of macroscopic realism (macrorealism), stating that the properties of macroscopic objects exist independent of and are not influenced by measurement. In analogy to Bell's theorem, they derived a necessary condition in terms of inequalities, which are now known as the Leggett-Garg inequalities. In this talk, a mathematical condition is introduced which is not only necessary but also sufficient for macrorealism. More importantly, the structure of this condition intuitively encompasses the physical meaning of macrorealism and allows for its experimental test in situations where the paradigm of Leggett-Garg inequalities might not be applicable.

2:54PM X30.00003 A quantum delayed-choice *gedanken* experiment¹, RADU IONICIOIU, Institute for Quantum Computing, University of Waterloo, DANIEL TERNO, Department of Physics & Astronomy, Macquarie University, Sydney — *Gedanken* experiments are important conceptual tools in the quest to reconcile our classical intuition with quantum mechanics and nowadays are routinely performed in the laboratory. An important open question is the quantum behaviour of the controlling devices in such experiments. We propose a framework to analyse quantum-controlled experiments and illustrate the implications by discussing a quantum version of Wheeler's delayed-choice experiment. The introduction of a quantum-controlled device (i.e., quantum beamsplitter) has several consequences. First, it implies that we can measure complementary phenomena with a single experimental setup, thus pointing to a redefinition of complementarity principle. Second, a quantum control allows us to prove there are no consistent hidden-variable theories in which "particle" and "wave" are realistic properties. Finally, it shows that a photon can have a morphing behaviour between "particle" and "wave"; this further supports the conclusion that "particle" and "wave" are not realistic properties but merely reflect how we "look" at the photon. The framework developed here can be extended to other experiments, particularly to Bell-inequality tests.

¹Work supported by ARC Centre for Quantum Computer Technology, Macquarie University and EC Project QUANTIP 244026

3:06PM X30.00004 The Pauli Exclusion Principle for electrons – a high sensitivity test in Gran Sasso underground laboratory, JOHANN MARTON, Stefan Meyer Institute, Austrian Academy of Sciences, VIP COLLABORATION — One of the fundamental rules of nature and a pillar in the foundation of quantum theory and thus of modern physics is represented by the Pauli Exclusion Principle. We know that this principle is extremely well fulfilled due to many observations like the order of the elements and the stability of matter. Numerous experiments were performed to search for tiny violation of this rule in various systems. The experiment VIP at the Gran Sasso underground laboratory is searching for possible small violations of the Pauli Exclusion Principle for electrons leading to an "anomalous" X-ray transition in copper atoms. VIP is aiming at a test of the Pauli Exclusion Principle for electrons with unprecedented accuracy, down to the level of 10^{-29} - 10^{-30} , thus improving the previous limit by 3-4 orders of magnitude. The experimental method, the setup, results obtained so far and future plans to further increase the precision by 2 orders of magnitude will be presented.

3:18PM X30.00005 Quantum metamaterials as a tool for investigating the quantum-classical transition, SERGEY SAVELIEV, ALEXANDRE ZAGOSKIN, MARK EVERITT, RICHARD WILSON, Department of Physics, Loughborough University, Loughborough LE11 3TU, UK — Quantum metamaterials are optical media comprised of individually controllable unit elements (e.g., qubits), which maintain quantum coherence for periods sufficient for an electromagnetic wave to pass through the system. They represent macroscopic, spatially extended quantum scatterers, which can be put in a superposition of states with different properties (e.g., different refractive indexes) and can thus provide new ways of testing different scenarios of quantum-classical transition. We consider an inverse of the classic double-slit experiment, where a classical electromagnetic wave is scattered by a quantum metamaterial in a superposition of states, and discuss the possibilities of its experimental realization.

3:30PM X30.00006 Progress towards a loophole-free test of nonlocality¹, KEVIN MCCUSKER, BRADLEY CHRISTENSEN, PAUL KWIAT, University of Illinois at Urbana-Champaign, JOSEPH ALTEPETER, Northwestern University — We report on our progress towards a loophole-free test of nonlocality using spontaneous parametric down-conversion (SPDC). While the timing loophole can be easily closed in such a system by moving the detectors far apart [1], closing the detector loophole is significantly more difficult. In the standard Bell entangled states with the maximal violation of the CHSH inequality [2], an overall efficiency of 83% is required. This limit can be lowered to 67% by using non-maximally entangled states (although sensitivity to noise is greatly increased) [3]. We are carefully engineering our source to achieve maximal heralding efficiency, by optimizing both the spatial and spectral filtering, while keeping noise low using high-extinction-ratio polarizing beamsplitters. Combined with high-efficiency detectors, either optimized visible-light photon counters [4] or transition-edge sensors [5], closure of the detection loophole is within reach.

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- [2] J. F. Clauser et al., Phys. Rev. Lett. 23, 880 (1969).
- [3] P.H. Eberhard, Phys. Rev. A 47, R747 (1993).
- [4] S. Takeuchi et al., Appl. Phys. Lett. 74, 1063 (1999).
- [5] A. E. Lita, A. J. Miller, and S. Nam, Opt. Exp. 16, 3032 (2008).

¹Supported by US-ISRAEL BSF GRANT #2008032.

3:42PM X30.00007 Loophole-free Quantum Steering¹, SVEN RAMELOW, BERNHARD WITTMANN, FABIAN STEINLECHNER, NATHAN K. LANGFORD, VCQ, Faculty of Physics, Univ. of Vienna and IQOQI Vienna, NICOLAS BRUNNER, Wills Physics Laboratory, Univ. of Bristol, HOWARD WISEMAN, Centre f. Quantum Computation and Communication Technology (ARC), Griffith University, RUPERT URSIN, ANTON ZEILINGER, VCQ, Faculty of Physics, Univ. of Vienna and IQOQI Vienna — Experiments testing quantum mechanics have provided increasing evidence against local realistic theories. However, a conclusive test that simultaneously closes all major loopholes (the locality, freedom-of-choice, and detection loopholes) remains an open challenge. An important class of local realistic theories can be tested with the concept of “steering.” Schrödinger introduced this term for entanglement seemingly allowing to remotely steer the state of a distant system [1]. Einstein called this “spooky action at a distance.” Steering was recently formalized by deriving steering inequalities allowing experimental tests. Here, we present the first loophole-free steering experiment [2]. We use entangled photons shared between two distant laboratories and close all loopholes by a large separation, ultra-fast switching and quantum random number generation, and high, overall detection efficiency. Beside its foundational importance loop-hole-free steering is relevant for is relevant for device-independent certification of quantum entanglement.

- [1] E. Schrödinger, Proc. Camb. , Phil. Soc. 31, 553 (1935)
- [2] B. Wittmann, S. Ramelow, F. Steinlechner, N. K. Langford, N. Brunner, H. Wiseman, R. Ursin, A. Zeilinger, arXiv:1111.0760, (2011)

¹Funding by FWF (CoQuS and SFB FoQus) and ERC (QIT4QAD)

3:54PM X30.00008 Conclusive quantum steering with superconducting transition edge sensors, MARCELO P. DE ALMEIDA, DEVIN H. SMITH, GEO GILLET, CYRIL BRANCIARD, ALESSANDRO FEDRIZZI, TILL J. WEINHOLD, School of Mathematics and Physics, University of Queensland, 4072 Brisbane, QLD, Australia, ADRIANA LITA, BRICE CALKINS, THOMAS GERTIS, SAE WOO NAM, National Institute of Standards and Technology, 325 Broadway, Boulder CO 80305, USA, ANDREW G. WHITE, School of Mathematics and Physics, University of Queensland, 4072 Brisbane, QLD, Australia — Quantum steering allows two parties to verify shared entanglement even if one measurement device is untrusted. A conclusive demonstration of steering through the violation of a steering inequality is of considerable fundamental interest and opens up applications in quantum communication. To date all experimental tests with single photon states have relied on post-selection, allowing untrusted devices to cheat by hiding unfavorable events in losses. Here we close this “detection loophole” by combining a highly efficient source of entangled photon pairs with superconducting transition edge sensors. We achieve an unprecedented ~62% conditional detection efficiency of entangled photons and violate a steering inequality with the minimal number of measurement settings by 48 standard deviations. Our results provide a clear path to practical applications of steering and to a photonic loophole-free Bell test.

4:06PM X30.00009 Experimental Violation of Heisenberg’s Precision Limit by Weak Measurements, ARDAVAN DARABI, LEE A. ROZEMA, DYLAN H. MAHLER, ALEX HAYAT, Centre for Quantum Information and Quantum Control, and Institute for Optical Sciences, Department of Physics, University of Toronto, YASAMAN SOUDAGAR, Ecole Polytechnique de Montreal, University of Toronto, AEPHRAIM M. STEINBERG, Centre for Quantum Information and Quantum Control, and Institute for Optical Sciences, Department of Physics, University of Toronto — Along with the uncertainty principle, Heisenberg postulated another set of relations, which set a lower limit on the disturbance caused by a measurement [1]. These relations were shown by Ozawa to be inaccurate [2], shedding doubt on widely accepted bounds on the information left in a system after a measurement, and offering new insights into the foundations of quantum physics and quantum information. A theoretical scheme for testing Ozawa’s precision-disturbance relations was proposed [3]. In this proposal the hurdle of destructive measurements is addressed by the weak value approach [4]. This scheme is based on a 3-qubit quantum circuit that requires two CNOT gates of variable strength with a common control qubit. Here, we present an experimental realization of Heisenberg’s precision limit violation based on weak value measurements. We implement a technique inspired by the one-way quantum computing using entanglement as the substrate for quantum gates. In this way, we demonstrate a violation of Heisenberg’s relation for measurement disturbance, confirming the revised bound due to Ozawa.

- [1] Z. Phys. 43 172(1927); [2] Ann. Phys. NY 311 350(2004); [3] New J. Phys. 12 093011(2010); [4] Phys. Rev. Lett. 60 1351(1988)

4:18PM X30.00010 The rise of long-distance entanglement within a linear chain of ions, THOMAS FOGARTY, Physics Department, University College Cork, Cork, Ireland, ENDRE KAJARI, BRUNO G. TAKETANI, Theoretische Physik, Universität des Saarlandes, D-66123 Saarbrücken, Germany, ALEXANDER WOLF, Institute of Quantum Physics, Ulm University, D-89069 Ulm, Germany, THOMAS BUSCH, Physics Department, University College Cork, Cork, Ireland, GIOVANNA MORIGI, Theoretische Physik, Universität des Saarlandes, D-66123 Saarbrücken, Germany — One stumbling block which limits our observation of quantum effects in the macroscopic world is decoherence. For this reason the study of decoherence and dissipation in open quantum systems has attracted a lot of attention. It has been shown that the generation of long distance entanglement is possible between oscillators via a harmonic crystal (Wolf et al, EPL, 95(2011) 60008). The aim of this current work is to propose an experimentally feasible setup to test the possibility of the creation of long distance entanglement. For this purpose we consider an ion chain in a linear Paul trap with two embedded impurities, whose transverse modes resemble the two degrees of freedom that we aim to entangle via the rest of the chain. With the aid of appropriately designed laser fields, the dynamics described in (Wolf et al, EPL, 95(2011) 60008) is reproduced. The resulting entanglement between the transverse modes of the impurities is analysed by means of the logarithmic negativity.

4:30PM X30.00011 Popper's Thought Experiment Reinvestigated, CHRIS RICHARDSON, JONATHAN DOWLING, Louisiana State University — Karl Popper posed an interesting thought experiment in 1934. With it, he meant to question the completeness of quantum mechanics. He claimed that the notion of quantum entanglement leads to absurd scenarios that cannot be true in real life and that an implementation of his thought experiment would not give the results that QM predicts. Unfortunately for Popper, it has taken until recently to perform experiments that test his claims. The results of the experiments do not refute QM as Popper predicted, but neither do they confirm what Popper claimed QM predicted. Kim and Shih implemented Popper's thought experiment in the lab. The results of the experiment are not clear and have instigated many interpretations of the results. The results show some correlation between entangled photons, but not in the way that Popper thought, nor in the way a simple application of QM might predict. A ghost-imaging experiment by Strekalov, et al. sheds light on the physics behind Popper's thought experiment, but does not try to directly test it. I will build the physics of Popper's thought experiment from the ground up and show how the results of both of these experiments agree with each other and the theory of QM, but disprove Popper.

4:42PM X30.00012 Positive Noise Cross Correlation in a Copper Pair Splitter., ANINDYA DAS, YUVAL RONEN, MOTY HEIBLUM, HADAS SHTRIKMAN, DIANA MAHALU, Weizmann Institute of Science, MOTY'S GROUP TEAM — Entanglement is in heart of the Einstein-Podolsky-Rosen (EPR) paradox, in which non-locality is a fundamental property. Up to date spin entanglement of electrons had not been demonstrated. Here, we provide direct evidence of such entanglement by measuring: non-local positive current correlation and positive cross correlation among current fluctuations, both of separated electrons born by a Cooper-pair-beam-splitter. The realization of the splitter is provided by injecting current from an Al superconductor contact into two, single channel, pure InAs nanowires - each intercepted by a Coulomb blockaded quantum dot (QD). The QDs impedes strongly the flow of Cooper pairs allowing easy single electron transport. The passage of electron in one wire enables the simultaneous passage of the other in the neighboring wire. The splitting efficiency of the Cooper pairs (relative to Cooper pairs actual current) was found to be $\sim 40\%$. The positive cross-correlations in the currents and their fluctuations (shot noise) are fully consistent with entangled electrons produced by the beam splitter.

4:54PM X30.00013 Scalable fiber integrated source for higher-dimensional path-entangled photons¹, ROBERT POLSTER, CHRISTOPH SCHAEFF, RADEK LAPKIEWICZ, ROBERT FICKLER, SVEN RAMELOW, ANTON ZEILINGER, University of Vienna — Higher dimensional Hilbert spaces are expected to show intriguing higher order effects. Examples are higher dimensional perfect correlations or the unsolved problem of finding a complete set of MUBs for dimension 6. Higher dimensional systems also have advantages for QKD protocols. Our approach is to build an easy to use platform to access these dimensions. We realized an in-fiber, high brightness and high fidelity source for path-entangled quNits in the telecom band. It is purely integrated in fiber and only standard off-shelf components are used. This results in high stability and scalability in terms of complexity with increasing dimension. In order to manipulate and transform the produced entangled states we implemented multiports in integrated optical technology, enabling us to perform any unitary transformation depending on its internal settings[1]. Results up to dimension 4 (ququarts) will be presented in the talk. [1] M. Reck, A. Zeilinger, H. J. Bernstein and P. Bertani, PRL 73, 1 (1994)

¹This work was supported by the ERC (QIT4QAD), the Vienna Doctoral Program on Complex Quantum Systems, and the Austrian Science Fund (FWF): SFB S40.

5:06PM X30.00014 New Near-Deterministic Teleportation Protocol with Linear Optics, MLADEN PAVICIC, University of Zagreb — We present a new near-deterministic method of separating all four photon Bell states by means of concatenated Mach-Zehnder interferometers. Realistic proposals for implementations of teleportation, superdense coding, and cryptographic ping-pong protocols will be presented. Discrimination of the Bell states is made possible by two two linear chains of concatenated Mach-Zehnder interferometers each fed with photons emerging from two opposite sides of a beam splitter. This amounts to detecting two Bell states $|\Phi^\pm\rangle$ while keeping the third one $|\Psi^+\rangle$ conditionally at bay—thus going around Vaidman-Lütkenhaus 50%-limit. Realistic implementation with an efficiency of 90% is feasible with today's technology. Channel capacity of 1.98 can be ideally achieved for superdense coding with 5 concatenated Mach-Zehnder interferometers but already with only two easily implementable ones we obtain 1.74 capacity. The setup is based on a revised and corrected method given in M. Pavičić, *Phys. Rev Lett.* **107**, 080403 (2011).

Thursday, March 1, 2012 2:30PM - 5:30PM –
Session X31 DMP: Focus Session: Topological Insulators: Synthesis and Characterization - Scanning Tunneling Spectroscopy 260

2:30PM X31.00001 Scanning tunneling spectroscopic studies of Dirac fermions and impurity resonances in the surface-state of a strong topological insulator Bi₂Se₃, H. CHU, M.L. TEAGUE, C.-C. HSU, N.-C. YEH, Caltech, L. HE, K.-L. WANG, UCLA, F.-X. XIU, Iowa State Univ. — Scanning tunneling spectroscopic studies of MBE-grown Bi₂Se₃ epitaxial films on Si (111) revealed surface-state (SS) characteristics of Dirac fermions and signatures of strong impurity resonances. The impurity resonances in this three-dimensional strong topological insulator (3D-STI) occurred near the Dirac energy (E_D) and diverged as the Fermi level (E_F) approached E_D . They were also highly localized within a region of radius ~ 0.2 nm, beyond which the SS spectra of the 3D-STI recovered quickly, suggesting robust topological protection against non-magnetic impurities. Similar spectral characteristics and separations between E_F and E_D were also observed in the MBE-grown Bi₂Se₃ films on CdS. For sufficiently thin samples, opening of an energy gap due to wave-function overlap between the surface and interface layers was observed. The Rashba-like spin-orbit splitting further gave rise to spin-preserving quasiparticle interferences. Finally, the effect of different impurities (e.g. Cr and Mn) on the SS spectra of Bi₂Se₃ as a function of magnetic field will be reported. This work was supported by FENA and DARPA.

2:42PM X31.00002 Scanning tunneling spectroscopy studies of Bi₂Te₂Se¹, ILYA DROZDOV, HAIM BAIDENKOPF, JUNGPIIL SEO, Department of Physics, Princeton University, SHUANG JIA, ROBERT CAVA, Department of Chemistry, Princeton University, ALI YAZDANI, Department of Physics, Princeton University — Topological insulators are a class of semiconductors characterized by the presence of current-carrying helical surface states lying within the bulk gap. The surface states of these materials possess massless Dirac-like dispersion. Helical spin texture of the surface states leads to suppression of backscattering in these materials. Results of scanning tunneling spectroscopy study of Bi₂Te₂Se (BTS) topological insulator will be presented. Similar to previously studied Bi₂Te₃ and Bi₂Se₃ the new material shows a relatively large band gap and a simple surface band structure. High bulk resistivity and high surface electron mobility make it a compound of interest for potential applications. Differential conductance mapping with scanning tunneling microscope is used to visualize surface states of this novel highest-bulk-resistivity topological insulator. These experiments enable us to assess the variation of local density of states in this compound under different growth conditions and to correlate the findings with transport properties

¹This work was supported by NSF, NSF-MRSEC, and DARPA

2:54PM X31.00003 Scanning tunneling spectroscopy of stripe induced spatial modulations in the electronic structure of $\text{Bi}_2\text{Te}_3+\text{d}$, YOSHINORI OKADA, WENWEN ZHOU, DANIEL WALKUP, CHETAN DHITAL, YING RAN, ZIQING WANG, STEPHEN WILSON, VIDYA MADHAVAN, Boston College — To take full advantage of the unique properties of topological insulators, a huge amount of effort has been spent in exploring the tunability of their charge carrier density or magnetism by chemical doping, creating an ever increasing need for probing and understanding the real-space electronic response. In this study, we investigate the effects of a 1D periodic modulation (stripes) on the electronic structure of $\text{Bi}_2\text{Te}_3+\text{d}$. Using a combination of spectroscopic mapping, Fourier transform spectroscopy and Landau level measurements we map out the energy-momentum dispersion of the surface state over a large energy range and show that the stripes have a non-trivial effect on the bulk and surface state band structure.

3:06PM X31.00004 Scanning tunneling microscopy study of ultrathin topological insulator Bi_2Te_3 nanoribbons, CAROLINA PARRA, DESHENG KONG, JASON C. RANDEL, ALEX W. CONTRYMAN, FRANCIS NIESTEMSKI, MING RUE D. THIAN, YI CUI, HARI C. MANOHARAN, Stanford University — Currently there is an increasing interest in the study of topological insulators (TI) nanostructures as a result of their large surface-to-volume ratio, which allows the manifestation of surface conduction states without masking by bulk carriers. We performed low-temperature scanning tunneling microscopy (STM) measurements of the surface of TI Bi_2Te_3 nanostructures grown on HOPG. Although surface states of TIs are inherently robust against almost any surface modifications, these materials are prone to various surface chemical reactions which are taken into account when preparing samples for devices and STM study. Our STM measurements reveal the presence of ultrathin nanostructures (nanoribbons and nanoplates) which show an important growth anisotropy, with lateral dimension growing much faster than the vertical thickness dimension. Nanoribbons group mainly in bunches, with an aspect ratio of 1:300 and thickness down to 6 nm (6 quintuple layers). Nanoplates with hexagonal morphology of lower than 20 quintuple layers thick were also found, suggesting both one- and two-dimensional preferential growth.

3:18PM X31.00005 The field dependence of quantized Landau levels on $\text{Bi}_2\text{Te}_3+\text{d}$ via scanning tunneling spectroscopy, DANIEL WALKUP, YOSHINORI OKADA, WENWEN ZHOU, CHETAN DHITAL, STEPHEN WILSON, VIDYA MADHAVAN, Boston College — Measurements of Landau level (LL) spectra by scanning tunneling spectroscopy can provide important information on quasi-particle lifetime, effective g-factor as well as the dispersion of surface state bands. We have studied the effect of magnetic fields on spatially inhomogeneous samples of the topological insulator $\text{Bi}_2\text{Te}_3+\text{d}$. Using spatial maps of Landau levels as a function of magnetic field, we show that the surface state electrons near the Dirac point are surprisingly sensitive to perturbations. The magnetic field dependence also allows us to obtain an upper limit to the effective g-factor for the surface state electrons.

3:30PM X31.00006 Landau quantization and the thickness limit of topological insulator thin films of Sb_2Te_3 , XUCUN MA, YEPEING JIANG, YILIN WANG, Institute of Physics, CAS, MU CHEN, Department of Physics, Tsinghua University, CANLI SONG, ZHI LI, LILI WANG, KE HE, Institute of Physics, CAS, XI CHEN, QI-KUN XUE, Department of Physics, Tsinghua University — We report the experimental observation of Landau quantization of molecular beam epitaxy grown Sb_2Te_3 thin films by a low-temperature scanning tunneling microscope. Different from all the reported systems, the Landau quantization in Sb_2Te_3 topological insulator is not sensitive to the intrinsic substitutional defects in the films. As a result, a nearly perfect linear energy dispersion of surface states as 2D massless Dirac fermion system is observed. We demonstrate that 4 quintuple layers are the thickness limit for Sb_2Te_3 thin film being a 3D topological insulator.

3:42PM X31.00007 Multiband quasiparticle interference in the topological insulator $\text{Cu}_x\text{Bi}_2\text{Te}_3$ ¹, ERIK VAN HEUMEN, van der Waals - Zeeman Institute, University of Amsterdam, S. JOHNSTON, IFW Dresden, Germany, E. RIENKS, A. VÁRYKHALOV, Helmholtz Institute Berlin, Germany, F. MASSEE, N. DE JONG, Y. HUANG, J. KAAS, J.B. GOEDKOOP, M.S. GOLDEN, van der Waals - Zeeman Institute, University of Amsterdam — One of the main interests in topological materials is their purported robustness against disorder. In the Bi_2X_3 family (X=Se,Te) cubic spin-orbit coupling terms play an important role through their effect on the dispersion of the surface states. The cubic terms are also responsible for the restoration of Friedel like oscillations around impurity sites, which may be important in surface transport processes. We have therefore investigated how impurity scattering affects the surface states using a combination of Fourier-transform scanning tunneling spectroscopy (FT-STs) and calculations of the charge density oscillations expected from the cubic spin-orbit coupling terms [1]. FT-STs allows us to map out the energy-momentum relation of the important scattering wave-vectors, which can be compared to scattering vectors predicted from a self-consistent single impurity scattering calculation. To fully explain the features observed in our experiments we need to take the conduction band into account. Namely, for energies where the surface states and the conduction band overlap, the dominant scattering process turns out to be interband impurity scattering.

[1] E. van Heumen et al., arXiv: 1110.4406

¹This work is funded by FOM and the VENI program (both part of NWO) and the EU (FP7/2007-2013, no. 226716).

3:54PM X31.00008 LT-STM study of the topological insulator Bi_2Se_3 with superconducting and/or magnetic over layers, RAMI DANA, ANITA ROYCHOWDHURY, University of Maryland, IREK MIOTKOWSKI, YONG P. CHEN, Purdue University, MICHAEL DREYER, University of Maryland — Superconducting and/or magnetic over layers structures on topological insulator (TI) surfaces were suggested as a potential candidate to create Majorana bound states and 1D Majorana fermions (spin $1/2$, particle = antiparticle). The latter can serve as a platform for topological quantum computation since two Majorana bound states equal one fermion bound state and two degenerate states (full/empty) forming one qubit. In this work we study the TI Bi_2Se_3 using a low temperature STM. The data shows the signature energy gap $\Delta \sim 0.3$ eV, metallic surface states and typical defects. Following the experimental challenges to create and detect Majorana bound or chiral edge states, we present our study of Nb and/or Fe films on the Bi_2Se_3 surface.

4:06PM X31.00009 Visualizing the inhomogeneous response of Dirac surface states to bulk disorder in topological insulators¹, HAIM BEIDENKOPF, PEDRAM ROUSHAN, JUNGPII SEO, LINDSAY GORMAN, ILYA DROZDOV, Joseph Henry Laboratory, Department of Physics, Princeton University, Princeton, New Jersey 08544, USA, YEW SAN HOR, ROBERT J. CAVA, Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA, ALI YAZDANI, Joseph Henry Laboratory, Department of Physics, Princeton University, Princeton, New Jersey 08544, USA — The Dirac dispersion and helical spin texture of surface states in topological insulators render them resilient to backscattering. This remarkable property, assured by time reversal symmetry, should give rise to enhanced surface conductivity as the Dirac states anti-localize in presence of disorder. We have used scanning tunneling microscopy (STM) and spectroscopy to study the response of the surface states to both magnetic and non-magnetic dopants [HB et al. Nat. Phys. doi:10.1038/nphys2108]. We find that helicity provides protection from scattering, irrespective of the magnetic nature of the individual scatterers and even of ferromagnetic correlations among them. However, the charged defects in the bulk induce pronounced fluctuations in energy, momentum and helicity of the surface states. Agreement with a theoretical model, derived for the response of Dirac states to charged disorder in graphene, further implies that such fluctuations limit the attainable surface mobility. Although we show that the potential energy landscape induced by the bulk defects does not localize the Dirac surface states, our results suggest that reducing charged defects content is essential for tuning the chemical potential to the Dirac energy and enhancing mobility of the novel surface states.

¹This work was supported by NSF, NSF-MRSEC, and DARPA

4:18PM X31.00010 Probing surface state conductance of topological insulator Bi_2Se_3 with scanning tunneling potentiometry, CHOCKALINGAM SUBBIAH, Department of Physics, Columbia University, NY, FRANCES ROSS, IBM T. J. Watson Research Center, Yorktown Heights, NY, MATTHEW BRAHLEK, SEONGSHIK OH, Department of Physics & Astronomy, Rutgers, The State University of New Jersey, ABHAY PASUPATHY, Department of Physics, Columbia University, NY — Topological insulators such as Bi_2Se_3 have unique surface states. How do electrons actually flow on the surface of a real Bi_2Se_3 sample? We study this question using scanning tunneling potentiometry. In this measurement, a lateral current flows in the sample while the local potential is mapped on the surface using a scanning tunneling microscope. This technique can be used to identify with atomic resolution the potential drops in the current-carrying pathways at the surface, and is ideally suited to measure the properties of quasi-2D materials such as graphene. Our topological insulator samples are MBE grown films of Bi_2Se_3 on a sapphire substrate. We will describe both the surface morphology and its effect on the current carrying pathways in the material.

4:30PM X31.00011 Probing high energy, unoccupied states on the surface of pristine and Fe doped Bi_2Te_3 by scanning tunneling spectroscopy, WENWEN ZHOU, YOSHINORI OKADA, DANIEL WALKUP, CHETAN DHITAL, Boston College, HSIN LIN, ARUN BANSIL, Northeastern University, STEPHEN WILSON, VIDYA MADHAVAN, Boston College — We probe the surface state of pristine and Fe-doped topological Insulator Bi_2Te_3 by using Fourier Transform Scanning Tunneling Spectroscopy (FT-STs). FT-STs allows us to probe the surface state dispersion far above the Fermi energy, a regime inaccessible to angle resolved photoemission spectroscopy. We report the observation of novel multi scattering channels that emerge at high energies along the ΓM and ΓK directions. The possible origins of these channels including spin-orbit scattering will be discussed.

4:42PM X31.00012 STS studies of the surface of Bi_2Se_3 , MEGAN ROMANOWICH, MAL-SOON LEE, S.D. MAHANTI, STUART TESSMER, Michigan State University, DUCK YOUNG CHUNG, JUNG-HWAN SONG, MERCOURI KANATZIDIS, Northwestern University; Argonne National Laboratory — We apply scanning tunneling spectroscopy to characterize the surface of the topological insulator Bi_2Se_3 . Spectroscopy reveals that the minimum in the local density of states (LDOS) does not actually vanish in the region where Dirac cone states exist. We demonstrate with density functional theory calculations that this can be understood in terms of an asymmetric addition to the LDOS associated with a contribution from the bulk valence band that overlaps in energy with the Dirac point. We will discuss the origin of the fluctuations in the LDOS seen in the experiment near 0.2 eV above the Dirac point, which are associated with tunneling into the lowest conduction band states.

4:54PM X31.00013 STM imaging of impurity resonances on Bi_2Se_3 , ZHANYBEK ALPICHSEV, Stanford University, RUDRO BISWAS, Harvard University, ALEXANDER BALATSKY, Los Alamos National Laboratory, JAMES ANALYTIS, JIUN-HAW CHU, IAN FISHER, AHARON KAPITULNIK, Stanford University — In this paper we present detailed study of the density of states near defects in Bi_2Se_3 . In particular, we present data on the commonly found triangular defects in this system. While we do not find any measurable quasiparticle scattering interference effects, we do find localized resonances, which can be well fitted by theory [1] once the potential is taken to be extended to properly account for the observed defects. The data together with the fits confirm that while the local density of states around the Dirac point of the electronic spectrum at the surface is significantly disrupted near the impurity by the creation of low-energy resonance state, the Dirac point is not locally destroyed. We discuss our results in terms of the expected protected surface state of topological insulators.

5:06PM X31.00014 Probing Dirac Fermions in Bi-based Semimetals by Cryomagnetic Scanning Tunneling and Point Contact Spectroscopy¹, J.Y.T. WEI, University of Toronto and Canadian Institute for Advanced Research, I. FRIDMAN, Y.T. YEN, University of Toronto, HECHANG LEI, KEFENG WANG, C. PETROVIC, Brookhaven National Laboratory — The topological semimetal Bi_2Se_3 is distinguished by the presence of two-dimensional Dirac fermions with strong spin-orbit coupling. The linear dispersion of Dirac fermions in Bi_2Se_3 was recently observed by scanning tunneling spectroscopy measurements of the Landau level spacing versus magnetic field. In this work we extend the field-dependent spectroscopy study of Dirac fermions to other Bi-based semimetals, for both topological and non-topological cases, using cryomagnetic scanning tunneling and point contact probes on single crystals down to 300 mK and up to 9 T. The spectral dependences on field strength and field direction are examined, in an effort to elucidate the role of spin-orbit coupling in each case.

¹Work supported by: NSERC, CFI-OIT and the Canadian Institute for Advanced Research. Work at Brookhaven supported by: the U.S. DOE under Contract No. DE-AC02-98CH10886 and in part by the Center for Emergent Superconductivity, an Energy Frontier Research.

5:18PM X31.00015 Thickness and Wave-Vector Dependence in the Inter-Surface Coupling of Topological Surface States of Sb(111) Films, GUANGGENG YAO, FENG PAN, ZIYU LUO, WENTAO XU, JIATAO SUN, ANDREW THYE SHEN WEE, YUANPING FENG, XUE-SEN WANG, Department of Physics, Faculty of Science, National University of Singapore — Sb is a semimetal but possesses topological surface states (SSs) [1]. Taking advantage of quantum confinement effect for bulk states and topological protection for SSs, an Sb thin film could be a topological insulator. We explore this possibility using Fourier-transform scanning tunneling spectroscopy (FT-STs) and *ab initio* calculations for Sb(111) films of thickness ≤ 30 bilayers (BL). Quasiparticle interference (QPI) patterns of SSs and calculated band structures exhibit dramatic dependence on film thicknesses, reflecting variation of inter-surface coupling of SSs with film thickness and wave vector $\mathbf{k}$. One Kramers-pair of SSs forming a Dirac point at $\mathbf{k} = 0$ exist on each surface for 6-BL or thicker films. The inter-surface coupling of SSs not far away from $\mathbf{k} = 0$ is significant in the QPI patterns at ~ 10 BL. Such coupling is due to a relative large penetration depth of these SSs results in unpolarized states with large wave function amplitude in the interior of the film. [1] D. Hsieh et al., Science 323, 919 (2009); K. K. Gomes et al., e-print arXiv:0909.0921 (2009); J. Seo et al., Nature 466, 343 (2010).

Thursday, March 1, 2012 2:30PM - 5:30PM –

Session X32 DMP DCOMP: Focus Session: Dielectric, Ferroelectric, and Piezoelectric Oxides - Elastic and Optical Properties 261

2:30PM X32.00001 Flexoelectricity in Nanoscale Ferroelectrics, GUSTAU CATALAN, ICREA and CIN2, Barcelona — All ferroelectrics are piezoelectric and thus have an intrinsic coupling between polarization and strain. There exists an additional electromechanical coupling, however, between polarization and strain gradients. Strain gradients are intrinsically vectorial fields and, therefore, they can in principle be used to modify both the orientation and the sign of the polarization, thanks to the coupling known as flexoelectricity. Flexoelectricity is possible even in paraelectric materials, but is generally stronger in ferroelectrics on account of their high permittivity (the flexoelectric coefficient is proportional to the dielectric constant). Moreover, strain gradients can be large at the nanoscale due to the smallness of the relaxation length and, accordingly, strong flexoelectric effects can be expected in nanoscale ferroelectrics. In this talk we will present two recent results that highlight the above features. In the first part, I will show how polarization tilting can be achieved in a nominally tetragonal ferroelectric (PbTiO_3) thanks to the internal flexoelectric fields generated in nano-twinned epitaxial thin films. Flexoelectricity thus offers a purely physical means of achieving rotated polarizations, which are thought to be useful for enhanced piezoelectricity. In the second part, we will show how the large strain gradients generated by pushing the sharp tip of an atomic force microscope against the surface of a thin ferroelectric film can be used to actively switch its polarity by 180° . This enables a new concept for “multiferroic” memory operation in which the memory bits are written mechanically and read electrically.

3:06PM X32.00002 Giant Flexoelectric Effect in Ferroelectric Epitaxial Thin Films, TAE WON NOH, DAESU LEE, Department of Physics and Astronomy, Seoul National University, A. YOON, M. KIM, Department of Materials Science and Engineering, Seoul National University, J.-G. YOON, Department of Physics, University of Suwon, J.-S. CHUNG, Department of Physics and CAMDRC, Soongsil University, J.F. SCOTT, Department of Physics, University of Cambridge, UK — The flexoelectric effect describes an electric field that is generated by a strain gradient. Owing to its universal nature, flexoelectricity has inspired broad scientific interest and has application potential, particularly in flexible systems. In solids, however, there has been little investigation into flexoelectricity, due to its minuscule magnitude by limited elastic deformation. In this presentation, we will develop a general framework for realizing and modulating the giant flexoelectric effect in epitaxial oxide thin films, emphasizing the key role of flexoelectricity in solids.¹ In epitaxial oxide thin films, a lattice mismatch between the film and the substrate can result in strain relaxation within tens of nanometers of the film/substrate interface, inducing a large strain gradient. We observed the nanoscale strain gradients in ferroelectric HoMnO_3 epitaxial thin films, which were 6 or 7 orders of magnitude larger than typical values reported for bulk oxides. Giant flexoelectric effect by the nanoscale strain gradient provides a means of tuning the physical properties of ferroelectric epitaxial thin films, such as domain configurations and hysteresis curves.²

¹D. Lee *et al.*, Phys. Rev. Lett. **107**, 057602 (2011).

²D. Lee *et al.*, Phys. Rev. B **81**, 012101 (2010).

3:18PM X32.00003 Thermal Stresses in Ferroelectric Thin Films and Their Role on the Dielectric, Pyroelectric, and Electrocaloric Properties, JIALAN ZHANG, S. PAMIR ALPAY, University of Connecticut — In-plane strains develop in thin films due to thermal stresses that arise from differences between the thermal expansion coefficients of the film and the substrate upon cooling from a growth temperature (T_G) to room temperature (RT). In ferroelectric (FE) films, there is a coupling between strain and polarization through electrostriction. Therefore, thermal strains may have profound effects on the dielectric, pyroelectric, and electrocaloric (EC) responses of FE films. We provide here a quantitative thermodynamic model to investigate the role of in-plane thermal strains on these properties. We show that there is a substantial degradation in the dielectric response and tunability of SrTiO_3 films on IC-friendly substrates such as Si and *c*-sapphire due to tensile thermal in-plane strains. Our analysis on (001)-textured polycrystalline $\text{Ba}_x\text{Sr}_{1-x}\text{O}_3$ (BST) films with different compositions indicates that for BST 60/40 and BST 70/30 films, the pyroelectric response does not display a significant dependence on T_G if the FE is in a paraelectric state. Furthermore, we show that for BaTiO_3 films on Si, the thermal stresses are sufficient to shift the zero-field Curie temperature to RT, resulting in a strong enhancement of the EC properties as compared to the bulk material.

3:30PM X32.00004 Polarization in Perovskite Manganites induced by Shear Stress¹, K. MIYANO, N. OGAWA, Y. IDA, R. TAMAKI, K. SHIMIZU, Y. NOMURA, R. ARITA, Univ. of Tokyo, Y. OGIMOTO, Univ. of Tokyo and Fuji Electr. Co. — We found static polarization in perovskite manganite films when they are under shear stress. The phenomenon is omnipresent in films deformed in (at least) monoclinic fashion due to the substrate-imposed strain, whereas it is absent in bulk crystals even though they are distorted in a similar manner in thermal equilibrium. The substrate stress of low symmetry is clearly the driving force for the appearance of the polarization. Optical second-harmonic generation (SHG) confirms the loss of inversion symmetry in strained films and pyroelectricity was detected in insulating films confirming the presence of the static polarization. DFT calculations show that the stable atomic positions in the experimentally observed structure is polar with the shift of the center of gravity of anions relative to that of cations as much as $10^{-2}\text{\AA}$. The calculated polar structure is consistent with the symmetry obtained from the SHG polarimetry.

¹JST-CREST

3:42PM X32.00005 Discovery of strain glass transition in non-metallic ferroelastic, PEI ZHANG, DEZHEN XUE, XIAOBING REN, MMRC, Frontier Institute of Science and Technology, Xi'an Jiaotong University, China, MMRC, FRONTIER INSTITUTE OF SCIENCE AND TECHNOLOGY, XI'AN JIAOTONG UNIVERSITY, CHINA TEAM, FERROIC PHYSICS GROUP, NATIONAL INSTITUTE FOR MATERIALS SCIENCE, TSUKUBA 305-0047, JAPAN COLLABORATION — Strain glass, a glassy state of lattice strain, has been identified in alloys with shuffle being the principle order parameter and strain being the secondary order parameter. However, it is well known that many non-metallic ferroelastic systems possess long range order with tilt being the first order parameter. But the existence of the glassy state of such strain caused by tilt remains unclear. In the present study, we report that the strain glass indeed exists in the non-metallic ferroelastic material, a Sr and Nb co-doped LaAlO_3 system, with randomly frozen tilt strain local order. With increasing defect concentration x in $\text{La}_{1-x}\text{Sr}_x\text{Al}_{0.95}\text{Nb}_{0.05}\text{O}_3$, the martensitic transition is gradually suppressed and finally strain glass transition occurs. The glassy transition is characterized by a typical frequency dispersion of modulus, a broken of ergodicity for static strain, as well as the formation of nano-domains with R local structure. Due to the strong local barrier caused by the randomly distributed point defects, the ideal freezing temperature T_0 of strain glass in this system increases with defect concentration, which can be well understood by a modified Landau free energy landscape.

3:54PM X32.00006 Enhanced Piezoelectricity in $\text{PbTiO}_3/\text{BaTiO}_3$ Superlattices, T. YUSUFALY, Rutgers University, B. ZIEGLER, University of Geneva, V.R. COOPER, Oak Ridge National Laboratory, S.J. CALLORI, J. SINSHEIMER, Stony Brook University, K.M. RABE, P. CHANDRA, Rutgers University, M. DAWBER, Stony Brook University — First-principles calculations by Cooper and Rabe predict an enhancement of the piezoelectric coefficient (d_{33}) in $\text{PbTiO}_3/\text{BaTiO}_3$ (PTO/BTO) superlattices for intermediate values of PTO concentration. PTO/BTO superlattices have been fabricated using an off-axis RF magnetron sputtering technique, enabling x-ray diffraction, electrical measurements and atomic force microscopy on this system. The experimental results agree with the calculated polarization, tetragonality and enhanced piezoelectricity as a function of PTO concentration. Additional first-principles calculations indicate that the enhancement in d_{33} is more pronounced in shorter-period superlattices. By applying a Landau-Devonshire model to this system, we find that the enhanced piezoelectricity is due to the combination of a bulk effect associated with the presence of finite electric fields in each layer and interfacial effects. Implications of our results for future experiments are discussed.

4:06PM X32.00007 Interpolation schemes for high-throughput prediction of new piezoelectric alloys, RICKARD ARMIENTO, Massachusetts Institute of Technology, BORIS KOZINSKY, Research and Technology Center, Robert Bosch LLC, MARCO FORNARI, Central Michigan University, GERBRAND CEDER, Massachusetts Institute of Technology — Systematic discovery of materials with optimized properties based on first principles methodologies requires well-defined descriptors, in addition to the automation infrastructure for calculations and data analysis. We have designed a set of computationally affordable descriptors for enhanced piezoelectric performances and analyzed the chemical space for oxides with the perovskite structure. Our results include phase stability for the most promising compositions and ad hoc interpolation schemes that have been exploited to identify 49 alloys with favorable properties.

4:18PM X32.00008 Piezoelectric characteristics of PZT thin films on polymer substrate, MIN-GYU KANG, YOUNH-HO DO, SEUNG-MIN OH, RHEZA RAHAYU, YIYEIN KIM, CHONG-YUN KANG¹, Korea Institute of Science and Technology, SAHN NAHM, Korea University, SEOK-JIN YOON, Korea Institute of Science and Technology — The goal of piezoelectric energy harvesting is to improve the power efficiency of devices. One of the approaches for the improvement of power efficiency is to apply the large strain on the piezoelectric materials and then many scientists approached using thin films or nano-structured piezoelectric materials to obtain flexibility. However, the conventional thin film processes available for the fabrication of piezoelectric materials as $\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3$ (PZT) are not compatible with flexible electronics because they require high processing temperatures ($>700^\circ\text{C}$) to obtain piezoelectricity. Excimer laser annealing (ELA) is attractive heat process for the low-temperature crystallization, because of its material selectivity and short heating time. In this study, the amorphous PZT thin films were deposited on polymer substrate by rf-sputtering. To crystallize the amorphous films, the ELA was carried out with various conditions as function of the applied laser energy density, the number of pulse, and the repetition rate. To evaluate the piezoelectric characteristics, piezoelectric force microscopy (PFM) and electrometer are used. As a result, we obtained the crystallized PZT thin film on flexible substrate and obtained flexible piezoelectric energy harvester.

¹Corresponding Author

4:30PM X32.00009 Characterizing the Angular Frequency of Radiative Polaritons using Infrared Spectroscopy, ANITA VINCENT-JOHNSON, GIOVANNA SCAREL, James Madison University Dept. of Physics and Astronomy — Polaritons are important for understanding the optical properties of oxide films and possibly also for energy conversion. The two known types of polaritons: surface phonon polaritons (SPP) and radiative polaritons (RP), form when infrared (IR) photons enter a crystal lattice material and couple with the phonons present. While SPP's are largely studied for their heat transfer properties, RP's are typically not studied; therefore, much is still not understood about RP's. It is known, however, that RP's have a complex angular frequency, which includes a real part, $\text{Re}(\omega)$, and an imaginary part, $\text{Im}(\omega)$. Investigations done by our Group suggests that $\text{Im}(\omega)$ indicates the frequency of the radiated field. What is unknown is the relationship between $\text{Re}(\omega)$ and $\text{Im}(\omega)$. Therefore, we experimentally compare three different oxides deposited on silicon and aluminum by atomic layer deposition (ALD). This allows us to characterize proportionality between $\text{Re}(\omega)$ and $\text{Im}(\omega)$ with respect to oxide film thickness.

4:42PM X32.00010 Dielectric and optical properties of SrTiO_3 films deposited from metallo-organic solution, M. SPIES, L.S. ABDALLAH, S. ZOLLNER, NMSU, C.V. WEISS, J. ZHANG, S.P. ALPAY, U of Connecticut, M.W. COLE, Army Research Lab — SrTiO_3 thin films on Si were grown by metallo-organic solution deposition. Spectroscopic ellipsometry was used to determine the ellipsometric angles ψ and Δ in the 0.6 to 6.6 eV spectral range at three angles of incidence. From the region below 3.5 eV (where the films are transparent), we are able to determine the refractive index and the film thickness, which ranges from 140 to 340 nm for different films. The refractive index is similar for all of our films, but 25% lower than that of bulk SrTiO_3 . By contrast, the low-frequency dielectric constant of similar films grown on metalized Si substrates is about the same as bulk SrTiO_3 . Using a B-spline parametrization, we are able to determine the dielectric function of our films from the ellipsometric angles. We find an onset of absorption (band gap) of about 3.7 eV and similar interband electronic transitions of our films as for bulk SrTiO_3 . For our films, the interband peaks are broadened due to poly-crystalline disorder and have a lower amplitude. The reason for the discrepancy between the low-frequency (vibrational) and the high-frequency (electronic) dielectric constant is unclear.

4:54PM X32.00011 Nonlinear photonic crystals of BaTiO_3 and their electro-optic properties, BRUCE WESSELS¹, Department of Materials Science and Engineering and Materials Research Center, and Department of Electrical Engineering and Computer Science, JIANHENG LI, ZHIFU LIU, Department of Materials Science and Engineering and Materials Research Center, Northwestern University, Evanston, IL 60208, USA, ELECTRONIC AND PHOTONIC MATERIALS GROUP TEAM — Future optical systems will require electro-optic (EO) modulators with bandwidths of 100 GHz and low drive voltage. To achieve this, non-linear photonic crystals using epitaxial BaTiO_3 have been proposed. In our work two-dimensional photonic crystal (PhC) structures with a hexagonal array were fabricated from an epitaxial BaTiO_3 thin film using focused ion beam milling. The PhC waveguides were based on $\text{Si}_3\text{N}_4/\text{BTO}/\text{MgO}$ multilayer epitaxial thin film structure. Simulation shows that sufficient refractive index contrast is achieved at 1550 nm to form a bandgap in the PhC structure by milling through the Si_3N_4 and BTO layers. The measured transmission spectrum of the PhC waveguide exhibited a stop-band centered at 1550 nm with well-defined band edges. Photonic crystal electro-optic modulators with a bandwidth of greater than 50 GHz have now been realized. The question of what dielectric properties limit the ultimate bandwidth of the PhC will be addressed.

¹Northwestern University, Evanston, IL 60208, USA

5:06PM X32.00012 Electro-optic contribution of optically generated small bound polarons in nominally undoped, thermally reduced LiNbO_3 ¹, MIRCO IMLAU, HAUKE BRUENING, Department of Physics, University of Osnabrueck, Germany — Recently we have shown that a spatial modulation of optically generated densities of small bound polarons can be applied for hologram recording in LiNbO_3 [1]. This new type of recording mechanism is of particular interest for the field of nonlinear and ultrafast photonics because of small bound polaron generation on the fs-scale. The grating recording via the photochromic response of small bound polarons was successfully applied to explain gratings recorded with a grating vector aligned orthogonal to the polar c-axis. In this contribution we study the relation of optically generated small bound polarons with pronounced index changes, that were found with values up to 10^{-4} and a grating vector parallel to the c-axis. The Pockels effect that must be driven by an internal electric space-charge field is taken into account. In contrast to the classical photorefractive effect, where slow and long-ranging transport mechanisms must be considered, we discuss the build-up of the space-charge field on the sub-ps-time scale in the model of optical absorption of small polarons, i.e., the optically generated polaron hopping to next-neighboring lattice sites.

[1] M. Imlau et al., Optics Express 19, 15322 (2011)

¹Financial support by the DFG (project IM37/5 and INST190/137-1) and DAAD (50445542) is gratefully acknowledged.

5:18PM X32.00013 Dispersive properties of small polaron-based hologram recording in nominally undoped, thermally reduced LiNbO_3 ¹, HAUKE BRUENING, MIRCO IMLAU, Department of Physics, University of Osnabrueck, Germany — We recently discovered a new type of hologram recording in nominally undoped, thermally reduced LiNbO_3 by means of a single intense ns-laser pulse ($\lambda = 532 \text{ nm}$) yielding short-lived volume phase-gratings with unique features [1]: a diffraction efficiency of more than 20% in the NIR spectral range ($\lambda = 785 \text{ nm}$), a stretched-exponential relaxation behavior of the grating efficiency with a lifetime in the ms-range at room temperature and a pronounced dependence on the orientation of the grating vector with respect to the polar c-axis. This type of hologram recording could be successfully modeled by taking into account an optically generated spatial modulation of small electron bipolarons, small bound and free electron polarons. In this contribution we face the unique dispersive properties of this type of hologram recording and particularly present our results for probing light in the blue-green spectral range ($\lambda = 488 \text{ nm}$). We show that the further contribution of small bound hole polarons must be taken into account. Furthermore, we conclude that a considerable diffraction efficiency at the telecommunication wavelength ($\lambda = 1550 \text{ nm}$) can be expected.

[1] M. Imlau et al., Optics Express 19, 15322 (2011)

¹Financial support by the DFG (IM37/5 and INST190/137-1) and DAAD (50445542) is gratefully acknowledged.

Thursday, March 1, 2012 2:30PM - 5:18PM – Session X33 GIMS: Focus Session: X-ray, Gamma Ray, and Electron Diffraction 106

2:30PM X33.00001 First-principles study of γ -ray detectors: Cs-based compounds¹, HOSUB JIN, JINO IM, ARTHUR FREEMAN, Department of Physics and Astronomy, Northwestern University, BRUCE WESSELS, Department of Materials Science and Engineering, Northwestern University, MERCOURI KANATZIDIS, Department of Chemistry, Northwestern University — In an effort to find good candidate materials for γ -ray detectors, Cs-based compounds containing heavy elements, such as in $\text{Cs}_2\text{Hg}_6\text{S}_7$, were investigated. We performed *ab-initio* density functional theory calculations using the full-potential linearized augmented plane wave method². The screened-exchange local density approximation (sX-LDA) scheme was employed to correct the underestimation of the band gap in the LDA method. As a result, the band gap of $\text{Cs}_2\text{Hg}_6\text{S}_7$ is predicted to be 1.23 eV by sX-LDA, corrected from 0.51 eV by LDA. Therefore, $\text{Cs}_2\text{Hg}_6\text{S}_7$ seems to be useful as a γ -ray detecting material in terms of the high density and the band gap. Not only the pristine bulk but also several defect configurations were calculated, which affects the transport properties. Defect formation energy determinations allow us to predict which defect configuration is most likely in $\text{Cs}_2\text{Hg}_6\text{S}_7$.

¹Supported by DTRA (Grant No. HDTRA1-09-1-0044)

²Wimmer, Krakauer, Weinert, Freeman, Phys. Rev. B, **24**, 864 (1981)

2:42PM X33.00002 ABSTRACT WITHDRAWN —

2:54PM X33.00003 Resolving Interface Interactions in Layered Structures in 3 Dimensions¹, ROZALIYA BARABASH, JON TISCHLER, JOHN BIDAI, Oak Ridge National laboratory, WENJUN LIU, Advanced Photon Source — 3D micro-Laue diffraction was used to probe interface interactions in layered structures. Indented Cr/NiAl composite with alternating submicron size Cr and NiAl lamellae was chosen as a model material. Differential aperture microscopy revealed a twin orientation relationship at the interface between the Cr and NiAl lamellae in the as grown state. The indentation-induced alternation of compressive/tensile residual strains in the neighboring Cr and NiAl lamellae was observed. Line broadening analysis found a two orders of magnitude increase of dislocation density in the near-surface zone in the center of the indent.

¹Research supported by the Division of Materials Sciences and Engineering, U.S. Department of Energy. Data collection was carried out on beamline ID-34-E at the Advanced Photon Source.

3:06PM X33.00004 X-ray Studies of Quantum Fluctuations in SrTiO_3 across its Quantum Paraelectric Phase Transition, SHIH-CHANG WENG, University of Illinois at Urbana-Champaign, RUQING XU, AYMAN SAID, HAWOONG HONG, Argonne National Laboratory, TAI-CHANG CHIANG, Univ. of Illinois at Urbana-Champaign — Strontium titanate (SrTiO_3), with a simple cubic perovskite structure at room temperature, displays a number of interesting phase transitions as a function of temperature and pressure. It exhibits an antiferrodistortive transition at $T_c = 105 \text{ K}$, resulting in a cubic-to-tetragonal structural distortion. This transition has been studied in detail by M. Holt and H. Hong using thermal diffuse scattering and inelastic x-ray scattering methods. Another phase transition takes place at 37 K, below which the system assumes a quantum paraelectric phase. It is generally believed that the classical free energy of the system favors a ferroelectric phase, but this transition never fully develops because of quantum fluctuation. Despite a large number of prior investigations, this quantum phenomenon is still not well understood in terms of the underlying lattice dynamics. Using inelastic x-ray scattering, we have obtained new information about this classic system, including mode softening as a function of temperature.

3:18PM X33.00005 X-ray nanotomography study of insulator-coated tips with sub-micron conducting apex for the combination of scanning probe microscopy and synchrotron radiation¹, VOLKER ROSE, Argonne National Laboratory, TEYU CHIEN, Northwestern University, JOHN FREELAND, DANIEL ROSENMANN, ROBERT WINARSKI, Argonne National Laboratory — Hard X-ray nanotomography provides an important three-dimensional view of insulator-coated “smart tips” that can be utilized for modern emerging scanning probe techniques. Tips, entirely coated by an insulating SiO_2 film except at the very tip apex, are fabricated by means of electron beam physical vapor deposition, focused ion beam milling and ion beam-stimulated oxide growth. Although x-ray tomography studies confirm the structural integrity of the oxide film, transport measurements suggest the presence of defect-induced states in the SiO_2 film [1]. The development of insulator-coated tips can facilitate nanoscale analysis with electronic, chemical, and magnetic contrast by synchrotron-based scanning probe microscopy.

[1] Rose et al., Appl. Phys. Lett. 99, 173102 (2011).

¹Work at the Advanced Photon Source, the Center for Nanoscale Materials, and the Electron Microscopy Center was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under contract DE-AC02-06CH11357.

3:30PM X33.00006 Grazing-incidence coherent x-ray imaging in true reflection geometry¹

TAO SUN, ZHANG JIANG, JOSEPH STRZALKA, JIN WANG, Argonne National Laboratory, APS SECTOR 8 TEAM — The development of the 3rd and 4th generation synchrotrons has stimulated extensive research activities in x-ray imaging techniques. Among all, coherent diffractive imaging (CDI) shows great promise, as its resolution is only limited by the wavelength of the source. Most of the CDI work reported thus far used transmission geometry, which however is not suitable for samples on opaque substrates or in which only the surfaces are the regions of interest. Even though two groups have performed CDI experiments (using laser or x-ray) in reflection geometry and succeeded in reconstructing the planar image of the surface, the theoretical underpinnings and analysis approaches of their techniques are essentially identical to transmission CDI. Most importantly, they couldn't obtain the structural information along sample thickness direction. Here, we introduce a reflection CDI technique that works at grazing-incidence geometry. By visualizing Au nanostructures fabricated on Si substrate, we demonstrate that this innovative imaging technique is capable of obtaining both 2D and 3D information of surfaces or buried structures in the samples. In the meanwhile, we will also explain the grazing-incidence-scattering based-algorithm developed for 3D phase retrieval.

¹ Use of the Advanced Photon Source was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357

3:42PM X33.00007 Soft x-ray absorption spectroscopy measurement methods with using x-ray scattering techniques

H. JANG, Department of Physics, POSTECH, Korea, J.-S. LEE, SSRL, SLAC, USA, W.-S. NOH, K.-T. KO, K.-B. LEE, Department of Physics, POSTECH, Korea, B.-G. PARK, J.-Y. KIM, PAL, POSTECH, Korea, S.H. CHUN, K.H. KIM, Dept. of Physics and Astronomy, Seoul National University, Korea, J.-H. PARK¹, Department of Physics, POSTECH, Korea — Methodology via x-ray absorption spectroscopy (XAS) has been actively employed for exploring the microscopic aspects of materials. In particular, such method within soft x-ray energy range is very useful for investigating strongly correlated systems, such as high T_C superconductor, and multiferroic, including heterostructures. While XAS approach on such materials has been used, however we sometimes confront a few of experimental difficulties; electron motion distortion under external fields, charging effect, and saturation effect. In this presentation, we introduce an alternative approach for overcoming the difficulties in conventional XAS measurement, which uses soft x-ray scattering techniques, i.e., reflection and diffraction. Due to photon-in and photon-out nature, probing depth becomes longer and possible to reduce several problems in conventional total electron yield method. The results of demonstrations on simple monoxide CoO and multiferroic Y-type hexaferrites will be given.

¹corresponding author: jhp@postech.ac.kr

3:54PM X33.00008 Structure uncovering from fluctuation x-ray scattering of randomly oriented nanoparticles¹

GANG CHEN, Lawrence Berkeley National Laboratory, MIGUEL MODESTINO, University of California, Berkeley, BILLY POON, ANDRE SCHIROTZEK, STEFANO MARCHESINI, Lawrence Berkeley National Laboratory, RACHEL SEGALMAN, University of California, Berkeley, ALEXANDER HEXEMER, PETER ZWART, Lawrence Berkeley National Laboratory — We have carried out a fluctuation x-ray scattering experiment on platinum coated gold nanoparticles randomly oriented on a substrate. A complete algorithm for determining the electron density of an individual particle from diffraction patterns of many particles, randomly oriented about a single axis is demonstrated. This algorithm operates on angular correlations among the measured intensity distributions and recovers the angular correlation functions of a single particle from measured diffraction patterns. Taking advantage of the cylindrical symmetry of the nanoparticles, we proposed a cylindrical model to reconstruct the structure of the nanoparticle by fitting both the experimental ring angular auto-correlation and the small angle scattering data. The physical meaning of the resulted structure is discussed in terms of their statistical distributions of the shape and electron density profile.

¹LBLN LDRD

4:06PM X33.00009 ABSTRACT WITHDRAWN —

4:18PM X33.00010 Hard X-ray resonance in sapphire crystal cavities using back diffraction

Y.-H WU, Y.-W TSAI, Y.-Y CHANG, Dept of Physics, National Tsing Hua University, C.-H CHU, National Synchrotron Radiation Research Center, DAVID G. MIKOLAS, C.-C FU, Institute of Nano Engineering and Microsystems, National Tsing Hua University, S.-L. CHANG, National Synchrotron Radiation Research Center & Dept of Physics, National Tsing Hua University, DEPT OF PHYSICS, NATIONAL TSING HUA UNIVERSITY TEAM, NATIONAL SYNCHROTRON RADIATION RESEARCH CENTER COLLABORATION, INSTITUTE OF NANO ENGINEERING AND MICROSYSTEMS, NATIONAL TSING HUA UNIVERSITY TEAM — The Fabry-Perot type resonators using back diffraction from sapphire crystals for hard X-ray was investigated. On the basis of its less absorption and hexagonal structure, the resonator in sapphire crystals underwent a pure 2-beam diffraction which could enhance the resonance interference and improve finesse compared with the one in silicon crystals. The resonators were manufactured from sapphire crystals using microelectronic lithography process with thickness of a few tens μm . With synchrotron radiation of energy resolution $\Delta E=0.82$ meV at 14.315 keV, X-ray back diffraction from two monolithic sapphire crystal plates shows resonance fringes clearly resulting from coherent interaction inside the energy gap of the (0 0 30) reflection. These experimental results of sapphire cavities imply the potential application for X-ray optics.

4:30PM X33.00011 X-ray wave guiding using three-beam Bragg-surface diffraction

SHIH-LIN CHANG, NSRRC, YAN-ZONG ZHENG, NTHU, WU TAI-SING TEAM, CHEN YI-CHUN TEAM, WU YU-HSIN TEAM, CHEN HSIN-YI TEAM, CHU PEI-CI TEAM — A diffraction-type of X-ray wave guide, in contrast to refraction-type, is proposed using three-beam diffraction geometry to generate a surface diffracted beam propagating along the direction of the wave guide. The three-beam Bragg-surface diffraction involves a symmetric Bragg reflection and a surface diffraction. The former is used to guide a wide-angle incident beam into a silicon crystal. The simultaneously occurring surface diffraction then guides the diffracted beam propagating along the direction of the wave guide that is parallel to the crystal surface. A wave guide with a shallow ditch is then manufactured along the direction of the surface diffraction using the conventional lithographic technique. As a whole the wave guide consists of a three-layer structure of tantalum/photon resist (PMMA)/tantalum, on the Silicon substrate. The surface diffracted X-rays can then be confined in and guided along the layer of photon resist. Details of the design of the wave guide and synchrotron diffraction experiments will be reported.

4:42PM X33.00012 Combined surface plasmon resonance and X-ray absorption spectroscopy¹

MIGUEL ANGEL GARCIA, Institute for Ceramic and Glass CSIC & IMDEA Nanociencia, AIDA SERRANO, Institute for Ceramic and Glass CSIC, Madrid, Spain, OSCAR RODRIGUEZ DE LA FUENTE, Dpt. Material Physics, Univ. Complutense at Madrid, Spain, GERMAN R. CASTRO, Spline Spanish CRG beamline at ESRF, Grenoble, France & ICMM CSIC — We present a system for the excitation and measurement of surface plasmons in metallic films based on the Kretschmann-Raether configuration that can be installed in a synchrotron beamline. The device was mounted and tested in a hard X-ray Absorption beamline, BM25 Spline at ESRF. With this device it is possible to carry on experiments combining surface plasmon and X-ray absorption spectroscopies. The surface plasmons can be used to monitor in situ changes induced by the X-rays in the metallic films or the dielectric overlayer. Similarly, the changes in the electronic configuration of the material when surface plasmons are excited can be measured by X-ray absorption spectroscopy. The resolution of the system allows to observe changes in the signals of the order of 10^{-3} to 10^{-5} depending on the particular experiment and used configuration. The system is available for experiments at the beamline.

¹This work was supported by the Spanish Ministry of Science and Education through the project FIS-2008-06249. We acknowledge the ESRF for provision of synchrotron radiation facilities and the SpLine beamline staff for assistance during XAS experiments.

4:54PM X33.00013 Probing of Strain Mediated Hybrid Multiferroic Devices, EDWIN FOHTUNG, J. KIM, M. MARSH, Department of Physics, University of California-San Diego, NA LEI, Institut d'Electronique Fondamentale, Universit Paris-Sud, S. CHEN, S. SINHA, Department of Physics, University of California-San Diego, D. RAVELOSONA, Institut d'Electronique Fondamentale, Universit Paris-Sud, ERIC FULLERTON, Center for Magnetic Recording Research, University of California-San Diego, OLEG SHPYRKO, Department of Physics, University of California-San Diego — Smart materials for sensor technology, (non) volatile device memories for information technology, and ultrasound generators in medical imaging have one thing in common, their active elements consist of ferroelectrics (FE) driven by voltages or ferromagnetics (FM) driven by magnetization. In the quest to design high functionality devices to meet today's consumer technological demands, high focus has been given to multiferroic [1]. However, the coexistence of magnetic order and ferroelectric polarization combined in a single-phase material has proven to be rare as most of these materials tend to have low magnetic ordering temperatures and are often antiferromagnets, in which the magnetoelectric (ME) coupling effect is intrinsically small. We utilize an alternative approach to design multiferroic-hybrid devices based on FE-FM composites where the ME coupling emerges from strain-mediated interaction between individual phases [2]. We develop a nonlinear thermodynamic theory for strain-mediated direct ME effect and Bragg Ptychographic Coherent Diffraction Imaging (BCDI) serves as the unique tool of choice for sub-nanometer resolution nondestructive probing of the order parameters in the devices [1] N. Spaldin and M. Fiebig, Science 309, 391 (2005). [2] E. Fohntung et al., submitted (2012)

5:06PM X33.00014 First-Principles Modeling for Low-Energy Electron Diffraction Spectra¹, JOHN MCCLAIN, University of New Hampshire, JIEBING SUN, Michigan State University, JAMES HANNON, IBM Thomas J. Watson Research Center, KARSTEN POHL, JIAN-MING TANG, University of New Hampshire — We present a computational method to incorporate density-functional theory (DFT) into the calculation of the reflectivity in low-energy electron diffraction (LEED). Rapid and accurate analysis of diffraction spectra will facilitate the development of low-energy electron microscopy. The dynamical analysis of the electron reflectivity is traditionally carried out using multiple scattering theory with spherically symmetric (muffin-tin) potentials. However, for directionally bonded materials, such as semiconductors, the actual crystal potentials in the interstitial region can be significant, particularly for very low energy electrons. DFT with nonlocal pseudopotentials yields the low-energy electronic structure more accurately. In typical DFT calculations for surfaces, a finite slab is set up in a large unit cell with periodic boundary conditions. By matching the plane waves representing the LEED beams to the Kohn-Sham wave functions at the boundaries of the supercell, we determine the diffraction intensities. To demonstrate that our matching approach is not limited by the finite size of the supercell, we first consider trial models with exact solutions. We then use this approach to analyze the electron diffraction from graphene and compare with features in the band structure.

¹ We acknowledge funding support from NSF DMR-1006863.

Thursday, March 1, 2012 2:30PM - 5:30PM – Session X34 DCP: Focus Session: Nano VI: Junctions and Transport 107A

2:30PM X34.00001 Electronic transport through a light-driven azobenzene molecule switch: A revisit by density functional theory study¹, YAN WANG, HAI-PING CHENG, Dept. of Physics and QTP, University of Florida, USA — Azobenzene, a molecule that changes conformation between *trans* and *cis* configurations, is a candidate light-driven molecule switch. Recent experiments showed that the “on” state with larger measured conductance is associated with the *cis* isomer, which is in contrast with our previous theoretical prediction. Here we reconsider the issue of the molecule-electrode and electrode-electrode coupling by performing a first-principles study of the electronic structures and transport properties of Au-azobenzene-Au molecule junctions. Specifically, we investigate the dependence of the conductance and the current-voltage characteristics in two types of Au electrode, 2-D Au(111) surface and 1-D Au STM tip. We find that, not only the *trans* to *cis* transformation of the molecule, but also the electrode-electrode coupling plays a critical role in determining the conductance near the Fermi level.

¹Supported by US/DOE/BES/DE-FG02-02ER45995.

2:42PM X34.00002 Reliable anchoring groups for single-molecule junctions, M. TERESA GONZÁLEZ, EDMUND LEARY, IMDEA-Nanoscience, CHARALAMBOS EVANGELI, CARLOS ARROYO, GABINO RUBIO-BOLLINGER, Universidad Autonoma de Madrid, NICOLÁS AGRAÏT, Universidad Autonoma de Madrid and IMDEA-Nanoscience — In the field of molecular electronics, thiols have been extensively used as the most common anchoring groups to bind molecules to gold electrodes. However, other anchoring groups as amines can provide interesting advantages. Recently, C60 has been also proposed as a possible very efficient binding group. In this talk, I will present our studies on molecular junctions formed by thiol-, amine-, and C60-terminated molecules. We use a STM (scanning tunneling microscope) break-junction technique to create and characterized single-molecule junctions both in ambient and liquid environment. We compare thiols and amines on the alkane family and an oligo(phenylene ethynylene). Our study of the molecular-junction stretching length allows us to conclude that thiols affect atomic rearrangement at the electrodes significantly more than amines. Using C60-terminated molecules, we have recently introduced a new technique for controllably wiring one molecule at a time. We first get STM images to located isolated molecules on a gold substrate, which are then specifically targeted and contacted using a STM gold tip. This technique offers a significant improvement over other techniques, as it guarantees that one and only one molecule is contacted at a time between the electrodes.

2:54PM X34.00003 Novel quantum interference effects in transport through molecular radicals, JUSTIN BERGFELD, Department of Chemistry, Northwestern University, GEMMA SOLOMON, NanoScience Center and Department of Chemistry, University of Copenhagen, CHARLES STAFFORD, Department of Physics, University of Arizona, MARK RATNER, Department of Chemistry, Northwestern University — In molecules with an unpaired electron (radicals), we predict a correlation-induced ‘Mott-node’ in the transmission spectrum arising from destructive interference between transport contributions from different charge states of the molecule. This class of quantum interference effect has no single-particle analog and cannot be described by effective single-particle theories. Large errors in the thermoelectric properties and nonlinear current-voltage response of molecular radical junctions are introduced when the complementary wave and particle aspects of the electron are not properly treated. A method to accurately calculate the low-energy transport through a radical-based junction using an Anderson model is given.

3:06PM X34.00004 Electron Transport through Porphyrin in Nanoscale Junctions, SWATILEKHA SAHA, GUOQUANG QIAN, KIM M. LEWIS, Rensselaer Polytechnic Institute — As electronic devices become exceedingly small, incorporation of molecules as circuit elements is an attractive option due to their small size and the new functions that molecules can bring to the existing microelectronics. To realize such devices we have fabricated nanogaps of size 2-3 nm on gold wires and positioned porphyrin molecules in the gap. I-V characteristics with and without molecules in the junction is performed and signatures of molecular transport has been identified. We measure inelastic electron tunneling spectra (IETS) from molecular junctions at 4K in ultra-high vacuum to study its vibrational modes. These measurements will be compared to Raman spectra. We discuss how IETS can provide valuable insight to the metal-molecule coupling and the role ligated atoms can play in electron transport properties.

3:18PM X34.00005 Modeling Surface and Stress-Anisotropy Effects on Transformations in Lead Sulfide Nanocrystals Under Pressure, CLIVE BEALING, RICHARD HENNIG, Cornell University — The semiconductor PbS, which displays a small band gap and large excitonic Bohr radius, presents an ideal candidate material for such devices as infrared photon detectors and nanocrystal solar cells.¹ This has motivated a number of studies into the effect of pressure on bulk PbS and PbS nanocrystals (NCs), which organize into highly periodic superlattices with interesting mechanical properties.² The ambient-pressure NaCl-type structure of PbS undergoes a transformation to an orthorhombic structure close to 2.5 GPa, which itself transforms to the CsCl-type structure at 21.5 GPa. We have identified competitive minimum energy paths between the different modifications of PbS using density-functional calculations, and have calculated the associated enthalpy barriers over a range of pressures. In empirical molecular dynamics simulations of the PbS NC transformation under pressure, the effect on the transformation of anisotropic stresses, applied perpendicular to the {100}- and {111}-type facets of the NC, has been investigated. The effect of the NC surface on the stability of metastable modifications in PbS NCs is also considered.

¹J. Choi, et al., Nano Lett., **9**, 3749 (2009)

²P. Podsiadlo, et al., Nano Lett., **11**, 579 (2010)

3:30PM X34.00006 Compositional Distribution and Electronic Structure of Ternary Compound Semiconductor Nanocrystals, SUMEET PANDEY, DIMITRIOS MAROUDAS, Department of Chemical Engineering, University of Massachusetts Amherst, MA 01003 — We present a first-principles-based theoretical study of compositional distribution and the resulting electronic structure of ternary quantum dots (TQDs) of compound semiconductor nanocrystals. The analysis is based on first-principles Density Functional Theory (DFT) calculations of atomic and electronic structure and on Monte Carlo (MC) simulations of compositional distribution according to DFT-parameterized valence force field models. We report results for $\text{ZnSe}_{1-x}\text{S}_x$ (type-I), $\text{ZnSe}_{1-x}\text{Te}_x$ (type-II), and $\text{In}_x\text{Ga}_{1-x}\text{As}$ (Reverse type-I) TQDs with nm-scale diffusion lengths and large surface-to-volume ratios. The equilibrium compositional distribution is predicted as a function of overall composition (x) and TQD diameter and its impact on the electron density distribution, electronic density of states, and band gap of the TQDs is analyzed. We find that thermodynamically stable atomic distributions allow for optimal band-gap tunability and wave function confinement in TQDs. Our findings explain the possibility for compositional redistribution that may cause, over time, favorable or adverse changes of the TQD electronic properties with far reaching implications for the synthesis and applications of such nanostructures in devices.

3:42PM X34.00007 The Role of morphology and interface in photoluminescent properties in CdSe/CdS Heterostructure Nanocrystals¹, ARNAUD DEMORTIERE, CHUNXING SHE, Argonne National Laboratory, DONOVAN N. LEONARD, Oak Ridge National Laboratory, SOMA CHATTOPADHYAY, MATTHEW PELTON, ELENA SHEVCHENKO, Argonne National Laboratory — Semiconductor core/shell colloidal nanocrystals (NCs) are promising materials for many applications such as luminescent solar concentrators and lasing media, due to their high PL quantum yield (PLQY) and their charge separation effect. The role of interface in PLQY and in band alignment type is studied in this nanoscale heterojunction. Rod-shaped CdSe/CdS NCs have been synthesized by colloidal chemical approach via epitaxial process, which gives us a fine-tuning of both the spherical core size and rod-like shell length. The modification of the relative morphology changes the effective core/shell band alignment, which impacts the electron and hole delocalization into the nanorods. The evolution of the PLQY and PL lifetimes has been studied as a function of the relative core/shell sizes. High PLQY of up to 80% and PL lifetime of 36 ns have been obtained for a shell-excitation wavelength of 450 nm with a large quasi-Stokes shift (~100nm). Radiative decay rates have been correlated with the rod volume and the band alignment type has been identified as being core size dependent. Finally, UltraSTEM and EXAFS analyses have been used to characterize the crystalline configuration at the core/shell interface and the lattice strain.

¹This work at the Center for Nanoscale Materials was supported by the U.S. Department of Energy.

3:54PM X34.00008 Electrostatic gating and single-molecule Raman spectroscopy, YAJING LI, JOSEPH HERZOG, DOUGLAS NATELSON, Rice University — SERS(surface enhanced raman spectroscopy) is a useful tool for single molecule spectroscopic investigations. We fabricated nanoscale Au bowtie structures to function as SERS substrates. Following electromigration, these metal nanostructures possess nanometer-scale interelectrode gaps that support highly localized surface plasmon resonances, resulting in SERS electromagnetic enhancements sufficient for single-molecule studies. These structures have also proven suitable for single-molecule electronic transport experiments, in which the underlying substrate can function as a gate electrode to shift molecular electronic levels relative to the metal source and drain. We will present preliminary results of the effect of gate modulation on the SERS and electrical properties of molecules in such junctions.

4:06PM X34.00009 Thermoelectricity and transmission eigenchannels in buckyball junctions¹, MICHAEL STEFFERSON, JARRED HUDSON, JOSHUA BARR, Department of Physics, University of Arizona, JUSTIN BERGFELD, Department of Chemistry, Northwestern University, CHARLES STAFFORD, Department of Physics, University of Arizona — Transmission through nanoscale junctions consisting of a single Buckminsterfullerene molecule between two Pt or Au electrodes is investigated in the Coulomb blockade regime using the nonequilibrium Green's function approach. The Green's function of the buckyball is calculated in the isolated-resonance approximation, including the degenerate HOMO and LUMO orbitals. Electron-electron interactions were included in a constant-interaction model derived from π -electron effective field theory. For junctions with Pt electrodes, we find two transmission channels (despite the 5-fold degenerate HOMO and 3-fold degenerate LUMO resonances) and a positive thermopower. For Au electrodes, the thermopower is strongly affected by quantum interference, and we find just one transmission channel.

¹This material is based upon work supported by the Department of Energy under Award Number DE-SC0006699.

4:18PM X34.00010 Study of Raman Stark Effect in Self-Aligned Nanojunctions, JOSEPH HERZOG, Rice University, DANIEL WARD, University of Wisconsin, DOUGLAS NATELSON, Rice University — Plasmonically-active nanojunctions have been used to study the electrical and optical properties of single molecules by using surface-enhanced Raman spectroscopy (SERS). A new, "self-aligned" fabrication technique has been developed to mass-produce more robust nanojunctions. Similar to nanogaps made by electromigration, these self-aligned nanojunctions have been shown to exhibit strong SERS signal. In addition to having the capabilities of fabricating SERS substrates on a massive scale, the self-aligned technique also produces devices with a longer shelf-life than those fabricated by electromigration. Preliminary studies of the electromigrated devices have demonstrated Raman Stark shifts under DC bias. This work aims to study the Stark effect more in-depth and with the self-aligned nanogaps geometry by integrating the self-aligned structures into electrical circuits. Initial findings and current progress of these simultaneous optical and electrical measurements of a single molecule's vibrational modes will be discussed.

4:30PM X34.00011 Hopping And Trapping of F4TCNQ on h-BN Nanomesh¹, HUANYAO CUN, SILVAN ROTH, ARI SEITSONEN, HAIFENG MA, JURG OSTERWALDER, THOMAS GREBER, None, PHYSICAL-CHEMISTRY INSTITUTE @ UZH COLLABORATION — A single layer of hexagonal boron nitride (h-BN) on Rh(111) (nanomesh) [1] is an excellent template for trapping and self-assembly of molecules. This hexagonal structure has a periodicity of 3.22 nm and an appearance with strongly bound h-BN regions called “pores” of about 2 nm in diameter surrounded by h-BN regions called “wires.” The trapping mechanism traces back to a corrugated electrostatic potential at the surface [2]. We have investigated the adsorption behavior of an electron acceptor molecule, tetrafluoro-tetracyano-quinodimethane (F4TCNQ) on nanomesh by combining XPS, UPS, STM and DFT calculation. The work function increase upon F4TCNQ adsorption indicates electron transfer to the molecules, and is in good agreement with the DFT result. At room temperature, F4TCNQ adsorbs on the “wires” and in the “pores” because of a high mobility. STM measurements allow us to detect the hopping rate of molecules. Upon cooling, molecules are trapped inside of pores, which gives insight into the behavior of a negatively charged molecule, compared to neutral species, in the trapping potential of h-BN nanomesh.

¹The project is supported by the Sinergia Program of the Swiss National Science Foundation.

4:42PM X34.00012 Quantum-Enhanced Thermoelectric Effects in Polycyclic Molecular Junctions¹, JOSHUA BARR, CHARLES STAFFORD, University of Arizona — We calculate the thermoelectric response of a polycyclic molecular junction including electron-electron interactions. To do this, the molecular Green's function is determined via a Lanczos-based technique and π -electron effective field theory is used to model the degrees of freedom most relevant to transport. In these junctions we find that the presence of multiple rings leads to higher order quantum interference features giving rise to dramatic enhancements of molecular thermoelectric effects, consistent with previous predictions based on Hückel theory, which neglected electron correlations.

¹This material is based upon work supported by the Department of Energy under Award Number DE-SC0006699.

4:54PM X34.00013 Decoherence Assisted Single Electron Trapping at Room Temperature, AHMED ELHALAWANY, MICHAEL LEUENBERGER, University of Central Florida — In this work, we theoretically investigate electron transport in heterostructure semiconductor nanowire (NW). We develop a new mechanism to trap an electron in a quantum dot (QD) by means of decoherence. There are six QDs in the NW. Bias voltage (V_b) is applied across the NW and gate voltage (V_g) is applied to the auxiliary QD to control single charge tunneling. The single electron dynamics along the NW is calculated by means of the generalized master equation based on the tight binding model taking into account electron LO phonon interaction (ELOPI) and thermal broadening inside the QDs. It is shown that the decoherence, which is in the pico-second (ps) regime, speeds up the trapping of the electron in the central QD with probability of 70% in less than 2 ps. Our results can be used for the implementation of high temperature single photon source (SPS) or single electron transistor (SET). We acknowledge support from NSF (Grant No. ECCS-0725514), DARPA/MTO (Grant No. HR0011-08-1-0059), NSF (Grant No. ECCS-0901784), AFOSR (Grant No. FA9550-09-1-0450), and NSF (Grant No. ECCS-1128597).

5:06PM X34.00014 First-Principles Studies on Photoinduced Charge Transfer in Functionalized Carbon Nanotubes¹, IEK-HENG CHU, DMITRI KILIN, HAI-PING CHENG, Department of Physics and the Quantum Theory Project, University of Florida, Gainesville, Florida — We have studied the binding energy, electronic structure, optical excitation, and relaxation of dinitromethane molecules ($\text{CH}_2\text{N}_2\text{O}_4$) on semiconducting carbon nanotubes (CNTs) of chiral index ($n, 0$) ($n=7,10,16,19$). The electronic structures calculated from density functional theory (DFT) show that the dinitromethane introduces a localized state inside the band gap of CNT systems of $n=10,16$ and 19 , which indicates that the state can trap an electron when the CNT is photoexcited. The dynamics of intra-band relaxations in such systems has been investigated using reduced density matrix formalism combined with DFT. For pristine CNTs, we have found that the calculated charge relaxation time constants agree well with the experimental time scales. Upon adsorption, these constants are modified and there is not a clear trend for the direction and magnitude of the change. However, our calculations predict that electron relaxation in the conduction band is faster than hole relaxation in the valence band, for CNTs with and without molecular adsorbates.

¹This work is supported by DOE/BES-DE-FG02-02ER45995. The computation is performed using facilities at NERSC.

5:18PM X34.00015 Understanding Crosstalk Between Parallel Molecular Wires, MATTHEW REUTER, Computer Science and Mathematics Division, Oak Ridge National Laboratory, TAMAR SEIDEMAN, MARK RATNER, Department of Chemistry, Northwestern University — Cooperative effects between molecular wires affect conduction through the wires, and studies have yet to clarify the conditions under which these effects enhance (diminish) conduction. Using a simple but general model, we attribute this crosstalk to the duality of energetic splitting and phase interference between the wires' conduction channels. In most cases, crosstalk increases (decreases) conductance when the Fermi level is far from (close to) an isolated wire's resonance. Finally, we discuss strategies for controlling crosstalk between parallel molecular wires.

[1] M. G. Reuter et al. J. Phys. Chem. Lett. 2, 1667-1671 (2011).

[2] M. G. Reuter et al. Nano Lett. 11, 4693-4696 (2011).

Thursday, March 1, 2012 2:30PM - 5:30PM –
Session X39 DMP DBIO DPOLY: Focus Session: Materials and Functional Structures for Biological Interfaces - Nanoscale Materials 109B

2:30PM X39.00001 ABSTRACT WITHDRAWN –

3:06PM X39.00002 Designing super-selectivity in multivalent nano-particle binding¹, FRANCISCO MARTINEZ-VERACOECHEA, DAAN FRENKEL, University of Cambridge — A key challenge in nano-science is to design ligand-coated nano-particles that can bind selectively to surfaces that display the cognate receptors above a threshold (surface) concentration. Nano-particles that bind monovalently to a target surface do not discriminate sharply between surfaces with high and low receptor coverage. In contrast, “multivalent” nano-particles that can bind to a larger number of ligands simultaneously, display regimes of “super-selectivity” where the fraction of bound particles varies sharply with the receptor concentration. We present numerical simulations that show that multivalent nano-particles can be designed such that they approach the “on-off” binding behavior ideal for receptor-concentration selective targeting. We propose a simple analytical model that accounts for the super-selective behavior of multi-valent nano-particles. We propose a simple rule of thumb to predict the conditions under which super-selectivity can be achieved. We validate our model predictions against the Monte Carlo simulations. Finally, we investigate the role of multi-component ligand-receptor interactions in the enhancement of targeting selectivity.

¹This work was supported by the ERC (Advanced Grant agreement 227758). Research partially carried out at the Center for Functional Nanomaterials, BNL, which is supported by the US DOE, Office of BES, under Contract No. DE-AC02-98CH10886.

3:18PM X39.00003 Nano-Engineered Cubic Zirconia for Orthopaedic Implant Applications¹

F. NAMAVAR, University of Nebraska Medical Center, A. RUBINSTEIN, University of Nebraska at Omaha, R. SABIRIANOV, UNO, G. THIELE, J. SHARP, U. POKHAREL, R. NAMAVAR, K. GARVIN, UNMC — Osseointegration failure of the prosthesis prevents long-term stability, which contributes to pain, implant loosening, and infection that usually necessitates revision surgery. Cell attachment and spreading in vitro is generally mediated by adhesive proteins such as fibronectin and vitronectin. We designed and produced pure cubic zirconia (ZrO₂) ceramic coatings by ion beam assisted deposition (IBAD) with nanostructures comparable to the size of proteins. Our ceramic coatings exhibit high hardness and a zero contact angle with serum. In contrast to Hydroxyapatite (HA), nano-engineered zirconia films possess excellent adhesion to all orthopaedic materials. Adhesion and proliferation experiments were performed with a bone mesenchymal stromal cells cell line (OMA-AD). Our experimental results indicated that nano-engineered cubic zirconia is superior in supporting growth, adhesion, and proliferation. We performed a comparative analysis of adsorption energies of the FN fragment using quantum mechanical calculations and Monte Carlo simulation on both types of surfaces: smooth and nanostructured. We have found that the initial FN fragment adsorbs significantly stronger on the nanostructured surface than on the smooth surface.

¹This work was supported by the Department of Energy

3:30PM X39.00004 Computational characterization of DNA/peptide/nanotube self assembly for bioenergy applications

VANESSA ORTIZ, RURIKO ARAKI, GALEN COLLIER, Department of Chemical Engineering, Columbia University — Multi-enzyme pathways have become a subject of increasing interest for their role in the engineering of biomimetic systems for applications including biosensors, bioelectronics, and bioenergy. The efficiencies found in natural metabolic pathways partially arise from biomolecular self-assembly of the component enzymes in an effort to avoid transport limitations. The ultimate goal of this effort is to design and build biofuel cells with efficiencies similar to those of native systems by introducing biomimetic structures that immobilize multiple enzymes in specific orientations on a bioelectrode. To achieve site-specific immobilization, the specificity of DNA-binding domains is exploited with an approach that allows any redox enzyme to be modified to site-specifically bind to double stranded (ds) DNA while retaining activity. Because of its many desirable properties, the bioelectrode of choice is single-wall carbon nanotubes (SWNTs), but little is known about dsDNA/SWNT assembly and how this might affect the activity of the DNA-binding domains. Here we evaluate the feasibility of the proposed assembly by performing atomistic molecular dynamics simulations to look at the stability and conformations adopted by dsDNA when bound to a SWNT. We also evaluate the effects of the presence of a SWNT on the stability of the complex formed by a DNA-binding domain and DNA.

3:42PM X39.00005 Engineering upconverting nanophosphors as biosensors and biotherapeutic agents

SHUANG FANG LIM, North Carolina State University — Contrast agents play an important role in the study of biological tissues and whole organisms, since they enable visualization of functional structures. Fluorescent contrast agents also enable specific targeting in therapeutic approaches. Developing optimized contrast agents is central to optimizing the performance of both imaging and therapy. Upconversion nanophosphors (UCNPs) are a class of nanoparticles which enable efficient 2-photon fluorescence. Their intrinsic properties of low toxicity, low excitation intensity, narrow fluorescence line width, multiplexing capability, zero fluorescent background, and absence of bleaching and blinking make them strong candidates as a contrast agent with wide applicability. I am working to develop these nanomaterials with biological significance as contrast agents in biolabels, in biosensors and as therapeutic agents in photodynamic therapy. This will be combined with the enhancement of brightness of the UCNPs through coupling to resonant gold nanostructures. The study is necessary in order to bring about a break through in upconversion luminescence enhancement, particularly at ever decreasing nanoparticle sizes necessary for biological applications.

4:18PM X39.00006 Optically Trappable Single Wall Carbon Nanotubes

SAMANTHA ROBERTS, Department of Physics, Cornell University, Ithaca NY, ARTHUR BARNARD, School of Applied and Engineering Physics, Cornell University, Ithaca NY, JOSHUA KEVEK, Department of Physics, Cornell University, Ithaca NY, ALEXANDER RUYACK, Materials Science and Engineering, Cornell University, Ithaca NY, IVE SILVESTRE, RODRIGO LACERDA, Department of Physics, Universidade Federal de Minas Gerais, Brazil, PAUL MCEUEN, Department of Physics, Kavli Institute at Cornell for Nanoscale Science, Cornell University, Ithaca NY — We are developing a single walled carbon nanotube (NT) force probe which would utilize an optical trap to manipulate NTs fitted with micron scale dielectric handles. With its nanometer diameter and micron length a NT harnessed in this way may eventually allow us to probe a cell's membrane and interior. In pursuit of this goal we have developed a method to create parallel arrays of aligned NT cantilevers. In this process we transfer highly aligned NTs to a substrate composed of alternating regions of Si separated by SiO₂. Patterning the NTs and etching away the oxide leaves behind ridges supporting arrays of NT cantilevers 0.7nm-2nm in diameter and up to 700nm in length with densities of over one cantilever per micron. We will discuss our work modifying this technique to pattern and release micron scale NT cantilever probes into solution. We have designed and optically tested lithographically patterned SiO₂ and SU-8 handles, shaped such that they can be manipulated with an optical trap in predictable orientations. We will focus on our current efforts in attaching these optically trappable dielectric handles to individual nanotubes so they can be implemented to make direct force measurements.

4:30PM X39.00007 Self-assembled peptide nanowires on single-layer graphene and MoS₂ with biomolecular doping effect¹

YUHEI HAYAMIZU, CHRISTOPHER R. SO, MEHMET SARIKAYA, Genetically Engineered Materials Science and Engineering Center, Materials Science and Engineering, University of Washington — Developing elegant hybrid systems of biological molecules on atomic single layers (ASLs), such as graphene, is a key in creating novel bio-nanoelectronic devices, where versatile biological functions are integrated with electronics of ASLs. Biomolecules self-assembling into ordered structures on ASLs offer a novel bottom-up approach, where organized supramolecular architectures spatially govern the ASL electronics. Despite the potential in bridging nano- and bio-worlds at the molecular scale, no work has yet realized a way to control electronic and optical properties of ASLs by the biomolecular structures. Here, we demonstrate that engineered dodecapeptides self-assemble into supramolecular networks of peptide nanowires on single-layer graphene and MoS₂. Peptide nanowires introduce electric charge into these ASLs via biomolecular doping. Abrupt boundaries of nanowires create electronic junctions in graphene, which manifest themselves within the single-layer as a self-assembled electronic network. Furthermore, the designed peptides modify both conductivity and photoluminescence of single-layer MoS₂. Controlling nano-electronics through engineered peptides potentially opens up new avenues in self-assembly of nanodevices for future bioelectronics.

¹Research supported by NSF-MRSEC, NIH-T32, NSF-BioMat and JST-PRESTO programs.

4:42PM X39.00008 *Ab initio* Calculations of Electronic Fingerprints of DNA bases on Graphene¹

TOWFIQ AHMED, JOHN J. REHR, Univ. of Washington, SVETLANA KILINA, North Dakota State University, TANMOY DAS, JASON T. HARALDSEN, ALEXANDER V. BALATSKY, Los Alamos National Laboratory — We have carried out first principles DFT calculations of the electronic local density of states (LDOS) of DNA nucleotide bases (A,C,G,T) adsorbed on graphene using LDA with ultra-soft pseudo-potentials. We have also calculated the longitudinal transmission currents $T(E)$ through graphene nano-pores as an individual DNA base passes through it, using a non-equilibrium Green's function (NEGF) formalism. We observe several dominant base-dependent features in the LDOS and $T(E)$ in an energy range within a few eV of the Fermi level. These features can serve as electronic fingerprints for the identification of individual bases from dI/dV measurements in scanning tunneling spectroscopy (STS) and nano-pore experiments. Thus these electronic signatures can provide an alternative approach to DNA sequencing.

¹Supported by the LANL CINT, DOE BES Grant DE-FG03-97ER45623, and DE-AC52-06NA25396

4:54PM X39.00009 Controlled Chemical Patterns with ThermoChemical NanoLithography (TCNL) , KEITH CARROLL, School of Physics, Georgia Institute of Technology, ANTHONY GIORDANO, School of Chemistry and Biochemistry, Georgia Institute of Technology, DEBIN WANG, Lawrence Berkeley National Laboratory, VAMSI KODALI, School of Physics, Georgia Institute of Technology, W.P. KING, Department of Mechanical Science and Engineering, University of Illinois Urbana-Champaign, S.R. MARDER, School of Chemistry and Biochemistry, Georgia Institute of Technology, E. RIEDO, J.E. CURTIS, School of Physics, Georgia Institute of Technology — Many research areas, both fundamental and applied, rely upon the ability to organize non-trivial assemblies of molecules on surfaces. In this work, we introduce a significant extension of ThermoChemical NanoLithography (TCNL), a high throughput chemical patterning technique that uses temperature-driven chemical reactions localized near the tip of a thermal cantilever. By combining a chemical kinetics based model with experiments, we have developed a protocol for varying the concentration of surface bound molecules. The result is an unprecedented ability to fabricate extremely complex patterns comprised of varying chemical concentrations, as demonstrated by sinusoidal patterns of amine groups with varying pitches ($\sim 5\text{--}15\ \mu\text{m}$) and the replication of Leonardo da Vinci's *Mona Lisa* with dimensions of $\sim 30 \times 40\ \mu\text{m}^2$. Programmed control of the chemical reaction rate should have widespread applications for a technique which has already been shown to nanopattern various substrates including graphene nanowires, piezoelectric crystals, and optoelectronic materials.

5:06PM X39.00010 Interface-Limited Spherulitic Growth of Hydroxyapatite/Chondroitin Sulfate Composite Enamel-like Films¹ , GUOBIN MA, YIFEI XU, XIYAN WANG, MU WANG, National Laboratory of Solid State Microstructures, and Department of Physics, Nanjing University, Nanjing 210093, China — Understanding and mimicking the growth of hard tissues such as tooth enamel may lead to innovative approaches toward engineering novel functional materials and providing new therapeutics. Up to now, *in vitro* growth of enamel-like materials is still a great challenge, and the microscopic formation mechanisms are far from well understood. Here we report synthesis of large-scale hydroxyapatite (HAP) and chondroitin sulfate (ChS) composite films by an efficient solution-air interface growth method. The products have the characteristic hierarchical prism structures of enamel and the mechanical properties comparable to dentin. We demonstrate that the films are assembled by spherulites nucleated at the solution surface. The growth of the spherulites is limited by the interfaces between them as well as between the solution and air, leading to the ordered prism structure. The results are beneficial for a clearer understanding of the fundamentals of tooth enamel formation.

¹Project supported by the National Science Foundation of China (Grant No.51172104) and the Ministry of Science and Technology of China (Grant No. 2010CB630705).

5:18PM X39.00011 Biomimetic Calcium Phosphate Crystallization: Synchrotron X-ray Studies¹ , AHMET UYSAL, BENJAMIN STRIPE, PULAK DUTTA, Physics and Astronomy, Northwestern University, BINHUA LIN, MATI MERON, CARS, The University of Chicago — The nucleation and growth of calcium phosphate by organic templates attract great attention due to its relevance to bone biomineralization. In spite of the vast studies in the field, the role of the organic templates in the process is still not well understood. One reason for this drawback is the lack of experimental tools to probe the organic template structure during the process. We studied the nucleation and growth of calcium phosphate under floating Langmuir monolayers, at the air/water interface, using two complementary X-ray scattering methods. We show that Grazing Incidence X-ray Diffraction (GID) and Grazing Incidence X-ray off-Specular Scattering (GIXOS) can reveal the organic-inorganic interface properties *in situ*. By using GID and GIXOS together, we can simultaneously determine the lateral interface structure and the electron density profile normal to the interface. Combined with *ex situ* methods, these techniques can improve our understanding of the role of the organic template during biomineralization.

¹This work was supported by the U.S. National Science Foundation under Grant No. DMR-1006432

Thursday, March 1, 2012 2:30PM - 5:30PM –
Session X40 DBIO DPOLY DCOMP: Focus Session: Single Molecule Biological Physics - Nucleic Acids 156A

2:30PM X40.00001 From force-fields to photons: MD simulations of dye-labeled nucleic acids and Monte Carlo modeling of FRET¹ , LORI GOLDNER, Physics Department, University of Massachusetts, Amherst — Fluorescence resonance energy transfer (FRET) is a powerful technique for understanding the structural fluctuations and transformations of RNA, DNA and proteins. Molecular dynamics (MD) simulations provide a window into the nature of these fluctuations on a different, faster, time scale. We use Monte Carlo methods to model and compare FRET data from dye-labeled RNA with what might be predicted from the MD simulation. With a few notable exceptions, the contribution of fluorophore and linker dynamics to these FRET measurements has not been investigated. We include the dynamics of the ground state dyes and linkers in our study of a 16mer double-stranded RNA. Water is included explicitly in the simulation. Cyanine dyes are attached at either the 3' or 5' ends with a 3 carbon linker, and differences in labeling schemes are discussed.

Work done in collaboration with Peker Milas, Benjamin D. Gamari, and Louis Parrot.

¹This work was supported by NSF grant MCB-0920139.

3:06PM X40.00002 Quantifying screening ion excesses surrounding stretched, charged polymers , JONATHAN LANDY, Materials Dept., UCSB, DUSTIN MCINTOSH, Physics Dept., UCSB, OMAR SALEH, Materials Dept., UCSB — We present the results of a combined theoretical/experimental study in which we have applied thermodynamic identities to infer – from single molecule force-extension curves taken at different salt concentrations – how the number of screening ions associated with a charged polymer changes as a function of its end to end extension. This number, which can change only through non-linear screening mechanisms, turns out to depend non-trivially on both the concentration of salt and the inherent rigidity of the polymer. In the case of a flexible polymer, such as ssDNA, our data indicates that the excess can change substantially between the fully extended and globule states. The effect is reduced for semi-flexible polymers, such as dsDNA, at physiologically-relevant salt concentrations, but it can again become substantial at lower salt concentrations. Based on these findings, we argue that small ion entropic effects should often contribute substantially to free energy differences between the competing conformational states of charged polymers – both *in vivo* and in certain polymer-based materials systems.

3:18PM X40.00003 Euler buckling and nonlinear kinking of double-stranded DNA , ALEXANDER FIELDS, KEVIN AXELROD, ADAM COHEN, Harvard University — Bare double-stranded DNA is a stiff biopolymer with a persistence length of roughly 53 nm under physiological conditions. Cells and viruses employ extensive protein machinery to overcome this stiffness and bend, twist, and loop DNA to accomplish tasks such as packaging, recombination, gene regulation, and repair. The mechanical properties of DNA are of fundamental importance to the mechanism and thermodynamics of these processes, but physiologically relevant curvature has been difficult to access experimentally. We designed and synthesized a DNA hairpin construct in which base-pairing interactions generated a compressive force on a short segment of duplex DNA, inducing Euler buckling followed by bending to thermally inaccessible radii of curvature. The efficiency of Förster resonance energy transfer (FRET) between two fluorophores covalently linked to the hairpin indicated the degree of buckling. Bulk and single-molecule measurements yielded distinctly different force-compression curves for intact DNA and for strands with single nicks, base pair mismatches, and damage sites. These results suggest that changes in local mechanical properties may play a significant role in the recognition of these features by DNA-binding proteins.

3:30PM X40.00004 Measuring fluctuations in shear stretched DNAs using site specific labeling

, ALLEN PRICE, Emmanuel College, Boston, MA, THOMAS GRAHAM, JOSEPH LOPARO, Harvard Medical School, Boston, MA, JOEL EAVES, University of Colorado, Boulder, CO — We report a new technique for measuring the internal dynamics of surface tethered DNAs in shear flow. Previous studies have used end labeling or intercalating dyes which label the entire length of the DNA. Neither prior method can resolve the internal longitudinal fluctuations of the DNA. Our technique accomplishes this by site specific labeling of five sites in lambda phage DNA using EcoRI labeled with fluorescent quantum dots. We used our technique to determine the two point cross correlation functions of the longitudinal and transverse fluctuations of the DNA under shear flow. Our technique allows us to test current models of the non-equilibrium fluctuations of DNA in shear flow in a way previously inaccessible.

3:42PM X40.00005 Electric-field Assisted Deposition of the DNA on Polymer Surface

, JUNHWAN RYU, Loomis Chaffee School, KE ZHU, JULIA BUDASSI, JONATHAN SOKOLOV, Stony Brook University — Recently, the interaction of DNA with surfaces has been widely studied for its range of applications, including mapping, sequencing and analyzing DNAs. In this study, the Lambda DNA molecules were aligned in 6:50(0.1M NaOH:0.02M MES) buffer solution with different electric fields and deposited onto polymethylmethacrylate (PMMA) surfaces by dipping and retracting PMMA coated silicon wafers into the solution. Electric field was set up with platinum wire and gold plated Si wafer. The DNA strands were dyed with YoYo-1 and observed using a fluorescence microscope. The efficiency of deposition was optimized with respect to DNA concentration, DNA length and electric field. The results indicate that the density and possibly the lengths of the DNA deposited on surface can be controlled by this method. Enhancement of adsorption density of greater than twenty-fold were found using electric field strengths of 10v/cm. This study is supported by NSF-DMR-MRSEC program.

3:54PM X40.00006 Using Microcontact Printing as a Novel Method for Patterned Dyeing of Surface-adsorbed DNA¹

, EMILY SHEA, Smithtown High School East, JULIA BUDASSI, KE ZHU, JONATHAN SOKOLOV, Stony Brook University — We use microcontact printing (MCP)¹ to stain individual DNA molecules adsorbed and combed onto a polymer-coated silicon surface. Polydimethylsiloxane (PDMS) stamps with micron-sized features have been used to selectively stain lambda DNA molecules with SyBr Gold dye. DNA was deposited out of dilute solution onto polymethylmethacrylate (PMMA) layers, 70nm thick, spun-coated on Si wafers, producing linearly stretched and aligned molecules. The stamps were soaked in dye solutions for one minute, followed by wiping of excess solution with a swap. The stamp was pressed onto the surface, varying the pressure and time of application (typically 5-10 minutes) to control the staining. The DNA molecules were imaged with a fluorescence microscope equipped with a cooled CCD camera. Single molecules of DNA were successfully dyed and imaged with stamps having a grating pattern either parallel to or perpendicular to the DNA orientation. Supported by NSF-DMR MRSEC program.

¹NSF-DMR MRSEC

4:06PM X40.00007 Stretching DNA Molecules on a Polymer Surface¹

, JONATHAN ROSENBERG, Torah Academy of Bergen County, KE ZHU, JULIA BUDASSI, JONATHAN SOKOLOV, Stony Brook University — DNA's stretched form is one of great importance to the study of its structural characteristics and sequence. In our experiment, we studied the effects of stretching on lambda DNA, deposited onto Polydimethyl siloxane (PDMS, silicone) using the evaporating drop method. The DNA was dyed with SyBr Gold dye, or YOYO dye, which does not drastically affect the stretching properties of the DNA molecules while being deposited. Different DNA concentrations were used to optimize the density of the DNA on the surface. Once deposited, the DNA was imaged using a confocal microscope, for further measurements and to image stretching, in situ. To stretch the DNA molecules after deposition onto PDMS, the PDMS sample was placed onto a modified linear stage, pinched at the ends. The DNA length was measured throughout stretching. The result shows we successfully stretched DNA strands by 68% without breakage of the strands and without the strands coming off of the PDMS surface. This study is supported by NSF-DMR-MRSEC program.

¹NSF-DMR MRSEC

4:18PM X40.00008 Polarization and Angle Dependence of Fluorescence from Aligned DNA¹

, ASHISH SRIDHAR, Brophy College Preparatory, SURI BANDLER, Ramaz Upper School, KE ZHU, YINGZHAN GU, JULIA BUDASSI, JONATHAN SOKOLOV, Stony Brook University — DNA molecules can be deposited and aligned on various surfaces and imaged by confocal microscopy when labeled with fluorescent dyes. SyBr Gold dye, is known to possess a high angle and polarization dependence. We measured the emission intensity for various incident angles as a function of incident polarization angle. Samples were created by means of dipping PMMA-coated silicon wafers into dyed DNA solutions with DC electric field setup or drop evaporation. The blue laser as the imaging light source was mounted on an optical rail with a polarizer with rotatable half wave plate to change the incident polarization relative to the DNA molecular orientation. When applied to samples dyed using SyBr Gold, a clear change in the intensity of imaged DNA strands was observed though a range of input polarization angle. We have shown that it is possible to optimize the conditions in which aligned DNA is imaged using confocal microscopy by varying the polarization and angle of incidence of laser light on the sample. This study is supported by NSF-DMR-MRSEC program.

¹NSF-DMR MRSEC

4:30PM X40.00009 Calorimetric and Low-Frequency Dielectric Studies of Mesoscopic Ordering in Solutions of Engineered DNA Hairpin Fragments

, K. KASHURI, H. KASHURI, G.S. IANNACCHIONE, WPI — Calorimetry (both AC and MDSC) from 20 to 100 °C, as well as low-frequency (0.1 to 100 kHz) isothermal dielectric measurements have been performed on solutions of DNA fragments as a function of concentration. Custom hairpin DNA fragments were obtained with 13-base unit length and samples made in solution at various concentration. Results show a reproducible heat capacity C_p signature on heating and cooling scans. This thermal behavior of a diluted oligonucleotide chain is very different from that seen for mesoscopic ordering of liquid crystals. The AC C_p peak vanishes and new features are revealed as the temperature scan rate is lowered to 0.017 K min⁻¹. The observed real, ϵ' , and imaginary, ϵ'' , permittivity of the suspended DNA show features indicating low-frequency dynamics that in turn suggests large-scale ordering or agglomeration of the DNA hairpin loops.

4:42PM X40.00010 Modeling of DNA zipper reaction rates

, PRESTON LANDON, CASEY SANCHEZ, ALEXANDER MO, RATNESH LAL, University of California, San Diego — DNA zippers are a thermodynamically driven system consisting of three DNA oligonucleotides. Two of the strands are designed to create a small helix the third is designed to invade and separated the helix. A zipper system consisting of a normal strand (N), a weak strand (W), and an opening strand (O). N is made up of normal DNA bases, while W is engineered with inosine bases substituted for guanine. Inosine forms one less hydrogen bond with cytosine than guanine. By varying the number and order of inosine, W is engineered to provide less than natural bonding affinities to N in forming the [N:W] helix. When O is introduced (a natural complement of N), it competitively displaces W from [N:W] and forms [N:O]. DNA zippers have been used to create new DNA devices such as springs and tweezers and to create functionalized DNA origami structures. Currently, The basic principles and interactions of DNA zippers are not well understood. Here we will report the results on an investigation of several different DNA zipper constructs designed to aid in the creation of a mathematical prediction of the reaction rate for DNA zippers.

4:54PM X40.00011 Moving Beyond Watson-Crick Models of Coarse Grained DNA, KEVIN DORFMAN, MARGARET LINAK, University of Minnesota - Twin Cities, RICHARD TOURDOT, University of Pennsylvania — DNA structure possesses several levels of complexity, ranging from the sequence of bases (primary structure) to base pairing (secondary structure) to its three-dimensional shape (tertiary structure) and can produce a wide variety of conformations in addition to canonical double stranded DNA. By including non-Watson-Crick interactions in a coarse-grained model, we developed a system that not only can capture the traditional B-form double helix, but also can adopt a wide variety of other DNA conformations. In our experimentally parameterized, coarse-grained DNA model we are able to reproduce the microscopic features of double-stranded DNA without the need for explicit constraints and capture experimental melting curves for a number of short DNA hairpins. We demonstrate the utility of the model by simulating more complex tertiary structures such as the folding of the thrombin aptamer, which includes G-quartets, and strand invasion during triplex formation. Our results highlight the importance of non-canonical interactions in DNA coarse-grained models.

5:06PM X40.00012 Direct comparison of the theory of molecular solvation with molecular dynamics and experiment, TYLER LUCHKO, IN SUK JOUNG, GEORGE GIAMBASU, BioMaPS Institute, Rutgers University, DARRIN YORK, DAVID A. CASE, BioMaPS Institute and Chemistry & Chemical Biology, Rutgers University — The reference interaction site model (RISM) provides complete equilibrium sampling of bulk solvent and solvent around a solute of arbitrary shape and size at a fraction of the computational cost of explicit solvent molecular dynamics (MD). Though based on first principles, approximations must be made to achieve numerical solutions. In this study, we first compare RISM to MD and experimental results for bulk solutions of aqueous monovalent ions using the Joung-Cheatham parameters with SPC/E and TIP3P water subject to several approximate closures. Then, using the same parameters and approximations, we evaluate the distribution of water and ions around a 24 base pair strand of DNA, once again, comparing to MD results and experimental observables. In both cases RISM gives the correct qualitative behavior and, often, the correct quantitative behavior. However, this strongly depends on the closure relation used, with higher order, HNC-like closures usually giving better results.

5:18PM X40.00013 Information-based measure of chirality for biomolecules, KAROL BACA LOPEZ, Faculty of Sciences, Autonomous University of the State of Mexico, B. ROY FRIEDEN, College of Optical Sciences, The University of Arizona, ROBERTO LOPEZ, MIGUEL MAYORGA, Faculty of Sciences, Autonomous University of the State of Mexico, ENRIQUE HENANDEZ LEMUS, Computational Genomics Department, National Institute of Genomic Medicine — Homochirality is a common property of biomolecules such as DNA, RNA and proteins. In particular, D-ribose and D-deoxyribose enantiomers are found within living cells, while their mirror images, the L-enantiomers, are not known to occur naturally even though the configurations are highly stable. On the other hand, proteins are formed by L-amino acids, not by their mirror images. Why? In this work, we propose the use of Fisher Information (FI) I as a measure of chirality or dissimilarity between enantiomers. We performed Hartree-Fock (HF) and Density Functional Theory (DFT) calculations to obtain the electronic wave function $\Psi(x, y, z)$ and corresponding density function $\rho(x, y, z)$ for each of the natural and synthetic forms of oligoribonucleotides and alanine amino acid. The four wave functions $\Psi(x, y, z)$ are used to compute the FI evaluated from two different viewpoints: a coherent viewpoint, which includes the phase part of each $\Psi(x, y, z)$, and an incoherent or classical viewpoint, which ignores the phase. Our goal is to describe the extent to which the information content in chiral molecules (D- and L-) plays a role in selecting one or the other isomer in nature.

Thursday, March 1, 2012 2:30PM - 5:30PM –

Session X41 DBIO DPOLY DCOMP: Focus Session: Physics of Proteins II: Folding and Structure 156B

2:30PM X41.00001 Simulations of the folding/unfolding of biomolecules under solvent, and pressure perturbations¹, ANGEL GARCIA², Rensselaer Polytechnic Institute — Proteins exhibit marginal stability, determined by the balance of many competing effects. This stability can be perturbed by changes in temperature, pH, pressure, and other solvent conditions. Osmolytes are small organic compounds that modulate the conformational equilibrium, folded (F) and unfolded (U), of proteins as cosolvents. Protecting osmolytes such as trimethylamine N-oxide (TMAO), glycerol, and sugars that push the equilibrium toward F play a crucial role in maintaining the function of intracellular proteins in extreme environmental conditions. Urea is a denaturing osmolyte that shifts the equilibrium toward U. We will describe calculations of the reversible folding/unfolding equilibrium, under various solution conditions that include urea, high pressure, and different charge states of the Trp-cage miniprotein. The folding/unfolding equilibrium is studied using all-atom Replica exchange MD simulations. For urea, the simulations capture the experimentally observed linear dependence of unfolding free energy on urea concentration. We find that the denaturation is driven by favorable direct interaction of urea with the protein through both electrostatic and van der Waals forces and quantify their contribution. Though the magnitude of direct electrostatic interaction of urea is larger than van der Waals, the difference between unfolded and folded ensembles is dominated by the van der Waals interaction. We also find that hydrogen bonding of urea to the peptide backbone does not play a dominant role in denaturation. The unfolded ensemble sampled depends on urea concentration, with greater urea concentration favoring conformations with greater solvent exposure.

¹This work has been funded by NSF MCB.

²Department of Physics, Applied Physics and Astronomy, 110 8th St, Troy, NY 12180

3:06PM X41.00002 Accurate prediction of explicit solvent atom distribution in HIV-1 protease and F-ATP synthase by statistical theory of liquids, DANIEL SINDHIKARA, NORIO YOSHIDA, FUMIO HIRATA, Institute for Molecular Science — We have created a simple algorithm for automatically predicting the explicit solvent atom distribution of biomolecules. The explicit distribution is coerced from the 3D continuous distribution resulting from a 3D-RISM calculation. This procedure predicts optimal location of solvent molecules and ions given a rigid biomolecular structure. We show examples of predicting water molecules near KNI-275 bound form of HIV-1 protease and predicting both sodium ions and water molecules near the rotor ring of F-ATP synthase. Our results give excellent agreement with experimental structure with an average prediction error of 0.45-0.65 angstroms. Further, unlike experimental methods, this method does not suffer from the partial occupancy limit. Our method can be performed directly on 3D-RISM output within minutes. It is useful not only as a location predictor but also as a convenient method for generating initial structures for MD calculations.

3:18PM X41.00003 Analysis and Interpretation of Single Molecule Protein Unfolding Kinetics

, HERBERT LANNON, JASNA BRUJIC, New York University — The kinetics of protein unfolding under a stretching force has been extensively studied by atomic force microscopy (AFM) over the past decade [1]. Experimental artifacts at the single molecule level introduce uncertainties in the data analysis that have led to several competing physical models for the unfolding process. For example, the unfolding dynamics of the protein ubiquitin under constant force has been described by probability distributions as diverse as exponential [2,3], a sum of exponentials, log-normal [4], and more recently a function describing static disorder in the Arrhenius model [5]. A new method for data analysis is presented that utilizes maximum likelihood estimation (MLE) combined with other traditional statistical tests to unambiguously rank the consistency of these and other models with the experimental data. These techniques applied to the ubiquitin unfolding data shows that the probability of unfolding is best fit with a stretched exponential distribution, with important implications on the complexity of the mechanism of protein unfolding.

[1] Carrion-Vazquez, et. al. Springer Series in Biophys. 2006

[2] Fernandez et. al. Science 2004

[3] Brujic et. al. Nat. Phys 2006

[4] Garcia-Manyes et. al. Biophys. J. 2007

[5] Kuo et. al. PNAS 2010

3:30PM X41.00004 Investigating protein structure and folding with coherent two-dimensional infrared spectroscopy

, CARLOS BAIZ, CHUNTE PENG, MICHAEL REPPERT, KEVIN JONES, ANDREI TOKMAKOFF, Massachusetts Institute of Technology — We present a new technique to quantitatively determine the secondary structure composition of proteins in solution based on ultrafast two-dimensional infrared (2DIR) spectroscopy. The percentage of residues in alpha-helix, beta-sheet, and unstructured conformations is extracted from a principal component analysis of the measured amide-I 2DIR spectra. We benchmark the method against a library of commercially-available proteins by comparing the predicted structure compositions with the x-ray crystal structures. The new technique offers sub-picosecond time resolution, and can be used to study systems that are difficult to study with conventional methods such as gels, intrinsically disordered peptides, fibers, and aggregates. We use the technique to investigate the structural changes and timescales associated with folding and denaturing of small proteins via equilibrium and transient temperature-jump 2DIR spectroscopy.

3:42PM X41.00005 Protein Folding and Functional Dynamics

, FENG GAI, University of Pennsylvania — Proteins are intrinsically flexible and dynamic objects. Thus, protein dynamics are intimately coupled to their function. In many cases, however, it is difficult to directly probe protein conformational dynamics occurring on either very fast or very slow timescales with high spatial resolution. In this talk, several examples will be discussed to show how ensemble and single-molecule spectroscopic methods can be used to follow protein folding events taking place on the nanosecond timescale and slow conformational dynamics associated with function.

4:18PM X41.00006 Folding a protein with equal probability of being helix or hairpin¹

, CHUNG-YU MOU, CHUN-YU LIN, National Tsing Hua University, Taiwan, ROC, NAN-YOW CHEN, National Center for High-Performance Computing, Taiwan, ROC — We explore the possibility for the native state of a protein being inherently a multi-conformation state in an ab initio coarse-grained model. Based on the Wang-Landau algorithm, the complete free energy landscape for the designed sequence 2D4X: INYWLAHAKAGYIVHWT A is constructed. It is shown that 2DX4 possesses two nearly degenerate native states: one has a helix structure, while the other has a hairpin structure and their energy difference is less than 2% of that of local minimums. Furthermore, the hydrogen-bond and dipole-dipole interactions are found to be two major competing mechanisms in transforming one conformation into the other. Our results indicate that degenerate native states are stabilized by subtle balance between different interactions in proteins; furthermore, degeneracy only happens for small proteins of sizes being around 18 amino acids or 40-50 amino acids. These results provide important clues to the study of native structures of proteins.

¹We acknowledge support of National Science Council of Taiwan.

4:30PM X41.00007 Generic transition hierarchies of lattice HP protein adsorption: A Wang-Landau study¹

, YING WAI LI, D.P. LANDAU, Center for Simulational Physics, University of Georgia, T. WÜST, Swiss Federal Research Institute — We have applied Wang-Landau sampling with appropriate trial moves² to investigate the thermodynamics and structural properties of the HP lattice protein model³ interacting with an attractive substrate. The conformational “phase transitions” of several benchmark HP sequences have been identified by a comprehensive canonical analysis of the specific heat and structural observables, e. g. radius of gyration and thermal derivatives of number of surface contacts. Three major “transitions”: adsorption, hydrophobic core formation, and “flattening” of adsorbed structures, are observed. Depending on the surface attractive strength relative to the intra-protein attraction among the H monomers, these processes take place in a different order upon cooling. We identify a small number of generic categories that are sufficient to classify the folding hierarchies for different HP chains consisting of assorted sequences and chain lengths, regardless of the monomer type that the surface attracts. We thus believe that this classification scheme is generally applicable to lattice protein adsorption problems.

¹Research supported by NSF.

²T. Wüst and D. P. Landau, Phy. Rev. Lett. **102**, 178101 (2009).

³K. A. Dill, Biochemistry **24**, 1501 (1985).

4:42PM X41.00008 Elucidating Structure and Catalytic Cycles of Anti- or Ferro-magnetic Iron Enzymes from Spin Density Functional Theory¹

, JORGE H. RODRIGUEZ, Department of Physics, Purdue University — Nature uses metal-containing enzymes to catalyze important biochemical reactions. Some enzymes, such as methane monooxygenase hydroxylase (MMOH), contain (anti)ferromagnetic binuclear iron centers that interact with dioxygen and/or other substrates to facilitate biochemical functions. We have studied the electronic and magnetic structures of several enzyme binuclear iron centers and predicted their spectroscopic properties. We have used spin density functional theory (SDFT) to predict ⁵⁷Fe Mössbauer and other spectral parameters of MMOH and structurally related iron-containing enzymes. Upon dioxygen binding, the diiron center of MMOH undergoes a ferromagnetic to antiferromagnetic transition which may play an important role in its catalytic activity. In addition, based on our ability to predict spectroscopic data, we have been able to predict the structure of a key reaction intermediate in the MMOH catalytic cycle for which there is no X-ray structure.

¹Funded, in part, by NSF CAREER award CHE-0349189

4:54PM X41.00009 AWSEM-MD: Coarse-grained Protein Structure Prediction Using Physical Potentials and Bioinformatically Based Local Structure Biasing, ARAM DAVTYAN, University of Maryland at College Park, WEIHUA ZHENG, NICK SCHAFER, University of California at San Diego, CECILIA CLEMENTI, PETER WOLYNES, Rice University, GAREGIN PAPOIAN, University of Maryland at College Park, PAPOIAN GROUP TEAM, WOLYNES GROUP COLLABORATION — The Associative memory, Water mediated, Structure and Energy Model (AWSEM) is a coarse-grained protein model. When combined with a sequence alignment method, AWSEM can be used to perform de novo protein structure prediction. Herein we present structure prediction results for a particular choice of sequence alignment method based on short residue sequences called fragments. We demonstrate the model's structure prediction capabilities for three variants on a standard sequence alignment protocol, all of which assume that the structure of the target sequence is not known. We show that the inclusion of structures from homologous sequences in the fragment memory search improves structure prediction only marginally. However, when the fragment search is restricted to only homologous sequences, AWSEM can perform high-resolution structure prediction.

5:06PM X41.00010 Combining first principles and replica exchange for the structure of two large peptides: Ac-Ala₁₉-LysH⁺ vs. Ac-LysH⁺-Ala₁₉¹, FRANZISKA SCHUBERT, MARIANA ROSSI, CARSTEN BALDAUF, VOLKER BLUM, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, D-14195 Berlin — Predicting the structure of peptides requires a high accuracy for “weak” interactions. We here focus on the predominant structure types of two alanine-based peptides *in vacuo* from first principles and in comparison to experimental IR spectroscopy¹: Ac-Ala₁₉-LysH⁺, which is expected to be α -helical [1,2], and Ac-LysH⁺-Ala₁₉, where globular monomers, helical dimers, and helices with non-standard protonation sites are expected [2]. Despite supposedly very different conformers, Ac-LysH⁺-Ala₁₉ and Ac-Ala₁₉-LysH⁺ yield very similar experimental IR spectra in the ≈ 1000 -2000 cm⁻¹ wavenumber range. We utilize a two-stage structure search approach: we begin by a force-field based replica exchange molecular dynamics (REMD) scan followed by further REMD scans based on density functional theory with the van der Waals corrected [3] PBE functional. We suggest plausible candidates for all likely structure prototypes. Helix-turn-helix motifs emerge as the most likely candidates and explain a subtle peak shift in experiment. [1] M. Rossi *et al.*, JPCL **1**, 3465 (2010); [2] M. Jarrold, PCCP **9**, 1659 (2007); [3] A. Tkatchenko, M. Scheffler, PRL **102**, 073005 (2009).

¹IRMPD experiments: G. von Helden, P. Kupser, K. Pagel, F. Filsinger, G. Meijer, Department of Molecular Physics, Fritz-Haber-Institut

5:18PM X41.00011 Enhanced Wang Landau Sampling of Adsorbed Protein Conformations, MITHUN RADHAKRISHNA, Columbia University, SUMIT SHARMA, Princeton University, SANAT K. KUMAR, Columbia University — Using computer simulations to model the folding of proteins into their native states is computationally expensive due to the extraordinarily low degeneracy of the ground state. In this paper, we develop an efficient way to sample these folded conformations using Wang Landau sampling coupled with the configurational bias method (which uses an unphysical “temperature” which is between the collapse and folding transition of the protein). This method speeds-up the folding process by roughly an order of magnitude over existing algorithms. We apply this method to study the adsorption of HP protein fragments on a hydrophobic surface, a model which is a close analog of one presented recently by Shea and coworkers. We are able to readily capture the fact that these fragments, which are unstructured in the bulk, acquire secondary structure upon adsorption onto a strong hydrophobic surface. Apparently, the presence of a hydrophobic surface allows these random coil fragments to fold by providing hydrophobic contacts that were lost in protein fragmentation.

Thursday, March 1, 2012 2:30PM - 5:30PM –
Session X42 DBIO DPOLY: Focus Session: The Physics of Genome Folding II: Chromosomes and Nucleosomes 156C

2:30PM X42.00001 Tensegrity, DONALD INGBER, Harvard School of Engineering and Applied Sciences and Harvard Med Sch — No abstract available.

3:06PM X42.00002 Polymer-nematic textures in spherical confinement: a coarse-grained model of DNA packing¹, GREGORY GRASON, Dept. of Polymer Science & Engineering, University of Massachusetts Amherst, HOMIN SHIN, Dept. of Materials Science & Engineering, University of Illinois at Urbana-Champaign — Inspired to understand the complex spectrum of space-filling organizations the dsDNA genome within the capsid of bacterial viruses, we study a minimal, coarse-grained model of single chains densely-packed into a finite spherical volume. We build the three basic elements of the model—i) the absence of chain ends ii) the tendency of parallel-strand alignment and iii) a preference of uniform areal density of chain segments—into a polymer nematic theory for confined chains. Given the geometric constraints of the problem, we show that axially symmetric packings fall into one of three topologies: the coaxial spool; the simple solenoid; and the twisted-solenoid. Among these, only the twisted-solenoid fills the volume without the presence of line-like disclinations, or voids, and are therefore generically preferred in the incompressible limit. An analysis of the thermodynamic behavior of this simple model reveals a rich behavior, a generic sequence of phases from the empty state for small container sizes, to the coaxial spool configuration at intermediate sizes, ultimately giving way, via a second-order, symmetry-breaking transition, to the twisted-solenoid structure above a critical sphere size, which we estimate to be within the range of bacteriophage capsid dimensions.

¹Supported by NSF CAREER Award DMR 09-55760

3:18PM X42.00003 Conformational Fluctuations of Chromosomal DNA in *E. coli*, CLARISSA FREEMAN, JENS-CHRISTIAN MEINERS, University of Michigan — We measured the conformational fluctuations of the bacterial chromosome in *E. coli* *in vivo* using fluorescence correlation spectroscopy (FCS). The chromosomal DNA was randomly decorated with a cell-permeable intercalating dye. Conformational fluctuations of the DNA move the fluorophores stochastically into the diffraction-limited excitation volume of a focused laser beam. The time correlation function of the fluorescence intensity reflects the underlying dynamics of the DNA on length scales down to ~ 200 nm. A comparison between live cells and dead yet structurally intact cells shows identical fluctuation spectra for short time scales, yet substantial differences for frequencies below 100 Hz. Live cells show much stronger fluctuations in this regime. This observation points to the crucial importance of active molecular motor action, as opposed to passive thermal noise, in driving larger conformational fluctuations in the chromosomal DNA, in particular on length scales exceeding ~ 500 nm.

3:30PM X42.00004 Spatial organization and dynamics of interphase yeast chromosomes¹ , BARIS AVSAROGLU, Dept of Physics, Brandeis Uni, Waltham MA, SUSANNAH GORDON-MESSER, Dept of Biology, Brandeis Uni, Waltham MA, MIRIAM FRITSCHKE, Inst fur Theoretische Physik, Heidelberg University, Heidelberg Germany, JUNGOH HAM, Dept of Biology, Brandeis Uni, Waltham MA, DIETER W. HEERMANN , Inst fur Theoretische Physik, Heidelberg University, Heidelberg Germany, JAMES E. HABER , Dept of Biology and Rosenstiel Center, Brandeis Uni, Waltham MA, JANE KONDEV, Dept of Physics, Brandeis Uni, Waltham MA — Understanding how the genome is spatially organized is an important problem in cell biology, due to its key roles in gene expression and DNA recombination. Here we report on a combined experimental and theoretical study of the organization and dynamics of yeast chromosome III which has a functional role in the yeast life cycle, in particular, it is responsible for mating type switching. By imaging two fluorescent markers, one at the spindle pole body (SPB) and the other proximal to the HML locus that is involved in DNA recombination during mating type switching, we measured the cell to cell distribution of distances and the mean square displacement between the markers as a function of time. We compared our experimental results with a random-walk polymer model that takes into account tethering and confinement of chromosomes in the nucleus, and found that the model recapitulates the observed spatial and temporal organization of chromosome III in yeast in quantitative detail. The polymer model makes specific predictions for mating-type switching in yeast, and suggests new experiments to test them.

¹This work was supported by NSF DMR-0706458 and MRSEC 0820492 at Brandeis University.

3:42PM X42.00005 Reverse-engineering Chromatin Folding via The Gaussian Polymer Model , MANJUL APRATIM, Physics and Astronomy, Rutgers, The State University of New Jersey, SWAGATAM MUKHOPADHYAY, Cold Spring Harbor Labs, ANIRVAN SENGUPTA, Physics and Astronomy, and BioMaPS Institute, Rutgers, The State University of New Jersey — Recent technological advancements in techniques exploring chromatin conformation, such as 3C and its derivatives, provide us with information about contact frequency between chromatin segments. There is an urgent need for systematic methods of reconstructing folding patterns of the chromatin from such data. Dekker et al have previously summarized this experimental data in the form of a so-called 'spatially averaged' conformation around which fluctuations occur. This would be accurate for regions where the chromatin is mostly frozen around one structure, but rather misleading for more dynamic euchromatin. To address the ill-posed problem of reconstruction of probability distribution from pairwise contact data, we propose a minimum relative entropy approach, which reduces to finding an interacting polymer model that reproduces the contact strengths, and allows for both very dynamic as well as frozen structures depending upon the indicated degree of interaction. While comparing contact frequencies computed from this model to observed data, we introduce the minimal number of interactions required as determined by criteria controlling model complexity. This technique allows us to reproduce known interactions for several biologically important regions like the beta-globin locus.

3:54PM X42.00006 Electrohydrodynamics of DNA in confinement , JONATHAN K. WHITMER, Department of Chemical and Biological Engineering, University of Wisconsin–Madison, JUAN P. HERNANDEZ-ORTIZ, Dept. of Materials, Universidad Nacional de Columbia, JUAN J. DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin–Madison — New methods of DNA sequencing aim to exploit the direct reading of individual DNA molecules. Such methods require one be able to elongate DNA molecules so that individual base-pairs may be accessed. In turn, this requires a detailed understanding of the mechanical and thermodynamic behavior of DNA, so that external manipulation and confinement successfully stretch the molecule. We aim to study the interplay between electrostatic and hydrodynamic interactions on the conformations of coarse-grained DNA through use of computer simulations with the general geometry Ewald-like method (GGEM), both in bulk and under geometric confinement.

4:06PM X42.00007 Susceptibilities to DNA Structural Transitions within Eukaryotic Genomes , DINA ZHABINSKAYA, CRAIG BENHAM, SALLY MADDEN, University of California at Davis — We analyze the competitive transitions to alternate secondary DNA structures in a negatively supercoiled DNA molecule of kilobase length and specified base sequence. We use statistical mechanics to calculate the competition among all regions within the sequence that are susceptible to transitions to alternate structures. We use an approximate numerical method since the calculation of an exact partition function is numerically cumbersome for DNA molecules of lengths longer than hundreds of base pairs. This method yields accurate results in reasonable computational times. We implement algorithms that calculate the competition between transitions to denatured states and to Z-form DNA. We analyze these transitions near the transcription start sites (TSS) of a set of eukaryotic genes. We find an enhancement of Z-forming regions upstream of the TSS and a depletion of denatured regions around the start sites. We confirm that these findings are statistically significant by comparing our results to a set of randomized genes with preserved base composition at each position relative to the gene start sites. When we study the correlation of these transitions in orthologous mouse and human genes we find a clear evolutionary conservation of both types of transitions around the TSS.

4:18PM X42.00008 Mechanics of DNA Sticky End Joints , EHSAN BAN, CATALIN PICU, Rensselaer Polytechnic Institute — Cohesive DNA sticky ends along with synthesis of stable branched DNA molecules have enabled self assembly of versatile new DNA structures including DNA crystals. Sticky end joints are formed by pairing of complimentary unpaired bases at the end of two DNA molecules. In this work mechanics of the DNA sticky end joints is investigated by using molecular dynamics simulations. Effects of base sequence, joint length, and salt concentration on the mechanical behavior of the joints is studied. The results have implications in understanding the mechanics of DNA crystals and other structures containing sticky end joints.

4:30PM X42.00009 Statistical physics of nucleosome positioning and chromatin structure¹ , ALEXANDRE MOROZOV, Department of Physics and Astronomy, Rutgers University — Genomic DNA is packaged into chromatin in eukaryotic cells. The fundamental building block of chromatin is the nucleosome, a 147 bp-long DNA molecule wrapped around the surface of a histone octamer. Arrays of nucleosomes are positioned along DNA according to their sequence preferences and folded into higher-order chromatin fibers whose structure is poorly understood. We have developed a framework for predicting sequence-specific histone-DNA interactions and the effective two-body potential responsible for ordering nucleosomes into regular higher-order structures. Our approach is based on the analogy between nucleosomal arrays and a one-dimensional fluid of finite-size particles with nearest-neighbor interactions. We derive simple rules which allow us to predict nucleosome occupancy solely from the dinucleotide content of the underlying DNA sequences. Dinucleotide content determines the degree of stiffness of the DNA polymer and thus defines its ability to bend into the nucleosomal superhelix. As expected, the nucleosome positioning rules are universal for chromatin assembled in vitro on genomic DNA from baker's yeast and from the nematode worm *C.elegans*, where nucleosome placement follows intrinsic sequence preferences and steric exclusion. However, the positioning rules inferred from in vivo *C.elegans* chromatin are affected by global nucleosome depletion from chromosome arms relative to central domains, likely caused by the attachment of the chromosome arms to the nuclear membrane. Furthermore, intrinsic nucleosome positioning rules are overwritten in transcribed regions, indicating that chromatin organization is actively managed by the transcriptional and splicing machinery.

¹AVM acknowledges support from the NIH grant HG00470 and from an Alfred P. Sloan Research Fellowship

5:06PM X42.00010 Interrogating Nucleosome Positioning Through Coarse-Grain Molecular Simulation¹, GORDON S. FREEMAN, DANIEL M. HINCKLEY, University of Wisconsin-Madison, VANESSA ORTIZ, Columbia University, JUAN J. DE PABLO, University of Wisconsin-Madison — Nucleosome positioning plays a crucial role in biology. As the fundamental unit in chromosome structure, the nucleosome core particle (NCP) binds to approximately 147 DNA base pairs. The location of bound NCPs in the genome, therefore, affects gene expression. The specific positioning of NCPs has been experimentally probed and competing viewpoints have been presented in the literature. Models for nucleosome positioning based on sequence-dependent flexibility (a genomic “code” for nucleosome positioning) have been demonstrated to explain available experimental data. However, so do statistical models with no built-in sequence preference; the driving force for NCP positioning therefore remains an open question. We use a coarse-grain model for the NCP in combination with advanced sampling techniques to probe the sequence preference of NCPs. We present a method for determining the relative affinity of two DNA sequences for the NCP and use this method to compare high- and low-affinity sequences. We discuss several coarse-grain protein models with varying level of detail to examine the impact of model resolution on the agreement of our results with experimental evidence. We also investigate the dynamics of the NCP-DNA complex and their dependence on system characteristics.

¹This work was supported by the National Science Foundation through the University of Wisconsin-Madison Nanoscale Science and Engineering Center, DMR-0832760.

5:18PM X42.00011 Dynamics of Histone Tails within Chromatin¹, MORGAN BERNIER, JUSTIN NORTH, MICHAEL PAGE, The Ohio State University Physics Department, CHRISTOPHER JARONIEC, The Ohio State University Chemistry Department, CHRISTOPHER HAMMEL, MICHAEL POIRIER, The Ohio State University Physics Department, CENTER FOR EMERGENT MATERIALS PROTO-INTERDISCIPLINARY RESEARCH GROUP COLLABORATION — Genetic information in humans is encoded within DNA molecules that is wrapped around histone octamer proteins and compacted into a highly conserved structural polymer, chromatin. The physical and material properties of chromatin appear to influence gene expression by altering the accessibility of proteins to the DNA. The tails of the histones are flexible domains that are thought to play a role in regulating DNA accessibility and compaction; however the molecular mechanisms for these phenomena are not understood. I will present CW-EPR studies on site directed spin labeled nucleosomes that probe the structure and dynamics of these histone tails within nucleosomes.

¹Center for Emergent Materials, a National Science Foundation Materials Research Science and Engineering Center

Thursday, March 1, 2012 2:30PM - 5:30PM – Session X43 DBIO DFD: Invited Session: Bacterial Swimming and Chemotaxis 157AB

2:30PM X43.00001 Bacterial Swimming and Accumulation at the Fluid Boundaries, JAY TANG, Physics Department, Brown University — Micro-organisms often reside and thrive at the fluid boundaries. The tendency of accumulation is particularly strong for flagellated bacteria such as *Escherichia coli*, *Vibrio alginolyticus*, and *Caulobacter crescentus*. We measured the distribution of a forward swimming strain of *Caulobacter crescentus* near a solid surface using a three-dimensional tracking technique based on darkfield microscopy and found that the swimming bacteria accumulate heavily within micrometers from the surface, even though individual swimmers are not trapped long enough to display circular trajectories. We attributed this accumulation to frequent collisions of the swimming cells with the surface, causing them to align parallel to the surface as they continually move forward. The extent of accumulation at the steady state is accounted for by balancing alignment caused by these collisions with the rotational Brownian motion of the micrometer-sized bacteria. We performed simulations based on this model, which reproduces the measured results. Additional simulations demonstrate the dependence of accumulation on swimming speed and cell size, showing that longer and faster cells accumulate more near a surface than shorter and slower ones do. Our ongoing experimental effort also includes observation of similar phenomena at the interfaces of either water-oil or water-air, noting even stronger trapping of the swimming bacteria than near a solid surface. These studies reveal a rich range of fluid physics for further analysis.

3:06PM X43.00002 Bacterial Motility Patterns and Their Chemotaxis Behaviors, XIAOLUN WU, University of Pittsburgh — No abstract available.

3:42PM X43.00003 Periplasmal Physics: The Rotational Dynamics of Spirochetal Flagella, GREG HUBER, University of Connecticut Health Center, and University of Connecticut Storrs — Spirochetes are distinguished by the location of their flagella, which reside within the periplasm: the tiny space between the bacterial cell wall and the outer membrane. In *Borrelia burgdorferi* (the causative agent of Lyme Disease), rotation of the flagella leads to cellular undulations that drive swimming. Exactly how these shape changes arise due to the forces and torques acting between the flagella and the cell body is unknown. By applying low-Reynolds number hydrodynamic theory to the motion of an elastic flagellum rotating in the periplasm, we show that the flagella are most likely separated from the bacterial cell wall by a lubricating layer of fluid. We obtain analytical solutions for the force and torque on the rotating flagellum through lubrication analysis, as well as through scaling analysis, and find results are in close agreement numerical simulations. (Joint work with J. Yang and C.W. Wolgemuth.)

4:18PM X43.00004 Microfluidics for bacterial chemotaxis, MINGMING WU, Biological and Environmental Engineering Department, Cornell University, Ithaca, NY 14853 — The emerging microfluidic technology opens up new opportunities for bacterial chemotaxis studies. In this talk, I will present our efforts in correlating molecular level events with cellular phenotypes in bacterial chemotaxis using microfabricated device. I will present results of bacterial chemotaxis in both single and dual chemical gradients. In single gradient experiments, we demonstrated that bacteria sense the chemical concentration at a logarithmic scale, similar to sensory system in higher organism. In dual gradient experiments, we showed that the number ratio of the two different types of receptor plays a critical role in bacteria's chemotactic decision making process. Experimental results based on single cell analysis will be presented. This work is supported by the National Science Foundation and the Cornell Nanobiotechnology Center.

4:54PM X43.00005 Directional swimming in bacteria: active and passive gradient responses, ROMAN STOCKER¹, MIT — The ability to swim directionally is paramount for bacteria, in their quest for nutrients and favorable microhabitats. This ability depends on both active and passive responses to gradients. Here we bring an example from each case, based on novel microfluidic experiments that quantify the swimming behavior of bacteria. First, we describe their active response to oxygen gradients - or aerotaxis - and show the unexpected consequences of competing oxygen gradients with nutrient gradients. Then, we present the first observations of directional swimming by bacteria in response to fluid velocity gradients - or rheotaxis. Combining experiments with mathematical modeling we demonstrate that, unlike in larger organisms such as fish, rheotaxis in bacteria is passive, resulting from a previously undetected torque that originates from the chirality of the bacterial flagellum.

¹Co-authors: Kwangmin Son, Yutaka Yawata, Marcos, Henry Fu, and Thomas Powers

Thursday, March 1, 2012 2:30PM - 4:54PM –
Session X44 DPOLY: Focus Session: Directed Assembly of Hybrid Materials - Nanoparticles in Micelles 157C

2:30PM X44.00001 Multigeometry nanoparticles and higher-order assemblies from block copolymer blends via kinetic control and chemical modification, JIAHUA ZHU, Department of Materials Science and Engineering, University of Delaware, SHIYI ZHANG, KAREN WOOLEY, Department of Chemistry, Texas A&M University, DARRIN POCHAN, Department of Materials Science and Engineering, University of Delaware — Multigeometry micellar structures, due to segregation of unlike hydrophobic domains trapped within the same micelle core, have been produced via self-assembly of block copolymer mixtures in tetrahydrofuran/water solution. The mixture is composed of two block copolymers with distinctive hydrophobic blocks but the same poly(acrylic acid) (PAA) hydrophilic block. By taking advantage of the complexation in the hydrophilic corona between the acid side chains of the PAA block and added organoamine molecules, unlike hydrophobic blocks can be trapped in the same micelle core. Locally, the unlike hydrophobic blocks can segregate into compartments and even express different interfacial curvatures, or geometries, within the same nanoparticle. Through controlled kinetic pathways, block copolymer design and mixing ratios, both micelle compartment size and shape can be controlled to generate sphere-sphere, sphere-cylinder, cylinder-cylinder, cylinder-bilayer, and bilayer-bilayer blended multigeometry nanoparticles. Furthermore, higher order assembly behavior of the micelles has been investigated by taking advantage of chemical modification on the hydrophilic PAA shells. New mixtures using functionalized-PAA-containing block copolymers produce nanoparticles with a compartmentalized surface. These patchy surfaces can be used as templates for asymmetric hybrid nanoparticles, but also as building blocks for hierarchical assembly of the nanoparticles to produce one-dimensional arrays or three dimensional networks.

2:42PM X44.00002 Polymer nano-particle hybrid micelles: Encapsulation of POSS into semi-fluorinated polymer micelles, DILRU RATNAWEERA, DVORA PERAHIA, Clemson University, SCOTT IACONO, Patrick Air Force Base, FL, JOSEPH MABRY, Edwards Air Force Base, CA, DENNIS SMITH, University of Texas, Dallas — Self-assembly of block copolymers in selective solvents was used to form a nanoparticle (NP)/polymer hybrid micelles. These micelles can be used as a cargo vehicle for other substances such as drug delivery, and as building blocks for polymer-nanocomposites with controlled NP distribution. Association of NPs into specific blocks of the copolymer depends on the compatibility between the NPs and the block as well as their preference to the solvent that micellization takes place. The current work introduces a small angle neutron scattering study of association of Polyhedral Oligomeric Silsesquioxane (POSS) NPs into micelles of a highly segregating random copolymer, Biphenyl Perfluorocyclobutane (BPh-PFCB), in toluene, which is a good solvent for BPh. Incompatibility between the blocks drives copolymer into micelles with PFCB in the core and BPh in swollen corona. Modification of NPs with polymer chains drives POSS cages into the micelle core and prevents the micelle dissociation at higher temperatures.

2:54PM X44.00003 Efficient Encapsulation of Gold Nanorods into Block Copolymer Micelles, DAE HWAN KIM, YOU-YEON WON, Purdue University — Gold nanorods (GNRs) have the potential to be used as an imaging and/or hyperthermia agent for cancer theragnosis. Clinical applications of as-synthesized GNRs (i.e., CTAB-coated CNRs) are currently limited by their cytotoxicity and insufficient colloidal stability. With an aim to address these problems, we developed a self-assembly processing technique for encapsulation of GNRs in block copolymer (BCP) micelles. This technique uses simple steps of solvent exchange processes designed based on the known principles of block copolymer self-assembly. It will be demonstrated that BCP-encapsulated GNRs are stable against aggregation under physiological conditions and non-toxic to cells.

3:06PM X44.00004 Kinetic pathways to organized polymer/nanoparticle assemblies, RYAN HAYWARD, University of Massachusetts Amherst — Processes that allow for controlled access to kinetically trapped non-equilibrium states have the potential to significantly expand the range of structures and properties that may be achieved by self-assembly. We will describe several recent examples from our group wherein new types of polymer/nanoparticle assemblies are enabled by designed processing pathways. In the first case, we study the formation of amphiphilic polymer micelles through hydrodynamic instabilities of solvent/water interfaces induced during emulsion processing. We show that this route allows for efficient co-encapsulation of multiple types of hydrophobic nanoparticles within the micelle cores. Second, we consider the influence of nanoparticles on spinodal decomposition of a polymer blend and find that the inclusion of aggregating particles provides a route to kinetically stabilize co-continuous structures through particle gelation in one of the polymer phases. Finally, we show how the structures of hybrid nanoparticle/conjugated polymer nanowires can be tuned using solution-state crystallization.

3:42PM X44.00005 A coarse-grained molecular dynamics approach to shear-directed assembly of nanoparticle arrays in amphiphilic block copolymer solutions, BRYAN ROLFE, Cornell University, JAEHUN CHUN, Pacific Northwest National Laboratory, YONG JOO, Cornell University, ENERGY AND ENVIRONMENT DIRECTORY PACIFIC NORTHWEST NATIONAL LABORATORY COLLABORATION — Experiments by Pozzo and Walker (2007) demonstrated shear ordering of binary nanoparticle block copolymer micelle crystals and its potential in the development of new nanostructured materials. Specifically, they have shown that nanoparticles occupying interstitial sites within the micelle crystal affect a low-shear, long-range order and that the shear type and rate are important to the crystal structure. However, the connection between macroscopic variables and resulting crystal structure is yet to be understood. We present results which elucidate the underlying mechanisms governing shear-directed assembly of these binary nanocrystals. Our approach employs a coarse-grained molecular dynamics model (CGMD) that includes the hydrodynamics of the solvent and preserves dynamic effects by making no assumptions regarding the micelle structure. In fact, micelle self-assembly of the amphiphilic block copolymers occurs in-situ with the nanoparticles along with the shear ordering of the binary crystal. Tunability of the crystal structure is determined by varying shear rates/types, nanoparticle size/concentration, and block copolymer chemistry as simulation parameters. The simulation predicted results of shear-directed assembly of nanoparticles will be compared to the experimental results.

3:54PM X44.00006 Nanoparticle Polymer Suspensions: Structure and Dynamics, SAMANVAYA SRIVASTAVA, LYNDEN ARCHER, Cornell University — We present structure and rheology measurements for model nanoparticle suspensions, which comprise of silica nanoparticles, densely grafted with small polyethylene glycol (PEG) chains and suspended in PEG oligomers. Structure characterization, using electron microscopy and X-ray scattering, reveals well-dispersed nanoparticles leading to stable suspensions across a range of particle volume fractions. At the same time, X-ray photon correlation spectroscopy studies reveal arrested dynamics and extremely small nanoparticle diffusivities in the high volume fraction suspensions, consistent with the expectations for a soft glass. The liquid-soft glassy solid transition is found to occur at strikingly low core volume fractions and the glassy suspensions are found to exhibit a range of unique features including strong shear thinning, presence of a zero shear Newtonian plateau, strain accelerated relaxation and prominent stress overshoots in flow startup. Comparisons of our experimental findings with the SGR model are provided and on this basis, we propose our suspensions as model systems for understanding the jamming transition and other properties of soft glasses. Further, we elucidate the form of particle interactions and compare them with models for spherical polymer brushes.

4:06PM X44.00007 Pristine graphene dispersions and solution-cast composites, SRIYA DAS, FAHMIDA IRIN, AHMED WAJID, ABEL CORTINAS, MICAH GREEN, Department of Chemical Engineering, Texas Tech University — Graphene holds potential as strong, conductive fillers in polymer nanocomposites; however, difficulties in dispersion quality and interfacial strength between filler and matrix have been a persistent problem for graphene-based nanocomposites, particularly for pristine, unfunctionalized graphene. We utilize a triphenylene based molecule (C10) to stabilize pristine graphene in water with a high graphene/stabilizer ratio. C10 molecules pi-pi stack with the graphene surface and prevent reaggregation. This dispersion can be reversibly destabilized based on pH and is stable against heat and lyophilization. Solution cast poly (vinyl alcohol) (PVA) composites prepared from these dispersions have enhanced mechanical and electrical properties (percolation threshold: 0.26 vol % graphene). Also, for the first time, pristine graphene/PVA dispersions are electrospun to form graphene/polymer composite nanofibers.

4:18PM X44.00008 Simulation of viscoelastic suspensions using regularized singularities, RONALD PHILLIPS, RYOTA AOKI, Chemical Engineering and Materials Science, UC Davis — Particles interacting through viscoelastic fluids exhibit behavior that differs qualitatively from corresponding systems with Newtonian suspending fluids. Depending on the type of fluid involved, the polymer contribution to the stress can induce clustering or particle chaining, and impede efforts to form a homogeneous suspension. We are using regularized singularities in conjunction with the finite volume method to calculate velocity fields, stress fields, and particle displacements in viscoelastic suspensions. These singularities consist of Stokelets and stresslets, or regions of enhanced body forces and stresses, and provide a simple model of suspensions of weakly deformable, non-neutrally buoyant particles. Simulations of hundreds of two-dimensional particles in multimode viscoelastic fluids show behavior similar to what is seen experimentally, and provide insight into the physical causes of particle aggregation in complex fluids.

4:30PM X44.00009 Polymer mediated solution self-assembly of nanorods, MIGUEL A. MODESTINO, RACHEL A. SEGALMAN, University of California, Berkeley — Control over the self-assembly of nanorods in polymer composites enables the design of hybrid materials in which the anisotropic properties of the nanocrystals can be harnessed efficiently. Here, we demonstrate that a delicate balance between entropic and enthalpic interactions controls the self-assembly behavior of nanorods in solutions and can lead to the formation of ordered nanorod arrays. Small angle X-ray scattering techniques were used to elucidate the phase behavior of CdSe nanorods in polymer solutions and to identify the concentration space that allows for the formation of nanorod superlattices. Furthermore, this work demonstrates that enthalpic interactions have strong effects on the nanorod self-assembly, and that the presence of reversible thermal transitions can allow for the growth of large nanorod arrays. The solution self-assembly behavior discussed in this study allows for the fabrication of solution processable composite thin films with vertically aligned nanorods over large areas.

4:42PM X44.00010 Quantifying the Thermodynamic Interactions in Carborane Nanoparticle Solutions, MARY MUTZ, University of Tennessee, ERIC EASTWOOD, Honeywell Kansas City Plant, MARK DADMUN, University of Tennessee and Oak Ridge National Laboratory — The dissolution of nanoparticles, particularly those containing boron, is an important area of interest for polymer nanocomposite formation and material development (1-2). In this work, the solubility of four boron cage molecules are quantified in toluene, THF, and methyl ethyl ketone with static light scattering, refractometry, UV-Vis spectroscopy, and physical observations. UV-Vis spectroscopy provides a method to determine the concentration and solubility limits of the solutions tested. Using light scattering, the second virial coefficient, A_2 , was determined and used to calculate χ , the solute-solvent interaction parameter. The Hildebrand solubility parameter, δ , was then extracted from this data using the Hildebrand-Scatchard solution theory (3-4). A list of potential good solvents based on the extracted δ value is provided for each nanoparticle. Of the systems tested, 1,3-di-o-carboranylpropane was shown to be a thermodynamically stable in toluene, with a χ less than 0.5, a solubility limit of 2.47 mg/mL, and all solutions remaining clear with no visible particle settling.

Thursday, March 1, 2012 2:30PM - 5:42PM –

Session X45 DPOLY: Focus Session: Soft Matter Physics of Drops, Bubbles, Foams, and Emulsions - Droplet spreading, colliding, wetting 159

2:30PM X45.00001 Ultrafast interference of splashing dynamics: where is the air?, MICHELLE DRISCOLL, University of Chicago — A drop impacting a solid surface with sufficient velocity will splash and emit many small droplets. While liquid and substrate properties obviously are important for determining the splashing threshold, it has also been shown that the surrounding gas is a crucial control parameter [1]. The mechanism underlying how the surrounding gas affects splashing remains unknown. One suggestion [2,3] has been that upon impact the liquid spreads outwards over a thin layer of gas that has been trapped beneath it during impact. In a sufficiently viscous liquid, splashing occurs at the edge of the drop several tenths of a millisecond after impact [4]. This large separation between impact and splashing, in both time and space, creates an ideal system in which to test whether the initial air pocket remains to influence splashing dynamics. We develop high-speed interference imaging to measure the air beneath all regions of a spreading viscous drop [5]. Although an initial air bubble is created on impact, no significant air layer persists up to the time a splash is created. This suggests that splashing in our accessible range of viscosities is not caused by the presence of a layer of air beneath the liquid, but rather it is initiated at the edge of the drop as it encroaches into the surrounding gas.

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- [5] M. M. Driscoll and S. R. Nagel, Phys. Rev. Lett. **107**, 154502 (2011).

3:06PM X45.00002 The drop impact dynamics of complex fluids on textured surfaces, KYOO-CHUL PARK, VIVEK SHARMA, ROBERT COHEN, GARETH MCKINLEY, Massachusetts Institute of Technology — The deposition of aqueous drops on non-wetting surfaces is an important canonical problem for many applications, including suppressing splash or rebound of sprayed herbicides on intrinsically hydrophobic plant leaves. The addition of a small amount of high molecular weight polymer has been demonstrated to suppress drop rebound on smooth hydrophobic surfaces. The high extensional viscosity of polymer solutions and the increased viscous dissipation near the receding contact line are cited as two distinct anti-rebound mechanisms. Using drop impact experiments on both micro- and nano-textured surfaces with controlled wetting characteristics we examine the roles of viscosity, elasticity and inertia on expansion, retraction, and rebound of well-characterized viscoelastic fluids. By adopting a stick-slip flow model on textured surfaces with various topographic length scales and solid area fractions, we rationalize the dynamics leading to complete rebound following drop impact on nanotextured surfaces even for highly viscoelastic fluids.

3:18PM X45.00003 Influence of nanoscale surface roughness on mechanism of dropwise water condensation¹, KONRAD RYKACZEWSKI, Material Measurement Laboratory, National Institute of Standards and Technology — Adversely to most potential applications of superhydrophobic coatings, only a few natural and artificial surfaces retain their superhydrophobic characteristics during water condensation. This work addresses the key question of why condensation on such surfaces leads to self-propelled dropwise condensation but causes wetting of other surfaces with water contact angles above 150 degrees. The effects of gradually varying nanoscale roughness of a hydrophobic surface on the mechanism of drop growth and coalescence are observed using electron and light microscopy. It is demonstrated that increasing the nanoscale surface roughness confines the base diameter of the nucleating droplets causing them to grow by increasing their contact angle. The increase in the nanoscale surface roughness also decreases triple line pinning during coalescence, thus allowing formation of nearly spherical drops after merging of two high contact angle drops. The role of the nanoscale roughness in the diameter confinement effect is explained through thermodynamic calculations. Lastly, confined base diameter growth model is derived and compared with experimental results.

¹This research was performed while K. Rykaczewski held a NRC ARRA fellowship at NIST. The author acknowledges J. Chinn from Integrated Surface Technologies Inc. for providing samples of superhydrophobic surfaces.

3:30PM X45.00004 Effect of Nano-Scale Roughness on Particle Wetting and on Particle-Mediated Emulsion Stability, ADRIANA SAN MIGUEL, SVEN BEHRENS, Georgia Institute of Technology — Colloidal particles can strongly adsorb to liquid interfaces and stabilize emulsions against droplet coalescence, the effectiveness of which depends crucially on the particle wettability. From the study of macroscopic solids, surface wetting is known to be influenced strongly by nano-scale roughness (as seen *e.g.* in the “Lotus effect” or in anti-fog coatings); similarly, strong effects of particle roughness on particle-stabilized emulsions should be expected. Here we report the first experimental study of particle wetting and particle-mediated emulsion stability in which particle roughness could be varied continuously without varying the surface chemistry. We demonstrate an enabling method for preparing particles and macroscopic substrates with tunable nano-roughness and correlate the extent of roughness quantitatively with surface wetting (measured *via* the three-phase contact angle) and with emulsion stability (quantifiable *via* the maximum capillary pressure). Our results confirm a dramatic influence of roughness on wetting, emulsion stability, and even the type of emulsion formed (o/w vs. w/o) upon mixing oil with an aqueous particle dispersion. Whether particle roughness benefits emulsion stability or not is seen to depend on both the size and shape of the surface features.

3:42PM X45.00005 ABSTRACT WITHDRAWN —

3:54PM X45.00006 Life Underneath a Leidenfrost Drop, AARON SHARPE, JUSTIN BURTON, ROELAND VAN DER VEEN, ANDRES FRANCO, SIDNEY NAGEL, The University of Chicago — Liquid drops deposited on a hot surface undergo a dramatic transition from boiling to levitating, a phenomena known as the Leidenfrost effect. The drops float on an insulating layer of evaporated vapor, which forms a pocket of high pressure underneath the drop and distorts the liquid-vapor interface. Experiments [1] have examined the lifetime and maximum size of such levitated drops. However, the interface beneath the drop has not been visualized or characterized. Using high-speed laser-light interference, we measure the geometry and fluctuations of the liquid-vapor interface. The interference fringes produced between the bottom surface of the liquid and the hot substrate provide information about the curvature of the vapor pocket beneath the drop as well as the azimuthal undulations along the rim that resides closest to the surface. We measure the speed, wavelength, and amplitude of the fluctuations as a function of the temperature of the substrate, as well as compare our results to recent theoretical predictions concerning the size of the vapor pocket for large drops [2].

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4:06PM X45.00007 Voltage Bursting Drops in Solids, QIMING WANG¹, DUKE UNIVERSITY, ZHIGANG SUO², HARVARD UNIVERSITY, XUANHE ZHAO³, DUKE UNIVERSITY — Droplets in air or liquids under electrical voltages appear in diverse processes from thunderstorm cloud formation, ink-jet printing, electrospinning nanofibers to electrospray ionization. In these processes, the electrostatic energy competes with surface energy of the drops and causes sharp tips to form on the ends of the drops. Here, we report a physically distinct scenario for droplets in solid matrices under voltages. We show that water drops in elastic polymers can form sharp tips and surprisingly burst into long tubes under applied voltages. The new phenomenon is governed by the elasticity and fracture of the solids, instead of the drops' surface energy as in previous cases. A new scaling is derived for the critical electrical field of the voltage-induced instability of drops in solids. The observations and analyses have significant practical impacts, as they illustrate the mechanism of a major failure mode, defect-induced breakdown, of dielectric polymers, which are widely used as insulating cables and polymer capacitors and transducers.

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4:18PM X45.00008 Spreading dynamics of a water droplet on a soluble polymer: glass transition effects, EMILIE VERNEUIL, JULIEN DUPAS, PPMD-SIMM, CNRS, UPMC, ESPCI ParisTech -Paris, France, MARCO RAMAIOLI, LAURENT FORNY, Nestlé Research Center, Lausanne - Switzerland, LAURENCE TALINI, FRANCOIS LEQUEUX, PPMD-SIMM, CNRS, UPMC, ESPCI ParisTech - Paris, France — We study the wetting dynamics of a droplet of solvent spreading on a soluble polymer coating. The complexity arises from the transfers of solvent and of soluble material through 3 processes: liquid evaporation and recondensation on the substrate, diffusion of the liquid in the substrate from the droplet, and substrate dissolution within the droplet. Indeed, when completely dry, the substrate, although soluble, is initially poorly wetting. Hydration enhances the wettability of the coating and the contact angle is found to decrease at higher humidity or at lower spreading velocity. In this paper, we explore experimentally the situation where hydration itself induces a sharp change in the diffusion coefficient of water in the polymer: this is what happens when the polymer undergoes a glass transition in water content. Diffusion coefficient changes by orders of magnitude upon glass transition, and we show that it results in a sharp effect on the course of the spreading as the hydration will be affected by the change in diffusion in the coating. We validate the previously derived model describing the various spreading regimes observed, and we expand it to account for the glass transition effects. It also successfully describes the results we obtain with other solvents and substrates.

4:30PM X45.00009 Water droplet spreading on a soluble polymer: what happens close to the contact line?, LAURENCE TALINI, JULIEN DUPAS, EMILIE VERNEUIL, FRANCOIS LEQUEUX, UPMC/CNRS/ESPCI, LAURENT FORNY, MARCO RAMAIOLI, Nestlé — We have studied the spreading of a water droplet on a water soluble substrate. Numerous coupled transfer processes are involved in such a situation, leading to complex wetting dynamics. In particular, previous studies have shown the major role of water evaporation from the droplet associated with water uptake by the substrate. However, the processes at stake close to the contact line, where the substrate properties set the wetting angle, have not been understood. We present an experimental study of the phenomena occurring within distances ranging from 10 to 1000 μm from the contact line of a water droplet spreading on a food polymer layer. We have evidenced a wrinkling pattern inside the droplet close to the contact line, and suggest it results from the swelling of the constrained polymer layer before it dissolves. In addition, using an optical method based on the analysis of Newton's rings, we have measured the hydration profile of the substrate ahead the contact line. We show that the profiles can be understood as a result of the evaporation/water uptake process through air combined with direct water diffusion in the substrate from the liquid wedge.

4:42PM X45.00010 Contact angle dependence of the resonant properties of sessile drops¹, JAMES SHARP, University of Nottingham — A simple optical deflection technique was used to monitor the vibrations of microlitre sessile drops of glycerol/water mixtures with glycerol compositions ranging from 0% to 75%. A photodiode was used to detect time dependent variations in the intensity of laser light reflected from the droplets. The intensity variations were Fourier transformed to obtain information about the resonant properties of the drops (frequency and width of the resonance). These experiments were performed on a range of different substrates where the contact angle formed by the droplets varied between $38 \pm 2^\circ$ and $160 \pm 4^\circ$. The measured resonant frequency values were found to be in agreement with a recently developed theory of vibrations which considers standing wave states along the profile length of the droplet. The widths of the resonances were also compared with theories which predict the influence of substrate effects, surface contamination effects and bulk viscous effects on the damping of capillary waves at the free surface of the droplets. These experiments indicate that the dominant source of damping in sessile liquid droplet is due to bulk viscous effects but that for small contact angles damping due to the droplet/substrate interaction becomes more important.

¹We acknowledge support from the EPSRC grant number EP/H004939/1

4:54PM X45.00011 Interfacial Effects on Droplet Dynamics in Poiseuille Flow, STEVEN HUDSON, NIST, JONATHAN SCHWALBE, MITRE, KENDRA ERK, FREDERICK PHELAN JR., NIST, PETIA VLAHOVSKA, Brown University — Many properties of emulsions arise from interfacial rheology. Here we advance theoretical understanding and experimental observation of the dynamics of isolated drops suspended in Poiseuille flow. Stokes flow is assumed in the bulk phases, and a jump in hydrodynamic stress at the interface is balanced by Marangoni forces (linearized with respect to local deviations of interfacial surfactant concentration) and surface viscous forces according to the Boussinesq–Scriven constitutive law. Interfacial diffusion is also included. Our analysis predicts slip, cross-stream migration and droplet-circulation velocities. These results and the corresponding interfacial parameters are separable, enabling a new droplet-based interfacial rheology method to determine interfacial viscosities and Marangoni elasticity. We illustrate such measurements by particle tracking velocimetry of surfactant-stabilized droplets in the Poiseuille flow of a microfluidic device. Small molecule and block copolymer surfactants are examined. This droplet-based interfacial rheology method is attractive since it mimics the natural geometry and length scale of practical emulsions and suspensions.

5:06PM X45.00012 Impact of liquid droplets on granular media, GILES DELON, DENIS TERWAGNE, STEPHANE DORBOLO, NICOLAS VANDEWALLE, HERVE CAPS, GRASP, Physics department B5, Université de Liège, Belgium — The crater formation due to the impact of a water droplet onto a granular bed has been experimentally investigated. Three parameters have been tuned: the impact velocity, the size of the droplet and the size of the grains. The shape of the crater depends on the Weber number at the moment the droplet starts to impact the bed. From the dynamical point of view, the spreading and the receding of the liquid during the impact have been carefully analyzed using image analysis of high speed video recordings. The different observed regimes are characterized by the balance between the impregnation time of the granular bed by the water contained in the droplet and the capillary time responsible for the receding of the drop.

5:18PM X45.00013 Droplet Rearrangement in a Sheared Dense Emulsion¹, S.K. DUTTA, D.L. BLAIR, Department of Physics, Georgetown University — The constituent particles of disordered colloidal dispersions compressed above the threshold for jamming flow with highly heterogeneous dynamics. Though this leads to the rich viscoelastic behavior that makes these materials so widespread, a clear description at the microscopic level has yet to emerge. We investigated the non-affine motion in a dense oil-in-water emulsion using a confocal rheometer, which can image individual droplets while applying a precisely controlled shear to the system. From these images, we identify the very fast rearrangements that accompany flow and determine the spatial and temporal distributions of the events as a function of the droplet volume fraction. In addition, it is possible to characterize the regions of the emulsion which are most susceptible to rearrangement.

¹This work is funded by the NSF through Grant DMR 0847490.

5:30PM X45.00014 Wetting Colloidal Particles at a Curved Interfaces, COLM KELLEHER, PAUL CHAIKIN, New York University Center for Soft Matter Research — At scales much smaller than the capillary length, surface tension plays a predominant role in the interactions that occur at an oil-water interface. When a spherical colloidal particle is adsorbed onto such an interface, two surface-tension-related effects occur: the adsorbed particle reduces the area of the interface, and the interface deforms in order to satisfy the requirement of constant contact angle at the three-phase contact line. If the interface is not flat or spherical, these effects depend on the position of the particle on the interface. In other words, the particle experiences an effective potential induced by the shape of the interface. [A. Wurger, PRE, 74, 041402 (2006).] We present results from an experiment in which a capillary bridge creates an interface of varying Gaussian curvature, onto which a colloidal particle is introduced. The shape of this interface is obtained by using confocal microscopy. We demonstrate that a shape-induced effective potential exists for this system, which attracts the wetting particle to the most curved regions. By tracking the motion of the particle in 3D, we are able to calculate the effective spring constant of this potential. We then compare our result to numerical and analytical predictions based on the geometry of the droplet.

Thursday, March 1, 2012 2:30PM - 5:30PM –

Session X46 DPOLY: Invited Session: Deformation and Fracture of Soft Materials 160AB

2:30PM X46.00001 Responsive Gel-Gel Phase Transitions in Artificially Engineered Protein Hydrogels, B.D. OLSEN, Massachusetts Institute of Technology — Artificially engineered protein hydrogels provide an attractive platform for biomedical materials due to their similarity to components of the native extracellular matrix. Engineering responsive transitions between shear-thinning and tough gel phases in these materials could potentially enable gels that are both shear-thinning and tough to be produced as novel injectable biomaterials. To engineer a gel with such transitions, a triblock copolymer with thermoresponsive polymer endblocks and an artificially engineered protein gel midblock is designed. Temperature is used to trigger a transition from a single network protein hydrogel phase to a double network phase with both protein and block copolymer networks present at different length scales. The thermodynamics of network formation and resulting structural changes are established using small-angle scattering, birefringence, and dynamic scanning calorimetry. The formation of the second network is shown to produce a large, nonlinear increase in the elastic modulus as well as enhancements in creep compliance and toughness. Although the gels show yielding behavior in both the single and double network regimes, a qualitative change in the deformation mechanism is observed due to the structural changes.

3:06PM X46.00002 Direct probes of molecular interactions at buried interfaces¹, ALI DHINOJWALA, The University of Akron — The molecular interactions at buried interfaces play an important role in adhesion, friction, and wetting. In my talk, I will discuss the use of interface-sensitive sum frequency generation (SFG) spectroscopy to study acid-base interactions at solid-liquid and solid-solid interfaces. The shift of the sapphire hydroxyl peak in contact with several polar and non-polar liquids and polymers can be used to determine the interaction energy. The magnitude of the interaction energies cannot be predicted based on measuring water contact angles. Molecular rearrangements at the sapphire interface, to maximize the interaction of the acid-base groups, play a dominant role and these effects are not accounted for in the current theoretical models. The importance of these interactions in controlling segregation of polymer blends and friction and adhesion of soft substrates will be discussed.

¹Funded by National Science Foundation

3:42PM X46.00003 Adhesion of hydrogels under water by hydrogen bonding: from molecular interactions to macroscopic adhesion¹, COSTANTINO CRETON, ESPCI ParisTech - UPMC - CNRS — Hydrogels are an essential part of living organisms and are widely used in biotechnologies, health care and food science. Although swelling properties, cell adhesion on gel surfaces and gel elasticity have attracted much interest, macroscopic adhesion of hydrogels on solid surfaces in aqueous environment is much less well understood. We studied systematically and in aqueous environment, the reversible adhesion by hydrogen bonding of macroscopic model hydrogels of polydimethylacrylamide (PDMA) or of polyacrylamide (PAAm) on solid surfaces functionalized with polyacrylic acid (PAA) polymer brushes. The hydrogels were synthesized by free radical polymerization and the brushes were prepared by grafting polytertbutyl acrylate chains and converting them by pyrolysis into polyacrylic acid. A new adhesion tester based on the flat punch geometry was designed and used to control the contact area, contact time, contact pressure and debonding velocity of the gels from the surface while the samples were fully immersed in water. The adhesion tests were performed at different pH and temperatures and the modulus of the gel and grafting density and molecular weight of the brushes was varied. Macroscopic adhesion results were compared with phase diagrams in dilute solution to detect molecular interactions. While the PDMA/PAA pair behaved very similarly in solution and in macroscopic adhesion tests, the PAAm/PAA pair showed an unexpectedly high adhesion level relatively to its complexation ability in dilute solution. Surprisingly, time dependent experiments showed that the kinetics of H-bond formation and breakup at interfaces was very slow resulting in adhesion energies which were very dependent on contact time up to one hour of contact. At the molecular level, neutron reflectivity showed that the equilibrium brush conformation when in contact with the gels was more extended at pH2 (H-bonds activated) than at pH9 (H-bonds deactivated) and that a certain applied pressure was necessary to bring the brush and the gel in contact. These combined results suggest that the mechanisms of formation and breakup of interactions at surfaces are more complex and cannot be understood from bulk interactions in solution alone.

¹We gratefully acknowledge support from the French ANR: project AdhGel

4:18PM X46.00004 Self-healing polymers and mechanochemistry¹, STEPHEN CRAIG, Department of Chemistry, Duke University — The forces that accompany macroscopic deformation and material failure are many orders of magnitude larger than the forces between the individual atoms of a molecule. The magnitude of macroscopic forces, in combination with the fact that they are directional, creates an opportunity to direct new, stress-responsive chemistry on demand in polymer materials. This talk will present studies of reactions under large, directional forces, and their applications in new classes of stress-responsive polymers, including a class of self-healing polymers in which mechanical activation of chemical reactions leads to improved structure and properties under conditions that are typically destructive to both.

¹This material is based on work supported by the U.S. Army Re-search Laboratory and the Army Research Office under Grant W911NF-07-1-0409.

4:54PM X46.00005 Soft active materials—when mechanics meets chemistry, ZHIGANG SUO, Harvard University — Soft materials, such as elastomers and gels, can mimic a salient feature of life: deformation in response to diverse stimuli. For example, an electric field can cause an elastomer to stretch several times its length. As another example, a change in pH can cause a gel to swell many times its volume. The deformation is large and reversible. These soft active materials are being developed for soft robots, adaptive optics, self-regulated fluidics, and programmable haptic surfaces. This talk describes recent work in my group on the mechanics of soft active materials. We formulate theories to answer commonly asked questions. How do mechanics, chemistry, and electrostatics work together to generate large deformation? What is the maximal energy that can be converted by a material? We also develop experimental methods to characterize nonlinear time-dependent mechanical behavior. Also described in this talk are hydrogels of exceptional toughness and stretchability.

Thursday, March 1, 2012 2:30PM - 5:18PM –

Session X47 DPOLY: Focus Session: Polymers for Energy Storage and Conversion - Nanostructures and Phase Separated Morphologies 160C

2:30PM X47.00001 Nanostructured Organometallic Polymers for Enzymatic Bioenergy, MOON JEONG PARK, JUNGPHIL LEE, Department of Chemistry, Division of Advanced Materials Science (WCU), Pohang University of Science and Technology (POSTECH) — The development of efficient enzymatic biofuel cell is a subject of considerable studies in past decades for potential applications such as biomedical devices and microchip systems. One of the key challenges in advancing the technology lies in the power densities of the system. Limitations have been arisen from the buried redox active sites within enzyme structure and poor interplay between redox reactions. In present study, a glucose oxidase is employed as a model enzyme and ferrocene-containing organometallic block copolymers are chosen for the electron mediators. Wiring of glucose oxidase into electrode surface was successfully achieved by cross-linked networks of organometallic polymers and remarkably, catalytic current densities of the fabricated electrodes have proven be a sensitive function of the morphologies of electron mediators. Different nanoscale morphologies, i.e., bicontinuous structure, nanowires, and nanoparticles, have been derived and the use of bicontinuous morphology confirms 2-50 times improved catalytic current response than the values obtained from other morphologies. The bio-sensing ability of the fabricated electrode with structural optimization was also exploited and good sensitivity is obtained at the physiological concentration of glucose in blood.

2:42PM X47.00002 Comparison of polymer-fullerene heterojunction morphology to bimolecular recombination kinetics, DEAN DELONGCHAMP, DEANNA RODOVSKY, NIST, JEFF PEET, Konarka, TRACEY CLARKE, ATTILA MOZER, University of Wollongong, LEE RICHTER, ANDREW HERZING, JOSEPH KLINE, NIST — One of the most important physical processes limiting the practical power conversion efficiency of bulk heterojunction (BHJ) organic photovoltaic devices is the bimolecular recombination of holes and electrons. Reduced recombination would permit the use of thicker BHJ layers, enabling greater light absorption without a penalty in device current. A few polymer light absorbers, when combined in a BHJ with a fullerene electron acceptor, exhibit recombination that is slower than Langevin-type, but the origins of this behaviour are not understood. This talk will describe our effort to determine whether slower-than-Langevin recombination can be attributed to features of the nanoscale morphology or crystalline microstructure within the BHJ film. In comparing BHJ films made from two silole-based monomers, one with Langevin recombination and one with slower-than-Langevin, we find many aspects of the BHJ material structure such as order, orientation, and nanoscale domain size and shape, to be surprisingly similar. We will compare the two materials and emphasize opportunities in data analysis and new measurements to determine whether a morphological basis underlies different recombination kinetics.

2:54PM X47.00003 Confinement effects on P3HT-PCBM Morphology for Bulk Hetero-Junction Polymer Solar Cells¹, ABUL HUQ, Department of Polymer Engineering, The University of Akron, DHARMARAJ RAGHAVAN, Department of Chemistry, Howard University, JOLANTA MARSZALEK, Department of Polymer Engineering, The University of Akron, DAVID BUCKNALL, Materials Science and Engineering, Georgia Institute of Technology, ALAMGIR KARIM, Department of Polymer Engineering, The University of Akron — Controlling morphology of the bulk hetero-junction in solar cell development is the key aspect for higher efficiency. We controlled the morphologies of phenyl-C61-butyric acid methyl ester (PCBM) and poly(3-hexylthiophene) (P3HT) blend thin films by tunable surface energy polydimethylsiloxane (PDMS) elastomer confinement. The advantages of replacing air-polymer interface with PDMS-polymer interface are its flexibility, easy detachability, facile tunability of surface energy by UVO exposure. We hypothesize that the confined annealing will suppress PCBM crystallinity, control crystallinity of P3HT, direct the vertical segregation of P3HT-PCBM blend, and thus influence the composition distribution of P3HT and PCBM at the interfaces. The annealed films were characterized by dark field optical microscopy, GISAXS, GIWAXS, AFM, and SANS. PCBM crystallization was indeed suppressed in the films during confinement annealing. On the other hand the phase separated interpenetrating network and favorable crystallinity of the P3HT evolved. The optimum surface energy of the confining PDMS yields the best structural features of the film. The morphology developed under different PDMS surfaces is an important step towards improvement of efficiency of OPV's.

¹DOE and BES

3:06PM X47.00004 The Role of P3HT Crystallization in the Morphological Development in P3HT/PCBM Thin Films Using Neutron Scattering, MARK DADMUN, WEN YIN, University of Tennessee — Small angle neutron scattering (SANS) provides an important method to characterize the morphology of PCBM/P3HT organic photovoltaics (OPVs), which is essential to improving the efficiency of plastic solar cell devices. Our recent SANS results indicate that fullerene derivatives and conjugated polymers employed in OPVs are significantly miscible, up to ~20%. In this work, the morphology of PCBM/P3HT composite *thin films* is investigated via SANS and analyzed to document their morphology and miscibility. These results indicate that both 20 and 50 vol% PCBM as-cast films exhibit relatively small low-Q scattering, suggesting an overall homogeneous mixture. After annealing at 150 °C for 30 minutes, P3HT undergoes further crystallization in both mixtures. However, the low-Q scattering of the 20 vol% PCBM sample remains low, indicating the film remains homogenous. On the other hand, 50% PCBM sample undergoes phase separation between amorphous PCBM and P3HT. These results therefore exemplify the importance of P3HT crystallization in the structure development of OPV active layers, showing that the crystallization of P3HT is not sufficient to induce phase separation.

3:18PM X47.00005 Understanding the Behavior of Poly(3-hexylthiophene) at Liquid/Vacuum Interfaces¹, YENENEH YIMER, MESFIN TSIGE, Department of Polymer Science, University of Akron, Akron, Ohio — Among semiconducting polymers used in opto-electronic devices, poly(3-hexylthiophene) (P3HT) is one of the better candidates because of its good electrical properties and ease of processing. The performance of these devices strongly depends on the structural, morphological, dynamic and interfacial properties of P3HT. Using molecular dynamics simulation and utilizing two different models - all-atom and united-atom - we have studied the dynamic and structural properties of free-standing P3HT thin films at liquid/vacuum interfaces. To quantify these properties, the temperature and chain-length dependence of surface roughness, interfacial width, surface tension, torsional defects, and several other surface properties have been investigated. The results we obtained from all-atom and-united atom models are in reasonable agreement.

¹This work is supported by the NSF (DMR0847580).

3:30PM X47.00006 Understanding Schroeder's Paradox, ADAM WEBER, AHMET KUSOGLU, Lawrence Berkeley National Laboratory — Schroeder's paradox is a well known, but not fully understood, phenomenon that exists in many polymers and gels. Essentially, the uptake of solvent in the polymer depends on the interaction with the boundary phase. Nafion, a polymer of interest for many electrochemical energy applications, is a classic example where the water uptake almost doubles by placement in liquid water versus saturated water vapor. In this talk, we examine the origin of this paradox through examination of Nafion morphology and water-uptake time constants using experiments in various solvents, vacuum, and small-angle X-ray scattering techniques. The results show that the interface controls the water uptake (even in bulk membranes) and that the interfacial morphology depends on the interactions of the different polymer moieties with the external environment including its density and dielectric constant. In addition, interactions with solid phases will be discussed which show similar impact on water uptake depending on whether they are hydrophilic or hydrophobic. Understanding the morphological changes and their associated impact on membrane properties is critical for optimizing polymers for use in energy applications.

3:42PM X47.00007 Ions in block copolymers: Effects on thermodynamics, structural changes and electric field induced alignment., THOMAS THURN-ALBRECHT, Martin-Luther-Universität Halle-Wittenberg — Block copolymers with added ions which selectively dissolve in one block are of interest as nanostructured polymeric ion conductors. In the microphase separated state such a system offers the possibility to simultaneously optimize different properties which would normally exclude each other. One block, being in the solid state, can give mechanical strength while the other block, typically in the liquid state, could be designed to achieve good ion transport. Oriented structures are especially interesting. We present two sets of experiments dealing with fundamental ion induced effects in block copolymers. It is generally observed that the addition of salt to a block copolymer leads to a strong increase of the order-disorder transition temperature and an increased domain spacing, i.e. conformational changes of the polymers. Based on a detailed analysis of small angle scattering data of two different copolymers (PS-b-PEO, PS-b-PVP) close to the order-disorder transition three contributions to the structural changes can be distinguished: an increased incompatibility between the different monomers, the additional volume of the added salt, and chain stretching due to coordination between polymer and salt. At the phase transition, i.e. at constant incompatibility χN , for low concentrations the increase in domain size is quantitatively explained by the volume of the added salt, at higher concentrations in addition chain stretching sets in. Structural and thermodynamic effects are considerably stronger in PEO than in P2VP. In a second experiment we study the effects of electric field induced interfacial polarization caused by the added salt. Impedance spectroscopy combined with orientation experiments at high fields enable a quantitative analysis of ionic polarization and a direct demonstration of its aligning effect on the interfaces. Field induced orientation effects are much stronger if the ionic charges come into play in comparison to much weaker dielectric effects. We present a physical model accounting for the differences.

4:18PM X47.00008 Does filler surface chemistry impact filler dispersion, polymer dynamics and conductivity in nanofilled solid polymer electrolytes?, LALITHA GANAPATIBHOTLA, JANNA MARANAS, The Pennsylvania State University — We study the impact of nanofiller surface chemistry on filler dispersion, polymer dynamics and ionic conductivity in acidic α -Al₂O₃ filled PEO+LiClO₄ solid polymer electrolytes (SPEs). SPEs are the key to light-weight and high energy density rechargeable Li ion batteries but suffer from low room temperature ionic conductivity. Addition of ceramic nanofillers improves conductivity of SPEs and their surface chemistry influences extent of conductivity enhancement. The ionic conductivity of acidic α -Al₂O₃ filled SPE is enhanced for salt concentrations at and below eutectic, while neutral γ -Al₂O₃ filler enhances conductivity only at eutectic composition. Li ion motion is coupled to segmental mobility of polymer and we study how this is affected by addition of α -Al₂O₃ using quasi-elastic neutron scattering. Aggregation extent of nanoparticles in SPE matrix, a less explored factor in filled SPEs, can affect segmental mobility of polymer. This can vary with surface chemistry of particles and we quantify this using small angle neutron scattering. All measurements are performed as a function of Li concentration, nanoparticle loading and temperature.

4:30PM X47.00009 Regular Arrays of Germanium Nanoparticles Assisted by Thermoset Polymer Composites for High Capacity Lithium Ion Battery, GYUHA JO, Pohang University of Science and Technology (POSTECH), MOON JEONG PARK, POSTECH (Pohang University of Science and Technology) — In recent years Li-batteries have attracted significant interests for a variety of applications such as portable electronics and electric vehicle (EV) batteries due to their high energy densities. Key challenges in advancing the technology lie in specific energy density, the long term cycle properties, and durability at elevated temperature. In present study, we were motivated to prepare high capacity Li-battery by creating regular arrays of germanium nanoparticles (GeNPs, 1600 mAh/g) to replace commercial graphite anode (370 mAh/g). Thermoset polymers were employed to prepare GeNPs/polymer composites with tunable NP loadings and spacings, followed by carbonization process to prepare GeNPs/carbon composite anode material. Due to the large volume change of GeNPs with charge/discharge cycles, the regular arrays of GeNPs are turned out to be a crucial parameter in obtaining enhanced cyclability. The GeNPs/carbon anode materials were cycle tested in a half cell configuration using Lithium foil as a counter electrode and lithium salt doped PS-PEO block copolymers as electrolytes. High capacity and rate capability were achieved, which demonstrate the role of nano-sized and regularly-arrayed anode active materials in obtaining the improved battery performance.

4:42PM X47.00010 Disorder – Order Transitions in Humidified Block Copolymer Electrolytes Studied by *In Situ* SAXS, KEITH BEERS, University of California, Berkeley, ANDREW JACKSON, European Spallation Source, NITASH BALSARA, University of California, Berkeley — The relationship between water uptake, proton conductivity and morphology in the dry and hydrated state for a series of poly(sulfonated styrene-*block*-ethylene) was investigated. Specifically, the disorder-to-order transition (DOT) and hydrated morphology was characterized by *in situ* humidity controlled small angle X-ray scattering (SAXS). The enhanced resolution afforded by SAXS allows for better characterization of the DOT than previous studies which have relied upon neutron scattering. The transition to an ordered state is found to display a coexistence of ordered and disordered states over a broad range of relative humidity values.

4:54PM X47.00011 Effects of lithium salts on the lamellar phase of diblock copolymers, ISSEI NAKAMURA, ZHEN-GANG WANG, California Institute of Technology — We study the effects of lithium salts on the lamellar phase of AB diblock copolymers by means of the self-consistent field theory. We consider a model in which the A and B blocks have different dielectric constants and account for the tight binding of Li^+ to one of the blocks, the preferential solvation energy of anions in the higher-dielectric polymer domain, the translational entropy of anions, and change in the χ parameter due to the binding of Li^+ . We study the effect of the strong polymer- Li^+ binding on the distribution of the salt ions. In particular, we show that local charge separation near the interface of the higher- and lower- dielectric polymers largely arises from the effect of the Born energy. We also examine the relationship between two definitions of the effective χ parameter, one based on the lamellar spacing and one based on the structure factor in the disordered phase, and show that these two definitions generally do not coincide.

5:06PM X47.00012 Structure of Block Copolymer Hydrogel Formed by Complex Coacervate Process, SOOHYUNG CHOI, JULIA ORTONY¹, DANIEL KROGSTAD, JASON SPRUELL, NATHANIEL LYND, SONGI HAN, EDWARD KRAMER, University of California, Santa Barbara — Complex coacervation occurs when oppositely charged polyelectrolytes associate in solution, forming dense micron-sized droplets. Hydrogels with coacervate block domains were formed by mixing two ABA and A'BA' triblock copolymer solutions in water where the A and A' blocks are oppositely charged. Small-angle neutron scattering (SANS) was used to investigate the structure of hydrogels formed by ABA triblock copolymers (A block: poly(allyl glycidyl ether) functionalized with guanidinium (A) or sulfonate (A'), B block: poly(ethylene oxide)). By using an appropriate fitting model, structural information such as coacervate core block radius and water volume fraction w can be extracted from SANS data. The results reveal that w in the coacervate core block was significantly higher than in conventional triblock copolymer hydrogels where microphase separation is driven by the hydrophobicity of the core-forming blocks.

¹Present affiliation: Northwestern University

Thursday, March 1, 2012 2:30PM - 5:42PM –
Session X48 DPOLY DBIO: Focus Session: Statistical Physics of Active Systems Away From Detailed Balance: Cytoskeleton, Flagella, and All That 161

2:30PM X48.00001 The Role of Dynein in Microtubule Mechanics, TONY LADD, University of Florida, GAURAV MISRA, Stanford University, JUN WU, ROBERT RUSSELL, TANMAY LELE, RICHARD DICKINSON, University of Florida — Experiments in Lele's group have shown that microtubules severed by laser ablation do not straighten, as would be expected from the large bending moments along their lengths. Instead, segments near newly created minus ends typically increased in curvature following severing, while segments near new microtubule plus ends depolymerize before any observable change in shape. However, in dynein-inhibited cells, segments near the cut straightened rapidly following severing. These observations suggest that microtubules are subject to significant tangential forces, and that lateral motion of the microtubule is primarily opposed by frictional rather than elastic forces. To interpret the experimental results, we have developed a numerical model for intracellular microtubule mechanics, accounting for dynein-generated forces on the microtubules. We have supplemented the Kirchhoff model for an elastic filament with the stochastic growth and collapse of microtubules, and by a model for dynein generated forces. I will present simulations of the dynamics of individual microtubules that show how motor forces result in the localization of short-wavelength buckles near the cell periphery. Our results suggest that microtubule shapes *in vivo* reflect a dynamic force balance, where bending moments are opposed by dynein-motor forces that include a large effective friction from the stochastic binding and unbinding of the motors. Simulations of the motion of the centrosome are consistent with a mechanism for centrosome centering driven by pulling forces exerted by dynein motors. I will explain how tension on the centrosome can be reconciled with buckled filaments near the cell periphery.

2:42PM X48.00002 Processivity and collectivity of molecular motors pulling membrane tubes, FRANCISCO FONTENELE ARAUJO, CORNELIS STORM, Eindhoven University of Technology — In every cell, directed transport involves proteins that convert chemical energy into mechanical work. Molecular motors responsible for this vital task are mostly too weak to carry biological cargo by themselves and some cannot even take more than a single step before unbinding from their cytoskeletal track. By acting collectively, however, they can muster the required forces. In this talk, we discuss interactions among motors and their collective effects on the extraction of membrane nanotubes. Via a force balance coupled to binding kinetics, we sketch the phase diagram of tube formation. Three regimes are identified: (1) tip clustering, in the sense that the driving force is concentrated at the tip of the tube, (2) viscous extraction, in which motors axially drag membrane, and (3) hybrid extraction, such that tip clustering and axial drag are equally important. Comparison with experiments indicates that synthetic membranes mostly fall into regime (1), while biological membranes tend to fall into regime (2). Our model suggests a unifying picture of tube extraction by both processive and nonprocessive motors.

2:54PM X48.00003 Carbon nanotubes as mechanical probes of equilibrium and non-equilibrium cytoskeletal networks, NIKTA FAKHRI, Third Institute of Physics - Biophysics, Georg-August-Universitaet, Goettingen, Germany, MATTEO PASQUALI, Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA, FREDERICK C. MACKINTOSH, Department of Physics and Astronomy, Vrije Universiteit, Amsterdam, The Netherlands, CHRISTOPH F. SCHMIDT, Third Institute of Physics - Biophysics, Georg-August-Universitaet, Goettingen, Germany — Networks of filamentous proteins underlie the mechanics of cells. The activity of motor proteins typically creates strong fluctuations that drive the system out of equilibrium. Understanding the behavior of such networks requires probes that ideally span the characteristic length-scales, from nanometers to micrometers. Single-walled carbon nanotubes (SWNTs) are nanometer-diameter filaments with micrometer length and tunable bending stiffness. On a Brownian energy scale they have persistence lengths of about 20-100 micrometers and show significant thermal fluctuations on the cellular scale of a few microns. Diffusive motion and local bending dynamics of SWNTs embedded in an active polymeric network reflect forces and fluctuations of the embedding medium. We study the motion of individual SWNTs in equilibrium and non-equilibrium networks by near infrared fluorescence microscopy. We show that SWNTs reptate in the network. We will discuss the possibility of using SWNTs as multi-scale probes relating their local dynamic behavior to the viscoelastic properties of the surrounding network.

3:06PM X48.00004 ABSTRACT HAS BEEN MOVED TO C1.00231 —

3:18PM X48.00005 The metaphase and anaphase dynamics is dominated by the physical and mechanical properties of both microtubules and chromatin, LUCA GRISA, MARIA KILFOIL, University of Massachusetts, Amherst — One of the most interesting problems in biophysics involves the physical separation of chromosomes and the mechanical properties of both microtubules (MT's) and chromatin. This process involves the polymers MT's and chromatin, each of which has unique physical properties that have been determined extensively in vitro. Of further interest for physicists is the out-of-equilibrium nature of this process involving several force generators from motor proteins and MT depolymerization. We follow the dynamics of spindle pole bodies and centromeres of yeast cells during mitosis in three-dimensions at high spatial resolution. Using this novel approach, we are able to observe spindle oscillations during metaphase, and the three-dimensional dynamics of spindle elongation and chromosome separation during anaphase. With these data, we can separate the dynamics caused by MT depolymerization from those caused by the motors. This allows us to determine the depolymerization rate of the kinetochore MT's in vivo. Furthermore, we determine the temporal profile of the chromatin extension during anaphase we combine with the known force-extension curve of chromatin in vitro, to infer the expected force-velocity curve of the collective motors in vivo, which has never been measured in vivo or in vitro.

3:30PM X48.00006 Effective temperature and spontaneous collective motion of active matter¹, SHENSHEN WANG, University of California, San Diego, PETER WOLYNES, Rice University — Spontaneous directed motion, a hallmark of cell biology, is unusual in classical statistical physics. Here we study, using both numerical and analytical methods, organized motion in models of the cytoskeleton in which constituents are driven by energy-consuming motors. Although systems driven by small-step motors are described by an effective temperature and are thus quiescent, at higher order in step size, both homogeneous and inhomogeneous, flowing and oscillating behavior emerges. Motors that respond with a negative susceptibility to imposed forces lead to an apparent negative temperature system in which beautiful structures form resembling the asters seen in cell division.

¹We gratefully acknowledge the financial support from the Center for Theoretical Biological Physics sponsored by the National Science Foundation via Grant PHY-0822283.

3:42PM X48.00007 An active matter analysis of intracellular Active Transport, BO WANG, KEJIA CHEN, SUNG CHUL BAE, STEVE GRANICK, University of Illinois Urbana-Champaign — Tens of thousands of fluorescence-based trajectories at nm resolution have been analyzed, regarding active transport along microtubules in living cells. The following picture emerges. Directed motion to pre-determined locations is certainly an attractive idea, but cannot be pre-programmed as to do so would sacrifice adaptability. The polarity of microtubules is inadequate to identify these directions in cells, and no other mechanism is currently known. We conclude that molecular motors carry cargo through disordered intracellular microtubule networks in a statistical way, with local cellular "noise" both in directionality and speed. Programmed random walks describe how local 1D active transport traverses crowded cellular space efficiently, rapidly, minimizing the energy waste that would result from redundant activity. The mechanism of statistical regulation is not yet understood, however.

3:54PM X48.00008 ABSTRACT WITHDRAWN —

4:06PM X48.00009 Constant torque in flagellar bacterial motors optimizes space exploration, CARLOS A. CONDAT, MARIO E. DI SALVO, IFEG-CONICET and National University of Cordoba, Cordoba, Argentina — Experiments indicate that the torque provided by the bacterial rotary motor is approximately constant over a large range of angular speeds. Constant torque implies that the power spent in active motion is proportional to the instantaneous bacterial speed, if the relation between angular speed and swimming speed is linear. Here we show that a constant torque maximizes the volume of the region explored by a bacterium in a resource-depleted medium. Given that nutrients in the ocean are often concentrated in separate, ephemeral patches, we propose that the observed constancy of the torque may be a trait evolved to maximize bacterial survival in the ocean. We also discuss the dependence of the explored volume with the particular features of the bacterial propulsion mechanism.

4:18PM X48.00010 Interplay between motor contractility and mechanical stability of active biopolymer networks, CHASE BROEDERSZ, Princeton University — The mechanical properties of cells are regulated in part by internal stresses generated actively by molecular motors in the cytoskeletal filamentous actin network. On a larger scale, collective motor activity allows the cell to contract the surrounding extracellular matrix, consisting also of biopolymer networks. Experiments show that such active contractility dramatically affects the networks' elasticity, both in reconstituted intracellular F-actin networks with myosin motors as well as in extracellular gels with contractile cells. We provide insight into this remarkable behavior with a model for the mechanics of contractile disordered networks consisting of simple straight fibers with linear bending and stretching elasticity. We find that these networks exhibit a low-connectivity rigidity threshold governed by fiber-bending elasticity and a high-connectivity threshold that controls a crossover between bending and stretching dominated network elasticity. Owing to their low connectivity, typical biopolymer networks fall below this upper threshold and their mechanical stability thus relies on the fibers' bending rigidity. The macroscopic elasticity of such networks is governed by soft fiber bending deformations. However, we find that motor-generated contractile forces can "pull out" these soft bending modes, thereby inducing a crossover to a mechanically more stable regime governed by stiff fiber stretching modes. Using scaling arguments and mean field theory, we show that this transition—induced by motor contractility—can be understood from the stress-dependence of the mechanical stability thresholds. These results suggest a physical principle by which active contractility can control biopolymer network mechanics, even when the fiber constituents are linear elastic elements.

4:54PM X48.00011 Propulsion of microorganisms by a helical flagellum, CHIH-HUNG CHEN, BRUCE RODENBORN, HARRY SWINNEY, Department of Physics and Center for Nonlinear Dynamics, University of Texas at Austin, BIN LIU, School of Engineering, Brown University, Providence Rhode Island, HEPENG ZHANG, Department of Physics and Institute of Natural Sciences, Shanghai Jiao Tong University — Many bacteria (e.g. *E. coli* and *Salmonella*) swim by rotating rigid helical flagella, which are typically several μm long and $0.4 \mu\text{m}$ in diameter. We investigate this propulsion in laboratory measurements on macroscopic rotating helices (typical diameter, 12 mm) in a fluid with viscosity 10^5 times that of water; thus the Reynolds number in the experiments is much less than unity, just as for bacteria. We measure the propulsive force and torque generated by a rotating flagellum, and the drag force on a translating flagellum; thus we can determine all elements of the propulsion matrices along the axial direction. We also compute force, torque and drag using the regularized Stokeslets method of Cortez et al. (2005). Our experimental and numerical results are in excellent agreement. However, these results differ significantly from the predictions of resistive force theories developed by Gray and Hancock (1953) and Lighthill (1975). The difference between our measurements and resistive force theory is especially large for helices with small pitch/diameter ratios, which is the regime of many bacteria.

5:06PM X48.00012 Energy Consumption of Actively Beating Flagella¹, DANIEL CHEN, Department of Physics, Brandeis University, DANIELA NICASTRO, Department of Biology, Brandeis University, ZVONIMIR DOGIC, Department of Physics, Brandeis University — Motile cilia and flagella are important for propelling cells or driving fluid over tissues. The microtubule-based core in these organelles, the axoneme, has a nearly universal “9+2” arrangement of 9 outer doublet microtubules assembled around two singlet microtubules in the center. Thousands of molecular motor proteins are attached to the doublets and walk on neighboring outer doublets. The motors convert the chemical energy of ATP hydrolysis into sliding motion between adjacent doublet microtubules, resulting in precisely regulated oscillatory beating. Using demembrated sea urchin sperm flagella as an experimental platform, we simultaneously monitor the axoneme's consumption of ATP and its beating dynamics while key parameters, such as solution viscosity and ATP concentration, are varied. Insights into motor cooperativity during beating and energetic consequences of hydrodynamic interactions will be presented.

¹We gratefully acknowledge support from the WM Keck Foundation.

5:18PM X48.00013 A particle based computational model for eukaryotic flagella, RAGHUNATH CHELAKKOT, MICHAEL HAGAN, Brandeis University — The structure of the eukaryotic flagella is very complex and the exact mechanisms responsible for flagellar beating are not clearly understood. Here we present a minimal model to study flagellar beating in two dimensions, which demonstrates that regular beating with a well defined characteristic frequency can arise spontaneously in the absence of external control. In this model, the flagella is represented by two stiff filaments clamped on a surface, on which model “molecular motors” take directed steps on one of the filaments and thereby apply a local force. The fluid medium is simulated using Multiparticle Collision dynamics (MPC), which is a particle based method for hydrodynamic simulations. Within a certain range of motor concentrations, large amplitude periodic oscillations with a well defined frequency are observed; other qualitatively different beating patterns arise outside of this range. We present a phase diagram that characterizes the beating behaviour as a function of relevant parameters such as filament length, motor density on the filament and motor velocity.

5:30PM X48.00014 Force generation in a regrowing eukaryotic flagellum¹, MARCO POLIN, DAMTP, University of Cambridge, BASTIEN BRUNEAU, Ecole Polytechnique, Paris, France, THOMAS JOHNSON, University of Birmingham, RAYMOND GOLDSTEIN, DAMTP, University of Cambridge — Flagella are whip-like organelles with a complex internal structure, the axoneme, highly conserved across eukaryotic species. The highly regulated activity of motor proteins arranged along the axoneme moves the flagellum in the surrounding fluid, generating forces that can be used for swimming or fluid propulsion. Although our understanding of the general mechanism behind flagellar motion is well established, the details of its implementation in a real axoneme is still poorly understood. Here we explore the inner working of the eukaryotic flagellum using a uniflagellated mutant of the unicellular green alga *Chlamydomonas reinhardtii* to investigate in detail the force and power generated by a moving flagellum during axonemal regrowth after deflagellation. These experiments will contribute to our understanding of the inner working of the eukaryotic flagellum.

¹MP acknowledges support from EPSRC

Thursday, March 1, 2012 2:30PM - 5:30PM –
Session X49 DMP DPOLY: Focus Session: Organic Electronics and Photonics - Polymer Di-
electrics and Charge Transport 162A

2:30PM X49.00001 Inhomogeneous deformation and instability in soft dielectric transducers, TIEFENG LI, SHAOXING QU, Zhejiang University, CHRISTOPH KEPLINGER, Johannes Kepler University, ZHIGANG SUO, Harvard University, WEI YANG, Zhejiang University — Dielectric elastomer (DE) is assembled by sandwich an elastomeric membrane with compliant electrodes on both sides. They are capable of converting mechanical into electrical energy (generator) or electrical into mechanical energy (actuator). The large actuation strain of DE has inspired intense development of dielectric elastomers as applications as actuators and generators. DE transducers are lightweight, compliant, rust-free, and can convert higher energy than those of conventional transducers. DE transducers often undergo inhomogeneous deformation and instability during operation. Inhomogeneous deformation can cause the DE membranes to have inhomogeneous fields distribution and fail locally. Instability during actuation highly affects the performance and safety of the DE transducer. We present an analytical model of a dielectric elastomer transducers undergoing inhomogeneous deformation and snap-through instability during operation.

2:42PM X49.00002 Dielectric Properties of Carbon, Silicon and Germanium Based Polymers: A First Principles Study, CHENCHEN WANG, GHANSHYAM PILANIA, CHUNSHENG LIU, RAMPI RAMPRASAD, University of Connecticut — The field of high energy density capacitors would benefit from the discovery of new insulating polymers with high dielectric constant, low loss, large band gap and high breakdown strength. The current standards for capacitive energy storage applications are polypropylene and polyethylene which have large band gap and high breakdown strength, but a small dielectric constant. As an initial step aimed at the discovery of new polymers with better dielectric properties, we consider a class of chemically-modified polymers based on polyethylene. These polymers are composed of $-XY_2-$ building blocks, with $X = C, Si$ or Ge , and $Y = H, F$ or Cl . We use density functional perturbation theory and exchange-correlation functionals that include van der Waals and/or nonlocal exchange interactions to accurately predict the structure, dielectric constant (electronic and ionic) and band gap of this class of polymers. The computed properties have been correlated to the underlying electronic structure and phonon modes, and tradeoffs between the band gap and dielectric constant are established. The time-consuming dielectric computations have been optimized using a new “single-chain” method to allow for future extensive explorations of the polymer chemical space via automated high-throughput computations.

2:54PM X49.00003 Paraelectric Crystalline Polymers for High Energy Density and Low Loss Dielectrics¹, LEI ZHU, Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, Ohio 44106-7202, RUN SU, College of Polymer Science and Engineering, Sichuan University, Chengdu, Sichuan 610065, JUNG-KAI TSENG, MAO-SHENG LU, Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, Ohio 44106-7202 — It is known that the high temperature phase above the Curie temperature (T_c) in poly(vinylidene fluoride-co-trifluoroethylene) [P(VDF-TrFE)] is a typical paraelectric phase. Frequency-dependent electric displacement-electric field (D-E) loop tests are used to study the dielectric/ferroelectric properties of this paraelectric phase. It is observed that normal ferroelectric hysteresis loops are observed at a poling frequency of 1 Hz, while narrow paraelectric loops are observed at a high poling frequency of 1000 Hz. The poling mechanism is revealed by an in-situ electric field-dependent Fourier transform infrared study. From this study, we consider that paraelectric crystalline polymers are good candidates for high energy density and low loss dielectrics.

¹Financial supports: Chinese Scholarship Council, National Science Foundation (DMR-0907580), and Army Research Office (W911NF-11-1-0534).

3:06PM X49.00004 Influence of Aqueous Electrolytes on Electrical Insulating Properties of Polyethylene, ADAM TORNHEIM, TOM DEVINE, UC Berkeley — Polyethylene is commonly used as electrical insulation in high voltage (3-35 kV), underground electrical distribution cables. During service conditions the insulation “ages” and may fail. One method of ageing is a consequence of long-time exposure of the polyethylene to humidity and groundwater. Chemical analyses by other researchers indicated iron was frequently detected in degraded areas of aged cable. In the current research we examine the effect of a ferric chloride electrolyte on the electrical insulating character of polyethylene. In earlier research we discovered that in the presence of high DC voltages (approximately 3kV-6kV) ferric chloride electrolytes markedly enhance electron injection into and subsequent electron transport through polyethylene. The present research shows that ferric chloride complexes in solution are likely responsible for electron injection. The effect of exposure to ferric chloride solution was permanent, causing an increase in current density when the polyethylene was subsequently exposed to other electrolytes. The effect of FeCl_3 exposure was observed in additive free polyethylene as well as commercially processed polyethylene.

3:18PM X49.00005 Theoretically guided design of efficient polymer dielectrics¹, PHILIP TAYLOR, ELSHAD ALLAHYAROV, Case Western Reserve University — We have used theory and molecular dynamics simulation as an aid to the development of polymeric materials with favorable properties for energy storage with low dielectric losses. We build on the principle that the stored energy in a capacitor is a sum of the intrinsic energy of the electric field and the energy of distortion of the molecular bonds within the dielectric. We have attempted to maximize the energy of bond distortion by increasing the polarization without introducing large losses. In this initial study we simulate the behavior of a system consisting of parallel chains of the antiferroelectric α phase of polyvinylidene fluoride that has been modified to increase the separation between chains through crosslinks that prevent chain rotation. By varying the crosslink density, we identify the optimum length of unlinked chain such that the polar entities that rotate when subject to a strong electric field will be neither so long that they rotate collectively with little stored energy, nor so short that the large distortion of bond angles necessary for dipole rotation reduces the polarizability. We have adopted a combined-atom model in order to make feasible the study of systems comprising up to 100 chains, each consisting of up to 500 monomers.

¹Work supported by the American Chemical Society Petroleum Research Fund

3:30PM X49.00006 Interface conductivity contribution in Co-Phthalocyanines capacitive type devices, CARLOS MONTON, ILYA VALMIANSKY, IVAN SCHULLER, Department of Physics and Astronomy, University of California San Diego, 9500 Gilman Dr., San Diego, La Jolla, CA 92093, U.S.A — Metal Phthalocyanines are flat organic semiconductors which exhibit interesting magnetotransport properties. Recent experimental studies in a particular system together with theoretical calculations have shown that the temperature and thickness dependence of the ohmic conductivity can be universally described by two independent contributions: the organic film and the electrode-film interface [1]. In order to explore the implications of this model we performed transport measurements in sandwich devices with different bottom electrodes materials. These devices are grown in-situ by Organic Molecular Beam Epitaxy to assure ultra clean electrode-film interfaces. A combination of structural and transport studies are used to investigate the reason for the drastic change in ohmic conductance at metallo-organic film thickness around 100nm.

[1] C. N. Colesniuc, R. R. Biswas, S. A. Hevia, A. V. Balatsky, and I. K. Schuller, Phys. Rev. B 83, 085414 (2011).

3:42PM X49.00007 Nanoscale Correlation of Heterogeneous Morphology and Electrical Transport in Nanostructured Organic and Hybrid Solar Cells, JIEBING SUN, SEAN WAGNER, XIAOYU LIU, PHILLIP DUXBURY, PENG PENG ZHANG, Michigan State University — The knowledge of correlation between morphology and electrical properties is essential both to understand fundamental physics and to facilitate device optimization. We report a systematic study of the organic blend of PCBM particles and P3HT fibers formed via the thermal annealing method. We use conductive atomic force microscopy (c-AFM) to simultaneously map the surface morphology and collect the electrical current. Cross-section AFM is attempted to get the internal 3D morphology so as to establish its correlation with the electrical properties. The obtained heterogeneity in the current map with a resolution up to 20 nm is attributed to the formation of cross-linked three dimensional fiber network, which is further supported by a three dimensional device model incorporating the geometry of nanowire and the c-AFM tip. Results on the hybrid cell of ZnO nanowires infiltrated with P3HT will also be discussed.

3:54PM X49.00008 Gigahertz Probing of Poly(3-hexylthiophene) With A Kilohertz Detection Scheme¹, JEFF WORNE, Department of Electrical and Computer Engineering, Rice University, COREY SLAVONIC, Department of Physics and Astronomy, Rice University, KEVIN KELLY, Department of Electrical and Computer Engineering, Rice University, DOUGLAS NATELSON, Department of Physics and Astronomy, Rice University — Organic semiconducting polymers have been well studied at DC and low-frequencies, giving important information about charge transport and metal-polymer interaction. However, comparatively little is known about the operation of these polymers at radio frequencies (1 GHz). RF frequencies can be a useful tool to investigate high-frequency mobility and charge carrier dynamics relevant for the possibility of using these polymers in RF applications. We present a novel technique that probes poly(3-hexylthiophene) (P3HT) response in the RF regime but allows for detection in the kHz regime. We show transport data of P3HT and discuss a theoretical framework for inferring behavior at GHz frequencies.

¹J.W. and D.N. acknowledge support from the National Science Foundation award ECCS-0901348

4:06PM X49.00009 Thickness dependence of hole mobility in regioregular poly(3-hexylthiophene) thin films, BINGYUAN HUANG, EMMANOUIL GLYNOS, BRADLEY FRIEBERG, PETER GREEN, University of Michigan-Ann Arbor — Methods of time of flight (TOF) and charge extraction by linearly increasing voltage (CELIV) are used to investigate the hole mobility in regioregular poly(3-hexylthiophene) (RR-P3HT) thin films. The film thickness was varied by changing the RR-P3HT solution concentration and spin-coating speed. The hole mobility is found to monotonically increase from 10^{-4} cm^2/Vs to 10^{-3} cm^2/Vs along with film thickness from 100 nm to 700 nm and saturate at 10^{-3} cm^2/Vs beyond 700 nm. X-ray diffraction and ellipsometry data showed that the film morphology changes with the thickness. The structural change supports the weak dependence of energetic and positional disorder on thickness analyzed by the Gaussian Disorder Model (GDM).

4:18PM X49.00010 Contribution of Increased Extraction Efficiency to Increased Photo-Luminescence in Strained Polymer Films, PO-JUI CHEN, Dept. of Photonics Engineering, Yuan Ze University, ARNOLD CHANG-MOU YANG, Dept. of Materials Science and Engineering, National Tsing Hua University, JUI-HUNG HSU, Dept. of Material Science and Opto-electronic Science, National Sun Yat-sen University, JONATHON D. WHITE, Dept. of Photonics Engineering, Yuan Ze University — Potential applications of Luminescent Conjugated Polymers in thin film diodes, solar cells and flat panel displays have been limited by low efficiency. Craze formation in MEH-PPV/polystyrene thin film leads to a factor of 2 or 3 increase in collected photo-luminescence (PL) due to a combination of factors such as MEH-PPV chain conformation and increased extraction efficiency of PL. In order to determine the contribution of the latter effect, we used Monte Carlo based Ray Tracing to analyze the trajectory of photons generated in the thin film under different strain conditions. Our results indicate that increased PL extraction due to the existence of crazes contributes ~15% of the observed increase in PL, the majority of this being due to light emitted near the craze edges.

4:30PM X49.00011 Modeling charge and energy transports in π -conjugated systems, YONGWOO SHIN, XI LIN, Boston University — A generic 3D model Hamiltonian is developed to simulate the charge and energy transports in π -conjugated composite materials. The intrachain interactions are described by our recently developed adapted Su-Schrieffer-Heeger Hamiltonian and the interchain $\pi\pi$ interactions are modeled using distance-dependent hopping integrals. Excellent agreements in their binding energetics and geometries with post-Hartree-Fock ab initio methods and experiments are found in the cases of a benzene dimer, graphene bi-layer, and poly(*p*-phenylene vinylene) (PPV) crystal. The computed photoinduced charge separated states and associated adsorption spectra of the PPV-C₆₀ and PPV-C₆₀-graphene agree perfectly with experimental measurements.

4:42PM X49.00012 NMR, magnetic susceptibility, and electrical conductivity investigation of doped poly-3-methylthiophene¹, W.G. CLARK, G. GAIDOS, UCLA Physics and Astronomy, K.J. SINGH, R. MENON, K.P. RAMESH, Physics, IISc Bangalore, India, A.P. REYES, P. KUHNS, NHMFL, Tallahassee, FL, J.D. THOMPSON, LANL, Los Alamos, NM — We report ¹H and ¹⁹F NMR spin-lattice relaxation rate (1/*T*₁) measurements over a wide range of temperature (3 K < *T* < 300 K) and magnetic field (0.9 T < *B* < 23.4 T for ¹H and 9.0 T for ¹⁹F) in the organic conductor poly-3-methylthiophene (P3MT) doped with hexafluorophosphate (PF₆). Also included are measurements of the electrical conductivity (σ) at *B* = 0 and 77 K < *T* < 300 K and the magnetic susceptibility (χ) at *B* = 0.1 T and 2 K < *T* < 350 K. The doping level has been varied to tune the conductivity value at 300 K in the fully doped sample to $\sigma \sim 120$ S/cm and in the dedoped one to $\sigma \sim 5$ S/cm. This range enables investigation of the roles of carrier density and electron-electron interactions in the mechanisms for 1/*T*₁. A correlation between χ and the relaxation mechanisms is observed in these samples. The results are analyzed using the modified Korringa relation. Also, the proton and fluorine spin relaxation data give insight into the role of both inter-chain and intra-chain conduction mechanisms.

¹This work was supported by the DST and NSF in Grants DMR-0334689 and OISE-0225578, at LANL from the DOE Office of Science, and at the NHMFL from NSF Grant DMR-0084173 and the State of Florida.

4:54PM X49.00013 Improving Order and Mobility in MEH-PPV Films by Reducing Polydispersity¹, JONATHON WHITE, Yuan Ze University — The effect of polydispersity on morphology and charge transport in drop cast films of poly[2-methoxy-5-(2'-ethylhexyloxy)-*p*-phenylene vinylene] (MEH-PPV) was investigated using grazing incidence X-ray diffraction and time-of-flight respectively. Morphologically, reducing polydispersity by removing short chain segments promoted the capability of crystallization. This resulted in higher hole mobility and non-dispersive transport down to lower temperatures for the lower polydispersity sample. The slope for the Poole-Frenkel relationship at 298 K was increased, and its change with temperature decreased, indicating reduced spatial inhomogeneity. Analysis using Bassler's Gaussian disorder model (GDM), found that the value for energy disorder ($\sigma \sim 53$ meV for both films) and infinite temperature zero field mobility ($\mu_0 \sim 3 \times 10^{-6}$ cm²/Vs) were similar for both films. However, a good fit for hopping site separation and spatial disorder was only possible for the lower polydispersity device, suggesting that the lower polydispersity films have less mesoscopic inhomogeneity.

¹Supported by the National Science Council of the Republic of China

5:06PM X49.00014 Charge Transport in Amorphous Polythiophene-Fullerene Blends, KIARASH VAKHSOURI, DEREK KOZUB, Department of Chemical Engineering, Pennsylvania State University, CHENCHEN WANG, ALBERTO SALLEO, Materials Science and Engineering, Stanford University, ENRIQUE GOMEZ, Department of Chemical Engineering and Materials Research Institute, Pennsylvania State University — Energy-filtered transmission electron microscopy studies revealed that amorphous mixed phases are ubiquitous within mesostructured polythiophene/fullerene mixtures. Nevertheless, the role of mixing within nanophases on charge transport of organic semiconductor mixtures is not fully understood. We have examined the electron mobility in amorphous blends of poly(3-hexylthiophene) and phenyl-C₆₁-butyric acid methyl ester. Our studies reveal that the miscibility of the components strongly affects electron transport within amorphous blends. Immiscibility promotes efficient electron transport by promoting percolating pathways within organic semiconductor mixtures. As a consequence, partial miscibility may be important for efficient charge transport in polythiophene/fullerene mixtures and organic solar cell performance.

5:18PM X49.00015 Modeling energy transport in π -conjugated dendrimers containing triple bonds, PAK KAU LIM, YONGWOO SHIN, XI LIN, Department of Mechanical Engineering and Division of Materials Science and Engineering, Boston University — An accurate, transferrable, and computational efficient adapted Su-Schrieffer-Heeger model Hamiltonian is developed to describe triple bonds in linear and fractal-dimensional π -conjugated systems. Chemical accuracy in the computed optical gaps is found for the cases of poly-(thiophene-ethynylene) and poly-phenylacetylene of arbitrary lengths, with all errors less than 3% as compared to existing UV-visible adsorption spectra. The computed exciton migration processes in the phenylacetylene dendrimers indicates that such conjugated Bethe tree structures are efficient energy transduction funnels.

Thursday, March 1, 2012 2:30PM - 5:30PM –

Session X50 DPOLY DFD: Focus Session: Micro and Nano Fluidics II: Structured or Active Surfaces and Electrotransport 162B

2:30PM X50.00001 Dynamics of self-oscillating cilia designed from active polymer gels, PRATYUSH DAYAL, AMITABH BHATTACHARYA, OLGA KUKSENOK, ANNA C. BALAZS, University of Pittsburgh — Using theory and simulations, we design active synthetic surfaces which are capable of replicating functionalities of biological cilia. In order to design such exquisite biomimetic systems we harness unique properties of polymer gels that undergo photosensitive Belousov-Zhabotinsky (BZ) reaction. Powered by internalized BZ reaction these polymer gels swell and de-swell autonomously by chemo-mechanical transduction and therefore are ideal materials for designing our system. In order to simulate the dynamics of the BZ cilia in surrounding fluid we have developed a nonlinear hybrid 3D model which captures elasto-dynamics of polymer gel and diffusive exchange of BZ reagents between the gel and the fluid. Here we show that the geometrical arrangement of cilia and the distribution of BZ activator in the fluid determine the dynamic response of the cilia. We further show that using light as an external stimulus we can sequentially modulate height of individual cilium and thereby create the “piano effect”. Finally, we demonstrate that synchronized oscillations in the cilia result from the distribution of BZ-activator in the surrounding fluid. Our findings can be used to design active surfaces which can be remotely tuned depending upon the magnitude of external stimuli.

2:42PM X50.00002 Using actuated synthetic cilia to enhance microscale heat transport, ZACHARY G. MILLS, ALEXANDER ALEXEEV, Georgia Institute of Technology — We used three dimensional computer simulations to examine heat transport in a microchannel that encompasses a periodic array of actuated synthetic cilia. The channel was filled with a viscous fluid and its walls were maintained at different temperatures. Elastic synthetic cilia were attached to the bottom channel wall and were actuated by a periodic external force applied horizontally to their free ends. To model this multi-component system, we employed a thermal lattice Boltzmann model coupled with the lattice spring model. We probed how the beating cilia affect the heat transfer between channel walls, and how the thermal transport coefficient changes depending on the oscillating frequency and the relative distance between actuated filaments. Our findings could be useful for developing new methods for temperature control in microscale devices.

2:54PM X50.00003 Transport of Micro-particles by Active Cilia Arrays, AMITABH BHATTACHARYA, Department of Chemical Engineering, University of Pittsburgh, GAVIN BUXTON, Department of Science, Robert Morris University, O. BERK USTA, Center for Engineering in Medicine, Massachusetts General Hospital, ANNA. C. BALAZS, Department of Chemical Engineering, University of Pittsburgh — Biological organisms are known to use hair-like filaments called cilia to manipulate and transport particles. The coordinated motion of cilia is known to be effective at propelling surrounding fluid. In this work, we show that adhesive interaction between the actuated cilia and particulates can be crucial towards controlling particle transport. We model transport of a microscopic particle via a regular array of beating elastic cilium, whose tips experience an adhesive interaction with the particle's surface. At optimal adhesion strength, the average particle velocity is maximized. Using simulations spanning a range of cilia stiffness, particle radius, and cilia-particle adhesion strength, we explore the parameter space over which the particle can be “released,” “propelled” or “trapped” by the cilia. We use a low-order model to predict parameters for which the cilia are able to attach themselves to the particle. We also study the effect of varying the particle size and stiffness on its transport properties. This is the first study that shows how both stiffness and adhesion strength are crucial for manipulation of particles by active cilia arrays.

3:06PM X50.00004 Fluid flows around nanoelectromechanical resonators, O. SVITELSKIY, V. SAUER, N. LIU, D. VICK, K.M. CHENG, M.R. FREEMAN, W.K. HIEBERT, University of Alberta Physics Department and National Institute for Nanotechnology, Edmonton AB Canada — To explore properties of fluids on a nanosize scale, we fabricated by a standard top down technique a series of nanoelectromechanical resonators (cantilevers and bridges) with widths w and thicknesses t from 100 to 500 nm; lengths l from 0.5 to 12 micron; and resonant frequencies f from 10 to 400 MHz. For the sake of purity of the experiment, the undercut in the widest ($w=500$ nm) devices was eliminated using the focused ion beam. To model the fluidic environment the devices were placed in the atmosphere of compressed gases (He , N_2 , CO_2 , Ar , H_2) at pressures from vacuum up to 20 MPa, and in liquid CO_2 ; their properties were studied by the real time stroboscopic optical interferometry. Thus, we fully explored the Newtonian and non-Newtonian flow damping models. Observing free molecular flow extending above atmospheric pressure, we find the fluid relaxation time model to be the best approximation throughout, but not beyond, the non-Newtonian regime, and both, vibrating spheres model and the model based on Knudsen number, to be valid in the viscous limit.

3:18PM X50.00005 Dynamic Similarity Principle for Nanoscale Resonant Devices in Gaseous Environments, CARYN BULLARD, MICHAEL ROUKES, California Institute of Technology, JOHN SADER, JIANCHANG LI, PAUL MULVANEY, The University of Melbourne — The mechanical performance of cantilevers on the nanoscale operating in atmosphere is dominated by gas damping. However, theoretical modeling of gas-solid interactions on the nanoscale is non-trivial due to the non-continuum nature of the gas flow. In addition, these gas-structure interactions can significantly affect the sensitivity of these devices. Instead of using numerical simulations to determine the gas flow and consequently, gas damping, of a nanoscale device, we used a general dynamic similarity principle to determine the gas damping of a nanoscale device by measuring the gas damping of a scaled up prototype device.

3:30PM X50.00006 Computational modeling of traveling wave electrophoresis¹, ROBERT CORRELL, JARROD SCHIFFBAUER, LLOYD CARROLL, West Virginia University — Traveling wave electrophoresis (TWE) is a microfluidic separation technique in which electrodes flanking a microchannel apply a traveling potential wave along the channel. Charged particles, including small molecules, proteins, and nanoparticles are differentially transported along the channel at a rate dependent on their mobility. TWE is ideally suited for application in lab-on-a-chip and field deployed sensor systems. In order to fully exploit this technology, a series of computational models have been developed, including 1-dimensional and 2-dimensional models. These models allow for testable predictions of single-particle motion, and the effects of factors such as pH and concentration upon separation efficiency. Efforts to include diffusive components within the model, and to consider the motion of bands, rather than single particles will be discussed.

¹This work is funded through NSF CBET-1066730 and the NSF RII award EPS-1003907, for which the WV EPSCoR Office and the WVU Research Corporation provided matching funds.

3:42PM X50.00007 Activated wetting dynamics in the presence of mesoscopic surface disorder, KRISTINA DAVITT, Laboratoire de Physique Statistique - ENS, MICHAEL PETTERSEN, Washington and Jefferson College, ETIENNE ROLLEY, Laboratoire de Physique Statistique - ENS — Although disorder is commonly used to explain contact angle hysteresis, it is often neglected when considering wetting dynamics. When viscous forces are negligible, contact-line velocity is modelled by the Molecular Kinetic Theory [1], which predicts an activated motion driven by molecular jumps on preferential adsorption sites. We believe that in the presence of mesoscopic disorder, this model can be reinterpreted and that the activation length is no longer molecular-sized but is related to depinning events on the surface. This hypothesis is supported by a study of the wetting of cesium by liquid hydrogen in which it was shown that the activation length is of the order of the expected roughness [2]. However, no systematic study between the activation area and the length scale of the disorder has previously been made. We study wetting dynamics on metal films evaporated under different conditions, allowing us to obtain films with lateral grain sizes ranging from 10 to 200 nm. We find that the activation area deduced from wetting experiments is coherent with these sizes; however, its precise relation to the scale of disorder is not clear.

[1] T.D. Blake and J.M. Haynes, J. Colloid Interface Sci. 30, 421 (1969)

[2] E. Rolley and C. Guthmann, PRL 98, 166105 (2007)

3:54PM X50.00008 Experimental test of Schrodinger's first-passage-time theory using colloids in micro-channels, SUNGCHEOL KIM, XINSHENG LING, Brown University — We report an experimental study of the first-passage-time problem of driven diffusion in micro-channels. Fluorescent microspheres of 190nm diameter are confined in channels of 1.0 micron in width and 1.0 micron depth and driven by an applied longitudinal electric field. The images are acquired by a fluorescent microscope. The time dependence of the particle positions is tracked using particle tracking algorithms. The first passage times at different electric field values are extracted from the real-time data and compared with the exact solution given by Schrodinger for the 1D biased diffusion equation with one absorbing boundary condition.

4:06PM X50.00009 Liquid-impregnated surfaces: overcoming the limitations of superhydrophobic surfaces for robust non-wetting and anti-icing surface, J. DAVID SMITH, RAJEEV DHIMAN, ERNESTO REZA-GARDUNO, GARETH MCKINLEY, ROBERT COHEN, KRIPA VARANASI, None — In this work we address fundamental limitations of superhydrophobic surfaces for non-wetting and anti-icing applications by impregnating them with a hydrophobic liquid. The impregnating liquid serves as a barrier to the penetration of impinging water droplets and forces preferential condensation and frost formation on texture tops. We predict the thermodynamically stable wetting states based on a free energy analysis, and model the behavior of rolling droplets on liquid-impregnating surfaces. We conducted droplet impact and roll-off experiments to assess the robustness of liquid-impregnated micro- and nano-scale textured surfaces and found that their ability to shed droplets was improved dramatically. Furthermore, environmental scanning electron microscope experiments demonstrated that frost formation as well as condensation occurs preferentially on these surfaces thereby limiting ice contact to texture tops only. Ice adhesion strength was quantified using a custom-built adhesion testing apparatus to demonstrate greatly enhanced anti-icing performance of the liquid-impregnating surfaces compared to superhydrophobic surfaces.

4:18PM X50.00010 Using Superhydrophobic Surfaces and Optical Caustics to Detect Nanoparticle Aggregation, ANTONIO GARCIA, JAMES LINDSAY, ERIC GILMORE, None — A 3-D envelope of refracted light known as an optical caustic, can be formed by shaping an aqueous drop on a superhydrophobic surface which is used to generate a signal that is very sensitive to changes in particle size. When the sample being detected is suspended in the drop, slow evaporation induces movement that segregates smaller from larger particles, enhancing the speed of detection via induced aggregation. While the unique properties of optical caustics have been used in engineering science to evaluate stress distributions and contact between material components, they have not been widely used in diagnostics or biological analyses. This paper demonstrates how this method can track aggregation of gold nanoparticles for rapid detection of molecular disease markers using immunoassays.

4:30PM X50.00011 Droplet condensation and growth on nanotextured surfaces impregnated with an immiscible liquid, SUSHANT ANAND, ADAM PAXSON, JONATHAN SMITH, RAJEEV DHIMAN, KRIPA VARANASI, Massachusetts Institute of Technology — For effective dropwise condensation, a surface that sheds droplets easily is desirable due to the enhancement in accompanying heat transfer. Incorporating nano-textures on the surface can enhance the droplet shedding or spreading. We demonstrate that droplet shedding can be further influenced by impregnating the nano-textured surface with a liquid which is immiscible with respect to the droplet. In this study, the dynamics of dropwise condensation on such immiscible liquid impregnated nano-textured surfaces have been investigated in pure quiescent water vapor conditions. Condensation experiments were conducted using an Environmental Scanning Electron Microscope by controlling the chamber water vapor pressure and substrate temperature. We show preferential sites for condensation and different modes under which droplets grow, depending upon the surface chemistry, surface texture, and the impregnating liquid properties. Concurrently, we show an evolution of apparent contact angles during the condensation process on the impregnated surfaces.

4:42PM X50.00012 Molecular diffusion and tensorial slip at surfaces with periodic and random nanoscale textures¹, NIKOLAI PRIEZJEV, Michigan State University — The influence of periodic and random surface textures on the flow structure and effective slip length in Newtonian fluids is investigated by molecular dynamics (MD) simulations. This study is motivated by the possibility to generate transverse flows in microfluidics devices to enhance mixing and separation processes. We consider a situation where the typical pattern size is smaller than the channel height and the local boundary conditions at wetting and nonwetting regions are characterized by finite slip lengths. In case of anisotropic textures, the interfacial diffusion coefficient of fluid molecules near heterogeneous surfaces correlates well with the effective slip length as a function of the shear flow direction with respect to the texture orientation. In addition, it was found that the angular dependence of the effective slip length obtained from MD simulations is in good agreement with hydrodynamic predictions provided that the pattern size is larger than several molecular diameters. These findings lend support for the microscopic justification of recently introduced tensor formulation of the effective slip boundary conditions in the case of noninertial flows of Newtonian fluids over smooth surfaces with nanoscale anisotropic textures.

¹Funding from NSF (CBET-1033662) is gratefully acknowledged.

4:54PM X50.00013 Wetting as a basis for a highly selective colorimetric indicator for organic liquids¹, IAN BURGESS, School of Engineering and Applied Sciences, Harvard University, KEVIN RAYMOND, NATALIE KOAY, Wyss Institute for Biologically Inspired Engineering, Harvard University, ANNA SHNEIDMAN, MATHIAS KOLLE, MARKO LONCAR, JOANNA AIZENBERG, School of Engineering and Applied Sciences, Harvard University — We present a colorimetric indicator for organic liquids that couples distinct macroscopic color patterns to minute differences in liquids' intrinsic wettability to a surface. We find that when a liquid percolates through the pores of large-area, defect-free silica inverse-opal films, a highly consistent re-entrant geometry leads to sharply defined threshold wettability for liquid infiltration, occurring at intrinsic contact angles near 20°. The structure also acts as a 3D photonic crystal, producing bright iridescent color that disappears when infiltrated with liquid, coupling the highly selective wetting observed to an easy-to-visualize colorimetric response. Combining a percolation model and FDTD optical simulations, we estimate the selectivity of the colorimetric response. In addition, we present a technique to generate precisely controlled spatial patterns of surface chemistry throughout the porous network. This lets us tailor the wettability threshold to specific liquids across a continuous range. Using these techniques, we demonstrate the applicability of this indicator to colorimetrically distinguish: i) ethanol-water mixtures varying by only 2.5% in concentration; ii) hexane, heptane, octane, nonane, and decane; and iii) samples of gasoline (regular unleaded) and diesel.

¹Supported by the AFOSR Award # FA9550-09-1-0669-DOD35CAP.

5:06PM X50.00014 Drag Measurements in Laminar Flows over Superhydrophobic Porous Membranes, OZGUR OZSUN, VICTOR YAKHOT, KAMIL L. EKINCI, Boston University — An anomalous hydrodynamic response has recently been observed in oscillating flows on mesh-like porous superhydrophobic membranes.¹ This effect was attributed to a stable Knudsen layer of gas at the solid-liquid interface. In this study, we investigate laminar channel flow over these porous superhydrophobic membranes. We have fabricated surfaces with solid area fraction ϕ_s , which can maintain intimate contact with both air and water reservoirs on either side. Typical structures have linear dimensions of 1.5 mm $\times$ 15 mm $\times$ 1 μ m and pore area of 10 μ m $\times$ 10 μ m. The surfaces are enclosed with precisely machined plastic microchannels, where pressure driven flow of DI water is generated. Pressure drop across the microchannels is measured as a function of flow rate. Slip lengths are inferred from the Poiseuille relation as a function of ϕ_s and compared to that of similar standard superhydrophobic surfaces, which lack intimate contact with an air reservoir.

¹S. Rajauria, O. Ozsun, J. Lawall, V. Yakhot, and K. L. Ekinci, Phys. Rev. Lett. 107, 174501 (2011)

5:18PM X50.00015 Thermo-super-hydrophobic effect, JERZY M. FLORYAN, The University of Western Ontario — Super-hydrophobic effect involves capture of gas bubbles in pores of solid wall. These bubbles separate moving liquid from the solid surface resulting in a substantial reduction of shear drag experienced by the liquid. The super-hydrophobic effect requires presence of two phases and thus drag reduction can be accomplished only for liquids. Thermo-super-hydrophobic effect takes advantage of the localized heating to create separation bubbles and thus can work with single phase flow systems. Analysis of a simple model problem shows that this effect is very strong in the case of small Re flows such as those found in micro-channels and can reduce pressure drop down to 50% of the reference value if the heating pattern as well as the heating intensity are suitably chosen. The thermo-super-hydrophobic effect becomes marginal when Re increases above a certain critical value.

Thursday, March 1, 2012 2:30PM - 5:18PM –
Session X52 GSNP DFD: Focus Session: Extreme Mechanics - Fracture, Friction, and Frequencies 153C

2:30PM X52.00001 Geometry of Tearing: crack propagation in brittle sheets¹, BENOIT ROMAN, JOSE BICO, PMMH CNRS/ESPCI/UPMC/Paris7 - Paris France, ENRIQUE CERDA, EUGENIO HAMM, FRANCISCO MELO, VICTOR ROMERO, Departamento de Física, Universidad de Santiago de Chile — We experiment the fracture of thin object everyday when trying to open a packaging. From a physics point of view, the propagation of cracks in thin brittle elastic sheets appears to be remarkably reproducible, with very regular crack path. We will present some examples where the crack path can be predicted using classical arguments in fracture and geometrical tools: this is another example where geometry plays a central role in the mechanics of thin sheets.

¹We thank ANR MecaWet

2:42PM X52.00002 Spiral and croissant crack in drying thin films, JOEL MARTHELOT, BENOIT ROMAN, JOSE BICO, PMMH ESPCI ParisTech, ETIENNE BARTHEL, JEREMIE TEISSEIRE, DAVY DALMAS, SVI CNRS Saint Gobain, FRANCISCO MELO, USACH — Drying mud or crazing in ceramics glaze leads to familiar hierarchical cracks network where a new crack connects perpendicularly to older ones. We report unusual spirals and croissants crack patterns in methylsiloxane drying thin films moderately adhering on a substrate. Such cracks are also observed in a very different situation when magnetron sputtering multilayers are under external tension. The amplitude and wavelength of the pattern are robust and are orders of magnitude larger than the thickness of the layer. The propagation of the spiral and croissant cracks occurs in a narrow range of adhesion energy between the film and the substrate and strain in the film. We will show how the propagation is driven by a cooperation between fracture and adhesion.

2:54PM X52.00003 Rupture of a highly stretchable acrylic dielectric elastomer, GEORGE PHARR, Harvard University, JEONG-YUN SUN, Seoul National University and Harvard University, ZHIGANG SUO, Harvard University — Dielectric elastomers have found widespread application as energy harvesters, actuators, and sensors. In practice these elastomers are subject to large tensile stretches, which potentially can lead to mechanical fracture. In this study, we have examined fracture properties of the commercial acrylic elastomer VHB 4905. We have found that inserting a pre-cut into the material drastically reduces the stretch at rupture from $\lambda_{rup} = 9.43 \pm 1.05$ for pristine samples down to only $\lambda_{rup} = 3.63 \pm 0.45$ for the samples with a pre-cut. Furthermore, using “pure-shear” test specimens with a pre-crack, we have measured the fracture energy and stretch at rupture as a function of the sample geometry. The stretch at rupture was found to decrease with sample height, which agrees with an analytical prediction. Additionally, we have measured the fracture energy as a function of stretch-rate. The apparent fracture energy was found to increase with stretch-rate from $\Gamma \approx 1500 \text{ J/m}^2$ to $\Gamma \approx 5000 \text{ J/m}^2$ for the investigated rates of deformation. This phenomenon is due to viscoelastic properties of VHB 4905, which result in an apparent stiffening for sufficiently large stretch-rates.

3:06PM X52.00004 How does adhesion impact the formation of telephone cord buckles?, ETIENNE BARTHEL, JEAN-YVON FAOU, SERGEY GRACHEV, CNRS / Saint-Gobain, GUILLAUME PARRY, SIMAP — Compressively stressed thin films with low adhesion frequently buckle into telephone cords. Although telephone cord buckles have been studied for decades, no complete understanding of their origin and propagation has so far been presented. Here, using Finite Element Analysis, we have coupled non-linear plate deformation with a cohesive zone model to simulate the kinematics of a propagating telephone cord buckle. On the experimental side, we have developed model thin films with a precise adjustment of both adhesion and residual stresses. From the comparison of the simulations with some experimental observations, we propose a generic mechanism for the formation of telephone cord buckles. Proper inclusion of the dependence of interfacial toughness upon mode mixity proved to be central to the success of the approach so that this clarification of the mechanism of telephone cord formation promises better understanding of interfacial toughness through the analysis of buckle morphology.

3:18PM X52.00005 Nonlinear modal interactions in a microcantilever¹, HIDDE WESTRA, HERRE VAN DER ZANT, WARNER VENSTRA, Kavli Institute of Nanoscience, Delft University of Technology — We study the nonlinear interactions between vibrational modes in a microcantilever. The flexural-flexural, torsional-torsional and torsional-flexural modal interactions are investigated theoretically and experimentally. In a cantilever, the nonlinearity arising from geometrical and inertial effects couples the different modes. The motion of one mode influences the resonance frequency of the other modes. We show that depending on the amplitude of one mode, both frequency stiffening and weakening of the other mode occurs. The modal interactions in clamped-clamped beam resonators is recently studied, and several applications have been proposed. Microcantilevers are frequently used in instrumentation, and the modal interactions presented here enable such schemes, including Q-factor tuning and self-detection.

¹The authors acknowledge financial support from the Dutch funding organization FOM (Physics for Technology)

3:30PM X52.00006 Effects of Roughness and Inertia on Precursors to Frictional Sliding¹, MARK O. ROBBINS, K. MICHAEL SALERNO, Johns Hopkins University — Experiments show that when a PMMA block on a surface is normally loaded and driven by an external shear force, contact at the interface is modified in discrete precursor slips prior to steady state sliding.[1] Our simulations use an atomistic model of a rough two-dimensional block in contact with a flat surface to investigate the evolution of stress and displacement along the contact between surfaces. The talk will show how local and global stress conditions govern the initiation of interfacial cracks as well as the spatial extension of the cracked region. Inertia also plays an important role in determining the number and size of slips before sliding and influences the distribution of stresses at the interface. Finally, the geometry of surface asperities also influences the interfacial evolution and the total friction force. The relationship between the interfacial stress state and rupture velocity will also be discussed. [1] S.M. Rubinstein, G. Cohen and J. Fineberg, PRL 98, 226103 (2007)

¹Supported by AFOSR FA9550-0910232

3:42PM X52.00007 Scratch test as a fracture process: from soft to hard materials, ANGE-THERESE

AKONO, Dept of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA, PEDRO MIGUEL REIS, Dept of Civil and Environmental Engineering & Dept of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA, NICHOLAS XAVIER RANDALL, CSM Instruments, Needham, MA, USA, FRANZ-JOSEF ULM, Dept of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA — The scratch test consists of driving a probe, at a certain depth, through a material and is most likely the oldest technique for the mechanical characterization of materials. Although it is widely used in strength testing, the presence of residual chips during the process suggests that a fracture mechanism is at play. We investigate the link between the material fracture properties, the probe geometry and the resulting forces using a combination of precision experiments and Linear Elastic Fracture Mechanics analysis. An analytical model is developed that is applicable both at the macro and micro scale, and that can take into account different probe geometries. Rationalizing the mechanics involved allows us to introduce a novel experimental technique to accurately determine the fracture toughness from scratch tests. Application of this technique to mechanical testing on metals, polymers and ceramics yields values for the fracture toughness that are in excellent agreement with conventional methods such as the three-point bending test, albeit in a way that is less destructive and more scalable. As such, our method to determine materials fracture properties represents an important new development in the field of mechanical micro-characterization.

3:54PM X52.00008 Sliding on a Nanotube: Interplay of Friction, Deformations and Defects, HSIANG-CHIH CHIU, SUENNE KIM, School of Physics, Georgia Institute of Technology, ERIO TOSATTI, International School for Advanced Studies (SISSA), and CNR-IOM Democritos, CHRISTIAN KLINKE, Institute of Physical Chemistry, University of Hamburg, ELISA RIEDO, School of Physics, Georgia Institute of Technology — Carbon nanotubes (CNT) have applications as composite material reinforcements and components in nanodevices due to their exceptional physical properties. However, CNTs have structural defects that can change their mechanical properties. For applications, CNTs have to be in contact with other surfaces, thus it is important to understand how defects change their frictional properties. Here, we show that defects can impact the frictional properties of supported Arc Discharge (AD) and Chemical Vapor Deposition (CVD) grown CNTs by sliding an AFM tip along (longitudinal) and across (transverse) the CNT axis. Larger friction coefficient is found during transverse sliding due to a lateral CNT deformation (called hindered rolling) that causes extra friction dissipation which is absent during longitudinal sliding.[1] A friction anisotropy, defined as the ratio of shear strength measured during both sliding directions, can be as high as 13.7 for AD CNTs but less than 6 for CVD CNTs. Extra defects in CVD CNTs couple both sliding motions, resulting in more energy dissipation and higher longitudinal friction. A simple analytical model is developed to explain the observed experimental behavior. Our finding provides a better understanding of tribological properties of individual CNT at the nanoscale. [1] M. Lucas et al., Nature Mater. 8, 876 (2009)

4:06PM X52.00009 Graphene Morphology on Nano-Patterned Electronic Substrates, GUANGXU LI, CIHAN YILMAZ, XIAOHONG AN, SIVASUBRAMANIAN SOMU, SWASTIK KAR, AHMED BUSNAINA, KAI-TAK WAN, Northeastern University, DEPARTMENT OF MECHANICAL AND INDUSTRIAL ENGINEERING COLLABORATION, NSF NANOSCALE SCIENCE AND ENGINEERING CENTER FOR HIGH-RATE NANOMANUFACTURING COLLABORATION, DEPARTMENT OF PHYSICS COLLABORATION — In order to get high quality of graphene for the application in electronic devices, good transfer of graphene prepared by mechanical exfoliation or chemical vapor deposition is always required and substrate with flat surface is preferred to avoid the crack and destruction of the thin sheets. Here, we studied the graphene morphology on nano-patterned electronic substrates by transferring graphene grown from chemical vapor deposition onto the gold nano pillar patterns on silicon substrate. The adhesion between the graphene and the gold surface makes the flexible thin membrane conform to the substrate geometry and form a series of blisters. By measuring the blister radius and height, the adhesion energy of graphene and gold substrate can be deduced. In the meantime, the morphology of graphene on the pillar patterns was found to strongly related to the adhesion energy, the height and separation of pillars. By changing these parameters, the blisters may decrease size or expand to coalesce. The critical separation between pillars and the critical height of pillars were predicted to avoid the coalescence of the blisters when the adhesion energy was fixed. The results obtained here can be useful to increase the performance and the durability of the graphene based device.

4:18PM X52.00010 Graphene Blister Adhesion Mechanics¹, NARASIMHA BODETTI, STEVEN KOENIG, JIAN-LIANG XIAO, SCOTT BUNCH, MARTIN DUNN, University of Colorado — We describe graphene blister configurations to study the elasticity of mono- and multi-layer graphene as well as the adhesion of the blister to an SiO₂ substrate. We create blisters by depositing graphene on a chip containing etched cavities of a prescribed volume. The chip is placed in a high-pressure chamber where the cavities are charged to a prescribed pressure. When the chip is removed from the chamber the pressure difference across the membrane causes it to bulge, while the number of gas molecules in the chamber remains constant. As the pressure is increased the membrane continues to bulge and at a critical pressure can delaminate (in a stable or unstable manner) permitting extraction of the adhesion energy from a combination of theory and measurements of the deformed blister configuration. We describe these experiments and develop a thermodynamic model of the system that identifies interesting nonlinear effects as the membranes deform including instabilities, delamination, and adhesion hysteresis, depending on the configurational parameters. We use the theory and experiments together to determine for the first time the adhesion energy between graphene and SiO₂, as well as explore the interesting mechanics that occur.

¹National Science Foundation, DARPA

4:30PM X52.00011 Novel method for simulation of structural post buckling, RACHMADIAN WULAN-DANA, Dept. of Mechanical Engineering and Materials Science, University of Pittsburgh, Pittsburgh, PA, SACHIN VELANKAR, Dept. of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA — A new FEM-based method for simulating the onset of buckling instabilities and the post-buckling evolution is developed. The method consists of creating a random spatial perturbation of the elastic modulus and applying a step-by-step loading to approach the critical state and beyond. Prior to buckling, the non-uniform modulus triggers micro bending and lateral deformation. As the compressive load progresses, the micro displacement grows non-linearly causing the system to be biased toward the mode that minimizes energy. The system buckles in that mode and the post-buckling deformation can be examined. The technique has been applied to several buckling cases. The results show quantitative agreement with theory and experiments. For problems with continuously-distributed buckling modes and critical values that are close from one to another, the method is able to automatically select the correct critical configuration. Unlike other perturbation methods that are inspired by either Eigen vectors or experimental data, the current method does not need a priori knowledge of the expected buckling mode. This is especially useful in complex problems (e.g. wrinkling of stretched films) for which linear eigenvalue analysis cannot predict the critical conditions.

4:42PM X52.00012 Buckling morphologies of crystalline shells with frozen defects, EE HOU YONG, Harvard University, PROF. L. MAHADEVAN (HARVARD UNI.) COLLABORATION — The crumpling of spherical crystalline lattices where the topological defects are frozen is studied. The geometry of the crumpled membrane is found to depend on the set of topological defects and more exotic defect sets can result in crumpled shapes resembling that of the Platonic and Archimedean solids. The phase diagram of the crumpled spheres can be categorized by two dimensionless numbers h/R (aspect ratio) and R/a (lattice ratio), where h is the thickness of the shell, R is the radius of the initial sphere and a is the average bond length of the triangulation. The shapes of the crumpled membrane can be understood using rotationally invariant quantities formed from spherical harmonics coefficients and a Landau free energy can be written, involving quadratic and cubic rotational invariants. Shells with different topological defects have qualitatively different hysteresis behaviors and the transitions appear to be first order in general.

4:54PM X52.00013 Do tidal stresses trigger large earthquakes early? , BRADEN BRINKMAN, MICHAEL LEBLANC, University of Illinois at Urbana-Champaign, JONATHAN UHL, None, YEHUDA BEN-ZION, University of Southern California, KARIN DAHMEN, University of Illinois at Urbana-Champaign — The effect of tidal or other periodic stresses on the timing of large earthquakes is a hotly debated topic in geophysics and rock-friction or granular physics communities. I discuss a simple probabilistic model which captures the main qualitative features of several rock-friction or granular experiments and may resolve some outstanding discrepancies between different experimental results. With sufficiently accurate measurements, quantitative predictions for real experiments are possible, including the number of measured events needed to detect correlations between periodic stresses and large slip events for given amplitudes and frequencies.

5:06PM X52.00014 Tattoo-Like Strain Gauges Based on Silicon Nano-Membranes , NANSHU LU, University of Texas at Austin, LU RESEARCH GROUP TEAM — This talk reports the in vivo measurement of tissue deformation through adhesive-free, conformable lamination of a tattoo-like elastic strain gauge consisted of piezoresistive silicon nano-membranes strategically integrated with tissue-like elastomeric substrates. The mechanical deformation in soft tissues cannot yet be directly quantified due to the lack of enabling tools. While stiff strain gauges for structural health monitoring have long existed, biological tissues are soft, curvilinear and highly deformable in contrast to civil or aerospace structures. An ultra-thin, ultra-soft, tattoo-like strain gauge that can conform to the convoluted surface of human body and stay attached during locomotion will be able to directly quantify tissue deformation without affecting the mechanical behavior of the tissue. While single crystalline silicon is known to have the highest gauge factor and best elastic response, it is intrinsically stiff and brittle. To achieve strain gauges with high compliance, high stretchability and reasonable sensitivity, single crystalline silicon nano-membranes will be transfer-printed onto polymeric support through carefully engineered stamps. The thickness and length of the Si strip will be chosen according to theoretical and numerical mechanics analysis which takes into account for the tradeoff between stretchability and sensitivity.

Thursday, March 1, 2012 2:30PM - 5:42PM –
Session X53 GSNP: Focus Session: Common Features of Soft Materials: Polymers, Colloids and Granular Media II 153B

2:30PM X53.00001 Shear thickening and jamming in suspensions of different particle shapes , ERIC BROWN, University of California, Merced, HANJUN ZHANG, NICOLE FORMAN, DOUGLAS BETTS, JOSEPH DESIMONE, University of North Carolina, Chapel Hill, BENJAMIN MAYNOR, Liquidia Technologies, HEINRICH JAEGER, The University of Chicago — We investigated the role of particle shape on shear thickening and jamming in densely packed suspensions. Various particle shapes were fabricated including rods of different aspect ratios and non-convex hooked rods. A rheometer was used to measure shear stress vs. shear rate for a wide range of packing fractions for each shape. Each suspensions exhibits qualitatively similar Discontinuous Shear Thickening, in which the logarithmic slope of the stress vs. shear rate has the same scaling for each convex shape and diverges at a critical packing fraction ϕ_c . The value of ϕ_c varies with particle shape, and coincides with the onset of a yield stress, a.k.a. the jamming transition. This suggests the jamming transition controls shear thickening, and the only effect of particle shape on steady state bulk rheology of convex particles is a shift of ϕ_c . Intriguingly, viscosity curves for non-convex particles do not collapse on the same set as convex particles, showing strong shear thickening over a wider range of packing fraction. Qualitative shape dependence was only found in steady state rheology when the system was confined to small gaps where large aspect ratio particle are forced to order.

2:42PM X53.00002 Fluctuations and Avalanche Statistics in Sheared Systems of Elliptical Particles¹ , SOMAYEH FARHADI, ROBERT P. BEHRINGER, Duke University — We have performed a series of 2D Couette shear experiment on a system of granular particles near jamming. In these experiments, the particles, which are photoelastic ellipses with aspect ratio 2, are confined between an inner rotating wheel and a fixed outer ring. The inner wheel rotation rate was varied between 0.01 and 0.1 rpm. Using photoelastic properties of the particles and two synchronized cameras, we are able to track the position, orientation and contact forces of each particle through the entire experiment. We determined the local mean, fluctuations, and correlations for various system properties, such as density (Voronoi volume), pressure, orientational order parameter and shear rate. A striking finding of this study is the fact that near jamming, the system can exist in an effectively shear jammed metastable state for very long times before relaxing to an unjammed state. We have also studied the dynamics of avalanches by analyzing the time series of global stress. This study gives us insight to the nature of failure in sheared systems of asymmetrical particles.

¹Grant Acknowledgement: NSF DMS-0835742, DMR-0906908

2:54PM X53.00003 Mapping From Soft to Hard-Core Disks Near the Athermal Shear Driven Jamming Transition¹ , PETER OLSSON, Department of Physics, Umeå University, 90187 Umeå, STEPHEN TEITEL, Department of Physics and Astronomy, University of Rochester, Rochester, NY 14627 — We examine the rheology of soft-core, bidisperse, frictionless disks in two dimensions at zero temperature with overdamped dynamics. For shear driven flow at a uniform strain rate $\dot{\gamma}$, we find a simple expression for an effective hard-core packing fraction, ϕ_{eff} , such that the pressure equivalent to the shear viscosity, $p/\dot{\gamma}$, for different shear rates, packing fractions, and different contact interactions all collapse onto a common curve when plotted as a function of ϕ_{eff} . This function is a characteristic of the hard-core limit as it describes the system in the limit of vanishing particle overlaps. This mapping recovers all the critical behavior found in earlier scaling analyses. We use this mapping to derive a duality relation that gives the exponent of the non-linear Herschel-Bulkley rheology *above* jamming in terms of the exponent of the diverging viscosity *below* jamming.

¹Work supported by Energy Grant No. DE-FG02-06ER46298 and Swedish Research Council Grant No. 2010-3725. Simulations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at PDC and HPC2N.

3:06PM X53.00004 Hot spots in an athermal system , JEROME CRASSOUS, AXELLE AMON, IPR UMR 6251, Université Rennes 1, France, VAN BAU NGUYEN, PMMH, ESPCI, UMR CNRS 7636 and Université Paris 6 & Paris 7, 75005 Paris, France, ARY BRUAND, ISTO, UMR 6113, 45000 Orléans, France, ERIC CLEMENT, PMMH, ESPCI, UMR CNRS 7636 and Université Paris 6 & Paris 7, 75005 Paris, France — We study experimentally the dynamical heterogeneities occurring at slow shear, in a model amorphous glassy material i.e. a 3D granular packing. The deformation field is resolved spatially using a Diffusive Wave Spectroscopy technique. The heterogeneities show up as localized regions of strong deformations spanning a mesoscopic size of about 10 grains and called the 'hot spots'. The spatial clustering of hot-spots is linked to the subsequent emergence of shear bands. Quantitatively, their apparition is associated with the macroscopic plastic deformation and their rate of occurrence gives a physical meaning to the concept of "fluidity," recently used to describe the local and non-local rheology of soft glassy materials.

3:18PM X53.00005 Effect of Inertial Mass on Velocity Correlations of Shear Driven Soft-Core Disks Approaching the Athermal Jamming Transition¹

, DANIEL VÅGBERG, PETER OLSSON, Umeå University, 90187 Umeå, Sweden, STEPHEN TEITEL, University of Rochester, Rochester, NY 14627 — It was found numerically that overdamped, frictionless, soft-core disks undergoing uniform shear driven flow, show differences in behavior depending on how the viscous dissipation is introduced into the numerical simulation. When dissipation is with respect to a sheared external reservoir (the so-called “mean-field” approximation), velocity correlations are found to determine a finite length scale ξ that diverges as the jamming transition is approached[1]. However, when dissipation is modeled by inter-particle inelastic collisions, the velocity correlations show no characteristic length other than the length of the system[2]. To study the relation between these two models of dissipation, we remove the overdamped constraint and consider particles with finite inertial mass m , and study how velocity correlations behave as the overdamped limit $m \rightarrow 0$ is approached.

[1] P. Olsson and S. Teitel, Phys. Rev. Lett. **99**, 178001 (2007).

[2] B. P. Tighe et al. Phys. Rev. Lett. **105**, 088303 (2010).

¹Work supported by Energy Grant No. DE-FG02-06ER46298 and Swedish Research Council Grant No. 2010-3725. Simulations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at PDC and HPC2N.

3:30PM X53.00006 Stretching dense colloidal suspensions: from flow to fracture

, MICHAEL SMITH, University of Nottingham, RUT BESSELING, ANDREW SCHOFIELD, University of Edinburgh, JAMES SHARP, University of Nottingham, MIKE CATES, University of Edinburgh, VOLFANGO BERTOLA, University of Liverpool — Concentrated suspensions of particles are commonly used in the pharmaceutical, cosmetic and food industries. Manufacture of these products often involves flow geometries that are substantially different from those studied by conventional shear rheology. Using a capillary break-up extensional rheometer we stretch fluids of different volume fraction at strain rates just below, at and above the critical rate required to induce jamming. We show that the jamming of a stretched colloidal column is closely related to that observed during shear rheology. However, fascinating additional effects due to the geometry are also observed. High speed photography of the filament shows evidence of dilatancy and granulation, leading finally to fracture at a critical strain rate. We also investigate an intriguing aspect of thin fluid filaments of the colloidal suspension, when stretched below the critical strain rate required to produce jamming. These filaments are observed to thin to a critical diameter before rupturing and displaying visco-elastic recoil. Finally, using fluorescent particles we visualise the flow fields inside these filaments to understand the dynamics.

3:42PM X53.00007 Fluctuations for Hopper Flow with Circular and Elliptical Particles¹

, JUNYAO TANG, Duke University — Recent studies have shown the importance of particle-scale fluctuations in granular flow, e.g. “stick-slip” and jamming. In this talk, we consider 2-D hopper flow, where we investigate how the mean and fluctuations of stress, velocity and density fields depend on hopper geometry (e.g. opening size and wall angle) and material properties (e.g. particle shape and initial filling height of materials). A particularly interesting observation is that the mean stress is a decreasing function of the filling height, even though the flux is nearly constant over the same range of material heights. We also find strong negative correlations between stress and velocity fluctuations. Also of interest is the effect of the particle orientation in the flow of elliptical particles. Related MD/DEM studies (supported by IFPRI and NSF) by Shattuck, Kondic and McCarthy et al. have found that good agreement between models and experiments for these flows.

¹This work is funded by IFPRI and the grant NSF-CBET-1010008

3:54PM X53.00008 Rheology and Jamming in Soft Colloidal System¹

, ANINDITA BASU, TIM STILL, Department of Physics and Astronomy, University of Pennsylvania, PAULO ARRATIA, Mechanical Engineering and Applied Mechanics, University of Pennsylvania, KERSTIN NORDSTROM, Department of Physics and Astronomy, University of Pennsylvania, JERRY GOLLUB, Department of Physics and Astronomy, Haverford College, DOUGLAS DURIAN, ARJUN YODH, Department of Physics and Astronomy, University of Pennsylvania — Recent simulations have proposed that the jamming transition can be understood in the framework of critical phenomena, and thus can be described by various asymptotic scaling laws. We use thermosensitive colloidal suspensions and a commercially available rheometer to study the shear response of soft colloidal glass across the jamming transition. We carry out steady-state (viscometry) and time-dependent (oscillatory) rheology experiments in the vicinity of the jamming transition. Both viscometry and oscillatory stress data exhibit asymptotic scaling and presence of critical exponents reminiscent of second-order phase transition, as reported in recent simulations. Critical scaling of frequency indicates the presence of a diverging time-scale associated with the jamming transition. We attempt to understand these critical exponents based on the microscopic interactions of the colloidal systems.

¹MRSEC DMR11-20901

4:06PM X53.00009 Local interactions and global rheology in disordered media

, ERIK WOLDHUIS, BRIAN TIGHE, Universiteit Leiden, KERSTIN NORDSTROM, DOUG DURIAN, Haverford College, JERRY GOLLUB, Haverford College, University of Pennsylvania, MARTIN VAN HECKE, Universiteit Leiden — We generalize our scaling model for the rheology of soft, frictionless repulsive spheres to include general local viscous and elastic interactions and come to a prediction of the effect on the global behavior of these local interactions. As our scaling model combines elastic and geometric ingredients and a power balance that depends on the local viscous law, we predict that the global rheology of disordered media depends on the details of the local interactions in a universal but non-trivial manner. We compare our predictions for the effect of different *elastic* interactions to recent experimental results on the interactions and rheology of NIPA particles.

4:18PM X53.00010 Jammed by shear: a new perspective of the jamming transition in frictional granular materials¹

, DAPENG BI, BULBUL CHAKRABORTY, Brandeis University — In the jamming diagram (*Nature* **396** 21 (1998)) for athermal systems jamming is induced only through compression, and jammed states exist above a packing fraction ϕ_J . Recent experiments in frictional disks clearly show shear induced jamming (D. Bi et al, *Nature* doi:10.1038/nature10667 (2011)). A minimum shear stress, τ_0 , is needed to create robust, shear-jammed (SJ) states with a strong force network percolating along both the compressive and dilational directions. This percolation transition is controlled by the fraction of force-bearing grains, a parameter not previously discussed in the context of jamming. The minimum anisotropy of SJ states vanishes as $\phi \rightarrow \phi_J$ from below in a manner reminiscent of an order-disorder transition. To shed light on the origin of shear jamming we have constructed a lattice gas model of force-bearing grains with nematic interactions between the force tiles (objects that reflect force balance on each grain). We will show that there are clear signatures of nematic ordering in SJ states, and present analysis of the nature of the shear-induced jamming transitions as a function of ϕ . We will also present numerical simulation results of sheared frictional particles.

¹This work has been supported by NSF.

4:30PM X53.00011 Deformation of inherent structures to detect short- and long-range correlations in supercooled liquids, EMANUELA DEL GADO, MAJID MOSAYEBI, PATRICK ILG, HANS CHRISTIAN OETTINGER, ETH Zurich, MICROSTRUCTURE AND RHEOLOGY, ETH ZURICH TEAM, POLYMER PHYSICS, ETH ZURICH TEAM — We use deformation of inherent structures as a tool for detecting structural changes and the onset of cooperativity in supercooled liquids. The non-affine displacement (NAD) field resulting from the applied deformation shows characteristic differences between the high temperature liquid and supercooled state, that are typically observed in dynamic quantities and correlated to normal mode structure. The average magnitude of the NAD is very sensitive to temperature changes in the supercooled regime and is found to be strongly correlated with the inherent structure energy. We can rationalize such changes in terms of a crossover from a viscous liquid to a regime dominated by elastic effects. In addition, the NAD field is characterized by a correlation length that increases upon lowering the temperature towards the supercooled regime. By analysing different measures of correlations in the direction of the NAD field, we discuss their analogies with observations in the cooperative dynamics.

4:42PM X53.00012 Experiments on ordering transitions in mechanically stable structures of granular rods, VIKRANT YADAV, Clark University, JEAN-YONNEL CHASTAING, Ecole Normale Supérieure de Lyon, ARSHAD KUDROLLI, Clark University — We investigated the evolution of granular rods from mechanically stable disordered to crystalline states in response to vibrations. We obtained positions and orientations of the rods in three dimensions using micro-focus X-ray Computed Tomography. Above a critical aspect ratio, we find that rods align vertically in layers with hexagonal order within a layer, independent of the shape of the container and details of the form of vibration. We also quantitatively study the evolution of local and global ordering using density pair correlation function $g(r)$ and orientational order parameter q_6 as a function of aspect ratio. As the system compacts, local structures emerge and grow, their size and orientation being dependent on volume fraction. Although the initial nucleation of order occurs along the boundaries, we show that the geometry of boundaries have little overall effect on the observed ordering transition. Finally we show that configuration entropy arguments do not play a significant role in the observed ordering, and the system evolves towards increasing stability under small perturbations.

4:54PM X53.00013 Elasticity of floppy amorphous systems, GUSTAVO DÜRING, EDAN LERNER, MATTHIEU WYART, New York University — Simple amorphous solids made of repulsive particles display curious properties when they are barely mechanically stable, in particular near the unjamming transition where pressure vanishes. Here we focus on another class of materials, including granular flows, covalent glasses or gels of semi-flexible polymers. In such materials the coordination associated with the dominant interaction is too weak to guarantee mechanical stability. This fact implies the presence of floppy modes, collective motions of particles that have no or very little restoring force, and that strongly affect the properties of these materials. We use analytical methods to derive the response of these systems, their length scale and frequency dependence, and test these numerically. If time permits our results will be compared with numerical observations in simplified suspension flows.

5:06PM X53.00014 Granular Matter, Foams, and Beyond: Applications of the Granocentric Model, KATHERINE NEWHALL, Courant Institute NYU — We present a local stochastic model that predicts the statistical fluctuations in jammed packings of monodisperse and polydisperse spheres revealed by confocal microscopy. Moreover, we find that this model can account for the properties of looser and denser random packings that result from depletion attraction between the particles or compression by an applied load, respectively. Finally, we extend the model to space-filling packings of cells in tissues and biliquid foams by testing analytic predictions for the dependence of the number of neighbors of a given cell on its volume. Interestingly, the model distinguishes between scenarios in which size or positional disorder in the packing dominate, in good agreement with experimental data. This versatile model can be put into the statistical mechanics framework proposed by Edwards in order to compute the entropy and compactivity of each packing.

5:18PM X53.00015 Force landscape for particulate systems¹, LOU KONDIC, New Jersey Institute of Technology, MIROSLAV KRAMAR, Rutgers University, ARNAUD GOULLET, New Jersey Institute of Technology, KONSTANTIN MISCHAIKOW, Rutgers University — We discuss the properties of force landscape for isotropically compressed particulate systems characterized by a wide range of packing fractions. The computational methods used are based on persistence diagrams which allow for clear identification of mathematical properties of force landscapes and help their physical interpretation. We find that using this technique which previously has not been applied to particulate matter, a significant new information can be extracted, going much beyond separation into 'strong' and 'weak' force networks. One result of this analysis is clear indication that for small packing fractions, polydispersity is a crucial parameter that defines the landscape, while for large packing fractions, friction, if present, becomes dominant. Preliminary results for dynamical features of force networks obtained from time-dependent analysis of force landscapes will be presented as well.

¹Supported by NSF Grant DMS-0835611 and DTRA Grant 1-10-1-0021

5:30PM X53.00016 Rearrangements in flow of foam, VIJAYAKUMAR CHIKKADI, ERIK WOLDHUIS, Instituut-Lorentz, Universiteit Leiden, PETER SCHALL, Institute of Physics, University of Amsterdam, MARTIN VAN HECKE, Kamerlingh Onnes Laboratory, Universiteit Leiden — The nonaffine deformation of amorphous solids has attracted considerable attention. Recent simulations and experiments have shown that the non-affine particle rearrangements under an applied stress are localised, and they generate a long-ranged quadrupolar strain field. Here we have investigated the particle rearrangements in flows of soft, viscous spheres near the jamming point. The characteristics of the particle rearrangements are extremely different as we move away from the jamming point.

Friday, March 2, 2012 8:00AM - 11:00AM –
Session Y1 GIMS: Measurement Science from Optics through Thermodynamics 203

8:00AM Y1.00001 Robustness of holographic particle tracking and characterization against defects in illumination, HENRIQUE W. MOYSES, BHASKAR JYOTI KRISHNATREYA, DAVID G. GRIER, Department of Physics and Center for Soft Matter Research, New York University — Images obtained with holographic video microscopy can be interpreted with predictions of the Lorenz-Mie theory of light scattering to track individual colloidal particle's motions with nanometer resolution in three dimensions over ranges extending to hundreds of micrometers, to measure their radii with nanometer resolution, and to characterize their complex refractive indexes with part-per-thousand precision. In this work we numerically and experimentally investigate how defects in the illumination system, such as divergence and tilt of the illuminating laser beam, and spherical aberrations in the optical train affect the measured properties of the particles. We show that for the usual conditions where the experiments are performed divergence and tilt of the laser beam do not affect the measured parameters significantly, while spherical aberration can introduce significant errors.

8:12AM Y1.00002 Quantification of metallic nanoparticle morphology with tilt series imaging by transmission electron microscopy¹, ANIRUDDHA DUTTA, BIAO YUAN, CHRISTOPHER J. CLUKAY, CHRISTOPHER N. GRABILL, HELGE HEINRICH, ANIKET BHATTACHARYA, STEPHEN M. KUEBLER, University of Central Florida — We report on the quantitative analysis of electrolessly deposited Au and Ag nanoparticles (NPs) on SU8 polymer with the help of High-Angle Annular Dark-Field Scanning Transmission Electron Microscopy (HAADF-STEM) in tilt series. Au NPs act as nucleating agents for the electroless deposition of silver. Au NPs were prepared by attaching Au^{3+} cations to amine functionalized SU8 polymeric surfaces and then reducing it with aqueous NaBH_4 . The nanoscale morphology of the deposited NPs on the surface of polymer has been studied from the dark field TEM cross sectional images. Ag NPs were deposited on the cross-linked polymeric surface from a silver citrate solution reduced by hydroquinone. HAADF-STEM enables us to determine the distances between the NPs and their exact locations at and near the surface. The particle distribution, sizes and densities provide us with the data necessary to control the parameters for the development of the electroless deposition technique for emerging nanoscale technologies.

¹This work was supported by NSF CAREER grant #0748712 and NSF-CHE grant #0809821.

8:24AM Y1.00003 Novel Imaging and Nano Fabrication with a Focused Beam of Helium Ions, JOHN NOTTE, Carl Zeiss, Microscopy — A newly introduced commercial instrument can produce a focused beam of helium ions with a focused probe size of 0.35 nm, and an energy range from 5 to 35 keV. While using only small beam currents (0.1 to 10 pA), it provides a means of generating images with high lateral resolution and surface specific information. The imaging is based up the generation of detectable particles (such as secondary electrons) as the beam interacts with the sample. Although similar to the scanning electron microscope, this instrument offers several unique imaging advantages. In addition to imaging, the focused helium beam has also been used for fabrication at the nanometer scale. Recent result have shown that this beam can be very effective for sputtering away materials to produce fine patterns for applications in biosensors, graphene, and plasmonic devices. The helium beam has also been used for lithographic purposes, producing 7 nm features with no apparent proximity effects. In another application, when the beam interacts with adsorbed molecules, the molecules are fixed – permitting the fabrication of three dimensional nano-structures. A review of the recent work, and future plans will be presented.

8:36AM Y1.00004 Neutral Atom Microscopy: A New Surface Imaging Probe, PHILIP WITHAM, ERIK SANCHEZ, Portland State University — Recent advances have made microscopy using scanned neutral atom beams a practical reality. This technique is also called Atomic DeBroglie Microscopy, Neutral Beam Microscopy, and Scanning Helium Microscopy. Using thermal energy (under 70 meV) gas particles with neutral charge results in a probe beam that scatters from the first atomic layer of samples, with little chance of beam damage. The technique presented eliminates any need to focus the beam by using an aperture in close proximity to the sample, and has produced the first published images from gas scattering. Resolution has reached $0.6\ \mu\text{m}$ and much higher resolution is possible¹. Now that NAM is a reality, a great deal of research can be done to show what it is uniquely useful for, and to explain the image contrast mechanisms. Molecular beam experiments show a wide range of surface properties that may be possible to image with such a microscope, some that are difficult to see otherwise. For example, thermal helium has a strong scattering interaction with surface hydrogens. Imaging un-coated surfaces with high electric fields is possible and imaging through high magnetic fields has been demonstrated. Recent image results and the basic instrument design will be presented. ¹A simple approach to neutral atom microscopy, Rev. Sci. Instrum. 82, 103705 (2011)

8:48AM Y1.00005 Imaging the solar cell p-n junction and depletion region using secondary electron contrast¹, JENNIFER HEATH, Linfield College, CHUN-SHENG JIANG, MOWAFAK AL-JASSIM, National Renewable Energy Laboratory — We report on secondary electron (SE) images of cross-sectioned multicrystalline Si and GaAs/GaInP solar cell devices, focusing on quantifying the relationship between the apparent n^+-p contrast and characteristic electronic features of the device. These samples allow us to compare the SE signal from devices which have very different physical characteristics: differing materials, diffused junction versus abrupt junction, heterojunction versus homojunction. Despite these differences, we find that the SE image contrast for both types of sample, and as a function of reverse bias across the diode, closely agrees with PC1D simulations of the bulk electrostatic potential in the device, accurately yielding the depletion edge and width. A spatial derivative of the SE data shows a local maximum at the metallurgical junction. Such data are valuable, for example, in studying the conformity of a diffused junction to the textured surface topography. These data also extend our understanding of the origin of the SE contrast.

¹This work was partially supported by the Petroleum Research Fund of the American Chemical Society

9:00AM Y1.00006 Resonant excitation of Rayleigh waves in a narrow fluid channel clad between two metal plates¹, NAGARAJ NAGARAJ, ARKADII KROKHIN, Center for Nonlinear Science, Univeristy of North Texas, JOSÉ SÁNCHEZ-DEHESA, VICTOR M. GARCIA-CHOCANO, Wave Phenomena Group, Universitat Politècnica de València, Spain — We study extraordinary absorption of acoustic energy due to resonant excitation of Rayleigh waves in a narrow water channel clad between two unidentical metal plates with Brass plate on one side of the channel and Aluminium plate on the other. The extraordinary absorption is observed at discrete resonant frequencies. From the elastic properties of the metal plates we derive a dispersion equation for coupled Rayleigh waves. Two different types of resonances, corresponding to different polarizations of the coupled waves, are studied for different channel widths and are experimentally confirmed. We also present the experimental confirmation of coupling through measurements of change in transmission minima with channel aperture. Experimental, theoretical, and numerical results are in a good agreement.

¹This work was supported by US Department of Energy Grant No. DE-FG02-06ER46312

9:12AM Y1.00007 Probing Heat Transfer in the Nanoscale Using Optomechanical Sensors., BRIAN BURG, JONATHAN TONG, POETRO SAMBEGORO, ANASTASSIOS MAVROKEFALOS, GANG CHEN, Massachusetts Institute of Technology — The transition from heat conduction to radiation at extremely small gaps cannot be captured by current theories. Experimentally researchers are only slowly starting to learn how to approach this domain. To this end, the development of a measurement platform based on the picowatt sensitivity of optomechanical sensors will be presented. The bending of a custom designed bimorph cantilever accurately allows the absolute amount of transferred heat to be extracted and temperature to be determined based on the response from thermal inputs. The versatility of the platform permits thermal radiation and conduction measurements, as well as the characterization of material thermal conductivities and absorptivities in nearly identical configurations. Results of this measurement platform for fundamental heat transfer measurements will considerably improve the current understanding of nanoscale energy transport and conversion, as well as lead to advanced design guidelines for energy capture and conversion devices, in particular thermophotovoltaic cells, (solar) thermoelectric generators and waste heat recovery heat exchangers.

9:24AM Y1.00008 Heat Capacity Measurements by Simultaneous Relaxation and AC-Calorimetry, H. KASHURI, K. KASHURI, G.S. IANNACCHIONE, WPI — A high-resolution method for measuring the heat capacity C_p using simultaneously AC and Relaxation Calorimetry techniques has been developed. This technique is useful for both first and second-order phase transitions of liquids and complex fluids. The difference of the C_p 's measured by the Relaxation and AC calorimetry is a direct measurement of a phase transitions' latent heat. As a test, the C_p of two cyanobiphenyl liquid crystals, 5CB and 8CB, were measured using a square wave modulation pulse train over a base temperature range from 300 to 320 K in which 5CB exhibits a first-order phase transition and 8CB exhibits a first and second-order phase transition. Fourier transform analysis allows for the direct C_p measurement at the fundamental frequency of the square wave pulse train (as well as higher frequency orders) as function of temperature (i.e., AC-mode). The heating and cooling relaxations at the beginning and end of the square pulse heating allows for a relaxation analysis of C_p by applying the dual slope-method that includes all enthalpic conversions.

9:36AM Y1.00009 The State of the Unit: A documentary film about the kilogram, AMY YOUNG¹, University of Illinois at Urbana-Champaign — The definition of the SI unit of mass is based on the international prototype of the kilogram, created in 1879 [1]. In the next years, metrologists will redefine the kilogram in relation to fundamental physical constants [2]. Intended for a general audience, the forthcoming documentary, *The State of the Unit: The Kilogram*, presents the history of the kilogram, interviews with researchers at national metrology institutes in the U.S., France, and Germany, and everyday mass measurement activities at varying scales. Excerpts of the film will be shown, and followed by a discussion with the filmmaker about the project to date. This film is supported in part by the Materials Computation Center at the University of Illinois at Urbana-Champaign, the California Institute of the Arts, Valencia, California, and La Fémis, Paris, France.

[1] The Kilogram and Measurements of Mass and Force, Z. J. Jabbour and S. L. Yaniv. J. Res. Natl. Inst. Stand. Technol. 106, 25–46 (2001).

[2] Redefining the SI Base Units, Peter Mohr. National Institute of Standards and Technology website. November 1, 2011. <http://www.nist.gov/pml/newsletter/siredef.cfm>. Accessed November 3, 2011.

¹California Institute of the Arts, Valencia, CA; La Femis, Paris, France

9:48AM Y1.00010 Wall friction measurement in the absence of mean shear¹, STEFANUS STEFANUS, JAMES CASTIGLIONE, RORY CERBUS, WALTER GOLDBURG, University of Pittsburgh — The dimensionless frictional force f between a pipe wall and a flowing turbulent fluid is $f = \nu \bar{s} / U^2$, where U is mean flow speed in the x -direction, ν is kinematic viscosity, and $\bar{s} = \frac{\partial u}{\partial y}$, where the y axis is perpendicular to the flow direction. The derivative is evaluated at the wall, $y = 0$. Described here a scheme for measuring f in a turbulent fluid where $\bar{s}$ is close to zero. Hence the source of frictional dissipation is from *fluctuations* in the shear about its mean, namely $\bar{s}^2$. This type of shear is encountered in turbulence in a closed container such as a food mixer. The scheme, which involves photon correlation spectroscopy, averages the shear rate over a laser spot size $w \simeq 100 \mu\text{m}$ or smaller. The scheme yields the probability density function (PDF) of components of the shear rate tensor and the moments of the PDF. The theory will be described briefly and measurements will be presented where $\bar{s} \simeq 0$. In that limit f is redefined to be $f = u' \bar{s}_{ij} / \nu$, where $\bar{s}_{ij}$ is the dominant component being measured, and u' is the rms fluctuations of the velocity.

¹Supported by the U. of Pittsburgh and NSF grant 0604477.

10:00AM Y1.00011 Mid-Infrared Photothermal Response in a Liquid Crystal Using a Quantum Cascade Laser¹, ALKET MERTIRI, Dept. Material Science, Boston University, MI HONG, Dept. Physics, Boston University, JEROME MERTZ, Dept. Biomedical Eng., Boston University, HATICE ALTUG, Dept. Electrical Eng., Boston University, SHYAMSUNDER ERRAMILLI, Dept. Physics, Boston University — We report on a new technique to measure the mid-infrared photothermal response induced by a tunable Quantum Cascade Laser (QCL) in the neat liquid crystal 4-Octyl-4'-Cyanobiphenyl (8CB), without using any intercalated dye. The modulated pump QCL range spanned a weak combination absorption band centered at 1912cm^{-1} . The thermally induced modulation of a Ti:Sapphire probe laser operating at 800 nm was measured by lockin detection. Heterodyne measurement of the response in the solid, smectic, nematic(N) and isotropic(I) liquid crystal phases allows direct detection of a weak mid-infrared normal combination mode absorption using an inexpensive room temperature silicon photodetector. The sensitivity of the response exceeds that of a conventional FTIR spectrometer equipped with a liquid nitrogen cooled detector. At high pump power in the nematic phase close to the N-I phase transition, we observe an interesting peak splitting in the photothermal response. The advent of tunable lasers that can access still stronger modes suggests that the photothermal mid-infrared response has the potential to detect ultralow concentration of absorbers.

¹We thank Thomas Jeys and Vladimir Liberman (MIT-Lincoln Labs) for helpful discussion.

10:12AM Y1.00012 Optical detection of thermal noise modes in torsional microelectromechanical oscillators¹, VINCENT VLAMINCK, JEFFREY R. GUEST, DARIO ANTONIO, DANIEL LOPEZ, JOHN E. PEARSON, AXEL HOFFMANN, Argonne National Laboratory — We present the optical detection of the thermal noise spectrum for different torsional MEMS that will be implemented in a study of magnetomechanical coupling at the nanoscale. The interferometric measurement yields the differential dynamic displacement between two diffraction-limited spots on the surface to sub-pm precision, allowing us to identify the thermal modes in the low MHz frequency range. Flexion and torsional modes from thermal noise at room temperature can be distinguished by different amplitudes at different positions of the probe beam. The different mechanical eigenmodes are identified with the help of finite element simulations. This study of the thermal oscillation serves to identify the torsional mode frequencies that can be matched to low frequency magnetization dynamics of magnetic domain wall oscillators. At this point we have fabricated torsional oscillators with a resonance frequency of 6.53 MHz and a Q-factor of 1030, which are at the same time compatible with magnetic domain wall oscillators.

¹Supported by DOE-BES under contract No. DE-AC02-06CH11357.

10:24AM Y1.00013 Advances in Surface Plasmon Resonance Imaging allowing for quantitative measurement of laterally heterogeneous samples, ADAM RAEGER, KYLE REITER, Department of Physics, University of Guelph, ANTHONY CLARKE, Department of Molecular and Cellular Biology, University of Guelph, JACEK LIPKOWSKI, Department of Chemistry, University of Guelph, JOHN DUTCHER, Department of Physics, University of Guelph — The Surface Plasmon Resonance (SPR) phenomenon is routinely exploited to qualitatively probe changes to materials on metallic surfaces for use in probes and sensors. Unfortunately, extracting truly quantitative information is usually limited to a select few cases – uniform absorption/desorption of small biomolecules and films, in which a continuous “slab” model is a good approximation. We present advancements in the SPR technique that expand the number of cases for which the technique can provide meaningful results. Use of a custom, angle-scanning SPR imaging system, together with a refined data analysis method, allow for quantitative kinetic measurements of laterally heterogeneous systems. The degradation of cellulose microfibrils and bundles of microfibrils due to the action of cellulolytic enzymes will be presented as an excellent example of the capabilities of the SPR imaging system.

10:36AM Y1.00014 Use of Cavity Ring Down Spectroscopy to Characterize Organic Acids and Aerosols Emitted in Biomass Burning¹

, SOLOMON BILILIGN, Department of Physics and NOAA-ISET Center North Carolina A&T State University, Greensboro, NC, MARC FIDDLER, NOAA-ISET Center, North Carolina A&T State University, Greensboro, NC, SUJEETA SINGH, Energy and Environmental Systems, North Carolina A&T State University, Greensboro, NC — One poorly understood, but significant class of volatile organic compounds (VOC) present in biomass burning is gas-phase organic acids and inorganic acids. These acids are extremely difficult to measure because of their adsorptive nature. Particulates and aerosols are also produced during biomass burning and impact the radiation budget of the Earth and, hence, impact global climate. Use cavity ring down spectroscopy (CRD) to measure absorption cross sections for OH overtone induced photochemistry in some organic acids (acetic acid and peracetic acid) will be presented and planned measurements of optical properties of aerosols composed of mixtures of different absorbing and non-absorbing species using CRD will be discussed.

¹The Authors acknowledge the support of the National Science Foundation under grant Number: 0803016.

10:48AM Y1.00015 Modeling large screening length effects in Electrostatic Force Microscopy

, P.L. LANG, LPEM, ESPCI-ParisTech-UPMC-CNRS, Paris, France; School of Science, BUPT, Beijing, China, A. MOTTAGHIZADEH, LPEM, ESPCI-ParisTech-UPMC-CNRS, Paris, France, L. CUI, LPEM, ESPCI-ParisTech-UPMC-CNRS, Paris, France; IOP and Beijing National Laboratory for Condensed Matter Physics, CAS, Beijing, China, A. ZIMMERS, H. AUBIN, LPEM, ESPCI-ParisTech-UPMC-CNRS, Paris, France, J. LI, D.N. ZHENG, IOP and Beijing National Laboratory for Condensed Matter Physics, CAS, Beijing, China — Electrostatic Force Microscopy (EFM) and its variants such as Kelvin Probe Microscopy (KPM) are ordinarily used to image charged states or electrochemical surface potentials. However, EFM can also be used to measure the local capacitance between the tip and the substrate. For perfectly metallic substrates, this capacitance is purely geometrical, i.e. it is set by the tip shape and substrate geometry. In semi-metals with long screening length, the measured capacitance contains a “quantum” component, which is set by the electronic compressibility. Using finite element calculations, we demonstrate that this quantum capacitance component can be measured by EFM. We apply these calculations to the analysis of EFM data on magnetite nanoparticles presented by A. Mottaghizadeh during this meeting.

Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y2 GMAG FIAP: Invited Session: Magnetic Materials and Magnetism Research for Energy Applications 204AB

8:00AM Y2.00001 Magnetic Materials in sustainable energy

, OLIVER GUTFLEISCH, Material Science, Technical University of Darmstadt Germany — A new energy paradigm, consisting of greater reliance on renewable energy sources and increased concern for energy efficiency in the total energy lifecycle, has accelerated research in energy-related technologies. Due to their ubiquity, magnetic materials play an important role in improving the efficiency and performance of devices in electric power generation, conversion and transportation. Magnetic materials are essential components of energy applications (i.e. motors, generators, transformers, actuators, etc.) and improvements in magnetic materials will have significant impact in this area, on par with many “hot” energy materials efforts. The talk focuses on the state-of-the-art hard and soft magnets and magnetocaloric materials with an emphasis on their optimization for energy applications. Specifically, the impact of hard magnets on electric motor and transportation technologies, of soft magnetic materials on electricity generation and conversion technologies, and of magnetocaloric materials for refrigeration technologies, will be discussed. The synthesis, characterization, and property evaluation of the materials, with an emphasis on structure-property relationships, will be examined in the context of their respective markets as well as their potential impact on energy efficiency. Finally, considering future bottle-necks in raw materials and in the supply chain, options for recycling of rare-earth metals will be analyzed.¹

¹O. Gutfleisch, J.P. Liu, M. Willard, E. Bruck, C. Chen, S.G. Shankar, Magnetic Materials and Devices for the 21st Century: Stronger, Lighter, and More Energy Efficient (review), Adv. Mat. 23 (2011) 821-842.

8:36AM Y2.00002 Spintronics Device for Stand-by Power Free Nonvolatile CMOS VLSI¹

, HIDEO OHNO, CSIS/RIEC, Tohoku University, Sendai, Japan — Recent progress in perpendicular magnetic-easy axis magnetic tunnel junctions (MTJs), a spintronics device, offers a high potential building block for constructing not only stand-alone fast and nonvolatile RAMs in the 30 nm feature size and beyond but also nonvolatile CMOS VLSI employing logic-in-memory architecture [1]. The shift from in-plane to perpendicular is prompted by the need for a high crystalline anisotropy that is available in perpendicular materials for reducing the device size. In addition, current-induced switching is inherently more efficient with perpendicular easy axis. However, satisfying both high tunnel magnetoresistance (TMR) ratio over 100% and low switching current was a challenge, because of the mismatch between MgO (100) - CoFe(B) bcc (100) structure needed to obtain high TMR and the crystal structure of perpendicular materials. It was shown that a strong perpendicular interface anisotropy exists at the MgO-CoFeB interface [2, 3], strong enough ($K_i = 1.3 \text{ mJ/m}^2$) to overcome demagnetization energy and make the easy axis perpendicular when the ferromagnetic electrode thickness is thin enough. First principle calculation by Nakamura *et al.* showed that the perpendicular anisotropy is due to the oxygen-iron bond that reduces contribution of in-plane crystalline anisotropy [4]. By the use of this perpendicular easy axis, a 40 nm ϕ MgO-CoFeB MTJ with high TMR (>100 %) and low switching current of 49 μA was realized [2]. It was also pointed out that activation volume for reversal plays an important role in determining the thermal stability of the MTJs [5]. I will discuss how the MTJs are incorporated in CMOS VLSIs to make them nonvolatile and stand-by power free.

[1] S. Ikeda, *et al.* IEEE Trans. Electron Devices, **54**, 991, 2007.

[2] S. Ikeda, *et al.* Nature Mat., **9**, 721, 2010.

[3] M. Endo, *et al.* Appl. Phys. Lett., **96**, 212503, 2010.

[4] K. Nakamura *et al.*, Phys. Rev. B, **81**, 220409(R), 2010

[5] H. Sato, *et al.* Appl. Phys. Lett. **99**, 042501, 2011.

¹This work is supported by the FIRST program of JSPS.

9:12AM Y2.00003 Optimized Magnetocaloric Materials¹ , VITALIJ PECHARSKY, Ames Laboratory US DOE and Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011-3020 — The discovery of the giant magnetocaloric effect in $\text{Gd}_5\text{Si}_2\text{Ge}_2$ and other R_5T_4 compounds (R = rare earth metal and T is a Group 14 element) generated a broad interest in the magnetocaloric effect and magnetostructural transitions. Reports on the giant magnetocaloric effect in other systems soon followed. These include $\text{MnFeP}_x\text{As}_{1-x}$ and related compounds, $\text{La}(\text{Fe}_{1-x}\text{Si}_x)_{13}$ and their hydrides, $\text{Mn}(\text{As}_x\text{Sb}_{1-x})$, $\text{CoMnSi}_x\text{Ge}_{1-x}$ and related compounds, Ni_2MnGa and some closely related Heusler phases, and a few other systems. A common feature is the enhancement of the magnetic entropy effect by the overlapping contribution from the lattice, regardless whether it is a massive structural change like in R_5T_4 compounds, or only a phase volume change as in $\text{La}(\text{Fe}_{1-x}\text{Si}_x)_{13}$. Both the magnetic and lattice entropies are, therefore, important and each contribution must be maximized in order to have the optimum magnetocaloric effect. Both of these entropy terms and the potential pathways towards a further enhancement of the giant magnetocaloric effect will be discussed.

¹This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Science and Engineering Division under contract No. DE-AC02-07CH11358 with Iowa State University.

9:48AM Y2.00004 High-Performance Permanent Magnets for Energy-Efficient Devices , GEORGE HADJIPANAYIS, Department of Physics and Astronomy, University of Delaware, Newark, DE, U.S.A. — Permanent magnets (PMs) are indispensable for many commercial applications including the electric, electronic and automobile industries, communications, information technologies and automatic control engineering. In most of these applications, an increase in the magnetic energy density of the PM, usually presented via the maximum energy product $(BH)_{max}$, immediately increases the efficiency of the whole device and makes it smaller and lighter. Worldwide demand for high performance permanent magnets has increased dramatically in the past few years driven by hybrid and electric cars, wind turbines and other power generation systems. New energy challenges in the world require devices with higher energy efficiency and minimum environmental impact. The potential of 3d-4f compounds which revolutionized the PM science and technology is almost fully utilized, and the supply of 4f rare earth elements does not seem to be much longer assured. This talk will address the major principles guiding the development of PMs and overview state-of-the-art theoretical and experimental research. Recent progress in the development of nanocomposite PMs, consisting of a fine (at the scale of the magnetic exchange length) mixture of phases with high magnetization and large magnetic hardness will be discussed. Fabrication of such PMs is currently the most promising way to boost the $(BH)_{max}$, while simultaneously decreasing, at least partially, the reliance on the rare earth elements. Special attention will be paid to the impact which the next-generation high- $(BH)_{max}$ magnets is expected to have on existing and proposed energy-saving technologies.

10:24AM Y2.00005 Soft Magnetic Materials for Improved Energy Performance¹ , MATTHEW WILLARD, U. S. Naval Research Laboratory — A main focus of sustainable energy research has been development of renewable energy technologies (e.g. from wind, solar, hydro, geothermal, etc.) to decrease our dependence on non-renewable energy resources (e.g. fossil fuels). By focusing on renewable energy sources now, we hope to provide enough energy resources for future generations. In parallel with this focus, it is essential to develop technologies that improve the efficiency of energy production, distribution, and consumption, to get the most from these renewable resources. Soft magnetic materials play a central role in power generation, conditioning, and conversion technologies and therefore promoting improvements in the efficiency of these materials is essential for our future energy needs. The losses generated by the magnetic core materials by hysteretic, acoustic, and/or eddy currents have a great impact on efficiency. A survey of soft magnetic materials for energy applications will be discussed with a focus on improvement in performance using novel soft magnetic materials designed for these power applications. A group of premiere soft magnetic materials – nanocrystalline soft magnetic alloys – will be highlighted for their potential in addressing energy efficiency. These materials are made up of nanocrystalline magnetic transition metal-rich grains embedded within an intergranular amorphous matrix, obtained by partial devitrification of melt-spun amorphous ribbons. The nanoscale grain size results in a desirable combination of large saturation induction, low coercivity, and moderate resistivity unobtainable in conventional soft magnetic alloys. The random distribution of these fine grains causes a reduction in the net magnetocrystalline anisotropy, contributing to the excellent magnetic properties. Recently developed $(\text{Fe,Co,Ni})_{88}\text{Zr}_7\text{B}_4\text{Cu}_1$ alloys will be discussed with a focus on the microstructure/magnetic property relationship and their effects on the energy efficiency of these materials for AC applications.

¹This work was funded in part by the Office of Naval Research under contract N0001410WX21681.

Friday, March 2, 2012 8:00AM - 11:00AM –
Session Y3 DCMP: Invited Session: Competing Phases and Quantum Criticality in Strongly Correlated Systems 205AB

8:00AM Y3.00001 Correlated Electron State in $\text{Ce}_{1-x}\text{Yb}_x\text{CoIn}_5$ Stabilized by Cooperative Valence Fluctuations¹ , LEI SHU², University of California, San Diego — Heavy fermion superconductivity has continuously attracted broad scientific attention. One of the important issues in this study is the relationship between quantum criticality, non-Fermi-liquid behavior (NFL), and unconventional superconductivity. It is generally thought that critical fluctuations associated with a magnetic quantum critical point (QCP) can provide a mechanism for NFL behavior and unconventional superconductivity in a narrow dome around the QCP. However, the precise nature of the relationship between these phenomena remains to be understood, particularly since many compounds have been reported where the NFL behavior persists over an extended region of the phase diagram in the absence of any identifiable QCP. Recently, intermediate valence phenomena has been found in the heavy fermion superconductor system $\text{Ce}_{1-x}\text{Yb}_x\text{CoIn}_5$. X-ray diffraction, electrical resistivity, magnetic susceptibility, and specific heat measurements reveal that many of the characteristic features of the $x = 0$ correlated electron state are stable for $0 \leq x \leq 0.775$, and that phase separation occurs for $x > 0.775$. The stability of the correlated electron state is apparently due to cooperative behavior of the Ce and Yb ions, involving their unstable valences. Low temperature NFL behavior is observed which varies with x , even though there is no readily identifiable quantum critical point. The NFL state is tuned by valence fluctuations. The strongly intermediate-valence state of Yb in $\text{Ce}_{1-x}\text{Yb}_x\text{CoIn}_5$ has recently been verified by angle-resolved photoemission spectroscopy, extended x-ray absorption fine structure, and x-ray absorption near-edge structure measurements.

¹This research was sponsored by the U.S. DOE under Research Grant No. DE-FG02-04ER46105 (crystal growth) and the NSF under Grant No. 0802478 (low temperature measurements).

²Current address: Fudan University, Shanghai, China

8:36AM Y3.00002 Tuning Correlations in Low-Dimensional Electron Systems: Fermi liquid versus non-Fermi-liquid behavior in organic conductors, MARTIN DRESSEL, 1. Physikalisches Institut, Universität Stuttgart — While the electronic properties of cuprates can be modified by electron or hole doping, organic conductors provide the opportunity to tune the strength of electronic correlations more directly. Varying the bandwidth by (physical or chemical) pressure, the κ -phase BEDT-TTF compounds cross over from a Fermi liquid to a Mott insulator by increasing effective correlations. We systematically investigate the electronic transport properties in organic conductors by dc resistivity and optical measurements in order to extract the temperature and frequency-dependent scattering rate $1/\tau = A(k_B T)^2 + B(\hbar\omega)^2$. We find corresponding temperature and frequency ranges in which the parabolic behaviors are observed. For the first time, we can quantitatively relate the two prefactors ($A/B = 56$) and their enhancement as correlations increase upon approaching the Mott transition. Conceptually low-dimensional organic conductors are also good candidates for quantum criticality because often an ordered state is located next to a metallic state when the system is tuned by pressure. Interestingly both are found, order in the spin as well as in the charge sector. Fermi-liquid behavior observed in the metallic state seems to be limited to certain regions of the phase diagram with non-Fermi-liquid properties evolving as the ordered phase is approached. It is not clear whether these deviations from Fermi liquid behavior are actually a signature of quantum criticality.

- [1] M. Dressel, *Quantum criticality in organic conductors? Fermi-liquid versus non-Fermi-liquid behavior*, J. Phys.: Condens. Matter **23**, 293201 (2011).
- [2] S. Yasin, M. Dumm, B. Salameh, P. Batail, C. Mézière and M. Dressel, *Transport studies at the Mott transition of the two-dimensional organic metal κ -(BEDT-TTF)₂Cu[N(CN)₂]Br_xCl_{1-x}*, Eur. Phys. J. B **79**, 383 (2011).
- [3] M. Dumm, D. Faltermeyer, N. Drichko and M. Dressel, *Bandwidth-controlled Mott transition in κ -(BEDT-TTF)₂Cu[N(CN)₂]Br_xCl_{1-x}: Optical studies of correlated carriers*, Phys. Rev. B **79**, 195106 (2009)
- [4] J. Merino, M. Dumm, N. Drichko, M. Dressel and R. H. McKenzie, *Quasiparticles at the verge of localization near the Mott metal-insulator transition in a two-dimensional material*, Phys. Rev. Lett. **100**, 086404 (2008)

9:12AM Y3.00003 Superconducting condensation energy of CeCu₂Si₂ and theoretical implications, STEFAN KIRCHNER, Max Planck Institute for Physics of Complex Systems — Unconventional superconductivity occurs in a broad range of strongly correlated electron systems including the newly discovered iron pnictides and chalcogenides, various intermetallic rare earth metals, the cuprates and the organic superconductors. These systems are not only of varying effective dimensionality but their parent compounds out of which superconductivity emerges ranges from metals to bad metals and Mott insulators. The only unifying characteristic features seems that unconventional superconductivity occurs in close vicinity of zero-temperature instabilities which are most often magnetic in nature. Heavy fermion compounds represent prototype systems to address the interplay between quantum criticality and unconventional superconductivity [1]. In CeCu₂Si₂, the magnetic quantum phase transition and superconductivity occur at ambient pressure which allows for a detailed study of the energetics across the superconducting transition. Based on an in-depth study of the magnetic excitation spectrum of CeCu₂Si₂ in the normal and superconducting state we obtain a lower bound for the change in exchange energy [2]. The comparison with the superconducting condensation energy demonstrates that the built-up of magnetic correlations near the quantum critical point does drive superconductivity in CeCu₂Si₂. In addition, our comparison establishes a huge kinetic energy loss which we relate to the competition of Kondo screening and superconductivity as the opening of the gap weakens the Kondo effect [2,3]. We discuss the relation between kinetic energy loss and the nature of the underlying quantum critical point [1,3]. Our unexpected findings sheds further light on the emerging global phase diagram of heavy fermion compounds [4] and are believed to be relevant to other families of superconductivity which are also located in close proximity to magnetism.

- [1] O. Stockert, S. Kirchner, F. Steglich, Q. Si, "Superconductivity in Ce- and U-based 122 heavy-fermion compounds," to be published in JPSJ (invited review paper).
- [2] O. Stockert, J. Arndt, E. Faulhaber, C. Geibel, H. S. Jeevan, S. Kirchner, M. Loewenhaupt, K. Schmalzl, W. Schmidt, Q. Si, F. Steglich, "Magnetically driven superconductivity in CeCu₂Si₂," Nature Physics, **7**, 119-124 (2011).
- [3] S. Kirchner and Q. Si, to be published.
- [4] Q. Si, "Quantum Criticality and Global Phase Diagram of Magnetic Heavy Fermions," Phys. Status Solidi B **247**, 476 (2010).

9:48AM Y3.00004 Quantum critical scaling in beta-YbAlB₄ and theoretical implications, ANDRIY NEVIDOMSKYY, Rice University, Houston, TX — Emergent phenomena in quantum materials are subject of intense experimental and theoretical research at present. A wonderful example thereof are the sister phases of YbAlB₄ - a newly discovered heavy fermion material [1]. While one phase (α -YbAlB₄) is a heavy Fermi liquid, its sibling β -YbAlB₄ is quantum critical, supporting an unconventional superconductivity with a tiny transition temperature of ~ 80 mK. Latest experiments [2] uncover the quantum critical T/B -scaling in β -YbAlB₄ and prove that superconductivity emerges from a strange metal governed by an extremely fragile quantum criticality, which apparently occurs at zero field, without any external tuning. Here, we will present a theoretical perspective on the quantum critical scaling in β -YbAlB₄ and will show that the critical exponents can be derived from the nodal structure of the hybridization matrix between Yb f -band and the conduction electrons. It follows that the free energy at low temperatures can be written in a scaling form $F \propto [(k_B T)^2 + (g\mu_B B)^2]^{3/4}$, which predicts the divergent Sommerfeld coefficient γ and quasi-particle effective mass as $B \rightarrow 0$: $\gamma \sim m^*/m \propto B^{-1/2}$. This is indeed observed in the experiment [1,2], which places a tiny upper bound on the critical magnetic field $B_c < 0.2$ mT. We will discuss theoretical implications of this fragile intrinsic quantum criticality in β -YbAlB₄ and discuss the possibility of a quantum critical phase, rather than a quantum critical point, in this material.

- [1] S. Nakatsuji *et al.*, Nature Physics **4**, 603 (2008).
- [2] Y. Matsumoto, S. Nakatsuji, K. Kuga, Y. Karaki, Y. Shimura, T. Sakakibara, A. H. Nevidomskyy, and P. Coleman, Science **331**, 316 (2011).

10:24AM Y3.00005 Chromium at High Pressure, RAFAEL JARAMILLO, Harvard University — Chromium has long served as the archetype of spin density wave magnetism. Recently, Jaramillo and collaborators have shown that Cr also serves as an archetype of magnetic quantum criticality. Using a combination of x-ray diffraction and electrical transport measurements at high pressures and cryogenic temperatures in a diamond anvil cell, they have demonstrated that the Néel transition (T_N) can be continuously suppressed to zero, with no sign of a concurrent structural transition. The order parameter undergoes a broad regime of exponential suppression, consistent with the weak coupling paradigm, before deviating from a BCS-like ground state within a narrow but accessible quantum critical regime. The quantum criticality is characterized by mean field scaling of T_N and non mean field scaling of the transport coefficients, which points to a fluctuation-induced reconstruction of the critical Fermi surface. A comparison between pressure and chemical doping as means to suppress T_N sheds light on different routes to the quantum critical point and the relevance of Fermi surface nesting and disorder at this quantum phase transition. The work by Jaramillo *et al.* is broadly relevant to the study of magnetic quantum criticality in a physically pure and theoretically tractable system that balances elements of weak and strong coupling.

- [1] R. Jaramillo, Y. Feng, J. Wang & T. F. Rosenbaum. Signatures of quantum criticality in pure Cr at high pressure. *Proc. Natl. Acad. Sci. USA* **107**, 13631 (2010).
- [2] R. Jaramillo, Y. Feng, J. C. Lang, Z. Islam, G. Srajer, P. B. Littlewood, D. B. McWhan & T. F. Rosenbaum. Breakdown of the Bardeen-Cooper-Schrieffer ground state at a quantum phase transition. *Nature* **459**, 405 (2009).

Friday, March 2, 2012 8:00AM - 10:48AM —
Session Y4 DAMOP: Cold Quantum Gases in Reduced Dimensions 205C

8:00AM Y4.00001 Tunneling-driven transitions in magnetization compressibility and density redistributions in a fermionic superfluid of cold atoms trapped in an array of one-dimensional tubes, KUEI SUN, C.J. BOLECH, University of Cincinnati — We study two-species fermion gases with attractive interactions in optical lattices that are made as an array of one-dimensional tube confinements. With the decrease in lattice depth, we find that the increase in tunneling between tubes leads to an incompressible-compressible transition in magnetization. The role of pair tunneling is considered, as well as the experimental implications.

8:12AM Y4.00002 Fermion Pairing in a One-Dimension Optical Lattice¹, ARIEL SOMMER, LAWRENCE CHEUK, MARK KU, WASEEM BAKR, MARTIN ZWIERLEIN, Department of Physics, MIT-Harvard Center for Ultracold Atoms, and Research Laboratory of Electronics, MIT, Cambridge, Massachusetts 02139, USA — Strongly correlated fermions in an array of two-dimensional planes coupled via tunneling serve as an important model system for high-temperature superconductors and layered organic conductors. We realize this model using ultracold fermionic ⁶Li atoms in a one-dimensional optical lattice near a Feshbach resonance. The depth of the lattice controls the interlayer coupling, and tunes the system between three and two dimensions. Pairing between fermions is studied using radio-frequency spectroscopy. The binding energy of fermion pairs is determined along the dimensional crossover and for different interaction strengths through the BEC-BCS crossover. Probes of superfluidity in the coupled layer system are also discussed.

¹This work was supported by the NSF, AFOSR-MURI, ARO-MURI, ONR, DARPA YFA, a grant from the Army Research Office with funding from the DARPA OLE program, the David and Lucile Packard Foundation and the Alfred P. Sloan Foundation

8:24AM Y4.00003 ABSTRACT WITHDRAWN —

8:36AM Y4.00004 Entanglement-based perturbation theory for highly anisotropic Bose-Einstein condensates, ALEXANDRE TACLA, CARLTON CAVES, University of New Mexico — We investigate the emergence of three-dimensional behavior in a reduced-dimension Bose-Einstein condensate trapped by a highly anisotropic potential. We handle the problem analytically by performing a perturbative Schmidt decomposition of the condensate wave function between the tightly confined direction(s) and the loosely confined direction(s). The perturbation theory is valid when the nonlinear scattering energy is small compared to the transverse energy scales. Our approach provides a straightforward way, first, to derive corrections to the transverse and longitudinal wave functions of the reduced-dimension approximation and, second, to calculate the amount of entanglement that arises between the transverse and longitudinal spatial directions. Numerical integration of the three-dimensional Gross-Pitaevskii equation for different cigar-shaped potentials and experimentally accessible parameters reveals good agreement with our analytical model even for relatively high nonlinearities. In particular, we show that even for such stronger nonlinearities the entanglement remains remarkably small, which allows the condensate to be well described by a product wave function that corresponds to a single Schmidt term.

8:48AM Y4.00005 Phase Diagram of the Bose Hubbard Model with Weak Links, KALANI HETTIARACHCHILAGE, VALY ROUSSEAU, KA-MING TAM, JUANA MORENO, MARK JARRELL, DANIEL SHEEHY, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, USA — We study the ground state phase diagram of strongly interacting ultracold Bose gas in a one-dimensional optical lattice with a tunable weak link, by means of Quantum Monte Carlo simulation. This model contains an on-site repulsive interaction (U) and two different near-neighbor hopping terms, J and t , for the weak link and the remainder of the chain, respectively. We show that by reducing the strength of J , a novel intermediate phase develops which is compressible and non-superfluid. This novel phase is identified as a Normal Bose Liquid (NBL) which does not appear in the phase diagram of the homogeneous bosonic Hubbard model. Further, we find a linear variation of the phase boundary of Normal Bose Liquid (NBL) to Superfluid (SF) as a function of the strength of the weak link. These results may provide a new path to design advanced atomtronic devices in the future.

9:00AM Y4.00006 The effective mass of ultracold atoms in one-dimensional optical lattices, FEDERICO DUQUE GOMEZ, J.E. SIPE, Department of Physics, University of Toronto — According to the effective mass theorem, in the presence of an external force the wavepacket associated with a crystal electron in one band accelerates as a particle with an effective mass. However, when the force is turned on suddenly, the expectation value of the acceleration initially behaves according to the electron's bare mass, and afterwards oscillates around the value given by the usual effective mass.¹ These oscillations are difficult to measure in typical solid state systems because they decay after a time of the order of femtoseconds.² We consider this oscillatory behaviour with ultracold atoms in a one-dimensional optical lattice where the time scale of the oscillations and the coherence times are much longer. Our theoretical analysis is based on a perturbation scheme that decouples the bands to any order in the external force.³ We check the validity of this perturbative approach, comparing its results with those obtained from a full numerical calculation. Experimental investigations are underway.⁴

¹D. Pfirsch and E. Spenke, Z. Physik **137**, 309 (1954).

²Y. M. Zhu, et al., phys. stat. sol. (c) **5**, 240 (2008).

³G. H. Wannier, Phys. Rev. **117**, 432 (1960).

⁴A. Steinberg, private communication.

9:12AM Y4.00007 Supercurrent decay via quantum nucleation of phase slips in one-dimensional lattice bosons¹, IPPEI DANSHITA, RIKEN, Wako, Saitama 351-0198, Japan, ANATOLI POLKOVNIKOV, Department of Physics, Boston University, Boston, MA 02215 — We study transport properties of one-dimensional (1D) Bose gases in a periodic potential. In 1D, superflow at zero temperature can decay via quantum nucleation of phase slips even when the flow velocity is much smaller than the critical velocity predicted by mean-field theories. We use instanton techniques to find that the decay rate G is algebraically increases with the flow momentum p as $G/L \propto p^{2K-2}$, where L is the system size, K the Luttinger parameter. We also discuss the relation between the nucleation rate and the quantum superfluid-insulator transition in order to present a physical interpretation of the scaling formula.

¹A. P. acknowledges support from NSF DMR- 0907039, AFOSR FA9550-10-1-0110, and the Sloan Foundation.

9:24AM Y4.00008 Compressibility and Entropy of One Dimensional Fermions in a combined Harmonic and Periodic Potential, ANDREW SNYDER, THEJA DE SILVA, Binghamton University — We solve the homogeneous Hubbard model for repulsively interacting fermions using thermodynamic Bethe ansatz method. Treating the harmonic potential in local density approximation, we calculate particle density, various compressibilities, double occupancy, and entropy as a function of temperature and interaction. These quantities show characteristic features that can be used to detect temperature, metal-insulator transition, and coexistence of metallic and insulating phases.

9:36AM Y4.00009 From GPE to KPZ: Finite temperature dynamical structure factor of the 1D Bose gas, MANAS KULKARNI, University of Toronto, AUSTEN LAMACRAFT, University of Virginia — Recent experiments on 1D Bose gases have raised interest in the investigation of dynamical properties at finite temperature such as the structure factor. For weak enough interaction and high enough temperature, we expect a classical description in terms of the Gross-Pitaevskii equation with thermally populated modes to be valid. Here, we present numerical results for the finite temperature dynamical structure factor and its universal anomalous scaling behavior, arising from resonant interactions between phonons. Our results are also relevant to sound damping in 1D classical fluids. Somewhat more surprisingly, there is a deep connection to systems in the Kardar-Parisi-Zhang universality class, describing growing fluctuating interfaces.

9:48AM Y4.00010 Photoinduced phase transition in one dimensional extended Hubbard model, HANTAO LU, SHIGETOSHI SOTA, Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto, 606-8502, Japan, HIROAKI MATSUEDA, Sendai National College of Technology, Sendai, 989-3128, Japan, TAKAMI TOHYAMA, Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto, 606-8502, Japan — We illustrate one interesting example of the photoinduced phase transitions due to a nonequilibrium process. The impact of laser pump on one dimensional half-filled extended Hubbard model in the spin-density-wave (SDW) phase is investigated by using time-dependent density-matrix renormalization group. With proper laser frequencies and strengths, we find that charge-density wave (CDW) can be observed during the pulse. Further, in some situations, for instance, near the boundary between SDW and CDW in the ground state, the CDW signature can be sustained even after the pulse turned off. The underlying physics and possible experimental realization are discussed.

10:00AM Y4.00011 Separation induced resonances in quasi-one-dimensional ultracold atomic gases, WENBO FU, Institute for Advanced Study, Tsinghua University, Beijing, 100084, ZHENHUA YU, Department of Physics, Ohio State University, Columbus, OH 43210, XIAOLING CUI, Institute for Advanced Study, Tsinghua University, Beijing, 100084 — We study the effective one-dimensional (1D) scattering of two distinguishable atoms confined individually by *separated* transverse harmonic traps. With equal trapping frequency for two s-wave interacting atoms, we find that by tuning the trap separations, the system can undergo *double* 1D scattering resonance, named as the separation induced resonance (SIR), when the ratio between the confinement length and s-wave scattering length is within $(0.791, 1.46]$. Near SIR, the scattering property shows unique dependence on the resonance position. Right at SIR, the universal property of a many-body system is manifested by studying the interaction effect of a localized impurity immersed in a Fermi sea of light atoms. The proposed SIR can be realized in cold atom experiment.

10:12AM Y4.00012 Boson pairing and unusual criticality in a generalized XY model, YIFEI SHI, University of Virginia — Motivated by the physics of condensates of boson pairs, we study the generalized XY model in two dimension, which has a term proportional to $\cos(2\theta)$ in addition to the normal XY Hamiltonian. This corresponds to having half vortices connected by solitons, as well as integer vortices. From both renormalization group analysis and Monte Carlo simulation using the worm algorithm, we find that the phase diagram includes Kosterlitz-Thouless transitions of half and integer vortices, together with an Ising transition. Remarkably, part of the Ising line is a direct transition from the quasi-long-ranged ordered state to the disordered state.

10:24AM Y4.00013 Pairing and pseudogap for ultracold fermions in two dimensions¹, J. TEMPERE², S.N. KLIMIN, J.T. DEVREESE, Theorie van Quantum en Complexe Systemen (TQC), Universiteit Antwerpen, Belgium — The T-matrix approach, straightforwardly applied to cold fermions in two dimensions, leads to a divergent fermion density for any finite temperature. We have shown that the Gaussian pair fluctuation theory, which is an improvement of the Nozières – Schmitt-Rink approach, provides a convergent density in the paired fermion state. In our work, special attention is paid to the pseudogap state above the BKT transition temperature. In the pseudogap state, the modulus of the order parameter is finite, while phase coherence is absent. The pairing crossover temperature in 2D has been determined. Owing to the fluctuations, this pairing temperature is considerably lower than the mean-field critical temperature. With increasing coupling strength, the pairing temperature behaves non-monotonically reaching a maximum before decreasing to a finite value. For an imbalanced Fermi gas, the fluctuations lower the critical value of the imbalance at which the superfluid or non-coherent paired state is formed. This effect exists even at zero temperature, where only the quantum fluctuations survive. The obtained pairing temperatures and spectral functions are in fair agreement with recent experimental results on pairing of fermionic atoms in strongly anisotropic optical lattices.

¹This work was supported by FWO-V projects G.0356.06, G.0370.09N, G.0180.09N, G.0365.08, the WOG WO.035.04N (Belgium).

²Also at Lyman Laboratory of Physics, Harvard University, USA

10:36AM Y4.00014 Excitation spectrum of two-dimensional cold fermionic gases in the dilute limit, C. BERTHOD, C. KOLLATH, T. GIAMARCHI, University of Geneva, Switzerland, M. FELD, B. FRÖHLICH, M. KOSCHORRECK, E. VOGT, M. KÖHL, University of Cambridge, United Kingdom — Two-dimensional gases of fermionic atoms have been recently realized, and cooled down to temperatures a few tenths of the Fermi temperature. Such ultracold atom systems are ideal tools to investigate the fundamental properties of Fermi ensembles subject to short-range interactions. One of the key questions is whether the interaction changes the ground state and excitation spectrum in a non-perturbative way, or whether the weak-coupling perturbation theory and Fermi-liquid idea remain valid in two dimensions. In contrast to condensed-matter systems, in atomic gases the perturbation theory must be carried out at finite temperature and far from the Fermi surface for a meaningful comparison with experiment. We have calculated the electronic self-energy of dilute two-dimensional Fermi gases at arbitrary temperature and momentum, using the ladder approximation. This scheme is expected to become exact (in a perturbative sense) in the low-density limit. For short-range attractive interaction, we study the evolution of the excitation spectrum as a function of temperature and interaction strength, and we compare our results with recent experiments.

Friday, March 2, 2012 8:00AM - 10:24AM – Session Y5 DCMF: Optical Properties and Excitations in Semiconductor Quantum Dots 206A

8:00AM Y5.00001 Elastic vs Inelastic Light Scattering from a Quantum Dot, K. KONTHASINGHE, J. WALKER, M. PEIRIS, University of South Florida, C.K. SHIH, University of Texas at Austin, Y. YU, M. LI, J. HE, L. WANG, H. NI, Z. NIU, Chinese Academy of Sciences, A. MULLER, University of South Florida — We spectrally resolve the light scattered by a single InAs semiconductor quantum dot and analyze in detail the contribution from elastic and inelastic scattering processes. The measurements are well described by the theoretical expression given by Mollow. High resolution measurements reveal that the elastically scattered light is highly phase coherent with the laser. Thus a quantum dot elastically scattering a pulsed laser may serve as a triggered single photon source. In this regime, spectral diffusion and other broadening mechanisms are not a bottleneck for obtaining transform-limited photons.

8:12AM Y5.00002 Polarized luminescence characterization of charged quantum dot molecules¹

, RAMANA THOTA, SWATI RAMANATHAN, KUSHAL C. WIJESUNDARA, ERIC STINAFF, Department of Physics and Astronomy, and Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, Ohio - 45701 - 2979, USA, ALLAN BRACKER, DAN GAMMON, Naval Research Laboratory, Washington, DC 20375, USA — Polarization sensitive spectroscopy of self assembled quantum dots (QDs) has been shown to yield important information about spins associated with the charge carriers in various excitonic states. As pairs of quantum dots are brought together, and the formation of molecular states via tunneling becomes relevant, the interactions that determine the polarization state can be modified. In this talk we will present polarization dependent photoluminescence and photoluminescence excitation studies on vertically stacked InAs QDs grown by molecular beam epitaxy. We will discuss the characterization of the Stokes parameters of singly and doubly charged exciton states in these coupled QDs and compare with the results reported for single QDs. This study will help in identifying appropriate charge states for potential spin manipulation and entanglement measurements.

¹This work has been supported by National Science Foundation (NSF) under the grant number DMR-1005525

8:24AM Y5.00003 Exciton fine structure splitting in self-assembled semiconductor quantum dots: Intrinsic and extrinsic effects

, RANBER SINGH, GABRIEL BESTER, Max Planck Institute for Solid State Research — We investigate the excitonic fine structure splitting (FSS) in InGaAs/GaAs and GaAs/AlGaAs quantum dots (QDs) of different shapes and sizes using an atomistic pseudopotential approach [1,2]. We consider intrinsic effects originating from the atomistic symmetry of the structure. We highlight the effects of the growth direction and the repercussions it has on the point group symmetry and the FSS. We give predictions for the cases where the semiconductor alloy has a certain degree of atomic order, and for the case, where the QDs are influenced by charged point defects. These effects are contrasted to the extrinsic effect of applied stress.

[1] R. Singh and G. Bester, *Lower bound for the excitonic fine structure splitting in self-assembled quantum dots*. Phys. Rev. Lett. **104**, 196803 (2010).

[2] R. Singh and G. Bester, *Nanowire Quantum Dots as an Ideal Source of Entangled Photon Pairs*. Phys. Rev. Lett. **103**, 063601 (2009).

8:36AM Y5.00004 Coulomb Enhanced Nonlinear Optical Properties of Strongly Confined Excitons in InAs/GaAs Quantum Dots

, HANZ RAMIREZ, JEFFERSON FLOREZ, ANGELA CAMACHO, Department of Physics, Universidad de los Andes — Nonlinear optical response in parametric crystals has become widely used in entanglement production; however, low generation rate is an undesirable feature of this technique. Self-assembled quantum dots arrays (QDAs) may be a promising alternative with a larger nonlinear coefficients respect to higher dimensionality systems. Previously, some works have dealt with nonlinear susceptibilities of InAs/GaAs quantum dots, studying intraband transitions of either electrons or holes. The second order susceptibilities found there, are substantially bigger than those in bulk samples, although interband excitations and Coulomb effects were not considered. In this work we study the effects of strong confinement and Coulomb interactions on exciton states in fully 3D axially symmetric QDs. By using partial CI approach, we obtain eigenenergies and envelope eigenfunctions. Second order optical susceptibilities and their dependence on quantum dot size and aspect ratio are calculated. As a main result, we observe a Coulomb related enhancement in the second order optical susceptibilities of exciton transitions as compared to those in bulk, 2D, and even 0D purely intraband systems. This increased nonlinear response suggests interband excited QDAs as efficient entanglement sources.

8:48AM Y5.00005 Diamagnetic Exciton Properties in Quantum Dot Molecules

, FINO PUERTO NELSON RICARDO, RAMIREZ HANZ YECID, Universidad de los Andes, CAMACHO ANGELA S, Profesor, GRUPO DE MATERIA CONDENSADA UNIVERSIDAD DE LOS ANDES TEAM — The magnetic properties of nanostructures like quantum dots and rings are the subject of intense research. In particular, magnetic control of coupled quantum dots (artificial molecules) has become subject of interest. The diamagnetic shift of confined excitons complexes has been used as a measured of the wave function spatial extent in semiconductor nanostructures. In weak magnetic field, the diamagnetic shift is expected to exhibit quadratic dependence. However, for exciton complexes the diamagnetic behavior is expected to exhibit more complicated features related to electron-hole asymmetry effects on Coulomb interactions. In this work we study the magnetic response of neutral and charged excitons in InAs/GaAs asymmetric artificial molecules By using a first order perturbation approach, and within the effective mass approximation, we calculate magnetic field dependent electronic structures of confined excitons and trions in vertically coupled quantum dots. These predicted regions, which show coexistence of crossing and anticrossing exciton states, because of allowing control of charge localization and polarization of emitted photons. .

9:00AM Y5.00006 ABSTRACT WITHDRAWN —

9:12AM Y5.00007 Observed Shifts in Unoccupied States for Cu Doped CdSe Quantum Dots Observed via Synchrotron Techniques

, JOSHUA JOSHUA, ROBERT MEULENBERG, University of Maine — Recent work has been targeted on examining the optical properties of guest ions in quantum dot (QD) lattice; however, very few studies have attempted to understand the effect the dopant has on the host electronic structure. In this talk, we will present data that suggests copper doping of CdSe QDs leads to trapped states below the conduction band (CB) minimum of the host CdSe particle. We propose that one possible reason for this could be hybridization between copper and cadmium, lowering the energy for the cadmium 5s states below the CB minimum of bulk CdSe. X-ray absorption near edge structure spectroscopy measurements at the Cd M_{3-} edge for bulk, undoped, and doped QDs are compared and an unexpected lowering in the CB minimum is observed. We also present a first order theoretical model, for describing our results considering the effects caused by confinement, doping, and hybridization. Numerical approximations for atomic interactions suggest the hybridization parameter can lead to a lowering of the CB minimum by as much as 1.5 eV, as observed experimentally. Future work will include more in depth modelling of hybridization starting from tight binding calculations, developing a predictive model, applicable to more than existing data.

9:24AM Y5.00008 Elementary electronic excitations in quantum wires made up of vertically stacked quantum dots

, M.S. KUSHWAHA, Rice University — We investigate the elementary electronic excitations in quantum wires made up of vertically stacked (self-assembled) InAs/GaAs quantum dots. The length scales (of a few nm) involved in the experimental setups prompt us to consider an infinitely periodic system of two-dimensionally confined (InAs) quantum dot layers separated by GaAs spacers. The resultant quantum wire is characterized by the Bloch functions and the Hermite functions. We make use of the Bohm-Pines' RPA in order to derive a general nonlocal, dynamic dielectric function. The theoretical framework is then specified to work within a two-subband model that enables us to scrutinize the single-particle as well as collective responses of the system. We also size up the importance of studying the inverse dielectric function in relation with the quantum transport phenomena. It is remarkable to notice how the variation in the barrier- and well-widths can allow us to tailor the excitation spectrum in the desired energy range. Given the foreseen applications in the single-electron devices and in the quantum computation, it is quite tempting to explore the electronic, optical, and transport phenomena in such systems.¹

¹M.S. Kushwaha, J. Chem. Phys. **135**, 124704 (2011).

9:36AM Y5.00009 Anomalous Suppression of Valley Splittings in Lead Salt Nanocrystals, ALEXANDER Poddubny, MIKHAIL NESTOKLON, Ioffe Institute, Russian Academy of Sciences, SERGUEI GOUPALOV¹, Jackson State University — Atomistic $sp^3d^5s^*$ tight-binding theory of PbSe and PbS nanocrystals is developed. It is demonstrated, that the valley splittings of confined electrons and holes strongly and peculiarly depend on the geometry of a nanocrystal. When the nanocrystal lacks a microscopic center of inversion and has T_d symmetry, the splittings are strongly suppressed as compared to the more symmetric nanocrystals with O_h symmetry, having an inversion center. This effect is quite unusual because typically a higher symmetry of a physical system implies a higher degeneracy of its energy levels, while in our case the suppression of the splittings occurs in NCs having lower symmetry. Nevertheless, we were able to explain this puzzling behavior using mathematical apparatus of the group theory.

¹Also with Ioffe Institute, Russian Academy of Sciences

9:48AM Y5.00010 First-principles spectroscopic characterization of PbSe nanoparticles passivated with Fe complexes, KEITH GILMORE, AARON HAMMACK, APRIL SAWVEL, EVELYN ROSEN, D. FRANK OGLETREE, JEFFREY URBAN, DELIA MILLIRON, BRETT HELMS, BRUCE COHEN, DAVID PRENDERGAST, Lawrence Berkeley National Lab, THE MOLECULAR FOUNDRY TEAM — Given that defining characteristics of nanoparticles – morphology, catalytic reactivity, optical and electronic properties – are often dictated by their surfaces, it is informative to investigate how surface chemistry and structure change as different ligands are introduced to the surface. Starting with oleate-passivated PbSe nanoparticles, we remove the oleate ligands and replace them with an organometallic complex: cyclopentadienyl iron dicarbonyl. Measured and calculated x-ray photoemission core-level shifts indicate a charge transfer between surface Pb atoms and Fe atoms. We investigate the nature of this charge transfer in more detail through analysis of x-ray absorption spectra (XAS) at the Fe L-edge. Fe XAS are calculated from first-principles using a GW-based Bethe-Salpeter approach. The spectra reveal that the extent to which pi-backbonding is possible between the Fe and associated carbonyls varies with the charge density on the Fe atom.

10:00AM Y5.00011 Preservation of the optical properties of small Si quantum dots in the face of oxidation¹, HUASHAN LI, ZHIGANG WU, MARK LUSK, Department of Physics, Colorado School of Mines — Rapid oxidation occurs when small, unpassivated Si quantum dots are subjected to ambient conditions, and it may at first seem that complete oxidation of 1-3 nm QDs is inevitable, since their initial oxidation rate is expected to be greater than that for bulk Si for a more open surface structure, and the oxide layers on bulk Si tend to be thicker than the dot radii. We use computations based on density functional theory show that sufficiently small, appropriately terminated dots might actually be able to resist oxidation better than their larger brethren. This is because, on well-passivated bulk surfaces, oxygen attacks silicon through vulnerable sites and defects, and defects are much less likely to be present as dot size decreases. Although the more open surface structure of these small dots does leave certain key sites more vulnerable to oxidation than their bulk counterparts, the oxygen atoms absorbed there are essentially immobile due to large hopping barriers. Furthermore, computations employing the many-body Green function perturbation theory show that the oxidation of these QDs has a relatively small impact on optical character. Therefore, the best defense against oxidation is to eliminate defects; a strategy that becomes increasingly reasonable as dot size decreases.

¹Renewable Energy Materials Research Science and Engineering Center (NSF Grant No. DMR-0820518) at the Colorado School of Mines and the National Renewable Energy Laboratory

10:12AM Y5.00012 Confinement effects on the vibrational properties of colloidal quantum dots, PENG HAN, GABRIEL BESTER, Max Planck Institute for Solid State Research — We present a first-principles study of the confinement effects on the vibrational properties of colloidal III-V and II-VI nanoclusters with thousand atoms and radii up to 16.2 Å. We describe the connection between the vibrational properties including surface-optical and -acoustic modes, coherent acoustic modes and the structural changes induced by the surface. We highlight the qualitative difference between III-Vs and II-VIs. We can clearly ascribe most of the observations to the large relaxation of the clusters dominated by an inward relaxation of the surface penetrating deep inside the cluster in case of the III-Vs and a large distribution of bond length at the surface of II-VIs. These strong confinement effects tend to disappear for clusters with more than 1000 atoms, where a small red shift of the Raman peaks remains, due to a softening in response to undercoordination. The coherent acoustic phonons are identified and found to be in good agreement with results from the Lamb model and experiment. We explain why the simple model by Lamb gives an accurate description in case of the breathing modes while the vibrational properties of small NCs are poorly described by continuum models in general.

Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y6 DMP: Carbon Nanotubes: Devices, Capacitors and Other Applications 206B

8:00AM Y6.00001 The Ultimate Electron Sources Using Millimeter Long Carbon Nanotubes¹, N. PEREA, Department of Physics, The Pennsylvania State University, USA, B. REBOLLO, J.A. BRIONES, A. MORELOS, D. HERNANDEZ, E. MUNOZ, F. LOPEZ-URIAS, Advanced Materials Department, IPICYT, Mexico, A.R. BOTELLO, J.C. CHARLIER, ICMN, Université Catholique de Louvain, Belgium, V. MEUNIER, Department of Physics, Rensselaer Polytechnic Institute, USA, G.A. HIRATA, CNYN-UNAM, Mexico, B. MARUYAMA, AFRL, Materials and Manufacturing Directorate, USA, M. TERRONES, Department of Physics, The Pennsylvania State University, USA and Exotic Nanocarbon Research Center, Shinshu University, Japan, H. TERRONES, Department of Physics, The Pennsylvania State University, USA — We are reporting the fabrication of a very efficient electron source using long and crystalline carbon nanotubes. These devices start to emit electrons at fields as low as 0.10 V/μm and reach threshold emission at 0.164 V/μm. In addition, these electron sources are very stable for long operation periods up to 200 hrs and can achieve peak current density of 2 Acm⁻² at only 0.28 V/μm. To demonstrate intense electron beam generation, these devices were used to produce white light by cathodoluminescence. Finally, to rationalize the measured properties in open carbon nanotubes of different lengths we used density functional theory. The modeling establishes a clear correlation between length and field enhancement factor.

¹JST-Japan, AFRL FA9550-08-1-0204, CONACYT: 63001, S-3908, 3072, S-3909, 60218-F1, 48300.

8:12AM Y6.00002 One-dimensional nature in transport property of SWNT thin film electrochemical transistor, HIDEKAZU SHIMOTANI, SATOSHI TSUDA, Tohoku Univ., HONGTAO YUAN, The Univ. of Tokyo, YOHEI YOMOGIDA, Tohoku Univ., RIEKO MORIYA, Tokyo Metropolitan Univ., TAISHI TAKENOBU, Waseda Univ., KAZUHIRO YANAGI, Tokyo Metropolitan Univ., YOSHIHIRO IWASA, The Univ. of Tokyo — Recent success in isolating single-walled carbon nanotubes (SWNTs) of narrow chirality distribution enabled making pure metallic (m-) and semiconducting (s-) SWNT films. Such films are expected to reflect the nature of individual SWNTs, that is their one dimensional subband structure. Therefore, it is interesting to investigate electronic transport in m- and s-SWNT films by controlling their Fermi level (E_F). Chemical doping or FET is unsuitable for the purpose because of the lack of precise and reversible E_F controllability, and the narrow controllable E_F range, respectively. The problems are solved by our electric double layer transistor technique,¹ where the gate voltage (V_G) is applied through an electrolyte. The conductance and optical absorption spectra of the resistance of s- and m-SWNT films were measured at various V_G . The conductance of the s-SWNT film showed stepwise change against V_G . The absorbance spectra indicate the steps correspond to reaching of the E_F to a vHs. Furthermore, even m-SWNT films showed steep increases of conductance, demonstrating that the conductance strongly depend on the subband filling. ¹ H. Shimotani et al., Appl. Phys. Lett. 88, 073104 (2006).

8:24AM Y6.00003 A general approach for high yield fabrication of CMOS compatible all semiconducting carbon nanotube field effect transistor, MUHAMMAD R. ISLAM, KRISTY KORMONDY, ELIOT SILBAR, SAIFUL KHONDAKER, Nanoscience Technology Center, Department of Physics, University of Central Florida, Orlando, Florida — We report strategies of achieving both high assembly yield of carbon nanotubes at selected position of the circuit via dielectrophoresis (DEP) and field effect transistor (FET) yield using semiconducting enriched single walled carbon nanotube (s-SWNT) aqueous solution. When the DEP parameters were optimized for the assembly of individual s-SWNT, 97% of the devices show FET behavior with a maximum mobility of $210 \text{ cm}^2/\text{Vs}$, on-off current ratio $\sim 10^6$ and on conductance up to $3 \mu\text{S}$, however with an assembly yield of only 33%. As the DEP parameters were optimized so that 1-5 s-SWNTs are connected per electrode pair, the assembly yield was almost 90% with $\sim 90\%$ of these assembled devices demonstrating FET behavior. Further optimization gives an assembly yield of 100% with up to 10 SWNT/site, however with a reduced FET yield of 59%. Improved FET performance including higher current on-off ratio and high switching speed were obtained by integrating a local Al_2O_3 gate to the device. Our 90% FET with 90% assembly yield is the highest reported so far for carbon nanotube devices. Our study provides a pathway which could become a general approach for the high yield fabrication of CMOS compatible carbon nanotube FETs.

8:36AM Y6.00004 Scanning Photocurrent Characterization of Absorption Resonances and Photocarrier Generation in Single-Walled Carbon Nanotubes, TRISTAN DEBORDE, TAL SHARF, Oregon State University, JOSHUA W. KEVEK, Cornell University, ETHAN D. MINOT, Oregon State University — We use a scanning photocurrent microscope (SPCM) in conjunction with a supercontinuum laser source to study resonant absorption in individual single-walled carbon nanotubes (SWNTs). Characterization by spectrally-resolved SPCM is much faster than using resonant Raman scattering. The technique also complements existing Rayleigh scattering techniques because measurements can be performed on SWNTs in a standard field-effect transistor geometry. The broad band light source (0.67 eV to 2.76 eV) is monochromated and then focused onto the SWNT. Resonant absorption is manifested as peaks in photo-induced conductivity as a function of excitation energy. The wide range of photon energies gives us access to the excitonic transitions E11 to E44 in typical semiconducting SWNTs. This allows us to access information about the diameter/chirality of the nanotube, as well as probing phenomena associated with photogenerated carriers in SWNTs at room temperature.

8:48AM Y6.00005 Local and broadband photovoltaic response of aligned carbon nanotube films, SEBASTIEN NANOT, DARIUS MORRIS, LISA A. HENDRICKS, JUNICHIRO KONO, ECE and Physics and Astronomy Department, Rice University, CARY PINT, ROBERT H. HAUGE, Smalley Institute, Rice University, FRANCOIS LEONARD, Sandia National Laboratories, Livermore — Although individual semiconducting single-walled carbon nanotubes (SWCNT) have exhibited clear photovoltaic responses, it remains unclear whether macroscopic films of carbon nanotubes can also behave this way. While some groups have explained finite photovoltages as Schottky barrier effects, other groups have proposed photo-thermoelectric effects in suspended films. Here, we have studied highly aligned SWCNT films that work well as photovoltaics. SWCNTs grown by CVD were transferred onto a SiO_2 substrate. There was a broad diameter distribution in the films to obtain a large wavelength range of interband absorption. The films were top-contacted with various metals. We made a systematic scanning photocurrent study of such samples at 660 and 1350 nm. A strong local photovoltage appeared at electrode-SWCNT interfaces. Detailed comparison with theoretical calculations of the dependence of photo-response on the nanotube orientation, metal electrode type, and temperature unambiguously revealed the photovoltaic nature of the observed photovoltage. We assign these effects to the doping of both metallic and semiconducting SWCNTs under the electrodes, in a similar fashion to graphene, its lineshape being determined by the diffusion of photoexcited carriers. Finally, to obtain a finite net signal under global illumination, we utilized different electrode combinations and studied their photoresponses from the visible up to mid-infrared and terahertz.

9:00AM Y6.00006 Separated Carbon Nanotube Macroelectronics for Active Matrix Organic Light-Emitting Diode Displays, YUE FU, JIALU ZHANG, CHUAN WANG, POCHIANG CHEN, CHONGWU ZHOU, University of Southern California — Active matrix organic light-emitting diode (AMOLED) display holds great potential for the next generation visual technologies due to its high light efficiency, flexibility, lightweight, and low-temperature processing. However, suitable thin-film transistors (TFTs) are required to realize the advantages of AMOLED. Pre-separated, semiconducting enriched carbon nanotubes are excellent candidates for this purpose because of their excellent mobility, high percentage of semiconducting nanotubes, and room-temperature processing compatibility. Here we report, for the first time, the demonstration of AMOLED displays driven by separated nanotube thin-film transistors (SN-TFTs) including key technology components such as large-scale high-yield fabrication of devices with superior performance, carbon nanotube film density optimization, bilayer gate dielectric for improved substrate adhesion to the deposited nanotube film, and the demonstration of monolithically integrated AMOLED display elements with 500 pixels driven by 1000 SN-TFTs. Our approach can serve as the critical foundation for future nanotube-based thin-film display electronics.

9:12AM Y6.00007 Semiconducting Enriched Carbon Nanotube Aligned Arrays of Tunable Density and Their Electrical Transport Properties¹, SAIFUL I. KHONDAKER, Nanoscience Technology Center, Department of Physics, School of Electrical Engineering and Computer Science, University of Central Florida, BIDDUT K. SARKER, SHASHAK SHEKHAR, Nanoscience Technology Center, and Department of Physics, University of Central Florida — Many proposed applications of semiconducting single walled carbon nanotubes (s-SWNT) require massively parallel array as they can average out inhomogeneity of individual tubes, provide larger on- currents and better transistor properties. Here, we report assembly of solution processed semiconducting enriched (99%) SWNT in an array with varying linear density via ac-dielectrophoresis and investigate electronic transport properties of the fabricated devices. We show that (i) the quality of the alignment varies with frequency of the applied voltage and that (ii) by varying the frequency and concentration of the solution, we can control the linear density in the array from 1 to 25 s-SWNT/ μm . We found that with increasing nanotube density the device mobility increases while the current on-off ratio decreases dramatically. For the dense array, the device current density was $16 \mu\text{A}/\mu\text{m}$, on-conductance was $390 \mu\text{S}$, and sheet resistance was $30 \text{ k}\Omega/\square$. These values are the best reported so far for any semiconducting nanotube array. Our study will have important implications in fabricating high quality devices for digital and analog electronics.

¹This work is partially supported by the U.S. National Science Foundation under Grant ECCS- 0748091 (CAREER).

9:24AM Y6.00008 Fully Transparent Separated Carbon Nanotube Based Thin-film Transistors and their Application in Display Electronics, JIALU ZHANG, CHUAN WANG, CHONGWU ZHOU, University of Southern California — Transparent electronics have attracted numerous research efforts in recent years due to its great potential to make significant commercial impact in a wide variety of areas such as transparent displays. High optical transparency as well as good electrical performance is required for this kind of applications. Pre-separated, semiconducting enriched carbon nanotubes are excellent candidates for this purpose due to their excellent mobility, high percentage of semiconducting nanotubes, and room-temperature processing compatibility. Here in this paper, we report fully transparent high-yield transistors based on separated carbon nanotube random network. High electrical performance is achieved by using large work function thin metal layer and indium-tin oxide (ITO) as contacts and all devices show excellent transparency ($\sim 82\%$). Furthermore, OLED control circuit has been demonstrated with transparent separated nanotube thin-film transistors and large range output light intensity modulation has been observed. Our results suggest the promising future of separated carbon nanotube based transparent electronics and can serve as the critical foundation for the next generation transparent display applications.

9:36AM Y6.00009 Fabrication of Carbon nanotube TFTs for pressure-sensing device by printing method, HIROYUKI ENDOH, NEC Corporation, FUMIYUKI NIHEY, HIDEAKI NUMATA, KAZUKI IHARA, Technology Research Association for Single Wall Carbon Nanotubes, TSUYOSHI SEKITANI, TAKAO SOMEYA, The University of Tokyo — Printing technology is very promising from many advantages, for example, low cost, flexible etc. We previously have developed a high-performance printed thin-film transistor (TFT) using single-walled carbon nanotube (CNT). A simple ink-jet printing system was used for drawing the device patterns. The maximum temperature was 200 degrees during nano-silver electrode fabrication. The temperature of CNT-channel patterning is under 50 degrees. The widths of the source and drain electrodes were about 1 mm and the channel length were about 150 μm . The thickness of the gate insulator was about 650 nm. The estimated mobilities using over 95% purified semiconductive-CNT were $\sim 5.1 \text{ cm}^2/\text{Vs}$ for the TFTs whose on/off ratio were more than 5,000. This time we fabricated CNT-TFT arrays for pressure-sensing sheet devices, using the printed-process on a plastic film. CNT-TFT sheet has a dimension of 16 x 16 TFTs. The average mobility of the TFTs is 4.6 cm^2/Vs . The pressure-sensing cell was prepared to combine Printed-TFT, a conductive rubber sheet and a film with a copper foil. Drain current changes in response to pressure applied to the current changes were observed up to 100nA from 10pA. These results were very promising for CNT-TFT applications to printable electronics.

9:48AM Y6.00010 Flexible Single-wall Carbon Nanotube Membrane Symmetric Aqueous Double Layer Electrochemical Capacitor¹, PRALAV SHETTY, Mechanical Engineering Department, The Pennsylvania State University, University Park, PA 16802, USA, JIM KAPULSON, RAMAKRISHNAN RAJAGOPALAN, Materials Research Institute, The Pennsylvania State University, University Park, PA 16802, USA, KOFI ADU, Department of Physics, The Pennsylvania State University, Altoona College, Altoona, PA 16601, USA — We present preliminary results on an aqueous symmetric double layer electrochemical capacitor (EDLC) constructed with flexible binder-free single wall carbon (SWCNTs) membrane as electrodes. The capacitors were cycled from 0 to 1V @ 10 A/g for 10,000 cycles with 99.9% coulombic efficiency and 94% energy efficiency, and 100% depth of discharge. The power performance of the aqueous symmetric SWCNTs membrane capacitor is almost 100 –1000 times better than commercial non-aqueous EDLC capacitors.

¹This Work is Funded by The Pennsylvania State University Materials Research Institute

10:00AM Y6.00011 Optimizing Efficiency in Conducting Polymer/Single-walled Carbon Nanotube Hybrids for Organic Photovoltaics, JOSH HOLT, Chemical & Materials Science Center, National Renewable Energy Laboratory, 1617 Cole Blvd., Golden, CO 80401 (USA), FRITZ PREHN, Department of Materials Science and Engineering, University of Wisconsin-Madison, 1509 University Ave., Madison, WI 53706 (USA), MARTIN HEENEY, Department of Chemistry, Imperial College London, South Kensington, SW7 2AZ, UK, NIKOS KOPI-DAKIS, GARRY RUMBLES, JEFFREY BLACKBURN, Chemical & Materials Science Center, National Renewable Energy Laboratory, 1617 Cole Blvd., Golden, CO 80401 (USA) — Several unique properties of single-walled carbon nanotubes (SWCNTs) have motivated their investigation as potential replacements for fullerene derivatives as the acceptor phase of organic photovoltaic (OPV) devices. Although replacement of the ubiquitous fullerene acceptors by SWCNTs in OPV devices has shown limited success thus far, better understanding of charge transfer between SWCNTs and conjugated polymers has promoted its viability. We provide experimental evidence that m-SWNTs limit the generation efficiency and lifetime of the charge-separated state in these composites. We also probe the photo-carrier generation and decay dynamics in poly(3-hexylthiophene) (P3HT) paired with a broad diameter range of SWCNTs. We witness electron transfer from the polymer to SWCNT and *selective* hole transfer from the SWCNT to polymer by varying the nanotube HOMO via its diameter. We finally extend our investigation to additional semi-conducting polymers that have contributed to high OPV efficiencies, pBTTT and PCDTBT.

10:12AM Y6.00012 Ultra-high density aligned Carbon-nanotube with controlled nano-morphology for supercapacitors, MEHDI GHAFARI, RAN ZHAO, YANG LIU, YUE ZHOU, JIPING CHENG, penn state univeristy, ROBERTO GUZMAN DE VILLORIA, B.L WARDLE, MIT, Q.M. ZHANG, penn state univeristy — Recent advances in fabricating controlled-morphology vertically aligned carbon nanotubes (VA-CNTs) with ultrahigh volume fraction create unique opportunities for developing unconventional supercapacitors with ultra-high energy density, power density, and long charge/discharge cycle life. Continuous paths through inter-VA-CNT channels allow fast ion transport, and high electrical conduction of the aligned CNTs in the composite electrodes lead to fast discharge speed. We investigate the charge-discharge characteristics of VA-CNTs with >20 vol% of CNT and ionic liquids as electrolytes. By employing both the electric and electromechanical spectroscopies, as well as nanostructured materials characterization, the ion transport and storage behaviors in porous electrodes are studied. The results suggest pathways for optimizing the electrode morphology in supercapacitors using ultra-high volume fraction VA-CNTs to further enhance performance.

10:24AM Y6.00013 Capacitance of highly ordered nanocapacitors arrays: Model and microscopy¹, ANDREA CORTES, CARLOS CELEDON, PABLO ULLOA, PATRICIO HABERLE, Departament of Physics, Universidad Tecnica Federico Santa Maria — It is described briefly the process used to build an ordered porous array in an anodic aluminum oxide (AAO) template, filled with multiwall carbon nanotubes (MWCNTs). The MWCNTs were grown directly inside the template through chemical vapor deposition (CVD). The role of the CNTs is to provide narrow metal electrodes with contact with a dielectric surface barrier, hence, forming a capacitor. This procedure allows the construction of an array of 10^{10} parallel nano-spherical capacitors/ cm^2 . A central part of this contribution is the use of physical parameters obtained from processing high-resolution transmission electron microscopy (HRTEM) images, to predict the specific capacitance of the AAO arrays. Electrical parameters were obtained by solving Laplace's equation through finite element methods

¹This research is partially funded by the following Grant 192 Nos.: MECESUP, No. FSM0605 and FONDECYT, Nos. 193 1100672 and 1110935, Chile.

10:36AM Y6.00014 Gecko inspired carbon nanotube based thermal gap pads¹, SUNNY SETHI, ALI DHINOJWALA, The University of Akron — Thermal management has become a critical factor in designing the next generation of microprocessors. The bottleneck in design of material for efficient heat transfer from electronic units to heat sinks is to enhance heat flow across interface between two dissimilar, rough surfaces. Carbon nanotubes (CNT) have been shown to be promising candidates for thermal transport. However, the heat transport across the interface continues to be a challenging hurdle. In the current work we designed free standing thermal pads based on gecko-inspired carbon nanotube adhesives. The pads were made of metallic carbon nanotubes and the structure was designed such that it would allow large area of intimate contact. We showed that these adhesive pads can be used as electrical and thermal interconnects.

¹Funded by Airforce Research Laboratory and NSF

10:48AM Y6.00015 Stiff and Multifunctional Carbon Nanotube Composites, YUNTIAN ZHU, XIN WANG, North Carolina State University, QINGWEN LI, Suzhou Institute of Nanotechnology and Nanobionics, PHILIP BRADFORD, FUH-GWO YUAN, North Carolina State University, DENNIS TUCKER, NASA Marshall Space Flight Center, WEI CAI, HSIN WANG, Oak Ridge National Laboratory — It has been a challenge for two decades to assemble the extremely strong carbon nanotubes (CNTs) into macroscopic CNT composites that break the strength ceiling of carbon fiber composites. Here we report the fast incorporation of long CNTs into polymer matrix using a novel approach, stretch-winding, to produce composites that are much stronger than any current engineering composite. The CNT composites reach a strength of 3.8 GPa, an excellent electrical conductivity and a high thermal conductivity. These superior properties are primarily derived from the long length, high volume fraction, good alignment and reduced waviness of the CNTs that are produced. The combination of high strength and excellent electrical and thermal conductivities makes CNT composites a promising enabler of new aerospace technologies and adventures.

Friday, March 2, 2012 8:00AM - 11:00AM – Session Y7 DCMP: Glassy Metallic, Semiconductor, Oxide and Chalcogenide Systems 207

8:00AM Y7.00001 Ion irradiation induced suppression of shear banding in amorphous ZrCuAl nanowires under simulated compression, QIRAN XIAO, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, HOWARD SHENG, School of Physics, Astronomy and Computational Sciences, George Mason University, YUNFENG SHI, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute — Metallic glasses (MG) are amorphous metallic solids which exhibit extraordinary mechanical properties including large elastic strain limit and high tensile strength; at the same time, MGs are generally brittle due to catastrophic failure of shear banding. Controversy remains, however, as to whether shear banding is size-dependent in MG nanopillar samples prepared using Focused Ion Beam (FIB) technique. Here we modeled Zr₅₀Cu₄₀Al₁₀ MG nanopillars under irradiation via molecular dynamic simulations (MD) and found a transition in deformation mode from dominant shear-banding to homogeneous shear-flow. Our results call for careful consideration of irradiation damage as a result of FIB sample-preparation-technique. In addition, we also show the amorphization of icosahedral structures as a result of irradiation, which might be responsible for the homogeneous deformation mode of irradiated MG nanowires upon compression tests.

8:12AM Y7.00002 Two Level Systems in Amorphous Silicon¹, DANIEL QUEEN, JULIE KAREL, University of California, Berkeley, XIAO LIU, Naval Research Laboratory, GREGORY HOHENSEE, DAVID CAHILL, University of Illinois, Urbana-Champaign, FRANCES HELLMAN, University of California, Berkeley — The specific heat of e-beam evaporated a-Si thin films prepared at various growth temperatures was measured from 2-300K. Below 20K, films with low density have a specific heat in excess of the predicted Debye value while higher density films do not. The excess heat capacity is typical of a glass with a linear contribution that is characteristic of two-level systems (TLS) and a T³ contribution that is in excess of the Debye specific heat calculated from the measured sound velocity. The excess specific heat is independent of the elastic properties of the materials as determined by shear modulus and sound velocity measurements but depends on film density. The density dependence suggests that the low energy excitations form in voids or low density regions and are not intrinsic to the amorphous silicon network. A correlation is found between the density of TLS and the excess T³ specific heat suggesting that they have a common origin. Comparisons will be made between the specific heat and internal friction.

¹This work supported by the NSF under Grant No. DMR-0907724

8:24AM Y7.00003 First principles calculations of the Urbach tail in the optical absorption of silica glass¹, BABAK SADIGH, Lawrence Livermore National Laboratory, PAUL ERHART, Chalmers University of Technology, DANIEL ABERG, ERIC SCHWEGLER, JEFF BUDE, Lawrence Livermore National Laboratory, OPTIC DAMAGE MODELING TEAM — We present density-functional theory calculations of the optical absorption spectra of silica glass for temperatures up to 2400 K. The calculated spectra exhibit exponential tails near the fundamental absorption edge that follow the Urbach rule, in good agreement with experiments. We also discuss the accuracy of our results by comparing to hybrid exchange correlation functionals. By deriving a simple relationship between the exponential tails of the absorption coefficient and the electronic density-of-states, we establish a direct link between the photoemission and the absorption spectra near the absorption edge. This relationship is subsequently employed to determine the lower bound to the Urbach frequency regime. Most interestingly, in this frequency interval, the optical absorption is Poisson distributed with very large statistical fluctuations. Finally, We determine the upper bound to the Urbach frequency regime by identifying the frequency at which transition to Poisson distribution takes place.

¹This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 with support from the Laboratory Directed Research and Development Program.

8:36AM Y7.00004 Substrate- and interface-mediated photocrystallization in a-Se films and multi-layers, G.P. LINDBERG, R.E. TALLMAN, B.A. WEINSTEIN, SUNY Buffalo, NY 14260-1500 USA, S. ABBASZADEH, K.S. KARIM, Univ. of Waterloo, Ontario, N2L 3G1 CA, A. REZNIK, TBRI, Thunder Bay, Ontario P7B 5E1 CA — Photocrystallization in a-Se films and layered a-Se structures is studied by Raman scattering as a function of temperature for photon energies near or slightly below the band gap. The samples are ~16.5 μm thick films of a-Se grown i) directly on glass, ii) on indium tin oxide (ITO) coated glass, iii) on glass that is spin coated with 800nm polyimide, and iv) on a Capton sheet. A low As-concentration (< 0.2 %) is present in several of the a-Se films. We compare the results on these samples to prior findings on a-Se HARP targets, and on a polymer-encapsulated a-Se film [1]. We observe strong evidence that the interface between the a-Se film and the underlying substrate and/or multi-layers plays an important role in the onset time and growth rate of photocrystallized Se domains. In some samples a discontinuous increase in the onset time with increasing temperature occurs near the glass transition (~310K), and there is a surprising "dead zone" of no crystallization in this region. Other samples merely show a minimum in the onset time at similar temperatures, but no discontinuity and no region where crystallization is absent. Soft intermediate layers appear to increase stability against crystallization in an overlying a-Se film. The competing effects of substrate shear strain and thermal driving forces on the photocrystallization process are considered to account for these findings.

[1] R.E. Tallman et. al. J. Non-crystalline Sols. **354**, 4577-81 (2008)

8:48AM Y7.00005 Lattice irreversibility and enhanced fragility under fatigue in amorphous solids, DESPINA LOUCA, PENG TONG, University of Virginia, GONGYAO WANG, PETER LIAW, University of Tennessee, YOSHIHIKO YOKOYAMA, Tohoku University, ANNA LLOBET, Los Alamos National Laboratory, YIMING QIU, NIST Center for Neutron Research — The enhanced brittleness observed in glassy ZrCuAl metallic alloys under mechanical cyclic fatigue loading is linked to a local atomic structure reorganization and suppression of atomic fluctuations. From the analysis of neutron scattering and the pair density function technique, an atomic cluster restructuring is observed that intensifies with increasing the compression cycles ex-situ. This is accompanied by an attenuation of the extended phonon-like lattice dynamics, beyond the region in the momentum space where the Boson peak appears, observed by inelastic neutron scattering. Together both effects most likely render the glass more fragile. These findings provide a direct link between the plasticity and the internal structure of metallic glasses under fatigue.

9:00AM Y7.00006 Probing the liquid behavior in La-based metallic glasses using NMR spectroscopy, MAGDALENA SANDOR, University of North Carolina, WEI XU, Huazhong University of Science and Technology, HAI-BO KE, XUE-KUI XI, Chinese Academy of Sciences, YUE WU, University of North Carolina, WEI-HUA WANG, Chinese Academy of Sciences — The nature of liquid structure and its temperature and/or pressure dependent behavior is currently an active area of scientific investigation. Temperature dependent ^{27}Al nuclear magnetic resonance (NMR) experiments were carried out above the liquid temperature in La-based metallic glasses. The strong coexistence of two liquid states was observed in addition to nonlinear liquid behavior. NMR results also provide thermodynamic insight for the structural changes observed.

9:12AM Y7.00007 Chemical ordering in Cu-Zr and Cu-Hf liquids and glasses, NICHOLAS MAURO, ADAM VOGT, MATT BLODGETT, JAMES BENDERT, KENNETH KELTON, Washington University, WASHINGTON UNIVERSITY DEPARTMENT OF PHYSICS TEAM — Evidence for chemical ordering in Cu-Zr and Cu-Hf metallic liquids and glasses is presented. High-energy X-ray diffraction data has been taken using the Beamline Electrostatic (BESL) technique and stationary scattering methods up to a high momentum transfer. From this data, we obtained the total pair-correlation functions. By examining the structural evolution in the equilibrium and undercooled liquid, and the glassy state, we find that ordering occurs, increasing the Cu-Zr (Cu-Hf) and Zr-Zr (Hf-Hf) correlations over a wide composition and temperature range. This ordering is evident by a judicious choice of scattering lengths and compositions. Growth is observed at two distinct r -space coordinates in the pair-correlation function, unique to these two metallic systems. These results will be discussed in the context of previous experiments which indicate that this ordering is chemical and topological in nature, likely due to the development of Cu-centered icosahedral clusters.

9:24AM Y7.00008 Molecular structure of $\text{Si}_x\text{Ge}_x\text{Te}_{100-2x}$ glasses¹, K. GUNASEKERA, P. BOOLCHAND, University of Cincinnati, S. MAMEDOV, Horiba Jobin Yvon Inc., New Jersey — Bulk glasses of the titled ternary have been synthesized in the $8\% < x < 16\%$ range by melt quenching. Glass transition temperatures, $T_g(x)$, increase linearly from 140°C at $x = 8\%$ to 200°C at $x = 12\%$, then decrease steadily to 160°C thereafter. The non-reversing enthalpy of relaxation at T_g shows a broad minimum near 9% but a maximum near 12% . Glasses appear to be fully polymerized at $x < 12\%$, but segregate as $x > 12\%$. The broad minimum near 9% , most likely, represents the opening of an Intermediate Phase. Raman scattering, excited using 785 nm radiation of a glass at $x = 10\%$, shows two modes, a broad one near 160 cm^{-1} and a narrow one near 127 cm^{-1} . A mode near 157 cm^{-1} has been previously² identified with polymeric Te_n chains of a-Te. Tentatively, we assign the 127 cm^{-1} mode with face-sharing³ GeTe_4 , and a mode near 170 cm^{-1} with edge-sharing SiTe_4 tetrahedra in these glasses. The nature of glass structure evolution with composition will be elucidated.

¹Supported by NSG grant DMR- 08-53957.

²M.Brodsky, Phys. Stat. Solidi(b) 52, 609 (1972)

³M. Malyj et al. Phys. Rev. B 31, 3672 (1985)

9:36AM Y7.00009 The sharpness of thermally reversing windows as a measure of glass network homogeneity¹, S. BHOSLE, K. GUNASEKERA, P. BOOLCHAND, University of Cincinnati, M. MICOULAUT, University of Paris IV, C. MASSOBRIO, University of Strassbourg — Reversibility windows(RWs) have been observed² in Chalcogenides, modified- and unmodified-oxides, and solid electrolytes. These are identified with isostatically rigid networks formed in narrow compositional windows between flexible and stressed-rigid elastic phases. Until recently, we found RWs in oxides and solid electrolytes to be sharper than in chalcogenides. Recently we introduced³ a Raman profiling method to track homogeneity of melts during synthesis, and found that the kinetics of homogenization of chalcogenide melts are slow. The enthalpy of relaxation at T_g measured in binary $\text{Ge}_x\text{Se}_{100-x}$ glasses show the RW to be intrinsically square-well like with sharp edges in homogeneous samples ($\Delta x \sim 0$), and becomes trapezoidal ($\Delta x = 1.5\%$), then triangular ($\Delta x = 3\%$) and eventually disappears as glass heterogeneity increases. The heterogeneity deduced from Raman profiling experiments provides the Ge-stoichiometry variation (Δx) across a batch composition, which can be used to predict the observed RWs.

¹Supported by NSF grant DMR-08-53907.

²Boolchand et al., Phil. Mag 85, 3823 (2005)

³Bhosle et al., Sol. St. Comm. 151, 1851 (2011)

9:48AM Y7.00010 Boson mode, Medium Range Structure and Intermediate Phase (IP) in $(\text{Na}_2\text{O})_x(\text{B}_2\text{O}_3)_{1-x}$ glasses¹, K. VIGNAROUBAN, P. BOOLCHAND, Univ of Cincinnati, M. MICOULAUT, Univ of Paris, M. MALKI, Univ of Orleans — Raman scattering of titled glasses are examined using a T64000 Dispersive system. Scattering strengths of the Boson mode (40 cm^{-1} , 70 cm^{-1}) and the Boroxyl ring (BR) mode (808 cm^{-1}) are found to decrease with increasing x at the same rate in the $0 < x < 20\%$ soda range. Apparently, the 2D character of BRs embedded in a 3D network gives rise to the Boson mode.² The triad of modes (705 , 740 , 770 cm^{-1}) near the 808 cm^{-1} mode are found to display a maximum in scattering strength near $x = 37\%$ (705 cm^{-1}), 33% (740 cm^{-1}) and 25% (770 cm^{-1}), suggesting that these are also ring modes of Na-tripentaborate (STPB), Na-diborate (SDB) and Na-triborate (STB) super-structures. Variations in Raman scattering strengths also suggest that STB percolate near $x = 20\%$, the *stress* transition, while the STPB and SDB percolate near $x = 40\%$, the *rigidity* transition. These transitions were inferred from m-DSC experiments that show an intermediate phase in the $20\% < x < 40\%$ range in dry and homogeneous glasses.

¹Supported by NSF grant DMR - 08-53957.

²M. Flores-Ruiz and G. Naumis, PRB, 2011. **83**: p. 184204

10:00AM Y7.00011 Boson mode, Intermediate Phase, and glass molecular structure of heavy metal Oxides¹, S. CHAKRABORTY, P. BOOLCHAND, U. of Cincinnati — We have synthesized bulk glasses of $(\text{B}_2\text{O}_3)_5(\text{TeO}_2)_{95-x}(\text{V}_2\text{O}_5)_x$ ternary and examined their thermal and optical properties as a function of composition “ x .” The enthalpy of relaxation at T_g shows a global minimum in the Vanadia concentration of $24\% < x < 26.5\%$, which we identify² as the intermediate phase (IP) with compositions at $x < 24\%$ to be in stressed-rigid and those at $x > 26.5\%$ in the flexible phase. Raman scattering reveals a rich lineshape including a Boson mode, whose scattering strength steadily decreases with increasing x , possibly due to bifurcation of weak (Te-O_{axial}) and strong ($\text{Te-O}_{equatorial}$) springs characteristic of TeO_2 building blocks.³ Vanadia alloying brings in isostatic building blocks, pyramidal $\text{V}(\text{O}_{1/2})_3$ and quasi-tetrahedral $\text{O}=\text{V}(\text{O}_{1/2})_3$ as suggested by present Raman scattering and recent ^{51}V NMR data.⁴ We describe the structure evolution of these glasses in terms of the Te-centered and V-centered local structures.

¹Supported by NSF grant DMR-08-53957.

²P. Boolchand et al. Phil. Mag. **85**, 3823 (2005)

³S. Sakida, J. Phys.: Condens. Matter **12** (2000)

⁴Ibid.

10:12AM Y7.00012 Identification of strong and weak interacting two-level systems in KBr:CN
 , ALEJANDRO GAITA-ARINO, Instituto de Ciencia Molecular, University of Valencia, MOSHE SCHECHTER, Department of Physics, Ben Gurion University of the Negev — Tunneling two-level systems (TLSs) are believed to be the source of phenomena such as the universal low temperature properties in disordered and amorphous solids, and $1/f$ noise. The existence of these phenomena in a large variety of dissimilar physical systems testifies for the universal nature of the TLSs, which however, is not yet known. Following a recent suggestion that attributes the low temperature TLSs to inversion pairs [M. Schechter and P.C.E. Stamp, arXiv:0910.1283] we calculate explicitly the TLS-phonon coupling of inversion symmetric and asymmetric TLSs in a given disordered crystal. Our work (a) estimates parameters that support the theory in M. Schechter and P.C.E. Stamp, arXiv:0910.1283 in its general form, and (b) positively identifies the relevant TLSs in a given system. Consequences to the understanding of the microscopic structure of amorphous solids will be discussed. A. Gaita-Arino and M. Schechter, Phys. Rev. Lett. **107**, 105504 (2011)

10:24AM Y7.00013 ABSTRACT WITHDRAWN —

10:36AM Y7.00014 Coulomb Glass: a Mean Field Study, SALVATORE MANDRA, MATTEO PALASSINI, Universitat de Barcelona — We study the Coulomb glass model of disordered localized electrons with long-range Coulomb interaction, which describes systems such as disordered insulators, granular metals, amorphous semiconductors, or doped crystalline semiconductors. Long ago Efros and Shklovskii showed that the long-range repulsion induces a soft Coulomb gap in the single particle density of states at low temperatures. Recent works suggested that this gap is associated to a transition to a glass phase, similar to the Almeida-Thouless transition in spin glasses. In this work, we use a mean field approach to characterize several physical properties of the Coulomb glass. In particular, following a seminal work of Bray and Moore, we show that the Edward-Anderson parameter q_{EA} and the spin glass susceptibility χ_{SG} are directly related to spectrum distribution of the Hessian matrix around free energy minima. Using this result, we show that no glass transition is associated to the gap formation.

10:48AM Y7.00015 Non-linear dielectric response of glass formers under oscillating temperature, TAKASHI ODAGAKI, MASATOSHI KURODA, HIDEAKI KATOH, Tokyo Denki University, YASUO SARUYAMA, Kyoto Institute of Technology — Exploiting a simple model we investigate linear and non-linear dielectric responses of glass formers under oscillating temperature. We demonstrate that three characteristic temperatures, Vogel-Fulcher, glass transition and cross-over temperatures, can be determined from the analysis of the dielectric response. We first show that the real part of the linear susceptibility at the static limit becomes a cusp below the cross-over temperature and its curvature changes at the glass transition temperature. We also analyze the non-linear susceptibility under oscillating temperature which contains information of the response of the system, in particular of the free energy landscape, against the temperature modulation. We find that the real part of the non-linear susceptibility shows anomalies at the characteristic temperatures similar to the linear susceptibility.

Friday, March 2, 2012 8:00AM - 10:36AM —

Session Y8 DMP GMAG: Focus Session: Frustrated Magnetism - Experiment 208

8:00AM Y8.00001 Magnetic ordering in SrEr_2O_4 and SrHo_2O_4 , O.A. PETRENKO, T.J. HAYES, O. YOUNG, G. BALAKRISHNAN, University of Warwick, UK, L.C. CHAPON, A. WILDES, ILL, Grenoble, France, P. MANUEL, ISIS, RAL, UK, P.P. DEEN, ESS, Lund, Sweden — Single crystal neutron diffraction reveals two distinct components to the magnetic ordering in geometrically frustrated compounds SrEr_2O_4 and SrHo_2O_4 . One component, a long-range ordered $\mathbf{k} = 0$ structure, is associated with the appearance of resolution limited Bragg peaks below the ordering temperature. Another component is a quasi 1D short-range structure which manifests itself by the presence of a strong diffuse scattering signal forming *planes* in reciprocal space. On cooling from higher temperatures down to 0.06 K, the partially ordered component develops gradually and does not undergo a pronounced phase transition. The magnetic moments in the long-range structure are pointing along the [001] axes in both compounds. In the short-range structure (which is incommensurate in SrEr_2O_4 and $\mathbf{k} \approx 1/2$ in SrHo_2O_4) the moments are predominantly pointing along the [001] and [010] axes in these two compounds respectively. The unusual coexistence of two magnetic structures is probed using XYZ-polarised neutron scattering techniques [1,2]. [1] T.J. Hayes *et al.*, to appear in Phys. Rev. B (2011). [2] O. Young *et al.*, in preparation (2011).

8:12AM Y8.00002 Magnetic order in GdBiPt studied by x-ray resonant magnetic scattering, A. KREYSSIG, M.G. KIM, Ames Laboratory, Dept. of Physics and Astronomy, Iowa State University, Ames, IA, J.W. KIM, Advanced Photon Source, ANL, Argonne, IL, S.M. SAUERBREI, S.D. MARCH, G.R. TESDALL, S.L. BUD'KO, P.C. CANFIELD, R.J. MCQUEENEY, A.I. GOLDMAN, Ames Laboratory, Dept. of Physics and Astronomy, Iowa State University, Ames, IA — Rare earth (*R*) half-Heusler compounds, *R*BiPt, exhibit a wide spectrum of novel ground states.[1] We have employed x-ray resonant magnetic scattering to elucidate the microscopic details of the magnetic structure in GdBiPt below $T_N = 8.5$ K. Experiments at the Gd L_2 absorption edge show that the Gd moments order in an antiferromagnetic stacking along the cubic diagonal [1 1 1] direction satisfying the requirement for an antiferromagnetic topological insulator as proposed previously[2] where both time-reversal symmetry and lattice translational symmetry are broken, but their product is conserved. The work at the Ames Laboratory was supported by US DOE, Office of Basic Energy Sciences, DMSE, contract DE-AC02-07CH11358. [1] P. C. Canfield *et al.*, J. Appl. Phys. **70**, 5800 (1991). [2] R. S. K. Mong *et al.*, Phys. Rev. B **81**, 245209 (2010).

8:24AM Y8.00003 X-ray resonance Exchange scattering study of Field induced meta-magnetic phases in TbNi_2Ge_2 ¹, R. DAS, Z. ISLAM, J.P.C. RUFF, Advanced Photon Source, Argonne National Laboratory, P.C. CANFIELD, Ames Laboratory, Iowa State University — Rare-earth inter-metallic compound, TbNi_2Ge_2 is an interesting material for its uniaxial anisotropy and the presence of a number of meta-magnetic phases (MP), which we have investigated using x-ray resonant exchange scattering techniques. Two distinct field induced MPs have been revealed at 5 K for fields below 3 T applied along the *c* axis. In zero field, the magnetic structure is characterized primarily by commensurate $q_1 = (0,0,0.75)$, $q_2 = (0.5,0.5,0)$ and $q_3 = (0.5,0.5,0.5)$ wave vectors, implying a complex sequence of FM and AFM planes. With increasing magnetic field, a weak (0,0,1) peak starts to evolve reaching a maximum in the first MP (1.2 T < H < 1.6 T) and sharply disappears on entering the second MP (H > 1.6 T). In the second MP, q_1 becomes incommensurate, (0,0,0.766), q_2 gets strongly suppressed, and q_3 peak splits into combination harmonics of q_1 and q_2 . The persistence of AF peaks imply that AF planes are quite robust to spin-flip transitions and MP phases are intricate in nature due to several competing interactions in this compound.

¹Use of the APS is supported by the DOE, Office of Science, under Contract No. DE-AC02-06CH11357, Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. DE-AC02-07CH11358

8:36AM Y8.00004 Inelastic neutron scattering of the itinerant magnets Cr₂Te₃ and tr-Cr₅Te₈

, ADAM ACZEL, GARRETT GRANROTH, Oak Ridge National Lab, NIRMAL GHIMIRE, University of Tennessee, MICHAEL MCGUIRE, Oak Ridge National Lab, DAVID MANDRUS, University of Tennessee, STEVE NAGLER, Oak Ridge National Lab — Itinerant magnets based on transition metal chalcogenide compounds are of current interest, in part due to their relationship to the parent compounds of Fe-based superconductors. Two particularly interesting systems in this family are the chromium tellurides Cr₂Te₃ and trigonal (tr) Cr₅Te₈. These materials crystallize in layered structures with alternating partially and fully-occupied planes of Cr atoms stacked along the c-axis. Magnetization measurements along different crystallographic directions show a net ferromagnetic response and large magnetic anisotropy. In addition, the saturation moments are smaller than predicted by an ionic model; consistent with itinerant behavior. Previous neutron diffraction results for Cr₂Te₃ revealed an ordered moment of $< 0.2 \mu_B$ in the partially-occupied planes. We examined the magnetic excitations in these materials by powder neutron spectroscopy measurements using the SEQUOIA instrument at the SNS. We find similar moment sizes for the magnetic Cr atoms of both systems. However, despite their similar crystal structures, ordered moment sizes, and chemical compositions, their magnetic excitation spectra are strikingly different. We compare our data to the predictions of various models in an effort to determine the relevant exchange parameters, put constraints on their magnitudes, and understand the differences between the inelastic magnetic spectra. We find that exchange along the c-direction is critical to explain our data.

8:48AM Y8.00005 Magnetic structure and site occupancies in Fe containing μ -phases AFe (A=Ta, Nb, Mo)¹

, NIRMAL GHIMIRE, University of Tennessee, OVIDIU GARLEA, MICHAEL MCGUIRE, Oak Ridge National Laboratory, DAVID MANDRUS, University of Tennessee and Oak Ridge National Laboratory — Binary μ -phases are intermetallic compounds occurring in numerous systems combining heavy and light transition metals. They have compositions close to AM where A is a 4d or 5d element (Nb, Ta, Mo, W) and M is a 3d element (Fe, Co, Ni, Zn). The possibility of mixed site occupancies results in stoichiometries ranging from A_7M_6 to A_6M_7 . Interestingly, only the Fe containing compounds have been found to show magnetic ordering. NbFe and TaFe are known to be antiferromagnetic, with Neel temperatures near 280 and 320 K, respectively. It has been reported that in these materials ferromagnetic kagome planes stacked antiferromagnetically along the rhombohedral (111) direction, but the exact site occupancies in these layers remain unclear. In our investigation we have found μ -phase of MoFe also to be antiferromagnetic, but with a unique magnetic structure and significantly lower transition temperature about 110 K. Here we discuss in detail the crystallographic and magnetic structures of TaFe, NbFe and MoFe μ -phases based on our recent neutron diffraction studies and physical property measurements on polycrystalline samples.

¹Research sponsored by the U.S. Department of Energy, Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Vehicle Technologies, as part of the Propulsion Materials Program, under Contract No. DE-AC05-00OR22725 with UT-Battelle, LLC.

9:00AM Y8.00006 Magnetic Excitations in the Nearly Localized, Itinerant Magnet Gd, Studied by Neutron Spectroscopy¹

, G.E. GRAROTH, A.A. ACZEL, J.A. FERNANDEZ-BACA, S.E. NAGLER, Oak Ridge National Laboratory — Many of the current questions about magnetic superconductors are present when these complex materials are in the normal state. Therefore studies of simpler itinerant magnets may help provide understanding of these phenomena. We chose to study an Itinerant magnet near to the fully localized limit. The system of choice, Gd has a total moment size of $\sim 7.6 \mu_B$ of which $\sim 0.6 \mu_B$ of that is itinerant. We used the SEQUOIA spectrometer, at the Spallation Neutron Source at Oak Ridge National Laboratory, to measure the magnetic excitations in a 12 gm ¹⁶⁰Gd single crystal. The fine resolution Fermi chopper was spun at 360 Hz and phased for $E_i = 50$ meV. The crystal was mounted with the $h0l$ plane horizontal and then rotated around the vertical axis in 1° steps. This method, and the large out of plane detector coverage of SEQUOIA, provided continuous coverage of a large region of reciprocal space allowing us to map the magnetic excitations. This map provides a measured structure factor for comparison to spin wave models with and without itinerancy effects. These measurements also more clearly resolve the excitations along the $h00$ direction than in previous studies (J. W. Cable, R. M. Nicklow and N. Wakabayashi Phys. Rev. B **32**, 1710 (1985)).

¹This research at Oak Ridge National Laboratory's Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

9:12AM Y8.00007 Magnetic and charge carriers properties of metamagnetic Fe₃Ga₄

, JOSHUA MENDEZ¹, YAN WU², BRADFORD FULFER³, JULIA CHAN⁴, JOHN DITUSA⁵, Louisiana State University — Single crystals of Fe₃Ga₄ were grown via an iodine vapor transport method. Previous investigations of arc-melted polycrystalline samples identify metallic conduction with a magnetic phase transition at 400 K and interesting temperature-dependent metamagnetic behavior. The single crystal samples allow a much fuller exploration of the magnetic properties and have yielded some interesting differences with the previous data. This includes a sharp reduction of the magnetization within the magnetically ordered phase associated with a sharp onset of the metamagnetic behavior in the field dependence near room temperature. A previously identified second phase transition occurs below 50 K where the metamagnetic behavior is replaced by a ferromagnetic magnetization with little hysteresis. We find substantial anisotropy in the magnetization which is particularly apparent between 50 and 300 K. Charge transport experiments are underway to explore the magnetoresistance and Hall effect of this magnet.

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9:24AM Y8.00008 Structural and magnetic characterization of the complete delafossite solid solution (CuAlO₂)_{1-x}(CuCrO₂)_x

, PHILLIP BARTON, RAM SESHADRI, Materials Department and Materials Research Laboratory, University of California, Santa Barbara, ANDREA KNÖLLER, Institut für Materialwissenschaft, Universität Stuttgart 70569, Germany, MATTHEW ROSSEINSKY, Department of Chemistry, University of Liverpool, England, UK — We have prepared the complete delafossite solid solution between diamagnetic CuAlO₂ and the t_{2g}^3 frustrated antiferromagnet CuCrO₂. The crystal structure and magnetism were studied with powder x-ray diffraction and magnetometry. The unit cell parameters follow the Végard law and μ_{eff} is equal to the Cr³⁺ spin-only $S = 3/2$ value. Θ_{CW} is negative and its magnitude increases with Cr substitution. For dilute Cr compositions, J_{BB} was estimated by mean-field theory to be 3.0 meV. Despite the sizable Θ_{CW} , long-range antiferromagnetic order does not develop until x is almost 1, and is preceeded by glassy behavior. For all samples, the 5 K isothermal magnetization is sub-Brillouin and does not saturate in fields up to 5 T. A scaled inverse susceptibility plot reveals that significant short-range antiferromagnetic interactions occur in CuCrO₂ above its Néel temperature. Additionally, the Al-substituted samples exhibit uncompensated short-range behavior and $x = 0.75$ shows glassy characteristics. It is suggested that reduction in magnetic frustration due to the presence of non-magnetic Al does not have as dominant an effect on magnetism as do chemical disorder and dilution of magnetic exchange.

9:36AM Y8.00009 Quasi-Spin Glass in a Geometrically Frustrated Magnet, ARTHUR RAMIREZ, ANDREW LAFORGE, University of California, Santa Cruz, BENNY CHAN, The College of New Jersey, GAVIN LAWES, Wayne State University — A spin glass state is observed in the B-spinel $\text{ZnCr}_{2(1-x)}\text{Ga}_{2x}\text{O}_4$ for $x < 0.05$ via low-temperature magnetization and specific heat. The spin glass phenomenology is conventional. The degrees of freedom (quasi-spins) that undergo freezing are unconventional, however, both in structure as well as their mutual interactions. In particular, below $x = 0.05$, the freezing temperature is independent of quasi-spin density, yielding a strong violation of mean field theory.

9:48AM Y8.00010 Thermodynamic tuning in the dilute Ising magnet $\text{LiHo}_{0.045}\text{Y}_{0.955}\text{F}_4$, D.M. SILEVITCH, M.A. SCHMIDT, University of Chicago, G. AEPPLI, University College London, T.F. ROSENBAUM, University of Chicago — The $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$ family of dipole-coupled Ising magnets has been found to exhibit a rich variety of magnetic phases, ranging from ferromagnet to spin glass to decoupled spin clusters. We examine the behavior for $x=4.5\%$ at dilution refrigerator temperatures as a function of thermal coupling to a heat reservoir. We show that by cooling the sample in different thermodynamic limits, we can select qualitatively different low temperature magnetic states with different quantum characters. Furthermore, we demonstrate that an external transverse magnetic field, which acts to tune the rate of quantum tunneling, can be used to switch the system between the two states.

10:00AM Y8.00011 High Pressure ^{31}P -NMR Study of the 2D Frustrated Square-Lattice Compound $\text{BaCdVO}(\text{PO}_4)_2$ at Low Temperatures¹, B. ROY, Ames Laboratory, Dept. of Phys. and Astro., Iowa State Univ., Y. KOMAKI, Graduate School of Science, Dept. of Phys., Chiba Univ., R. NATH, D.C. JOHNSTON, Y. FURUKAWA, Ames Laboratory, Dept. of Phys. and Astro., Iowa State Univ. — $\text{BaCdVO}(\text{PO}_4)_2$ is a $S=1/2$ frustrated square-lattice (FSL) compound with a nearest neighbor exchange coupling $J_1 \sim -3.36$ K and a next-nearest neighbor exchange coupling $J_2 \sim 3.53$ K bearing $J_2/J_1 \sim 1.05$. Based on the J_2/J_1 ratio, the system is known to be located close to the disordered ground state (known as 'nematic state') regime of the phase diagram. We have carried out ^{31}P -NMR measurements under high pressure (~ 1 GPa) and at low temperatures using dilution refrigerator to investigate the pressure effects on the magnetic properties of the system. Under ambient pressure at $H=2.67$ T, we observed a sharp peak in ^{31}P spin lattice relaxation rate ($1/T_1$) at $T_N \sim 1.05$ K, which corresponds to the antiferromagnetic ordering temperature. On the other hand, under a pressure of 1 GPa, the peak in $1/T_1$ is suppressed and $1/T_1$ shows a sudden decrease below ~ 0.75 K. This indicates that T_N decreases with the application of pressure. We will report the temperature dependence of the NMR spectra and of the $1/T_1$ under different magnetic fields and pressures.

¹Supported by USDOE under the Contract No. DE-AC02-07CH11358.

10:12AM Y8.00012 Triplet state and in-gap scattering from the spin- $1/2$ quantum antiferromagnet Ba_2YMoO_6 , J.P. CARLO, Villanova University, J.P. CLANCY, University of Toronto, T. AHAREN, University of Ottawa, Z. YAMANI, National Research Council Canada, J.P.C. RUFF, Argonne National Laboratory, J.J. WAGMAN, G.J. VAN GASTEL, H.M.L. NOAD, McMaster University, G.E. GRANROTH, Oak Ridge National Laboratory, J.E. GREEDAN, H.A. DABKOWSKA, B.D. GAULIN, McMaster University — The double perovskite material Ba_2YMoO_6 is known to exhibit an absence of long-range and short-range magnetic order down to at least 2K, indicating a high degree of geometric frustration of its tetrahedrally-coordinated spin- $1/2$ Mo^{5+} moments, and NMR results have implied the existence of a spin-singlet ground state. Though geometric frustration in both 3D and quasi-2D systems has been of intense interest in recent years, comparatively little attention has been given to FCC systems, which may exhibit geometric frustration as the FCC lattice can be viewed as a network of edge-sharing tetrahedra. We have conducted inelastic neutron scattering measurements using triple-axis and time-of-flight instruments, revealing a band of scattering at 28 meV which disappears above ~ 125 K; we identify this scattering band as the triplet excitation out of a singlet ground state. We also identify a weaker population of in-gap states which are reminiscent of spin-polaron states induced by weak disorder.

10:24AM Y8.00013 Magnetothermal transport in monoclinic $\text{Nd}_2\text{Ti}_2\text{O}_7$ ¹, HUI XING, Department of Physics, University at Buffalo-SUNY, HONGWANG ZHANG, University at Buffalo-SUNY, HANJIE GUO, Department of Physics, Zhejiang University, CHUNMU FENG, GUANGHAN CAO, ZHUAN XU, Zhejiang University, HAO ZENG, University at Buffalo-SUNY — The monoclinic $\text{Nd}_2\text{Ti}_2\text{O}_7$ is an interesting material due to the existence of a novel field-induced slow spin relaxation (SSR) in the paramagnetic state. The SSR is attributed to the cooperative relaxation mode formed through the spin-spin interactions between partially polarized spins. Here we report the magnetothermal transport measurement on $\text{Nd}_2\text{Ti}_2\text{O}_7$ single crystals. The zero field thermal conductivity is dominated by the phonon contribution. The magnetothermal conductivity reveals significant field dependence. The field and temperature dependence is discussed in connection with the field-induced slow spin relaxation. .

¹Research supported by NSF DMR0547036

Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y9 DMP GMAG: Focus Session: Complex Bulk Oxide: Orbital Physics 209

8:00AM Y9.00001 Temperature dependence of Photoinduced dynamics in the orbital-ordered state of $\text{AV}_{10}\text{O}_{15}$ ($A = \text{Ba}, \text{Sr}$), AYAKA NOGAMI, YUYA ONISHI, KOU TAKUBO, TAKUROU KATSUFUJI, Dept. of Physics, Waseda University — In $\text{AV}_{10}\text{O}_{15}$ ($A = \text{Ba}, \text{Sr}$), the V ions with mixed-valence states, $\text{V}^{2+}/\text{V}^{3+}$ ($3d^3/3d^2$), are located on the triangular lattice. $\text{BaV}_{10}\text{O}_{15}$ exhibits a structural phase transition with V trimerization caused by the orbital ordering of V ions at $T_c = 123$ K, whereas $\text{SrV}_{10}\text{O}_{15}$ does not exhibit such a phase transition. We performed a femtosecond pump-probe reflection spectroscopy on $\text{BaV}_{10}\text{O}_{15}$ and $\text{SrV}_{10}\text{O}_{15}$ to clarify their photoinduced dynamics. For $A = \text{Ba}$, a photoinduced melting of V trimerization, i.e. a photoinduced phase transition, was observed at 10 K ($< T_c$). At $T = 200$ K ($>> T_c$), the photoinduced reflectivity change ($\Delta R/R$) for $A = \text{Ba}$ shows an oscillation with the period of several tens picoseconds, similarly to the behavior for $A = \text{Sr}$ at 10 K. This oscillation can be explained by assuming that the photoinduced state at the sample surface propagates into the inside of the sample. At $T = 135$ K, immediately above T_c , we found that $|\Delta R/R|$ for $\text{BaV}_{10}\text{O}_{15}$ increases with time, suggesting that the area of the photoinduced state on the sample surface increases with time.

8:12AM Y9.00002 Chemical pressure effects on structural, magnetic, and transport properties of $\text{Mn}_{1-x}\text{Co}_x\text{V}_2\text{O}_4$ ¹, ANDHIKA KISWANDHI, JAMES BROOKS, JUN LU, JEFFREY WHALEN, THEO SIEGRIST, HAIDONG ZHOU, National High Magnetic Field Laboratory — The low-temperature x-ray diffraction, susceptibility, specific heat, and resistivity of the single crystal $\text{Mn}_{1-x}\text{Co}_x\text{V}_2\text{O}_4$ have been investigated. With increasing Co-doping, the chemical pressure related to the decreasing V-V distance drives the system towards the itinerant electron limit, accompanied with the increase of the ferrimagnetic transition temperature and the suppression of the structural distortion. These effects are compared to the effects from the application of physical pressure, and show that the V-V distance is the critical parameter controlling the properties of AV_2O_4 .

¹This work is supported by NSF-DMR-0654118 and the State of Florida. A. Kiswandhi is supported in part by NSF-DMR-1005293

8:24AM Y9.00003 Thermal conductivity of spinel MnV_2O_4 with doping, TAKURO KATSUFUJI, T. OMURA, T. ISHIKAWA, Y. ISHITSUKA, Department of Physics, Waseda University — Spinel MnV_2O_4 exhibits a structural phase transition and ferrimagnetic ordering simultaneously at 57 K. The crystal symmetry in the low-temperature phase obtained by the x-ray diffraction of a single crystal indicates an antiferro-orbital ordering of V t_{2g} states [1]. It was also found that Al doping into the V site suppresses the orbital-ordering temperature (T_{oo}) but barely affects the ferrimagnetic-ordering temperature (T_N); thus two transition temperatures are separated in the Al-doped samples. We measured the thermal conductivity of $\text{Mn}(\text{V}_{1-x}\text{Al}_x)_2\text{O}_4$, and found that thermal conductivity sharply increases (thermal resistivity decreases) below T_{oo} . It was also found that, with applied magnetic field, thermal resistivity increases above T_{oo} but decreases below T_{oo} . These results indicate that thermal conductivity is dominated by the fluctuation of orbital ordering. [1] T. Suzuki *et al.*, Phys. Rev. Lett. 98, 127203 (2007).

8:36AM Y9.00004 Magnetic properties driven by local structure in quasi-1D Ising chain system cobaltate system, BONGJAE KIM, BEOM HYUN KIM, KYOO KIM, HONG CHUL CHOI, SANG-YEON PARK, Y.-H JEONG, B. I. MIN, Department of Physics, POSTECH, Pohang, 790-784, Korea — Using *ab-initio* band structure method and the microscopic model calculation, the origins of the large orbital magnetic moment and unique magnetic anisotropy in the quasi-1D magnetic cobaltate, $\alpha\text{-CoV}_2\text{O}_6$, is investigated. Unique crystal electric field effect in $\alpha\text{-CoV}_2\text{O}_6$ is combined with the strong spin-orbit coupling, results in intriguing magnetic properties of the system. Based on the estimated strengths of the intra- and the inter-chain exchange interaction, experimentally found 1/3 magnetization plateau in the MH curve can be attributed to spin-flop mechanism. Origin of the reduced magnetic entropy behavior is found to be the strong uniaxial magnetic anisotropy in the quasi-1D Ising chain system.

8:48AM Y9.00005 A Comparative Study of Magnetic and Structural Transitions Focusing on Dielectric and RF Measurements¹, LAUREL WINTER, JAMES BROOKS, NHMFL/FSU, HAIDONG ZHOU, NHMFL — High frequency inductive and dielectric measurements were used to study the magnetic and structural transitions of a number of compounds, including a series of spinel vanadates of the form $\text{Mn}_{1-x}\text{Co}_x\text{V}_2\text{O}_4$. We then compared the results to those found using other measurement techniques, such as resistivity and specific heat. The high frequency inductive measurements were conducted using a tunnel diode oscillator (TDO), and proved to be an effective and simple way to observe the magnetic transitions. From capacitance and dissipation measurements we were able to observe both magnetic and structural transitions, but only in the more insulating samples.

¹NSF-DMR-0602859

9:00AM Y9.00006 MicroRaman study of orbitonphonon coupling in YbVO_3 , BENOIT ROBERGE, SERGE JANDL, Université de Sherbrooke, THOMAS T.M PALSTRA, A.A. NUGROHO, University of Groningen — Owing to their strong electron correlation, transition-metal oxides with perovskite related structures display a variety of interesting properties such as Mott transition, high- T_c superconductivity and colossal magnetoresistance. YbVO_3 belong to this family and exhibits magnetic and orbital orderings at low temperatures. In this communication, we present a study of its first order and multiphonon Raman active excitations as a function of temperature. Impact of various orbital, magnetic and structural transitions is analyzed and possibilities of orbiton-phonon coupling in the observed phonon combinations around 1400 cm^{-1} are discussed.

9:12AM Y9.00007 Controlling Magnetism in Multiferroic BiFeO_3 , VALERY KIRYUKHIN, Rutgers University — BiFeO_3 (BFO) is a room-temperature multiferroic combining large electric polarization with an antiferromagnetic structure with a superimposed long-wavelength (62 nm) cycloidal modulation. Large single crystals of BFO have become available recently, opening up new opportunities for experiments. In this talk, we discuss various ways of controlling magnetism in BFO single crystals using coupling between the ferroelectric and magnetic order parameters. Electric field can rotate the electric polarization and Fe spins simultaneously, and a chiral magnetic monodomain state can be obtained. Populations of the 3 equivalent cycloidal magnetic domains can be controlled by an electric field through piezoelectric coupling. Alternatively, they can be controlled via the inverse effect by applying uniaxial pressure. Very small (~ 50 bar) pressures producing tiny elastic strain ($\sim 10^{-5}$) are needed to move the magnetic domain walls. Using polarized small-angle neutron scattering, we show for the first time that the spins in the cycloid are tilted, producing local weak ferromagnetism ($0.06\ \mu_B$ rms value), confirming a long-standing theoretical prediction. This shows that intrinsic macroscopic ferromagnetism could be expected in strained BFO, in which the cycloid is suppressed. Combined with the ability to control the magnetic domains by an electric field or tiny deformation, this observation accentuates the potential of BFO for room-temperature applications involving magnetoelectric effects.

9:48AM Y9.00008 Pressure-driven changes in electronic structure of BiCoO_3 ¹, SUDIPTA KANUNGO, TANUSRI SAHA-DASGUPTA, S.N Bose National Centre for Basic Sciences — Using first-principles DFT based calculations, carried out on the recently measured crystal structure data [Oka *et al.* J. Am. Chem. Soc. 132, 9438 (2010)], we study the changes in the electronic structure of BiCoO_3 between the ambient-pressure and the high-pressure conditions. Our study shows that the application of high pressure drives the high-spin-to-low-spin transition at the Co site. The obtained results for the ambient pressure phase shows C-type AFM alignment of Co high spins, while the electronic structure at the high-pressure phase shows the presence of a finite energy gap at E_f in contrast with previously reported metallic or semimetallic character with low-spin state of Co. This semiconducting behavior in the nonmagnetic BiCoO_3 with LS state of Co is found to be driven by the presence of the GdFeO_3 type of orthorhombic distortion which arises due to finite mixing of Bi lone-pair states with O-p states, as opposed to previously predicted cubic or tetragonal symmetry of the high-pressure. The ambient pressure phase shows an order of magnitude larger energy gap arising due to the AFM alignment of Co in the high-spin state than the energy gap at the high pressure phase, explains the observed 3-order of magnitude jump in resistivity.

¹Ref: Sudipta Kanungo and T. Saha-Dasgupta, Phys.Rev.B 83,104104(2011)

10:00AM Y9.00009 Long Range Ordering in Oxygen Doped SrCoO_x ¹, F.J. RUECKERT, University of Connecticut, F.Z. HE, Canadian Light Source, H. MOHOTALLA, University of Hartford, J.I. BUDNICK, W.A. HINES, University of Connecticut, B. DABROWSKI, Northern Illinois University, B.O. WELLS, University of Connecticut — Recent investigations have shown magnetic phase separation in polycrystalline samples of SrCoO_x ($2.5 \leq x \leq 3.0$).² As the samples are oxidized electrochemically, distinct ferromagnetic phases are formed at $\text{SrCoO}_{2.75}$ ($T_C = 165\text{ K}$), $\text{SrCoO}_{2.88}$ ($T_C = 220\text{ K}$), and SrCoO_3 ($T_C = 280\text{ K}$). In the polycrystalline bulk samples, two magnetic phases are seen at oxygen concentrations between 2.875 and 3.0, always occurring in only a single structural phase. The distinct phases are also evident in epitaxial 100 nm films, but the mixed magnetic phase at intermediate concentrations is suppressed. The occurrence of separate magnetic phases at concentrations of 2.75 [3-1/4], 2.88 [3-1/8], and 3.0 imply an electronic ordering commensurate with the lattice. Using resonant x-ray diffraction in thin film samples, we have discovered the existence of a superlattice peak at (1/4, 1/4, 1/4), revealing a previously hidden order with a periodicity four times the basic perovskite cell in all directions.

¹This work is supported by the NSF through contract # DMR-0907197 (UConn) and DMR-0706610 (NIU).

²Xie *et al.* Appl. Phys. Lett 99, 052503 (2011)

10:12AM Y9.00010 Structural and magnetic properties of $\text{Nd}_{1-x}\text{Ca}_x\text{BaCo}_2\text{O}_{5.5}$, OMAR CHMAISSEM, Physics Department - Northern Illinois University and Materials Science Division - Argonne National Laboratory, IL USA, STANISLAW KOLESNIK, Physics Department - Northern Illinois University, IL USA, BOGDAN DABROWSKI, Physics Department - Northern Illinois University and Materials Science Division - Argonne National Laboratory, IL USA, SEVDA AVCI, Materials Science Division, Argonne National Laboratory, IL USA, MAXIM AVDEEV, Bragg Institute, ANSTO, Australia, JASON HODGES, Spallation Neutron Source, Oak Ridge National Laboratory, TN USA — $\text{R}_{1-x}\text{A}_x\text{BaCo}_2\text{O}_{5.5}$ (R = rare earth, A = alkaline metal) is a relatively new class of complex oxide materials that exhibit a wide range of magnetic attributes in addition to metal/insulator switching properties, structural transitions and superstructure order parameters. In many ways, this family exhibits behaviors similar to those of the famous colossal magnetoresistive manganites; however, more complex properties have also been identified owing to the fact that the oxidation state of the cobalt ions often behave in unpredictable ways depending on the chemical composition of the investigated material and the corresponding Co local environment. Thus, Co^{3+} and Co^{4+} ions with high, intermediate and low spin states may be produced offering an additional degree of freedom to be accounted for when designing new materials with tunable magnetic properties. In this talk, I will discuss the effects of calcium substitution at the Nd sites and the various structural and magnetic models as determined by neutron powder diffraction and complementary magnetic measurements.

10:24AM Y9.00011 Peculiarities of spin and charge degrees of freedom in strongly correlated layered cobaltates, FRANK LECHERMANN, LEWIN BOEHNKE, I. Institute for Theoretical Physics, University of Hamburg, Germany, ANTOINE GEORGES, Ecole Polytechnique, Centre de Physique Theorique (CPHT), Palaiseau, France, OLEG E. PEIL, CHRISTOPH PIEFKE, I. Institute for Theoretical Physics, University of Hamburg, Germany — The layered cobaltate systems stand for the rare case of metallic quasi-2D triangular lattices at doping x . While $x=0$ corresponds to a half-filled scenario, $x=1$ marks the band-insulating limit. Surprisingly, the phase diagram displays especially for $x > 0.5$ a rich competition between different spin-orderings as well as intriguing charge-ordering processes. Though already at high doping, strong electronic correlations are mainly responsible for the complex physics [1-4]. By means of combinations of band-structure techniques with many-body approaches it is shown that various cobaltate features may be tackled successfully. For instance the in-plane crossover from antiferromagnetic spin correlations towards the onset of ferromagnetism as well as charge ordering tendencies favoring an effective kagome lattice close to $x=0.67$ in agreement with experiment. The charge order also substantially effects the spectral and transport properties, giving rise to a specific low-energy scale susceptible to nonlocal correlations.

[1] F. Lechermann, Phys. Rev. Lett. 102, 046403 (2009).

[2] C. Piefke, L. Boehnke, A. Georges and F. Lechermann, Phys. Rev. B 82, 165118 (2010).

[3] L. Boehnke and F. Lechermann, arXiv:1012.5943.

[4] Oleg E. Peil, A. Georges and F. Lechermann, arXiv:1107.437

10:36AM Y9.00012 Stability of Multiferroic Transition in FeVO_4 against Transition Metal Doping, AKILA KUMARASIRI, Wayne State University, Detroit, MI, AMBESH DIXIT, Indian Institute of Technology, Rajasthan, India, GAVIN LAWES, Wayne State University, Detroit, MI — FeVO_4 is a recently discovered multiferroic material which undergoes successive antiferromagnetic phase transitions at $T_{N1} \sim 22$ K and $T_{N2} \sim 15$ K, with ferroelectricity developing at the T_{N2} transition. FeVO_4 is a type II multiferroic where the ferroelectricity is magnetically driven. We have studied the effect of transition metal doping on these two phase transitions in order to explore how the multiferroic order is affected by introducing perturbations into the lattice. We synthesized polycrystalline $\text{M}_x\text{Fe}_{1-x}\text{VO}_4$ samples (M = Zn, Mn, Cr) using a standard solid state reaction method, and we used magnetic, dielectric, and heat capacity measurements to track the transition temperatures. Both magnetic and heat capacity measurements show clear peaks at the two transitions, enabling us to map how the transitions are suppressed as the doping fraction is changed. On doping with non magnetic Zn, we find only a minimal suppression of both transition temperatures, indicating the magnetic interactions producing the multiferroic order are surprisingly robust against non-magnetic perturbations. We will also present preliminary results of the effects of magnetic dopants, specifically Mn and Cr.

10:48AM Y9.00013 ^{51}V single-crystal NMR Study on multiferroic FeVO_4 , JINSHAN ZHANG, School of Energy, Power and Mechanical Engineering, North China Electric Power University, Beijing, China, LONG MA, WEIQIANG YU, Department of Physics, Renmin University of China, Beijing, China, ZHANGZHEN HE, State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Science, Fujian, China — The multiferroicity in FeVO_4 is so far not well understood because its spin-orbit coupling is probably very weak. In this talk, we report our ^{51}V single crystal NMR study on FeVO_4 under zero field and a finite field. The double magnetic transitions with $T_{SDW} \approx 19$ K and $T_{helical} \approx 13$ K are clearly shown by NMR spectra and the spin-lattice relaxation rate $1/T_1$. Two nonequivalent ^{51}V sites are identified with different hyperfine couplings. Just below $T_{helical}$, a large RF enhancement is seen, which indicates rich magnetic domain walls formed in the helical state and not in the SDW state. Based on our results, we discuss the coupling between the magnetism and the ferro-electricity in FeVO_4 .

Friday, March 2, 2012 8:00AM - 11:00AM –
Session Y10 DCOMP: Invited Session: Modeling & Simulation of the Impact of Space Radiation on Electronic Systems (Avionic and Astronautic) 210A

8:00AM Y10.00001 Mitigation of Space Radiation Effects, WILLIAM ATWELL¹, The Boeing Company — During low earth orbit and deep space missions, humans and spacecraft systems are exposed to high energy particles emanating from basically three sources: geomagnetically-trapped protons and electrons (Van Allen Belts), extremely high energy galactic cosmic radiation (GCR), and solar proton events (SPEs). The particles can have deleterious effects if not properly shielded. For humans, there can be a multitude of harmful effects depending on the degree of exposure. For spacecraft systems, especially electronics, the effects can range from single event upsets (SEUs) to catastrophic effects such as latchup and burnout. In addition, some materials, radio-sensitive experiments, and scientific payloads are subject to harmful effects. To date, other methods have been proposed such as electrostatic and electromagnetic shielding, but these approaches have not proven feasible due to cost, weight, and safety issues. The only method that has merit and has been effective is bulk or parasitic shielding. In this paper, we discuss in detail the sources of the space radiation environment, spacecraft, human, and onboard systems modeling methodologies, transport of these particles through shielding materials, and the calculation of the dose effects. In addition, a review of the space missions to date and a discussion of the space radiation mitigation challenges for lunar and deep space missions such as lunar outposts and human missions to Mars are presented.

¹Boeing Research & Technology 13100 Space Center Blvd., MS: HB 2-30 Houston, TX 77058 cell #: 281/804-3673

8:36AM Y10.00002 The Space Radiation Environment in Energetic Particles at the Earth ,

GARY ZANK, Center for Space Plasma and Aeronomic Research (CSPAR) and Physics Department, University of Alabama in Huntsville — Understanding the radiation environment in energetic particles at the Earth is critical to the stability, integrity, and longevity of satellite subsystems. The radiation environment comprises particles trapped in the Earth's radiation belts and magnetosphere, those generated by solar energetic particle events (SEPs), and galactic and anomalous cosmic rays. Of these different populations, the most highly variable, and consequently difficult to anticipate, is the SEP population. This is also the population that can often cause the most damaging effects. SEP events can be either impulsive or gradual (sometimes a mixture of the two) with the gradual events being larger, much longer lasting, and often with higher particle energies. Diffusive shock acceleration at a coronal mass ejection driven shock wave is generally invoked to explain gradual SEP events. The detailed [plasma] physics of the acceleration mechanism remains to be elucidated. We are fortunate in that very detailed observations of particle acceleration at shock waves, particularly in the guise of Space Weather, are providing considerable experimental insight into the basic physics of particle acceleration at a shock wave. Detailed interplanetary observations are not easily interpreted in terms of simple steady-state models of particle acceleration at shock waves. Three fundamental aspects make the interplanetary problem much more complicated than the typical astrophysical problem: the time dependence of the acceleration and the solar wind background; the geometry of the shock; and the long mean free path for particle transport away from the shock wave. An interplanetary shock is not steady, as it decelerates and expands into an expanding, temporal solar wind. Furthermore, the shock geometry varies from quasi-parallel to quasi-perpendicular along a shock front, and multiple shocks can be present simultaneously in the solar wind. Consequently, the shock itself introduces a multiplicity of time scales, ranging from shock propagation time scales to particle acceleration time scales at parallel and perpendicular shocks, and many of these time scales feed into other time scales (such as determining maximum particle energy scalings, escape time scales, etc.). We will discuss the basic physics of particle acceleration via scalings, their relationship to particle acceleration models, observations and geometry in both an astrophysical and space physics context. This will include discussing the physics of perpendicular and parallel shocks, upstream turbulence, particle spectra, and particle injection and the seed population. After acceleration of particles at an interplanetary shock, the transport of energetic particles is non-diffusive because of their large mean free path in the quiet solar wind. We will address the coupled acceleration and transport of heavy ions, Fe/O ratios, the variability among individual events, and seed particle populations. We will discuss theoretical models and address recent modeling efforts.

9:12AM Y10.00003 Monte Carlo Simulation of Radiation Effects in Microelectronics¹ , ROBERT

A. WELLER, Vanderbilt University — Microelectronic devices are susceptible to disruption by ionizing radiation, and with the scaling of devices to ever-smaller dimensions they are increasingly vulnerable to single event effects. Single event effects are transient errors in active devices, usually although not exclusively in digital logic, that are caused by the interaction of ionizing particles with the materials from which the devices are made. This presentation describes a Monte Carlo approach for predicting the rate of single event effects from knowledge of radiation environments and device structure. The approach combines detailed physical modeling of discrete radiation events, semiconductor device simulation to estimate charge transport and collection, and circuit simulation to determine the macroscopic electrical effects of collected charge. Details of the Monte Carlo simulation will be presented, and a mathematical analysis that establishes its relationship to earlier single event rate prediction methods will be discussed. Recent experimental and computational results on the rate of single event effects in highly scaled devices will be reviewed.

¹Work supported by NASA and the Defense Threat Reduction Agency Basic Research Program.

9:48AM Y10.00004 Data-driven Three-Dimensional (3D) Global Magnetohydrodynamic (MHD) Model with Radiation to Study the Solar Atmospheric Dynamics¹ , SHI WU, The University of

Alabama in Huntsville — In this presentation, we describe a self-consistent, three-dimensional, global compressible, and resistive magnetohydrodynamic (MHD) model together with time-dependent boundary conditions based on the projected method of characteristics at the source surface (photosphere) to accommodate the observations. The additional physics included in this model are differential rotation, meridional flow, effective diffusion, and cyclonic turbulence effects in which the complex magnetic field structure can be generated through the nonlinear interactions between the plasma flows and magnetic field. To illustrate the capability of this model, we selected GONG's global transverse velocity measurements of synoptic chart CR2009 near the photosphere and SOLIS full-resolution LOS magnetic field maps of synoptic chart CR2009 on the photosphere as the inputs to drive the model to simulate the equilibrium state and compute the energy transport across the photosphere. To show the advantage of using both measured magnetic field and transverse velocity data, we have investigated two cases: (1) with the inputs of the LOS magnetic field and transverse velocity measurements, and (2) with the input of only the LOS magnetic field. For these two cases, the simulation results presented here are a three-dimensional coronal magnetic field configuration, density distribution on the photosphere and 1.5 solar radii, and the solar wind in the corona. The deduced physical characteristics are the total current helicity and the synthetic emission.

¹Work performed by STW is supported by NSF grant ATM0754378.

10:24AM Y10.00005 Multi-Scale Modeling of the Plasma Flow and Magnetic Fields in the Entire Heliosphere , NIKOLAI POGORELOV, Physics Department, University of Alabama in Huntsville — Numerical model of the solar wind (SW)

interaction with the local interstellar medium (LISM), developed in UAHuntsville and implemented in the Multi-Scale Fluid-Kinetic Simulation Suite, treats ions with MHD equations while the transport of neutral atoms is performed kinetically by solving the Boltzmann equation. Pickup ions are treated as a separate fluid or kinetically. The evolution of SW turbulence is addressed on the differential equation level. Time-dependent, based on observational data, modeling of the SW in the entire heliosphere is critical for the space weather modeling and interpretation of the spacecraft data. We choose LISM properties using remote observations and appropriate numerical modeling which allows us to constraint them by matching the ribbon of the energetic neutral atom flux detected in different energy bands by the Interstellar Boundary Explorer. We used the Ulysses data to model the SW-LISM interaction during the period of the mission and matched rather well the timing of the termination shock crossing by Voyager 1 and Voyager 2. The SW boundary conditions include those provided by the interplanetary scintillation measurements and obtained by numerical modeling of the inner heliosphere from the Sun's surface to the Earth orbit. Numerical results are extracted as time series along real spacecraft trajectories and compared with in situ measurements.

Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y11 DMP: Focus Session: Graphene Devices - Fabrication 210B

8:00AM Y11.00001 Lattice-Nanotomy for Large-Scale Production of Transferrable and Dispersible Graphene-Nanostructures of Controlled Shape and Size¹ , BALABALAJI PADAVALA, NIHAR MOHANTY,

Kansas State University, DAVID MOORE, University of Kansas, ZHIPING XU, Tsinghua University, ASHVIN NAGARAJA, ALFREDO A. RODRIGUEZ, VIKAS BERRY, Kansas State University, DR. MOORE'S TEAM TEAM, DR. XU'S TEAM TEAM — In this talk, we will present a novel graphite-lattice-nanotomy (nanoscale-cutting) process for high throughput production of monodispersed graphene nanostructures (GNs) with controlled shape (square, rectangle, ribbons and triangle), dimensions (sizes at 5 nm resolution with a range of 5–600 nm) and chemical-construct. We demonstrate that this versatile process enables the realization of unprecedented graphene-nanostructures, which exhibit the evolution of semiconductor-characteristics and electrical transport mechanism. Further, we will present in detail the size and shape-dependent electrical and optical properties of these GNs via various microscopic and spectroscopic techniques. This nanotomy process can provide access to virtually-infinite and unprecedented GNs for development of fundamental optical/electrical/structural correlations and novel applications.

¹NSF-CAREER, Office of Naval Research and KSU-Startup

8:12AM Y11.00002 Direct Writing of Graphene-based Nanoelectronics via Atomic Force Microscopy, MICHAEL HAYDELL, ELENA CIMPOIASU, US Naval Academy, Physics Dept., Annapolis, MD, 21402, WOO KYUNG LEE, RORY STINE, Naval Research Laboratory, Surface Nanoscience and Sensor Technology, Washington DC, 20375, WILLIAM P. KING, Univ. of Illinois at Urbana-Champaign, Dept. of Mech. Science and Eng., Urbana, IL, 61801, PAUL SHEEHAN, Naval Research Laboratory, Surface Nanoscience and Sensor Technology, Washington DC, 20375 — We use direct writing with an atomic force microscope (AFM) to fabricate simple, graphene-based electronic components to explore their electronic properties and the feasibility of manufacturing electronic devices via AFM. The process being studied, thermochemical nanolithography (TCNL), involves flowing current through an AFM cantilever to provide thermal energy to a chemically modified graphene (CMG) film, either graphene oxide or graphene fluoride. The heat reduces the insulating CMG film back into conductive graphene. Thus, these nanoribbons can be used to fabricate nano-scale electronic components such as resistors, capacitors, and transistors. The technique, as compared to other attempts to produce graphene-based devices, is simple, does not involve solvents or other complicated fabrication steps, and allows for the exact placement of the devices on the substrate. The electronic properties of the devices produced using the two materials, measured using current-voltage characteristics at various temperatures down to 2 K and in variable magnetic fields up to 9 T, will be discussed. This work was partially supported by the US Naval Academy Research Office and the Nanoscience Institute at NRL.

8:24AM Y11.00003 A study on tapered graphene nanoribbons with controlled angle: Fabrication and conductivity studies¹, SREEPRASAD THERUVAKKATTIL SREENIVASAN, BALABALAJI PADAVALA, PHONG NGUYEN, VIKAS BERRY, Kansas State University — Graphene, the newest member in the nanocarbon family, is a perfect single atom thick 2D sheet made up of carbon with exceptional electrical and mechanical properties. It is well-known that the band-gap of graphene nanoribbons (GNRs) can be controlled via their width. Here we demonstrate that GNRs with tapered morphology have semiconducting-to-metallic continuum along its length, and thus exhibit unique electrical properties. The device is fabricated from a single layer graphene grown on a Cu foil via the standard CVD process. Here, the graphene is transferred on a silica substrate and electron beam lithography etching is performed to produce a tapered graphene GNR device, followed by with Pd-Au electrode-deposition. We demonstrate the unique carrier transport properties, electrical rectification and carrier modulation in these novel devices.

¹Office of Naval Research, KSU-Start up

8:36AM Y11.00004 Toward graphene based electronics from homogeneous top-gated graphene devices, JINSEONG HEO, HYUNJONG CHUNG, HEEJUN YANG, DAVID SEO, HYUN JAE SONG, KYOUNG-EUN BYUN, SEONGJUN PARK, Samsung Advanced Institute of Technology, GRAPHENE TEAM — We report high quality top-gated graphene field effect devices integrated on 150mm substrate, which involves unprecedented homogeneous chemical vapor deposition growth of monolayer graphene on Ni/Cu. Statistics of maximum resistance, dirac voltage and also mobility over a thousand devices are shown for the first time, in which 5% of measurable devices are in 3,000~5,000 cm²/V·s of mobility. Furthermore, logic gates such as NOT and AND based on top-gated graphene devices were demonstrated. Our results imply a route toward graphene based electronics with complementary metal-oxide-semiconductor (CMOS) compatible process.

8:48AM Y11.00005 Gate-Tunable Superconductor-Insulator Transition in Bilayer-Graphene Josephson Junctions, DONGCHAN JEONG, GIL-HO LEE, Pohang University of Science and Technology, YONG-JOO DOH, Korea University, HU-JONG LEE, Pohang University of Science and Technology — Bilayer graphene shows opening of electric-field-induced band gap, the size of which is proportional to the intensity of the electric field. We report electronic transport measurements on superconducting proximity effect in planar dual-gated bilayer-graphene Josephson junction with Pb_{0.93}In_{0.07} (PbIn) electrodes ($\Delta_{PbIn} \sim 1.1$ meV, $T_c = 7.0$ K). The junction resistance along the charge-neutral point (CNP) increases as we modulate top- and back-gate voltages away from the zero-gap CNP. The resistive state near the CNP shows a variable-range-hopping-type insulating behavior in R - T curve with lowering temperature crossing the superconducting transition of PbIn electrodes. However, a highly doped regime shows metallic R - T behavior and junction becomes superconducting below T_c . Moreover, magnetic-field-induced Fraunhofer supercurrent modulation, microwave-induced Shapiro steps, and multiple Andreev reflection (MAR) are observed, which indicate the formation of genuine Josephson coupling across the planar junctions below T_c with sufficiently transparent superconductor–bilayer graphene interface. The separatrix of the superconductor-insulator transition corresponds to the square junction conductance of $G_{sq} \sim 6-8e^2/h$.

9:00AM Y11.00006 Characterization of graphene quantum dot hybrid structures¹, TING-FUNG CHUNG, JIUNING HU, LUIS A. JAUREGUI, LIANGLIANG CHEN, QING ZHAO, XIULIN RUAN, YONG P. CHEN, Purdue University — We report electrical transport, photo-electric response and Raman spectroscopy measurements in macroscopic samples of graphene decorated with inorganic quantum dots (CdSe QDs). QDs are deposited on chemical vapor deposition (CVD) graphene by spin-coating. Raman measurements of graphene decorated with QDs on Si wafer show very similar spectra with clear G and 2D peaks that reveal no degradation of graphene during the QDs deposition process. Furthermore, two types of device architectures (QDs-graphene and graphene-QDs-graphene) are fabricated with graphene as a transparent electrode and QD as a light absorbent for electrical photoresponse characterization. Upon application of either a broadband light source or a 532-nm monochromatic laser source, graphene-QDs-graphene devices demonstrate photoconducting response, but not in the case of QDs-graphene devices.

¹This work is partially supported by Day & Associate LLC.

9:12AM Y11.00007 Fabrication of nanometer-scale suspended graphene transistors, VAHID TAYARI, JOSHUA O. ISLAND, SERAP YİĞEN, JAMES PORTER, A.R. CHAMPAGNE, Department of Physics, Concordia University, Montreal, Quebec, Canada — We present a method to fabricate suspended ultra-short graphene transistors. We define narrow bowtie gold junctions on exfoliated graphene, and then use an oxygen plasma to etch away the graphene except under the gold junctions. The next step is to wet etch the SiO₂ under the junctions to suspend the devices. Finally, we use a feedback-control electromigration procedure to break the gold junctions and expose sections of graphene which are 100 to 300 nm wide and as short as ≈ 10 nm. Using electron transport, we show that these suspended graphene nanocrystals form ballistic two-dimensional Dirac electron gas systems. We study them as a function of temperature and charge carrier density. These ultra-short NEMS transistors offer the prospect of exploring the coupling between flexural vibrons and charge carriers in graphene.

9:24AM Y11.00008 Implementation of embedded-gate graphene field effect transistors on flexible substrates, JONGHO LEE, LI TAO, MILO HOLT, DEJI AKINWANDE, University of Texas at Austin — In this work we present embedded-gate graphene field effect transistors (GFETs) on flexible polyimide films for high frequency RF and sensor applications. Graphene transistors with gate lengths from 1μm to 4μm and width of 8μm have been realized by e-beam lithography. Chemical vapor deposited monolayer graphene with negligible defects is transferred to flexible polyimide substrates for device fabrication. The electrostatic measurement reveals that fabricated device shows a mobility of over 1000cm²/Vs at room temperature, the highest reported among graphene FETs implemented on flexible films. Surface roughness and impurity doping are of crucial importance in fabricating flexible graphene devices since its charge transport is limited by mobility degradation due to surface roughness and doping related with the chemical transfer process. The stack of atomic layer deposited Al₂O₃ as gate dielectric and gate pads underneath provides smooth surface for graphene to sit on as confirmed by atomic force microscopy. This results in a field effect mobility of an embedded gate GFET twice that of a top gated GFET on polyimide substrates. The minimum conduction point is close to zero, indicating the impurity induced doping for the device is negligible.

9:36AM Y11.00009 Molecular Layer-seeded Ultra-thin Top-gate Dielectrics for High Transconductance Graphene Transistors, VINOD SANGWAN, DEEP JARIWALA, HUNTER KARMEL, JUSTICE ALABOSON, LINCOLN LAUHON, Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, TOBIN MARKS, Department of Materials Science and Engineering and Department of Chemistry, Northwestern University, Evanston, Illinois 60208, MARK HERSAM, Department of Materials Science and Engineering, Department of Chemistry and Department of Medicine Northwestern University, Evanston, Illinois 60208 — The potential of graphene in integrated analog and digital circuits can only be fully realized through incorporation of ultra-thin gate dielectrics to enable large-scale small-channel graphene field-effect transistors (GFETs). Atomic-layer deposition (ALD) is a viable technique to fabricate gate-dielectrics, however, it requires a seeding layer on otherwise inert graphene. Here, we demonstrate a single molecule thick perylene-3,4,9,10-tetracarboxylic dianhydride overlayer as an effective seeding layer to grow high- κ Al_2O_3 on mechanically exfoliated graphene for high-performance GFETs. Using an ultra-thin ($< 1\text{nm}$) seeding layer, in contrast to polymer films (5-10 nm), we demonstrate fabrication of the thinnest ALD-grown gate-dielectric (4 nm) reported to date in top-gated GFETs. This yields high performance GFETs with the intrinsic transconductance parameter approaching 2.4 mS and the field-effect mobility $\sim 3000\text{ cm}^2/\text{Vs}$. We also demonstrate generalization of this molecular layer seeded-ALD growth method to higher- κ gate dielectrics, yielding further enhanced GFET transconductance for possible application to radio-frequency circuits.

9:48AM Y11.00010 Conductance through two-terminal graphene junctions with wetting metal contacts, SALVADOR BARRAZA-LOPEZ, University of Arkansas, MARKUS KINDERMANN, MEI-YIN CHOU, Georgia Institute of Technology — Metallic contacts become a relevant factor for the behavior of nanoscale graphene devices. A thin layer of a wetting metal—a metal that forms covalent bonds to graphene—is customarily placed in between graphene and bulk leads. The most common choices for this wetting metal are Titanium, Chromium, and Palladium. We will present the equilibrium conductance through crystalline (defect- and impurity-free) two-terminal graphene junctions attached to normal, spin-unpolarized Titanium metal leads. In addition, we discuss the equilibrium potential profile across the junctions, and the presence of Fabry-Perot oscillations. The conductance shows pronounced noise, and the Fano factor near the Dirac point is seen to fluctuate, as in experiment [1]. The distribution of transmission eigenvalues is bimodal, indicating a disordered-metal-like charge transport through nanoscale two-terminal graphene junctions with wetting metals.

[1] L. DiCarlo, J. R. Williams, Y. Zhang, D. T. McClure, and C. M. Marcus. Phys. Rev. Lett. 100, 156801 (2008).

[2] S. Barraza-Lopez, M. Kindermann, and M.-Y. Chou. (Manuscript in preparation.)

10:00AM Y11.00011 Fabrication of a tunable quantum point contact in bilayer graphene, PATRICK MAHER, CARLOS FORSYTHE, Columbia University, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS, PHILIP KIM, Columbia University — The realization of a quantum point contact (QPC) in graphene is of interest for both physical and technological reasons. Fabricating a tunable QPC thus far, however, has been technologically challenging due to the inability to electrostatically deplete graphene. Recent advances have allowed for the creation of high mobility dual-gated bilayer samples sandwiched in hexagonal boron nitride. These samples display a robust, tunable band gap, which opens the door to electrostatically defining the conductance channel. In this presentation, we report the fabrication and characterization of point contact structures in high mobility dual-gated bilayer graphene samples employing hBN as both the top and bottom dielectric layer.

10:12AM Y11.00012 Surperconducting Graphene Nanodevice in Ballistic Regime, JOEL I-JAN WANG, Harvard School of Engineering and Applied Sciences, Harvard University/ Department of Physics, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, PABLO JARILLO-HERRERO, Department of Physics, Massachusetts Institute of Technology — Superconductivity carried by Dirac fermion can be realized through induced superconductivity in graphene. Observation of novel phenomena anticipated by theories requires superconducting graphene devices with low disorder so that the transport is ballistic. In this talk we present the fabrication and characterization of superconducting graphene nanodevices that are built on hexagonal Boron Nitride. The ultra flatness and lack of dangling bond in the boron nitride substrate reduces the disorder in graphene, opening the door to the study of ballistic Dirac fermion in superconducting regime.

10:24AM Y11.00013 Scanning Tunneling Potentiometry Mapping of Electron Transport in Graphene on SiC^1 , KENDAL CLARK, SHENGYONG QIN, XIAO GUANG ZHANG, Oak Ridge National Laboratory, GUOWEI HE, Carnegie Mellon University, GONG GU, University of Tennessee, RANDALL FEENSTRA, Carnegie Mellon University, AN-PING LI, Oak Ridge National Laboratory — Single layers of graphene formed on SiC look to be a promising system for the realization of graphene electronics. To utilize the full potential of graphene on SiC a complete understanding of the physical and electronic properties of this system is needed. Scanning Tunneling Microscope (STM) images along with scanning tunneling spectroscopy is used to characterize the sample surface. STM images clearly show the distinction between 1 monolayer (ML) and 2ML regions and this transition is further confirmed by point spectroscopy and spectroscopic mapping across the boundary. Defects, grain boundaries, step edges and other potential scattering centers are thought to play a major role in the electronic properties, especially in transport, along the graphene sheets. Using a low temperature four-probe scanning tunneling microscope, potentiometry measurements are performed on the epitaxial graphene grown on 4H-SiC. Potentiometry maps spanning the transition from 1ML to 2ML graphene show a contrast change indicating a potential change at this interface. Preliminary results of the transport along this potentially revolutionary new electronic system will be presented.

¹This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Office of Basic Energy Sciences, U.S. Department of Energy.

10:36AM Y11.00014 Atomic Force Microscopy-Based Local Tunable Oxidation of Graphene, SATORU MASUBUCHI, IIS University of Tokyo, INQIE University of Tokyo, MIHO ARAI, IIS, University of Tokyo, TOMOKI MACHIDA, IIS University of Tokyo, INQIE University of Tokyo, PRESTO-JST — We have fabricated graphene/graphene oxide/graphene (G/GO/G) junctions by local anodic oxidation lithography using atomic force microscopy (AFM). The conductance of the G/GO/G junction decreased with the bias voltage applied to the AFM cantilever V_{tip} . For G/GO/G junctions fabricated with large and small $|V_{tip}|$, GO was semi-insulating and semiconducting, respectively. AFM-based LAO lithography can be used to locally oxidize graphene with various oxidation levels and achieve tunability from semiconducting to semi-insulating GO [S. Masubuchi *et al.*, Nano Lett. 11, 4542 (2011).]

10:48AM Y11.00015 High mobility Single Layer Epitaxial Graphene on 4H-SiC (000-1), YIKE HU, ZELEI GUO, MING RUAN, JOHN HANKINSON, JAMES PALMER, BAIQIAN ZHANG, RUI DONG, JAN KUNC, CLAIRE BERGER, WALT DEHEER, Georgia Institute of Technology — Multi-layer Epitaxial Graphene on 4H-SiC (000-1) has demonstrated very high mobility up to $\sim 27,000\text{ cm}^2/\text{Vs}$ [1]. Recently single layer graphene grown by the Confinement Control Growth method [2] exhibits mobility up to $\sim 25,000\text{ cm}^2/\text{Vs}$ at 4K and $13,000\text{ cm}^2/\text{Vs}$ at 300K with $p=3 \times 10^{12}\text{ cm}^{-2}$. The relation between Raman G peak features (FWHM and position) and carrier density of Epitaxial Graphene on carbon face is revealed. Quantum Hall Effect [3] is observed both for p and n type carriers on top gated sample. This indicates that top gated single layer graphene can be produced on the Carbon face with high quality and high carrier mobility.

[1] Science 312, 1191 (2006)

[2] PNAS 108 (41) 16900 (2011)

[3] APL 95, 223108 (2009)

Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y12 DCMP: Graphene: Electronic Structure and Interactions - STM and Nanoribbons

210C

8:00AM Y12.00001 Mapping Dirac Quasiparticles near a Single Coulomb Impurity on Graphene

, YANG WANG, VICTOR BRAR, Physics Department, UC Berkeley and LBNL, ANDREY SHYTOV, School of Physics, University of Exeter, QIONG WU, WILLIAM REGAN, Physics Department, UC Berkeley and LBNL, HSIN-ZON TSAI, Physics Department, UC Berkeley, ALEX ZETTL, Physics Department, UC Berkeley and LBNL, LEONID LEVITOV, Department of Physics, Massachusetts Institute of Technology, MICHAEL CROMMIE, Physics Department, UC Berkeley and LBNL, PHYSICS DEPARTMENT, UC BERKELEY TEAM, LBNL TEAM, SCHOOL OF PHYSICS, UNIVERSITY OF EXETER COLLABORATION, DEPARTMENT OF PHYSICS, MASSACHUSETTS INSTITUTE OF TECHNOLOGY COLLABORATION — We have locally mapped the response of charge carriers to a single Coulomb potential placed on a gated graphene device. Scanning tunneling microscopy and spectroscopy were used to fabricate a tunable charge impurity and to measure how Dirac fermions screen it. By mapping spatial variation in the electronic structure of graphene we have directly probed the strength of screened electronic interactions, obtaining a value of $\epsilon = 3$ for the intrinsic graphene dielectric constant. This small value suggests that microscopic electron-electron interactions contribute significantly to intrinsic graphene properties.

8:12AM Y12.00002 Graphene Tunneling Heterostructures

, BENJAMIN HUNT, JAVIER SANCHEZ-YAMAGISHI, PABLO JARILLO-HERRERO, R. C. ASHOORI, MIT — We have fabricated tunneling heterostructures comprising graphene on boron nitride (BN) substrates and tunnel barriers constructed of exfoliated BN or MoS_2 . We present measurements of the low-temperature tunneling spectrum as a function of the tunneling energy and the carrier density in the graphene, with the latter controlled by a back-gate voltage. We observe a series of tunneling resonances, reminiscent of those seen in STM and planar tunneling experiments on graphene, whose energies disperse with the back-gate voltage.

8:24AM Y12.00003 Scanning Tunneling Spectroscopy of Graphene on Hexagonal Boron Nitride

, MATTHEW YANKOWITZ, JIAMIN XUE, DANIEL CORMODE, Physics Department, University of Arizona, JAVIER SANCHEZ-YAMAGISHI, PABLO JARILLO-HERRERO, Department of Physics, Massachusetts Institute of Technology, K. WATANABE, T. TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, PHILIPPE JACQUOD, BRIAN LEROY, Physics Department, University of Arizona — Recent work has found hexagonal boron nitride (hBN) to be a good substrate for graphene devices due to its ability to screen charged impurities in the underlying substrate and increase graphene mobility. We investigated graphene on hBN heterostructures using scanning tunneling microscopy and spectroscopy. Because hBN has the same bond structure as graphene with a slightly longer lattice constant, a rotationally dependent Moiré pattern is formed in graphene on hBN heterostructures. The Moiré pattern creates a weak periodic potential for the charge carriers in graphene. We performed an experimental and theoretical investigation of its effect on the local density of states. We observed a Moiré wavelength dependent modification of the local density of states in good agreement with theory predictions.

8:36AM Y12.00004 Local spontaneous time-reversal symmetry breaking and interacting Dirac fermions in strained CVD-grown graphene on copper

, R.T.-P. WU, M.L. TEAGUE, H. CHU, D.A. BOYD, N.-C. YEH, Dept. of Physics, Caltech, Pasadena, CA 91125, M.W. BOCKRATH, Dept. of Physics and Astronomy, Univ. of California, Riverside, CA 92521 — Atomically resolved imaging and spectroscopy of CVD-grown graphene on Cu are studied using scanning tunneling microscopy and spectroscopy. Under strain-induced giant pseudo-magnetic fields (B_S), quantized Landau levels are manifested by peaks of density of states (DOS) at quantized energies. While global time-reversal symmetry is preserved, local spontaneous time-reversal symmetry breaking (TRSB) for the two inequivalent lattice sites due to opposite B_S directions is evidenced by the presence or absence of the zero-mode tunneling conductance peak, confirming theoretical predictions for gauge fields in graphene causing local TRSB while preserving the chiral symmetry. Additionally, the finding of both integer and fractional quantum Hall states due to strain-induced B_S may be attributed to significant short-range Coulomb interactions of Dirac fermions in graphene mediated by the underlying Cu substrate, which yields an onsite Coulomb interaction $U \sim 3.2$ eV larger than the nearest-neighbor hopping energy $t \sim 2.8$ eV. Finally, effects on the DOS of graphene due to pseudo-magnetic fields are compared with those due to applied fields. This work was supported by NSF.

8:48AM Y12.00005 Real-Space Magnitude and Spatial Extent of the Surface Charge Density of Graphene¹

, P. XU, Y. YANG, S.D. BARBER, M.L. ACKERMAN, J.K. SCHOELZ, SALVADOR BARRAZA-LOPEZ, I. BELLAICHE, P.M. THIBADO, Department of Physics, University of Arkansas, IGOR A. KORNEV, Propriétés et Modélisation des Solides, France — The discovery of graphene, a unique two-dimensional electron system with extraordinary physical properties, has ignited tremendous research activity in both science and technology. One such extraordinary property is its enormous current-carrying capacity of $1\mu\text{A}$ per atomic row. Fundamentally, this suggests that graphene possesses an unusually large electronic density of states (DOS). Surprisingly, a detailed atomic-scale investigation of the DOS has yet to be completed. Here we present, for the first time, variable-current scanning tunneling microscopy (STM) images, which reveal an unusual three-dimensional picture of graphene's orbitals. Furthermore, density functional theory was used to simulate the variable-current STM images. From this we found that the orbitals expand to fill the holes in the honeycomb structure, making atomic-resolution STM more difficult at lower currents. Also, we discovered that the wavefunctions expand into the vacuum an unusually large amount. Identical studies were performed on graphite, revealing that the DOS of graphene is 300% larger. Other significant differences found between graphite and graphene will be discussed.

¹Support provided by ONR N00014-10-1-0181, N00014-08-1-0915, NSF 0855358, 0701558, DoE 46612.

9:00AM Y12.00006 Direct Imaging of Intrinsic Molecular Orbitals Using Graphene-based Moiré Pattern¹

, HAITAO ZHOU, GENG LI, JINHAI MAO, YELIANG WANG, SHIXUAN DU, HONGJUN GAO, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES, BEIJING 100190, CHINA TEAM — Direct imaging of the intrinsic electronic structure at high resolution is of both fundamental and technological importance for investigating molecular interaction and mechanisms. Metallic or semiconducting materials are commonly used as substrates for molecular adsorption. Generally, the strong interactions between molecules and these substrates significantly change the intrinsic electronic and geometric structures of the adsorbed molecules. In order to overcome this problem, much effort has been made by passivating substrates with various buffer layers, for instance, thin organic films, NaCl, and oxides. We demonstrate the graphene grown epitaxially on Ru(0001) can be used as a buffer layer to study the intrinsic electronic properties of adsorbed molecules. The intrinsic molecular orbitals of C60, pentacene and perylene-3,4,9,10-tetracarboxylic dianhydride molecules were imaged by scanning tunneling microscope (STM). High resolution STM images of the molecules reveal that the graphene layer decouples the individual molecules electronically from the metallic substrate, which is also verified by density functional theory calculations.

¹This work was financially supported by the NSFC (10834011, 60976089) and MOST (2009CB929103, 2010CB923004) of China.

9:12AM Y12.00007 Tip Induced doping effects in the local tunnel spectra of graphene, ANJAN K. GUPTA, SHYAM K. CHOUDHARY, Physics Department, IIT Kanpur — We report on tip induced carrier density changes in local tunnel spectra of single layer graphene (SLG) with backgate using room-temperature scanning tunneling microscopy (STM) and spectroscopy. The SLG samples, prepared by exfoliation method and verified by Raman spectra, show atomically resolved honeycomb lattice. Local tunnel spectra show two minima with the two moving in opposite directions along the bias axis. One minimum shows nearly a square-root dependence, and the other shows a linear dependence on the gate voltage. We understand these features as arising from the STM tip induced and bias voltage dependent change in carrier density in SLG. Other than the tip induced doping we also see the effect of charge inhomogeneity on the local tunnel spectra of SLG. The charge inhomogeneity is also seen in bilayer graphene but no new features due to tip induced doping are observed in the local spectra.

9:24AM Y12.00008 Electronic Structures of Graphene on Ru(0001): Scanning Tunneling Spectroscopy Study, WON-JUN JANG, JEUNG-HUM JEON, JONG KEON YOON, SE-JONG KAHNG¹, Department of Physics, Korea University — Graphene has inspired remarkable advances in nanotechnology due to its unusual electronic band structures represented by massless Dirac cones. Graphene can be epitaxially grown on metal surfaces by chemical vapor deposition method. Due to the lattice mismatch, epitaxial graphene grown on Ru(0001) shows hexagonal Moiré patterns with subatomic height variations. We studied local electronic structures of the epitaxial graphene using low-temperature scanning tunneling microscopy (STM) and spectroscopy (STS). Different spectra were observed at top, bridge, and hollow regions of the Moiré patterns. Observed STS data will be explained with structural models.

¹corresponding author

9:36AM Y12.00009 Fourier transform-STM: signatures of impurity scattering in graphene ribbons, ANDERS BERGVALL, TOMAS LOFWANDER, Department of Microtechnology and Nanoscience - MC2, Chalmers University of Technology, SE-41296 Goteborg, Sweden — We report results of a theoretical investigation of the effects of impurity scattering on the Fourier transformed local density of states (FT-LDOS) in graphene ribbons. We derive analytic expressions, within the Dirac approximation, for the Green's functions for armchair ribbons. Utilizing these, we show that the FT-LDOS contains distinct features that can be understood in terms of intra- and intersubband scattering processes. The ribbon band structure can then be reconstructed from the FT-LDOS. This makes the FT-LDOS a valuable spectroscopic tool. These predictions can be directly confirmed by Fourier transform scanning tunneling microscopy.

9:48AM Y12.00010 Tunable gap graphene micro-ribbons for terahertz plasmonics, DANHONG HUANG, Air Force Research Laboratory, Space Vehicles Directorate, Kirtland Air Force Base, NM 87117 USA, GODFREY GUMBS, OLEKSIY ROSLYAK, Department of Physics and Astronomy, Hunter College of the City University of New York, 695 Park Avenue, New York, NY 10065 USA — Maxwell's equations are solved for an array of graphene micro-ribbons located at the interface between a vacuum half-space and a half-space of a dielectric substrate. Our calculations include mode-mixing in the optical-response function. A closed-form analytic expression is obtained for the nonlocal optical-response function of a graphene layer with an induced energy gap which is then employed in our calculations beyond the long-wavelength approximation. Both the reflectivity and transmissivity spectral functions are calculated. Specifically, we obtain their dependences on the period of the array, the ribbon width, chemical potential of doped graphene, energy gap between the valence and conduction bands, substrate refractive index, and incident angle of a plane-wave electromagnetic field. Additionally, a qualitative comparison is made between our calculated results in this paper and the recent experimental data given by Ju, *et al.*, [Nature Nanotechnology, 6, 630 (2011)].

10:00AM Y12.00011 Electron-phonon coupling effects in the (8-5-5) line defect of graphene nanoribbon, HENG LUO, YONGWOO SHIN, XI LIN, Boston University — A “metallic” line defect in graphene nanoribbon consisting of alternating units of octagon and a pair of pentagons (8-5-5) is modeled using the adapted Su-Schrieffer-Heeger model Hamiltonian to include explicit electron-phonon coupling effects. Our results indicate that the 8-5-5 line defect has a finite optical gap of 0.4 eV with a broken charge conjugation symmetry, the bottom conduction band state mimic the nanoribbon edge case and the top valence state identical to the polyacetylene case. Upon photoexcitation, a small self-localized polaron state is found along one zigzag side of the line defect and a soliton-antisoliton pair is found on the other side. When the line defect is sandwiched between two graphene nanoribbons, the finite optical gap and photo-induced self-localized states persist as long as the nanoribbon width is smaller than 2 nm.

10:12AM Y12.00012 One Dimensional Massless Dirac Fermions in Functionalized Graphene Nanoribbons¹, R. TUĞRUL SENER, OZAN ARI, Department of Physics, İzmir Institute of Technology, İzmir, Turkey — Low-energy excitations of graphene are massless Dirac fermions due to presence of linear bands crossing at the Fermi level. Zigzag-edged nanoribbons of graphene (ZGNR), however, being semiconducting, do not possess this property. Using ab initio density-functional theory calculations we find that it is possible to close the band gap of ZGNRs through edge-functionalization with Na atoms. Moreover, the resulting band structure displays tilted-v-shaped linear bands crossing at the Fermi level, corresponding to one-dimensional massless Dirac fermions. We discuss mechanism of formation of such a band structure and its consequences in terms of electronic and transport properties.

¹Supported by TÜBİTAK, Project No: 111T318

10:24AM Y12.00013 Band Structure Measurements of Bottom-up Fabricated Graphene Nanoribbons, CHRISTOPHER BRONNER, FELIX LEYSSNER, STEPHAN MEYER, Fachbereich Physik, Freie Universität Berlin, Berlin, Germany, MANUEL UTECHT, TILLMANN KLAMROTH, PETER SAALFRANK, Universität Potsdam, Institut für Chemie, Potsdam, Germany, PETRA TEGEDER, Fachbereich Physik, Freie Universität Berlin, Berlin, Germany — Along with the growing interest in graphene, other low-dimensional carbon nanostructures are currently in the focus of research since these materials offer a wide variety of properties interesting e.g. for nanotechnology application. Among these carbon systems, quasi-one-dimensional graphene nanoribbons (GNR) introduce a possibility to tune the electronic structure - for example, GNRs exhibit a band gap which is inversely proportional to their width and can thus be adjusted over a wide range. While many theoretical studies have been published on the band structure of GNRs, experiments are usually limited by the quality of the GNRs' fabrication, e.g. using lithography or unzipping of carbon nanotubes. In order to avoid defects and irregular edges that are inevitable in these methods, lately a surface-assisted bottom-up synthesis has been demonstrated which yields quasi-perfect GNR structures. [1] In the present study we employ complementary surface-sensitive spectroscopies to investigate occupied and unoccupied bands and the band gap in an armchair GNR which has been synthesized on the Au(111) surface. DFT calculations were performed to obtain a thorough understanding of the nature of the observed states.

[1] J. Cai *et al.*, Nature (London) 466, 470-473 (2010)

10:36AM Y12.00014 Synthesis and characterization of nitrogen-doped graphitic nanoribbons, JOSUE ORTIZ, M. LUISA GARCIA, IPICT, Mexico, XIAOTING JIA, Massachusetts Institute of Technology, U.S.A., RAFAEL MARTINEZ, Universidad Autonoma de Barcelona, Spain, MIGUEL A. PELAGIO, Universidad Federal de Pernambuco, Brazil, DAVID SWANSON, Augustana College, U.S.A., A. LAURA ELIAS, HUMBERTO GUTIERREZ, The Pennsylvania State University, U.S.A., FERNANDO RODRIGUEZ, EMILIO MUNOZ, IPICT, Mexico, MILDRED DRESSELHAUS, Massachusetts Institute of Technology, U.S.A., HUMBERTO TERRONES, MAURICIO TERRONES, The Pennsylvania State University, U.S.A. — Nitrogen doping of carbon nanostructures such as nanotubes and graphene is a practical approach for tailoring their electronic and chemical properties. However, the doping of graphene nanoribbons still remains to be a challenge. Here we discuss a novel synthetic route to N-doped graphitic nanoribbons using chemical vapor deposition. The morphology of the new nanomaterial resembles the observed for the undoped graphitic nanoribbons, with particular differences specially at the ribbons' edges. We performed scanning and transmission electron microscopy as well as Raman and X-ray photoelectron spectroscopies in order to confirm the nitrogen presence within the nanoribbons. In addition, the electrical response for individual nanoribbons was obtained. We observed that N-doped nanoribbons exhibit a clear semiconductor-like behavior depending on the amount of nitrogen embedded in the hexagonal carbon network (undoped nanoribbons always showed a metallic response). These doped nanostructures could find applications in the fabrication of electronic devices.

10:48AM Y12.00015 Graphyne- and Graphdiyne-based Nanoribbons: Density Functional Theory Calculations of Electronic Structures¹, LIDA PAN, LIZHI ZHANG, BOQUN SONG, SHIXUAN DU, HONGJUN GAO, Institute of Physics, Chinese Academy of Sciences, Beijing — Graphdiyne, a carbon allotrope, which has the same symmetry as graphene and has butadiyne linkages between its nearest-neighbor hexagonal rings, has recently synthesized and fabricated on copper, showing experimentally the semiconductor property with conductivity of $2.516 \times 10^{-4} \text{ S m}^{-1}$, which is comparable to silicon. We investigate the configurations and electronic properties of graphyne and graphdiyne nanoribbons with armchair and zigzag edges by using first principles calculations. Our results show that all the nanoribbons are semiconductors with suitable band gaps similar to silicon. And their band gaps decrease as widths of nanoribbons increase. We also find that the band gap is at the Γ point for all graphdiyne ribbons and it is at the X point for all graphyne ribbons. Of particular interest, the band gap of zigzag graphyne nanoribbons show a unique "step effect" as the width increases. This property is good for tuning of the energy band gap, as in a certain range of the ribbon width, the energy gap remains constant and in reality the edge cannot be as neat as that in a theoretic model. Graphyne and graphdiyne with tunable gaps are promising candidates for future carbon-based electronic devices.

¹the Natural Science Foundation of China (NSFC) (Grant No.10834011), the MOST "973" projects of China (Grant No. 2011CB932700, 2011CB921702)

Friday, March 2, 2012 8:00AM - 11:00AM –
Session Y13 DMP GMAG: Focus Session: Low-Dimensional and Molecular Magnetism - Nano-
magnetism on Surfaces - Magnetic Adatoms and Clusters 211

8:00AM Y13.00001 Magnetism of single-vacancy defects in graphene and boron-nitride nanoflakes¹, SILVIA FERNANDEZ-SABIDO, CARLOS RAMOS, EDUARDO CIFUENTES-QUINTAL, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico — In this work we have used the hexagonal zigzag graphene and boron-nitride nanoflakes as a simple systems for studying the new class of magnetic materials obtained by structural vacancies in nonmagnetic s-p nanostructures. We have shown that for these systems, it is possible to predict the total spin moment from an electron counting analysis. Employing DFT calculations based on the LCAO approximation and the Fixed Spin Moment method, we have determinate the ground state spin multiplicity and the spin magnetic distribution for these structures. We have found that the ground state multiplicity of graphene nanoflakes is triplet, corresponding to a spin magnetic moment of $M = 2\mu_B$. Analyzing the spin orbital distribution we have determinate that the spin-polarized for the graphene nanoflakes is equally distributed in the sp^2 and p_z orbitals. For the boron-nitride nanoflakes we have obtained a quartet state ($M = 3\mu_B$) in the case of a boron vacancy, and a doublet state ($M = 1\mu_B$) for a nitrogen vacancy. We have found that for the boron-vacancy the spin-polarized is mainly localized on the sp^2 orbitals of nitrogen atoms. In contrast, for the nitrogen-vacancy the spin-polarized is concentrated at the p_z orbitals of boron atoms.

¹This research was supported by Conacyt-Mexico, Grant 83604.

8:12AM Y13.00002 Dynamical magnetic excitations in adatoms and dimers on metallic surfaces¹, SAMIR LOUNIS, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, ANTONIO T. COSTA, ROBERTO B. MUNIZ, Instituto de Física, Universidade Federal Fluminense, 24210-340 Niterói, RJ, Brazil, DOUG L. MILLS, Department of Physics and Astronomy, University of California Irvine, Irvine, California, 92697 USA — There is hardly any method which has shaped nanoscience and nanotechnology more profoundly than the scanning tunneling microscope. Such a tool is used nowadays to probe spin-excitations in nano-objects[1,2,3,4]. A key quantity describing these excitations is the transverse dynamical magnetic susceptibility that we calculate using the Korringa-Kohn-Rostoker Green function method within the framework of time-dependent density functional theory[5]. The behavior of adatoms and dimers will be discussed and comparison to experimental works will be provided when available.

[1] C. F. Hirjibehedin *et al.*, Science 317, 1199 (2007)

[2] T. Balashov *et al.*, Phys. Rev. Lett. 102, 257203 (2009)

[3] A. A. Khajetoorians *et al.*, Phys. Rev. Lett. 106, 037205 (2011)

[4] B. Chilian *et al.*, Arxiv:1108.2443

[5] S. Lounis *et al.*, Phys, Rev, Lett. 105, 187205 (2010); Phys. Rev. B 83, 035109 (2011)

¹S. L. acknowledges the support of the HGF-YIG Programme VH-NG-717. The research of D. L. M. and A. T. C. was funded by the U. S. Dept. of Energy, via grant DE-FG03-84ER-45083

8:24AM Y13.00003 Real Space Observation of Inelastic Kondo Effect and Interorbital Spin-Coupling in Molecule-Metal Contacts, AITOR MUGARZA, CORNELIUS KRULL, Catalan Institute of Nanotechnology, ROBERTO ROBLES, NICOLAS LORENTE, RICHARD KORYTAR, Centre d'Investigacions en Nanociència i Nanotecnologia, CIN2 (ICN-CSIC), SEBASTIAN STEPANOW, GUSTAVO CEBALLOS, PIETRO GAMBARDILLA, Catalan Institute of Nanotechnology — We present a comparative scanning tunneling spectroscopy study of four different types of MPc complexes ($M = \text{Fe, Co, Ni, Cu}$) adsorbed on the Ag(100) surface. Their magnetic properties are studied via the Kondo interaction with the substrate. Whereas the spectra of FePc and CoPc near the Fermi level is featureless, CuPc and NiPc show a Kondo resonance arising from the interaction of a ligand spin with conduction electrons. The spin at the organic macrocycle is induced by charge transfer from the Ag substrate. In CuPc, the coexistence of ion and ligand spin gives rise to interorbital coupling and spin excitations. The latter are observed via inelastic tunneling, where the Kondo interaction appears coupled to spin and vibrational excitations. By using the tip as a mobile electron we find that each type of excitation occupy mutually exclusive regions within the molecule, and result in different spin relaxation dynamics, reflecting the need of an atomic control of the molecule-metal interface to obtain reproducible transport properties. Finally, we study the influence of intermolecular interactions on the electronic and magnetic properties by creating artificial clusters in a controlled manner by manipulation of individual molecules.

8:36AM Y13.00004 Emerging magnetic stability in atomically assembled spin arrays, SEBASTIAN LOTH, Max Planck Research Group - Dynamics of Nanoelectronic Systems, Hamburg, Germany, SUSANNE BAUMANN, CHRISTOPHER P. LUTZ, D.M. EIGLER, ANDREAS J. HEINRICH, IBM Research - Almaden, San Jose, CA, USA — Magnetic stability is usually created by the interaction of a large ensemble of atomically small magnetic moments that are themselves unstable. We make use of the Scanning Tunneling Microscope's ability to move individual atoms and construct arrays of interacting spins. Owing to their smallness, the magnetic states of these spin arrays are quantized and we probe their energies by inelastic electron tunneling spectroscopy [1]. To gain access to the equally important dynamical properties we employ an all-electronic pump-probe measurement scheme with which we follow the evolution between the spin states at nanosecond speed [2]. The combination of energetic and dynamical information allows identification of the relevant spin interaction and spin relaxation mechanisms at the atomic level. We design arrangements of atoms that suppress quantum tunneling of magnetization and drastically stabilize different spin configurations. Tracing the emergence of magnetic stability in the progression from individual atoms to arrays of spins points to new avenues for spintronic applications at atomic dimensions.

[1] A. J. Heinrich, J. A. Gupta, C. P. Lutz, D. M. Eigler, Science 306 466 (2004).

[2] S. Loth, M. Etzkorn, C. P. Lutz, D. M. Eigler, A. J. Heinrich, Science 329 1628 (2010).

8:48AM Y13.00005 Magnetocrystalline anisotropy of 3d transition metal atoms on graphene, JUN HU, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA 92697-4575 — Graphene has attracted most attention in the field of condensed matter physics, chemistry and material science since the first day when it was produced in lab. It's an ideal material for two-dimensional electron gas (2DEG). Most intriguingly, the electronic and magnetic properties can be easily engineered by decorating with external elemental atoms ranging from nonmetal to transition metal. Especially, graphene is attractive for spintronics due to its long spin life time and high mobility. So far, ultrathin Co films have been deposited on graphene which exhibit perpendicular magnetic anisotropy. In this work, first-principles calculations are performed to systematically study the magnetic properties of graphene decorated by 3d transition metal atoms with several covering patterns. We find that Fe/graphene always exhibits in-plane anisotropy regardless the coverage, while Mn/graphene and Co/graphene tend to have perpendicular easy axis for most range of coverage. The spin moments of Ni atoms are largely quenched for Ni/graphene. Moreover, the Mn atoms on graphene prefer ferromagnetic exchange coupling which are totally different from the pure counterpart without graphene support. The strong hybridization between 3d orbitals of transition metal atoms and π states of graphene are responsible for the modification of magnetic properties. **Acknowledgement.** This work was supported by DOE Grant DE-FG02-05ER46237.

9:00AM Y13.00006 Exploring Kondo Phenomena in Physisorbed Nitric Oxide, RYAN REQUIST, SISSA, Trieste, Italy, ALEXANDER SMOGUNOV, CEA Saclay, France, PIERPAOLO BARUSELLI, MICHELE FABRIZIO, ERIO TOSATTI, SISSA, Trieste, Italy — The NO molecule is a $S=1/2$ system that can be physisorbed on gold surfaces. As there are presently no data indicating whether or not physisorbed NO retains its spin and displays an observable Kondo effect, we investigate that question by means of our ab-initio based DFT+NRG approach [1]. DFT calculations for NO/Au(111) confirm that at low coverage the on-top adsorption site is the most stable, with the NO molecule forming an angle of approximately 60 degrees with the surface normal. Spin-polarized DFT calculations reveal that the molecule retains one unpaired electron in an antibonding π orbital that hybridizes, albeit moderately, with the surface. Based on these ingredients, we discuss the possibility of observing a zero-bias Kondo anomaly in scanning tunneling spectroscopy above NO/Au(111). The influence of gold surface states and vibronic motion of the molecule are also investigated. [1] P. Lucignano et al., Nature Mat. 8, 563 (2009).

9:12AM Y13.00007 Magnetic Interaction between Surface Engineered Rare-earth Atomic Spins, BARBARA JONES, IBM Almaden Research Center, San Jose, CA, CHIUNG-YUAN LIN, National Chaio Tung University, Taiwan — We report an ab initio study of rare-earth adatoms (Gd) on a surface, where it has been demonstrated previously that the STM can build and manipulate spin-coupled transition-metal atoms on such a surface one atom at a time, and have their spin excitation measured to be antiferromagnetic. The present work is the first attempt of studying rare-earth spin-coupled adatoms, the geometry effect of spin coupling, and the underlying mechanism of ferromagnetic coupling. The exchange coupling between Gd atoms on the surface is calculated to be antiferromagnetic in one geometry and ferromagnetic in another, by considering their collinear spins and using the PBE+U exchange correlation. We also find the Gd dimer in these two geometries is similar to nearest-neighbor and next-nearest-neighbor Gd atom pairs in GdN bulk. We analyze how much direct exchange, superexchange, and RKKY interactions contribute to the exchange coupling for the ferromagnetic arrangement by additional first-principles calculations of alternative model systems. Our calculations also show that the Gd spin of these structures is $7/2$, the same as that of a GdN bulk.

9:24AM Y13.00008 Atom-by-atom engineering and atomic magnetometry of tailored nano-magnets with SP-STM¹, ALEXANDER A. KHAJETOORIANS, JENS WIEBE, BRUNO CHILIAN, Institute of Applied Physics, Hamburg University, Hamburg, Germany, SAMIR LOUNIS, STEFAN BLÜGEL, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany, ROLAND WIESENDANGER, Institute of Applied Physics, Hamburg University, Hamburg, Germany — Nanomagnets, namely arrays of a few exchange coupled atomic magnetic moments, possess a rich variety of magnetic properties and are explored as constituents of nano-spintronics technologies. They have been realized as magnetic clusters or molecular nanomagnets. Individual nanomagnets, built from magnetic atoms adsorbed onto a non-magnetic surface (adatoms) coupled by Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange, exhibit a high level of versatility resulting from distance-dependent interactions. Here, we combine spin-resolved scanning tunneling microscopy (SP-STs), atom manipulation and simulations to tailor nanomagnets ranging from linear chains to complex two-dimensional arrays and perform magnetometry in an atom-by-atom fashion. Distinct ground states of each chain, depending on even or odd numbers of constituent atoms, and magnetic frustration within the arrays have been observed directly. Our work demonstrates real space access to the magnetic states of tailored nanostructures providing an approach to tackling open fundamental questions in magnetism.

¹ERC Advanced Grant "FUORE", DFG-SFB668, LEXI-cluster "Nanospintronics," HGF-YIG Programme VH-NG-717

9:36AM Y13.00009 First-principles study of magnetic exchange interactions in scanning probe microscopy, STEFAN HEINZE, CESAR LAZO, PAOLO FERRIANI, Institute of Theoretical Physics and Astrophysics, University of Kiel, Germany — In the last years, spin-polarized scanning tunneling microscopy (SP-STM) has been established as a technique to resolve complex magnetic structures down to the atomic scale. More recently, it has even become possible to detect the exchange interactions between tip and sample by magnetic exchange force microscopy (MExFM). However, the interpretation of such measurements is non-trivial, especially on the atomic scale. Here, we use density functional theory in order to study the effect of exchange interactions in SP-STM and MExFM measurements. First, we demonstrate the occurrence of a spin-valve effect for single Co and Cr atoms on Fe islands on W(110) contacted by an SP-STM tip as a result of the spin-dependent orbital symmetry of the states in the vicinity of the Fermi energy [1]. We find that the exchange interaction between tip and adsorbed atoms affects the magnetoresistance in the tunneling regime. Second, we explain the quantitative measurement of the exchange interaction across a vacuum gap using MExFM applied to an Fe monolayer on W(001) [2]. We show how the chemical tip composition influences the magnitude and distance dependence of the exchange forces.

[1] M. Ziegler et al., New J. Phys. 13, 085011 (2011).

[2] R. Schmidt et al., Phys. Rev. Lett. 106, 257202 (2011).

9:48AM Y13.00010 Evidence of Kondo effect in organic radical nanoassemblies, MOHAMMAD RASHIDI, STEFAN MULLEGER, MICHAEL FATTINGER, REINHOLD KOCH, Solid state physics division, Johannes Kepler University, Linz, Austria — The outstanding spatial resolution of low temperature (LT) scanning tunneling microscopy (STM) and spectroscopy (STS) enables to probe the frontier orbital electronic structure of single magnetic molecules and clusters adsorbed on substrates. Here, we study self-aligned nanostructures of (spin-1/2) hydrocarbon radicals on a metal surface by means of LT-STM and STS. Pronounced involvement of surface state electrons is observed in the frontier molecular orbital (MO) resonances. An empty hybrid state closely above the substrate Fermi level exhibits the characteristic properties of surface Kondo effect reported for similar systems in the literature. By identifying three electronic states as hybrids of molecular orbitals and surface state electrons (two of them directly related to the Kondo effect), we are able to present a modified picture of the surface Kondo effect. It is based on a valence-bond model, where the bonding state represents Kondo's virtual bound state and the antibonding state is the so called 'Kondo resonance' reported in STM studies of the surface Kondo effect. Furthermore, double occupation of the originally singly unoccupied MO by tunneling electrons leads to the third state well above the Fermi level due to Coulomb repulsion as described by the Anderson model.

10:00AM Y13.00011 Spin inelastic electron transport through magnetic nanostructures, AARON HURLEY, NADJIB BAADJI, STEFANO SANVITO, Trinity College Dublin — Recent experimental advances in scanning tunneling microscopy make the measurement of the conductance spectra of isolated and magnetically coupled atoms on nonmagnetic substrates possible. Notably, these spectra are characterized by a competition between the Kondo effect and spin-flip inelastic electron tunneling. In particular they include Kondo resonances and a logarithmic enhancement of the conductance at voltages corresponding to magnetic excitations, two features that cannot be captured by second order perturbation theory in the electron-spin coupling. We have now derived a third order analytic expression for the electron-spin self-energy, which can be readily used in combination with the non-equilibrium Green's function scheme for electron transport at finite bias. We demonstrate that our method is capable of semi-quantitative description of the competition between Kondo resonances and spin-flip inelastic electron tunneling at a computational cost significantly lower than that of other approaches. The examples of Co and Fe on CuN are discussed in detail. We also explain the theoretical origin of the conductance asymmetry that is present for both spin and non-spin polarized STM tips in the experimentally determined spectra of these atoms.

10:12AM Y13.00012 Real-space imaging of inelastic Kondo effect in a single O₂ molecule, YING JIANG, International Center for Quantum Materials, Peking University, Beijing 100871, China, WEI JI, Department of Physics, Renmin University of China, Beijing 100872, China, QING HUAN, ARTHUR YU, SHAOWEI LI, Department of Physics and Astronomy, University of California, Irvine, CA 92697-4575, WILSON HO, Department of Physics and Astronomy and Department of Chemistry, University of California, Irvine, CA 92697-4575 — Inelastic Kondo effect of the single O₂ molecule physisorbed on Ag(110) surface is investigated in real space using a low-temperature scanning tunneling microscope (STM) at 10 K. The O₂ molecule carries an unpaired spin, as supported by density functional theory, showing a Kondo resonance at the Fermi energy. The coupling between the vibrations and the unpaired electron in the O₂ molecule results in the inelastic Kondo effect, which is manifested as striking side peaks at finite biases in the dI/dV spectra, in clear contrast to the normal vibrational inelastic tunneling spectroscopy (IETS). Spectroscopic imaging shows that two vibrational modes are coupled to the Kondo resonance with different strengths, which arises from the symmetry match between the Kondo state and the vibrational modes.

10:24AM Y13.00013 Scanning Tunneling Microscopy and Spectroscopy of Fe[H₂B(Pz)₂]₂(bipy) Spin-Crossover Complex on Au(111)¹, ALEX PRONSCHINSKE, GEOFF LEWIS, YIFENG CHEN, North Carolina State University, ROBERT BRUCE, WEI YOU, University of North Carolina, MARCO BUONGIORNO-NARDELLI, DAVID SHULTZ, DANIEL DOUGHERTY, North Carolina State University — Spin crossover compounds have externally-tunable magnetic moments that will be useful for spintronic applications if they result in correspondingly tunable electronic properties. In order to assess this electronic tunability, we have performed variable temperature scanning tunneling microscopy and spectroscopy on a known Fe(II) spin crossover compound, Fe[H₂B(Pz)₂]₂(bipy), thermally-evaporated onto a single crystal Au(111) surface. We report on the surface assembly of this molecule in few layer films including imaging with submolecular resolution. In addition, we use STS to probe the local density of electronic states across a temperature range spanning the low spin to high spin transition and compare with first principles electronic structure calculations.

¹Funding Provided by NSF Center for Chemical Innovation: Center for Molecular Spintronics (CHE-0943975)

10:36AM Y13.00014 Frustration in the Magnetic Molecules W₇₂V₃₀ and Pr₁₃ Probed by NMR and Tunnel-diode Resonator, STEVEN YENINAS, M. LUBAN, R. PROZOROV, Y. FURUKAWA, The Ames Laboratory, C. SCHRÖDER, University of Applied Sciences, Bielefeld, Germany, J. SCHNACK, University of Bielefeld, Germany — The magnetic molecules Pr₁₃ and W₇₂V₃₀ have been studied by DC and AC magnetic susceptibilities and NMR. These molecules exhibit geometrical frustration resulting from antiferromagnetic intramolecular coupling of nearest neighbor paramagnetic ions. In Pr₁₃, 12 Pr^{III} ions (S=1) interact along edge sites of an icosahedron centered about an additional Pr^{III} ion. For W₇₂V₃₀, 30 V^{IV} ions (S=1/2) interact along corner sharing sites of a near perfect icosidodecahedron, a spherical representation of a 2-D Kagome Lattice. Characterizing the DC magnetic response requires a distribution of exchange constants for both molecules at low temperatures. Results are compared to similar frustrated systems which feature a variety of magnetic phenomena - metamagnetic phase transitions, magnetic hysteresis without anisotropy, spin glass behavior, and superparamagnetism.

10:48AM Y13.00015 Unification of ultrafast, laser-driven and slow, phonon-driven spin-flip scenarios in the three-magnetic-center cluster Ni₃Na₂, HONGPING XIANG, GEORGIOS LEFKIDIS, WOLFGANG HÜBNER, Dept. of Physics and Research Center OPTIMAS, University of Kaiserslautern — Recently the use of the three-magnetic-center Ni₃Na₂ on a fictitious, inert surface as a prototypical system for ultrafast, laser-driven spin manipulation and logic functionalization was reported [1]. Here we extend this investigation of spin dynamics on the same system by including vibronic motion and recalculating all electronic states for each structural distortion. The first immediate finding is that the system exhibits an unexpectedly rich set of magnetic phases (geometry sets with different orientations of the highly localized spin-density). Exploiting those phases allows us (a) to establish the combination of spin dynamics and phonons as an unprecedentedly accurate sensor of the bond length between metallic centers, and (b) to present for the first time a unified picture of ultrafast (fs), laser-driven and slow (ps), phonon-driven spin dynamics in molecular magnets.

[1] W. Hübner, S. Kersten, G. Lefkidis, Phys. Rev. B **79**, 184431 (2009).

Friday, March 2, 2012 8:00AM - 11:00AM —

Session Y14 DMP GMAG: Focus Session: Spins in Carbon - Organic Spintronics 212

8:00AM Y14.00001 A new twist on organic spintronics: Controlling transport in organic sandwich devices using fringe fields from ferromagnetic films¹, MARKUS WOHLGENANNT, University of Iowa, Department of Physics and Astronomy — Organic spintronics studies the physics of spin-injection and magnetic-field dependent transport phenomena in organic semiconductors, possibly leading to devices with added functionality. So far, studies have focused on spin-valve architectures as well as entirely non-magnetic devices that nevertheless show large room-temperature magnetoresistance through the so-called organic magnetoresistive effect. We demonstrate a new method of controlling the electrical conductivity of an organic film at room temperature, using the spatially-varying magnetic fringe fields of a magnetically-unsaturated ferromagnet. A large variation from hopping site to hopping site of the nuclear hyperfine field is known to dramatically affect electronic transport in organics, whose resistances are very sensitive to small applied magnetic fields, so the ferromagnet's fringe fields might act as a substitute either for the applied magnetic field or for the inhomogeneous hyperfine field. The size of the effect, magnetic field dependence, and hysteretic properties rule out a model where the fringe fields from the ferromagnet provide a local magnetic field that changes the electronic transport properties through the hyperfine field, and show our effects originate from electrical transport through the inhomogeneous fringe fields coming from the ferromagnet. Surprisingly these inhomogeneous fringe fields vary over length scales roughly two orders of magnitude larger than the hopping length in the organic materials, challenging the fundamental models of magnetoresistance in organic layers which require the correlation length of the inhomogeneous field to correspond roughly to the hopping length. Our devices, which do not rely on spin injection, tunneling anisotropic magnetoresistance or spin-valve behavior, may provide a simple approach to integrating magnetic metals and organics for hybrid spintronic devices. These devices may find application as high-voltage readouts of the magnetic state of low-impedance ferromagnetic films.

¹I would like to acknowledge the contributions to this work by M.E. Flatte, F. Wang (University of Iowa), F. Macia, and A. D. Kent (New York University) and financial support by Army MURI Grant No. W911NF-08-1-0317

8:36AM Y14.00002 Magnetic Field Effects: Triplet-Charge Annihilation versus Triplet-Triplet Annihilation in Organic Semiconductors, BIN HU, MING SHAO, LIANG YAN, MINGXING LI, University of Tennessee — Triplet-charge reaction and triplet-triplet annihilation are two important processes in generating magnetic field effects in organic semiconductors. This presentation reports experimental studies on triplet-charge annihilation (TCA) versus triplet-triplet annihilation (TTA) in organic semiconductors. Specifically, we separately adjust the triplet-charge and triplet-triplet interactions towards the generation of TCA and TTA by changing triplet density, charge confinement, and charge/exciton ratio based on organic light-emitting diodes. We then use magnetic field effects of electroluminescence (MFE_{EL}) to study the TCA and TTA through spin interactions. We observe that the electroluminescence can clearly show negative response to applied magnetic field when triplets and charges are simultaneously confined within close proximity. On contrast, the electroluminescence only exhibits positive MFE_{EL} when triplets are confined within close proximity. Therefore, it can be concluded that the TCA is a major process to annihilate triplets through Coulomb interaction in organic semiconductors.

8:48AM Y14.00003 Electron Spin Relaxation: The Role of Spin-Orbit Coupling in Organic Semiconductors, M. WILLIS, L. NUCCIO, Queen Mary University of London, L. SCHULZ, University of Texas at Austin, USA, W. GILLIN, T. KREOUZIS, Queen Mary University of London, F. PRATT, J. LORD, ISIS Muon Facility, UK, M. HEENEY, Imperial London, UK, S. FRATINI, Institut Neel Grenoble, FR., C. BERNHARD, University of Fribourg, CH, A. DREW, Queen Mary University of London — Rapid development of organic materials has lead to their availability in commercial products. Until now, the spin degree of freedom has not generally been used in organic materials. As well as engineering difficulties, there are fundamental questions with respect to the electron spin relaxation (eSR) mechanisms in organic molecules. Muons used as a microscopic spin probe, localized to a single molecule, can access information needed to identify the relevant model for eSR. In this presentation I will introduce the ALC-MuSR technique describing how eSR can be extracted and the expected effects. I will show how the technique has been applied to small organic molecules such as the group III Quinolate series and functionalized molecules with a pentacene-like backbone. Lastly I will present the Z-number and temperature dependence in these organic molecules and show strong evidence for a spin-orbit based eSR mechanism.

9:00AM Y14.00004 Using quantum spin-phase to elucidate weakly coupled pair hopping rates in organic semiconductors, WILLIAM BAKER, University of Utah, DANE MCCAMEY, TOM KEEVERS, University of Sydney, JOHN LUPTON, University of Regensburg, CHRISTOPH BOEHME, University of Utah, UTAH SPIN ELECTRONICS GROUP COLLABORATION, LUPTON GROUP COLLABORATION, SYNDEY QUANTUM PHYSICS GROUP COLLABORATION — We have carried out electrically detected spin echo experiments on recombining electron-hole pairs (polaron pairs)¹ in MEH-PPV organic light emitting diodes at different temperatures and device currents. We find long spin-phase relaxation times [$T_2 = 324(18)$ ns] at room temperature and less than twice this value [$T_2 = 611(39)$ ns] at $T = 10$ K. Next to this very weak temperature dependency, we also observe nearly no dependency of T_2 on the free carrier density in the material. We attribute this coherence decay behavior to charge carrier hopping transitions between localization sites which are exposed to differing hyperfine fields. Although the nuclear spin relaxation times in our material are much longer than the time scale of our experiments, the stochastic movement through this random environment leads to a time dependent fluctuating field causing an irreversible phase loss. We have simulated the echo experiments with this hopping process incorporated, and find good agreement with experimental data. The results of our study contrast free polaron transport processes which show an Arrhenius-type activation in time-of-flight experiments.

¹McCamey, D. R. *et al.*, *Nat Mater* **7**, 728 (2008).

9:12AM Y14.00005 Spin-flip induced magnetoresistance in positionally disordered organic solids¹, NICHOLAS HARMON, MICHAEL FLATTÉ, University of Iowa — A theory for magnetoresistance in positionally disordered organic materials is presented and solved using percolation theory. The model describes the effects of spin dynamics on hopping transport by considering changes in the effective density of hopping sites, a key quantity determining the properties of percolative transport. Faster spin-flip transitions open up 'spin-blocked' pathways to become viable conduction channels and hence produce magnetoresistance. Features of this percolative magnetoresistance can be found analytically in several regimes, and agree with previous measurements, including the sensitive dependence of the magnetic-field-dependence of the magnetoresistance on the ratio of the carrier hopping time to the hyperfine-induced carrier spin precession time. Studies of magnetoresistance in known systems with controllable positional disorder would provide an additional stringent test of this theory.

¹This research was made possible by an ARO-MURI

9:24AM Y14.00006 Magnetoresistance in organic spin-valve devices with low work-function metal, H.-JAE JANG, Semiconductor and Dimensional Metrology Div., NIST & Dept of Physics, WFU, KURT P. PERNSTICH, DAVID J. GUNDLACH, Semiconductor and Dimensional Metrology Div., NIST, OANA D. JURCHESCU, Dept. of Physics, Wake Forest Univ., CURT A. RICHTER, Semiconductor and Dimensional Metrology Div., NIST — Organic thin-films have recently generated interest for studies related to spin-based phenomena. Long spin transport through organic semiconductors has been predicted due to their weak spin-orbit and small hyperfine interactions. This property gives them great potential for spintronic applications. While magnetoresistance (MR) has been reported by multiple research groups, controversy still remains over whether the basic mechanism is the transport of spin-polarized carriers through the organic semiconducting thin films or transport via unintended tunneling paths through the devices. We investigate the MR of organic thin-film spin valve devices fabricated from tris[8-hydroxyquinoline]aluminum (Alq3), high Tc transition ferromagnetic metals, and low work-function metals. The devices are fabricated without the exposure to the air to minimize the oxidation. We observe the MR as large as 3 % at 4.5K in devices containing Alq3 as thick as 150 nm.

9:36AM Y14.00007 Origin of magnetoresistance in organic spin-injection structures, ZHI-GANG YU, SRI International — Spin injection into organic materials is usually inferred from the device resistance difference between antiparallel and parallel magnetic configurations (magnetoresistance, or MR) in an organic spin valve (OSV). The common features of the observed MR in OSVs include: 1) the MR is pronounced only at a low bias, where the device I-V characteristic is essentially linear; 2) the MR quickly decreases with bias and temperature while the decrease in device resistance is insignificant; 3) the MR is usually negative for OSVs with thick organic films, particularly when the two ferromagnets are similar in electronic structure. Despite superficial resemblance between OSVs and inorganic spin-injection structures, the MR in the former cannot be explained by theories developed for the latter. Here we show that the resistance of an OSV is controlled by the carrier density deep inside the organic and the MR is due to the difference in the carrier density for the two magnetic configurations. The sign of MR is determined by the electron spin polarization at a finite energy above the Fermi level in the electrodes. This picture explains common features of MR and suggests new strategies for probing and manipulating spin in organic spintronic structures.

9:48AM Y14.00008 Magnetoresistance in an all-organic-based spin valve, BIN LI, CHI-YUEH KAO, JUNG-WOO YOO, YU LU, MENGQI ZHOU, VLADIMIR PRIGODIN, ARTHUR EPSTEIN, The Ohio State University — We demonstrate spin injection and detection in an all-organic-based magnetic tunnel junction using two layers of organic-based magnet V[TCNE]_x (x~2, TCNE: tetracyanoethylene) as the magnetic contacts and organic semiconductor rubrene (C₄₂H₂₈) as the spacer. For the V[TCNE]_x film growth, we exploited two different growth techniques, chemical vapor deposition and molecular layer deposition, which result in different coercivities of V[TCNE]_x films. The spin valve devices show negative magnetoresistance (MR), the sign of which does not change with temperature and bias. To explain the unusual negative MR, we propose a simple phenomenological bias-enhanced selective tunneling (BEST) model based on the different spin polarizations of the molecular energy levels of V[TCNE]_x. Our results show the significance of bias induced energy level shift in organic spintronic devices due to relatively narrow spin polarized bandwidths. This work was supported in part by AFOSR Grant No. FA9550-06-1-0175, DOE Grant Nos DE-FG02-01ER45931, DE-FG02-86ER45271, NSF Grant No. DMR-0805220, the Center for Emergent Materials (an NSF-MRSEC; Award Number DMR-0820414) at The Ohio State University and the Institute for Materials Research at The Ohio State University.

10:00AM Y14.00009 Manganese Phthalocyanines on manganese surfaces: An ab-initio approach to the tunneling magnetoresistance, MARIA SORIANO, JUAN JOSE PALACIOS, Universidad Autonoma de Madrid — We have performed computational studies of spin polarized transport based on Density Functional Theory (DFT) using a non-equilibrium Green's functions formalism implemented in our ANT code [1] to compute tunneling magnetoresistance (TMR) on different manganese based systems. Specifically we present results for STM tips on a clean manganese surface, which is well known to show an antiferromagnetic coupling between layers when grown on an iron surface. In this system we have studied the dependence of the TMR on the tip-surface distance, the position of the tip, and on the bias voltage. Also we present a comparison between the Landauer formalism and the Tersoff-Hamman approach, usually used in this context. Finally we analyse the interaction between Manganese Phthalocyanine (MnPc) molecules on the manganese surface, focusing on the TMR signature and its dependence on the different adsorption sites.

[1] J.J. Palacios et. al. Ab-initio Quantum Transport (ANT). alacant.dfa.ua.es

10:12AM Y14.00010 Spin injection in cobalt and copper phthalocyanines¹, DAVID CIUDAD, Massachusetts Institute of Technology, MARCO GOBBI, CIC nanoGUNE Consolider, DARIO A. ARENA, National Synchrotron Light Source, Brookhaven National Lab, JAGADEESH S. MOODERA, Massachusetts Institute of Technology — An organic light emitting diode (OLED) is a heterojunction comprising two different organic semiconductors (OS): one for hole and another one for electron transport. Electrons and holes recombine at the interface between them. Depending on their total spin the recombination may (singlet state) or may not (triplet state) produce visible light. The efficiency of OLEDs could be doubled by injecting a spin-polarized current (Spin-OLED).² One obstacle to attain a spin-OLED is the lack of studies of spin diffusion lengths (λ_s) and injection efficiencies on hole-transport OS. We investigate spin injection in phthalocyanines (Pcs). The Pcs are ideal candidates to reach the above goal because: 1) of their high hole mobility; 2) Cu-Pc in particular is currently used in OLEDs; 3) their high thermal and chemical stability; 4) these molecules contain a single metal atom making them a unique system to study its effect on the spin injection. To determine λ_s we investigate multilayer structures having transition metal/ Cu-Pc or Co-Pc interfaces including magnetic tunnel junctions with OS as barriers. Further characterization of these interfaces has been performed by soft X-Ray measurements at the NSLS-BNL facility.

¹Work supported by European Marie Curie Fellowship (FP7-PEOPLE-2010-IOF, no 275176), ONR grant N00014-09-1-1847, UNLFR 09-0532-01(NSF), RLE-MIT, EFRC and DOE.

²I. Bergenti et al. Organic Electronics, 2004, 5, 3

10:24AM Y14.00011 The role of thin MgO(100) epilayer for polarized charge injection into top-emitting OLED¹, TAE HEE KIM, NYUN JONG LEE, YU JEONG BAE, Department of Physics, Ewha Womans University, Seoul, South Korea, HYUNDUK CHO, CHANGHEE LEE, School of Electrical Engineering and Computer Science, Seoul National University, Seoul, South Korea, EISUKE ITO, Fluoro-Order Functions Research Team, RIKEN Advanced Science Institute, Wako, Saitama 351-0198, Japan — A new top-emitting OLED (TOLED) structure, which is formed on an Si(100) substrate and an epitaxial MgO(100)/Fe(100)/MgO(100) bottom electrode, was investigated. Our TOLED design included a semi-transparent cathode Al, a stack of conventional organic electroluminescent layers (α -NPD/Alq₃/LiF) and a thin Cu-Phthalocyanine (CuPc) film to enhance the hole injection into the luminescent layers. At room temperature (RT), magnetoluminescence of ~5 % was observed in low magnetic field up to 1 Tesla, which is obviously larger than that of the OLEDs with epitaxial and polycrystalline Fe anodes without MgO(100) covering layer. Our results indicate that the magnetic field effect on the electroluminescence could be strongly related to the magnetic properties of bottom electrode, more precisely the interfacial properties between CuPc layer and the anode. Therefore, we focused on understanding interface electronic states and energy alignment by using x-ray photoemission spectroscopy and ultraviolet photoemission spectroscopy. Our results showed that the use of appropriate oxide layers could represent a new interface engineering technique for improving reliability and functionality in organic semiconductor devices.

¹This work is supported by National Research Foundation of Korea Grants (NRF-2011-0017209 and 2011-0005908).

10:36AM Y14.00012 Spin Polarized Scanning Tunneling Microscopy of Alq₃ on Cr(001)¹, DANIEL DOUGHERTY, ZHENGANG WANG, ALEX PRONSHINSKE, Department of Physics, North Carolina State University — The field of organic spintronics has been strongly motivated in recent years by the observation of giant magnetoresistive effects in tris-(8-hydroxyquinoline) aluminum (Alq₃) films and nanostructures. It is crucial to understand the spin- dependent electronic structure at metal-Alq₃ interfaces. We have carried out spin polarized scanning tunneling microscopy to measure the local density of electronic states for submonolayer films of Alq₃ grown on the layered antiferromagnetic Cr(001) surface. We report an energy-dependent tunneling conductance asymmetry for single molecules adsorbed on differently magnetized (001) terraces and discuss its connection with metal-molecule hybridization and magnetoresistive effects in Alq₃ spintronic devices.

¹Funding provided by: NSF Center for Chemical Innovation: Center for Molecular Spintronics (CHE-0943975)

10:48AM Y14.00013 Ferroelectric control of the spin polarization in an organic spin valve, DALI SUN, Oak Ridge National Laboratory / The University of Tennessee, Knoxville, XIAOSHAN XU, Oak Ridge National Laboratory, LU JIANG, Oak Ridge National Laboratory / The University of Tennessee, Knoxville, HO NYUNG LEE, Oak Ridge National Laboratory, HANGWEN GUO, Oak Ridge National Laboratory / The University of Tennessee, Knoxville, PAUL C. SNIJDERS, T. ZAC WARD, Oak Ridge National Laboratory, ZHENG GAI, X.-G ZHANG, Oak Ridge National Laboratory / Center for Nanophase Materials Science, JIAN SHEN, Fudan University/ The University of Tennessee, Knoxville — Recently engineering the spin propagation in organic spin valves has shown increasingly interesting properties. In this work we demonstrate novel ferroelectric control of the spin polarization in an organic spin valve. By inserting a thin ferroelectric buffer layer between a bottom $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$ (LSMO) electrode and the organic Alq_3 layer, a controlled spin polarization through the ferroelectric interface is achieved. The spin valve exhibits both positive and negative magnetoresistance depending on the applied bias. We conclude that this results from the energy level shift by the ferroelectric dipoles between Alq_3 and LSMO (Research sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy).

Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y15 DMP FIAP GMAG: Focus Session: Spins in Metals: Spin Torque Theory, Spin Dependent Transport 213

8:00AM Y15.00001 Newtonian reciprocity between spinmotive forces (SMF) and spin-torque-transfer (STT), STEWART BARNES, Physics Department, University of Miami, Coral Gables, FL — An SMF and the STT effect are reflected in definitions

$$\vec{p} = m\vec{v} + e\vec{A}_s \quad \text{and} \quad H = H_0 + e\Phi_s + eA_{0s},$$

valid beyond the adiabatic approximation, where the momentum $m\vec{v}$ is mechanical, while $\vec{p}$ is that conjugate to the position $\vec{r}$, H is the full Hamiltonian while H_0 is that for uniform magnet. Here $(\vec{A}_s, A_{0s})$ is the four vector which reflects the *linear* momentum of the magnetic system. The spin magnetic and electric fields

$$B_i = -\frac{im^2}{\hbar}\epsilon_{ijk}[v_j, v_k] \quad \text{and} \quad E_i = -\frac{im^2}{\hbar}[v_i, v_0]; \quad i = \{x, y, z\}$$

where $i\partial_t = mv_0 + eA_0$, and involve commutators. The Landau-Lifshitz equations are an *emergent*. They correspond to

$$[S_z, (H_0 + e\Phi_s + eA_{0s})] = 0$$

as required to separate the *slow* magnetic and *fast* electronic degrees of freedom. E.g. $L = (enAz - \dot{q})\frac{\hbar}{e}\phi + g\mu_B BnAx - q\mathcal{E}$ is the Lagrangian for simple domain wall connected to a battery emf $\mathcal{E}$. SMF-STT reciprocity reflects Newtonian third law and *not* an Onsager relationship between transport coefficients. Experiment for spin-valves and MTJs will be reviewed.

8:12AM Y15.00002 Theoretical investigation of the dynamics of a magnetic bilayer in the presence of spin transfer torque, LYDIA NOVOZHIOVA, Western Connecticut State University, SERGEI URAZHIDIN, Emory University — Magnetoelectronic nanodevices, such as magnetic memory cells and spin torque nano-oscillators, generally utilize at least two magnetic layers, the “reference” and the “free” layer. While most previous studies focused only on the behaviors of the “free” layer, the dynamics of the “reference” layer can also be important due to the coupling between the layers. We utilize Landau-Lifshitz-Slonczewski equations in the macrospin approximation to analyze the dynamics of a magnetic bilayer driven by a dc current. We show that even in the absence of magnetic or RKKY interactions, coupling between the layers is efficiently mediated by the spin transfer torque. We use an axially symmetric approximation to derive an analytical stability condition for the bilayer. The stability is determined by the physical characteristics of the bilayer and two control parameters - the dc current and the external time-independent magnetic field. Additionally, we use an averaging technique to find synchronized precessional motions of the two nanomagnets. Finally, we show that for some conditions, the dynamics of the bilayer becomes chaotic. Such chaotic dynamics is prohibited for a single macrospin due to the limitations imposed by the dimensionality of the system.

8:24AM Y15.00003 Interplay between conduction electron spin current and magnon spin current¹, SHULEI ZHANG, SHUFENG ZHANG, Department of Physics, University of Arizona — Spin current is a flow of angular momentum that can be carried by conduction electrons as well as magnons. In conducting ferromagnets, both electron spin currents and magnon currents are present. By using a semiclassical description for conduction electrons and magnons, we evaluate the distribution functions of the non-equilibrium electrons and magnons in the presence of electron-magnon interactions. In some interesting limiting cases, we have derived novel diffusion equations for both electrons and magnons. We then apply our formalisms to study the spin currents for various bilayer and trilayer systems. In particular, we predict how an electron spin current in a metallic layer can be converted into a pure magnon current in a ferromagnetic insulator layer at interface. We also discuss possible experimental realizations for non-equilibrium magnon currents.

¹This work is supported by NSF (ECCS-1127751).

8:36AM Y15.00004 A Unified Quantum Theory of Spin Transfer Torque and Electron Transport in Magnetic Nanostructures¹, YONG WANG, Department of Physics, The University of Hong Kong, Hong Kong — Dynamical control of nanoscale magnetization by spin-polarized current has attracted intensive studies due to its vast potential applications in spintronics. The magnetization dynamics driven by spin transfer torque is usually described by the semiclassical theory, where the quantum nature of the magnet is neglected. Here, we present a unified theory which describes the magnetization and the spin-polarized electrons at the full quantum level. The quantum state of the magnetization is given by the coherent state in angular momentum space, and is driven by the continuous scatterings with the electrons in the stochastic nature. Based on this picture, the Monte Carlo simulation is applied to get the mean trajectory and fluctuations of the magnetization, and also the electric current and the current shot noise. We also analyze the different sources which contribute to the magnetization noise and current noise, and show that the quantum noise due to the scattering can be comparable to the thermal noise at low temperature. An analytic theory is also formulated in terms of the density matrix technique. We obtain the master equation of the density matrix of the magnet driven by spin transfer torque, and find that it becomes a Fock-Planck equation in the coherent representation. Solutions from this approach is highly consistent with the results from the Monte Carlo method. We foresee that our theory will play an important role when the quantum nature of the nanomagnet emerges in the spintronics devices. For references, see [1] Yong Wang and L.J. Sham, Quantum Dynamics of a Nanomagnet driven by Spin-Polarized Current, arxiv : 1106.2359. [2] Yong Wang and L.J. Sham, A Quantum Theory of Spin Transfer Torque, to be submitted.

¹We acknowledge support of this work by the U. S. Army Research Office under contract number ARO-MURI W911NF-08-2-0032.

9:12AM Y15.00005 Spin-population inversion in magnetic point contacts under non-equilibrium conditions¹, TORSTEN PIETSCH, STEFAN EGLE, ELKE SCHEER, None — The creation of a novel type of spin-based electronics is one of the most intensively researched topics in current solid-state physics. The unifying characteristics in this advancing field is that the spin degree of freedom of the electron rather than its charge is exploited to achieve a specific device functionality. Recently, theoretical predictions suggest that spin-inversion in metallic point contacts under strong non-equilibrium conditions may enable the design of novel types of radiation sources. These radiation sources are highly tunable and of giant intensity compared to cutting-edge semiconductor devices, due to the much larger electron density in metals. Moreover, the accessible frequency range covers both, microwave (GHz) and THz radiation. Especially the later one is of great interest, since up to date there is no miniaturized, high intensity THz source available. Therefore, the experimental demonstration of this lasing effect in metallic systems is an important breakthrough in solid state physics. Presently the concept of spin-flip lasing in magnetic point contacts rests on theoretical predictions and first proof of principle studies. Herein we present detailed investigations on the magneto-transport properties of magnetic heterostructures and -point contacts. In particular, we study the complex interplay between magnetization, current density and the influence of high frequency (GHz and THz) fields on the magneto-transport properties of magnetic point contacts. The results illustrate that a successful spin-population inversion can be detected via transport spectroscopy.

¹We acknowledge the financial support of the ICT FET Open project (FP7-ICT-FET - 225955 STELE)

9:24AM Y15.00006 Two-channel resonant tunneling in the presence of spin-orbit coupling¹, T.V. SHAHBAZIAN, L.S. PETROSYAN, Jackson State University — We study resonant tunneling through a pair of localized states independently coupled to two-dimensional electron gas (2DEG) in the leads. The shape of tunneling conductance is determined by the coherent coupling of localized states via electron continuum in the leads. We show that spin-orbit coupling (Rashba and Dresselhaus) in 2DEG leads to a splitting of the narrow (subtunneling) peak by the amount proportional to spin-orbit coupling constant. The conductance lineshape is highly sensitive to the magnitude and orientation of in-plane magnetic field.

¹Supported by NSF

9:36AM Y15.00007 Non-equilibrium coherent potential approximation for electron transport, ALAN KALITSOV, University of Puerto Rico, MAIRBEK CHSHIEV, SPINTEC, JULIAN VELEV, University of Puerto Rico — Treatment of disorder in extended systems presents essential difficulties because the disorder breaks the periodicity of the system. The coherent potential approximation (CPA) solves this problem by replacing the disordered medium with a periodic effective medium [1]. However, calculating the electron current within CPA requires summing scattering diagrams to infinite order, the so called vertex corrections. In this work we reformulate CPA for non-equilibrium electron transport (NE-CPA). This approach, based on the non-equilibrium Green function formalism, provides an efficient and precise way to solve the transport problems in the presence of disorder. We demonstrate that the NE-CPA current is equivalent to the CPA current with vertex corrections to infinite order. [1] B. Velicky, Phys. Rev. 184, 614 (1969).

9:48AM Y15.00008 Semiclassical dynamics of Bloch electrons to second order in electromagnetic fields, YANG GAO, SHENGYUAN YANG, QIAN NIU, University of Texas at Austin — Berry curvature appears in the semi-classical theory of Bloch electrons already to first order in electromagnetic fields, resulting in profound modification of the carrier velocity and phase space density of states. Here we derive the equations of motion for the physical position and crystal momentum to second order in the fields. The dynamics still has a Hamiltonian structure, albeit with noncanonical Poisson brackets between the physical variables. We are able to expand both the carrier energy and the Poisson brackets to second order in the fields with terms of clear physical meaning. To demonstrate the utility of our theory, we obtain with much ease the electromagnetic response and orbital magnetic susceptibility.

10:00AM Y15.00009 Zero bias STS Kondo anomalies of Co impurities on Cu surfaces: do ab initio calculations work?, PIER PAOLO BARUSELLI, SISSA, Via Bonomea 265, Trieste 34136, Italy, ALEXANDER SMOGUNOV, SISSA, Via Bonomea 265, Trieste 34136, Italy, CEA Saclay, MICHELE FABRIZIO, SISSA, Via Bonomea 265, Trieste 34136, Italy, ICTP Trieste, RYAN REQUIST, SISSA, Via Bonomea 265, Trieste 34136, Italy, ERIO TOSATTI, SISSA, Via Bonomea 265, Trieste 34136, Italy, ICTP Trieste — Transition metal atoms such as Co on Cu (111), (100), and (110) surfaces produce STS I-V spectra showing different zero bias Kondo anomalies [1] but these differences have been neither quantitatively predicted nor fully explained theoretically. We apply to this problem the DFT+NRG scheme of Lucignano et al [2], where one solves by NRG an Anderson model built from ab initio phase shifts provided by DFT. For Co/Cu(100) and Co/Cu(110) our calculations describe correctly the experimental trend of Kondo temperatures, and fairly the lineshapes too. By contrast, they fail to describe Co/Cu(111) where in particular the anti-lorentzian lineshape found in experiment remains unexplained. This failure underscores the role of surface states, probably relevant for Co/Cu(111) [3] but not correctly described by our thin slab calculations. Future efforts to quantitatively include Kondo screening by surface states are therefore called for. 1. N. Knorr et al PRL 88, 096804 (2002); M. Ternes et al 2009 J. Phys.: Cond. Matt. 21, 053001 (2009); A. Gumbsch et al PRB81, 165420 (2010). 2. P. Lucignano et al Nature Mat. 8, 563 (2009); P.P. Baruselli et al, Physica E, doi:10.1016/j.physe.2011.05.005. 3. C. Lin et al. PRB 71, 035417 (2005).

10:12AM Y15.00010 ABSTRACT WITHDRAWN —

10:24AM Y15.00011 Linear magnetoresistance as a Berry phase effect, HUA CHEN, University of Tennessee at Knoxville, University of Texas at Austin, DI XIAO, Oak Ridge National Lab, ZHENYU ZHANG, University of Science and Technology of China, Harvard University, University of Texas at Austin, QIAN NIU, University of Texas at Austin — Conventional theory of charge carrier dynamics in metals and semiconductors predicts a quadratic field dependence in the magnetoresistance (MR) in the weak field limit. A linear dependence is usually explained as a quantum effect known as weak localization. However, in systems with time reversal symmetry breaking, a linear dependence can be observed even above room temperature, where quantum coherence is absent. Here we show that linear MR can arise from the Berry curvature modified semiclassical dynamics of the charge carriers, and evaluate its magnitude in several model systems and make preliminary comparisons with experimental results.

10:36AM Y15.00012 Theory of conducting electrons in textured antiferromagnets, RAN CHENG, QIAN NIU, The University of Texas at Austin — The dynamics of conducting electrons in antiferromagnetic texture is shown to exhibit an SU(2) geometric phase in the iso-spin that characterizes a locked spin-sublattice degree of freedom. The iso-spin rotation is purely geometrical and can be expressed in terms of the flux of a novel Berry curvature jointing the real and momentum space, a crucial quantity that has been overlooked in conventional transport theory. We provide an example of one dimensional domain wall, where the iso-spin rotation is topologically quantized. Scattering by skyrmion centers in two dimensions are also discussed, where a Mott like scattering of the iso-spins is predicted.

10:48AM Y15.00013 Exchange field induced large magnetoresistance in the correlated insulator phase of ultrathin Beryllium films¹, TIJIANG LIU, YIMING XIONG, SHANE STADLER, JOSEPH PRESTIGIACOMO, PHILIP ADAMS, Louisiana State University, LOUISIANA STATE UNIVERSITY COLLABORATION — We present a detailed study of low-temperature magnetotransport properties of ultrathin, amorphous Be films in the EuS/Be bilayers. Significant magnetoresistance (MR) of pure insulating Be films can only be observed in fairly high magnetic field ($> \sim 5$ tesla), but by depositing insulating ferromagnetic EuS on top of Be film, one can obtain the same value of MR at low magnetic field (~ 0.2 tesla). We argue that this shift of MR from high field to low field may be caused by the exchange field in the Be component of Be/EuS bilayers.

¹DOE under Grand No. DE-FG02-07ER46420

Friday, March 2, 2012 8:00AM - 11:00AM – Session Y16 DCMP: Strongly Correlated Electrons - Experiment and Theory 251

8:00AM Y16.00001 Electronic Excitations in CuO from a Many-Body Point of View, CLAUDIA RÖDL, FRANCESCO SOTTILE, LUCIA REINING, Laboratoire des Solides Irradiés, Ecole Polytechnique, 91128 Palaiseau cedex, France — The insulating transition-metal oxide CuO is considered a key to understanding the electronic structure of high-temperature superconducting cuprates, since it features similar bonding geometries. The photoemission spectra of this oxide, which is usually termed to be strongly correlated, have not been explained satisfactorily by first-principles calculations up to now. Special difficulties arise from the close entanglement of the structural and electronic degrees of freedom in this compound, which is due to the unoccupied Cu 3d orbitals. In contrast to the local-density approximation of density-functional theory (DFT), which predicts CuO to be a metal, we obtain finite band gaps by means of hybrid functionals containing screened exchange and the DFT+*U* method. Starting from these qualitatively correct band structures, we perform many-body calculations in the *GW* approximation. The various approaches to the one-particle excitation spectra are compared to experimental results. We discuss whether or not the peaks occurring in the photoemission data are quasiparticle excitations or satellite structures, respectively.

8:12AM Y16.00002 Pressure Effects on the Vanadium Oxides V₆O₁₁, V₇O₁₃, and V₈O₁₅¹, STELLA KIM, ESTELLE COLOMBIER, NI NI, SERGEY BUD'KO, PAUL CANFIELD, Iowa State University and Ames Laboratory — Members of the V_NO_{N-1} Magneli Series ($3 < N < 9$) exhibit metal to insulator transitions (MIT) as well as antiferromagnetic (AFM) transitions at ambient pressure, with the exception of V₇O₁₃ which remains metallic to lowest measured temperatures. In this talk we present pressure and temperature dependent measurements of electrical resistivity for V₆O₁₁, V₇O₁₃ and V₈O₁₅ samples. For V₆O₁₁ and V₈O₁₅ MIT can be suppressed by 4 and 1.3 GPa respectively. For V₇O₁₃ and V₈O₁₅ *T*_{SDW} can be suppressed by 3.5 GPa. Composite phase diagrams will be presented and low temperature data, focusing on the possibility of quantum criticality will be discussed.

¹Supported by U.S. DOE (DE-AC02-07CH11358)

8:24AM Y16.00003 Magnetic properties of Fe_{1-y}Co_ySi near insulator-metal transition¹, YAN WU, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, BRADFORD FULFER, JULIA CHAN, Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803, DAVID YOUNG, JOHN DITUSA, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803 — FeSi is a nonmagnetic narrow gap insulator with interesting temperature-dependent magnetic and optical properties. When doped with Mn, holes are introduced to the FeSi system along with S=1 magnetic moments. As a result, a non-Fermi liquid metallic state is observed due to the underscreening of the S=1 moments. Here we investigate the effects of Co doping of FeSi (Fe_{1-y}Co_ySi, $0 \leq y \leq 0.03$) to explore the insulator-to-metal transition and to compare with Mn-doped effects. We find a systematic increase of the Curie constant and Weiss temperature of the impurity-induced low temperature susceptibility with *y*. The Curie constant and saturated magnetization indicates that there is an underlying competition between screening of the magnetic moments at low *y* and ferromagnetic ordering at higher Co-concentrations. Transport measurements are underway to explore the associated charge carrier properties in this semiconducting system on the verge of ferromagnetism.

¹This work is supported by NSF DMR.

8:36AM Y16.00004 Signatures of Correlation Effects and Thermopower in FeSi, JAN TOMCZAK, KRISTJAN HAULE, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — Correlated semiconductors have been studied intensively over the years, because they exhibit an unusual metalization process which is poorly understood. At low temperatures FeSi behaves as an ordinary semiconductor, while at high temperatures the system is a bad metal with a Curie like susceptibility. Analogies with heavy fermion Kondo insulators and mixed valence compounds, and anomalous electron phonon coupling have been invoked to account for this behavior, but lacking quantitative methodologies applied to this problem, a consensus remained elusive to date. Here, we use realistic many-body methods to elucidate the metalization of FeSi. Our methodology accounts for all substantial anomalies observed in FeSi: lack of conservation of spectral weight in optics, Curie susceptibility and an anomalous thermoelectric power. Having quantitatively validated our approach, we propose a new scenario. In correlated insulators such as FeSi the metalization is induced by the emergence of non-quasiparticle incoherent states in the gap. This coherence-incoherence crossover is accompanied by a massive reorganization of the spin excitations. Besides the fundamental interest of our theory, our work is relevant to the design of thermoelectric materials based on correlated insulators.

8:48AM Y16.00005 FeGa3 – a strongly correlated insulator?, MONIKA GAMZA, Brookhaven National Laboratory, MEIGAN ARONSON, Stony Brook University and Brookhaven National Laboratory — FeGa3 is one of few Fe-based nonmagnetic semiconductors, in which a small gap is produced by the hybridization of Fe 3d states with p states of a group 13 or 14 element. The role of strong electron-electron correlation effects in formation of the gap is unclear. In case of FeSi and FeSb2, a metal-insulator transition was observed at temperatures low relative to the gap energy, which is a hallmark of a Kondo nature of the gap. For FeGa3, a combination of photoemission data and DFT-based electronic structure calculations indicated a rather strong on-site effective Coulomb repulsion within the Fe 3d shell *U*_{eff}~3 eV and a sizable *U*_{eff}/*W* ~ 0.6 (*W* – band width) [1]. Interestingly, recent ARPES measurements revealed a Fe 3d derived state located around 0.4 eV away from the top of the valence band [1]. Thermodynamic and transport measurements do not give any sign of a metal-insulation transition up to 1000 K [2]. To get insight into the importance of e-e correlation effects in formation of the gap in FeGa3, we drive the system towards a metallic state by doping. The results of resistivity, specific heat and magnetization measurements on doped single crystals of FeGa3 grow by Ga-flux technique will be discussed.

[1] Arita M et al., Phys. Rev. B 83, 245116 (2011)

[2] Hadano Y et al., J. Phys. Soc. Jpn. 78, 013702 (2009)

9:00AM Y16.00006 Hybridization wave as the cause of the metal-insulator transition in rare earth nickelates¹, HYOWON PARK, Department of Physics, Columbia University, CHRIS A. MARIANETTI, Department of Applied Physics, Columbia University, ANDREW J. MILLIS, Department of Physics, Columbia University — The metal-insulator transition driven by varying rare earth (*Re*) ion in *ReNiO₃* has been a longstanding challenge to materials theory. Experimental evidence suggesting charge order is seemingly incompatible with the strong Mott-Hubbard correlations characteristic of transition metals. We present density functional, Hartree-Fock and Dynamical Mean field calculations showing that the origin of the insulating phase is a hybridization wave, in which a two sublattice ordering of the oxygen breathing mode produces two *Ni* sites with almost identical *Ni* *d*-charge densities but very different magnetic moments and other properties. The high temperature crystal structure associated with smaller *Re* ions such as *Lu* is shown to be more susceptible to the distortion than the high temperature structure associated with larger *Re* ions such as *La*.

¹This work was supported by the U. S. Army Research Office via grant No. W911NF0910345 56032PH.

9:12AM Y16.00007 Non-thermal dynamics of the spin and charge order in striped nickelates, WEI-SHENG LEE¹, SLAC National Accelerator Lab. — In the striped nickelate $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$, spin order coexists with charge order, whose periodicity is half of spin order. So far, most of the studies on the stripe phase were performed in the thermal equilibrium state by varying temperatures; the dynamics of stripe phase in the time domain when the system is driven-out-of-equilibrium has not yet been studied. Using the x-ray free electron laser (XFEL) at LCLS, we performed time-resolved optical-pump and resonant soft x-ray diffraction probe experiments to study the dynamics of the spin and charge order. Comparisons of charge and spin order dynamics will be discussed.

¹This work is a collective contributions of 33 researchers from several institute. Full list of the author will be acknowledged in the presentation.

9:24AM Y16.00008 The temperature evolution of NiO_6 octahedral tilts as a probe to study charge stripes in $\text{Ln}_{1.67}\text{Sr}_{0.33}\text{NiO}_4$ ($\text{Ln}=\text{La}/\text{Nd}$)¹, MILINDA ABEYKOON, EMIL BOZIN, GENDA GU, JOHN HILL, JOHN TRANQUADA, Brookhaven National Laboratory, SIMON BILLINGE, Brookhaven National Laboratory, Columbia University — $\text{Nd}_{1.67}\text{Sr}_{0.33}\text{NiO}_4$ and $\text{La}_{1.67}\text{Sr}_{0.33}\text{NiO}_4$ exhibit long range ordered (LRO) charge stripes below $T_{\text{co}} \sim 240\text{K}$. When the charge stripes are static and long-range ordered, they have been seen as superlattice Bragg peaks in single crystal neutron and x-ray diffraction. We used neutron atomic pair distribution function (NPDF) technique to investigate the possibility of existence of localized charges above T_{co} , where, the LRO of the stripes disappears. Rigid body type NiO_6 octahedral tilts were used as a probe to study the local and average structural response to charge order. The amplitude of rotation of the octahedral units was used to investigate the observed large apical oxygen thermal ellipsoids (anisotropic thermal displacement parameters) in the a-b crystal plane. We measured enhanced tilt amplitudes in the local structure, compared to the average. We will discuss the temperature dependence of the tilt amplitudes and of the correlation length of the local tilt order and explore the potential relationship to local stripe order.

¹This work was supported by DE-AC02-98CH10886.

9:36AM Y16.00009 Time-Dependent Recovery of Charge and Spin Order in Striped Nickelate¹, Y.F. KUNG, C.-C. CHEN, A.F. KEMPER, Stanford University, W.-S. LEE, B. MORITZ, Stanford University and SLAC National Accelerator Laboratory, A.P. SORINI, Lawrence Livermore National Laboratory, Z.-X. SHEN, T.P. DEVEREAUX, Stanford University and SLAC National Accelerator Laboratory — Using time-dependent Ginzburg-Landau theory, we study the melting and recovery of charge and spin order in the striped nickelate $\text{La}_{1.75}\text{Sr}_{0.25}\text{NiO}_4$ in response to an ultrashort pump pulse that destroys the order. Treating the behavior of both the amplitudes and phases of the order parameters, we examine their effects on the recovery time scales of the charge and spin order. We compare the temporal dynamics of our model to experimental observations at the Linac Coherent Light Source (LCLS).

¹National Defense Science and Engineering Graduate Fellowship

9:48AM Y16.00010 ARPES studies on metal-insulator-transition in $\text{NiS}_{2-x}\text{Se}_x$, GARAM HAN, Y.K. KIM, W.S. KYUNG, CHUL KIM, Y.Y. KOH, Institute of Physics and Applied Physics, Yonsei University, Korea, K.D. LEE, Department of Physics, Inha University, Korea, C. KIM, Institute of Physics and Applied Physics, Yonsei University, Korea — Understanding Metal insulator transition (MIT) is one of the most challenging issues in condensed matter physics. $\text{NiS}_{2-x}\text{Se}_x$ (NSS) is a well known system for band width controlled MIT studies while most of High- T_c superconductors (HTSCs) are described within band filling MIT picture. Cubic pyrite NiS_2 is known as a charge-transfer (CT) insulator and easily forms a solid solution with NiSe_2 , which is a good metal even though it is isostructural and isoelectronic to NiS_2 . MIT is induced by Se alloying and is observed at a low temperature for $x=0.5$. The important merit is that there is no structure transition which often accompanies MIT. In spite of the importance of the system, even the experimental band dispersion is not known so far along with many controversies. For this reason, we performed angle resolved photoemission spectroscopy on high quality single crystals and successfully obtained Fermi surface maps of $x=0.5$, $x=0.7$ and $x=0.8$ systems (the metallic side). By doping dependent systematic studies on NSS and comparison with LDA calculation, we try to explain the relationship between band width and the MIT.

10:00AM Y16.00011 Quantum criticality at a Mott-Hubbard Metal-Insulator Transition, ARNAB BANERJEE, DANIEL SILEVITCH, ALEXANDER PALMER, The University of Chicago, YEJUN FENG, The Argonne National Laboratory, THOMAS ROSENBAUM, The University of Chicago — The Mott insulator nickel disulfide undergoes an insulator to metal transition that can be driven by either hydrostatic pressure or doping-induced chemical pressure. Previously, NiS_2 doped with selenium to just below the quantum critical point showed anomalous critical exponents as a function of pressure. Doping, however, introduces positional disorder and charge transfer effects from the selenium orbitals, potentially altering the critical behavior. We report here on a set of transport experiments on pure NiS_2 , where the pressure and temperature scales for the critical regime require the use of a diamond anvil cell integrated with a helium dilution refrigerator, allowing us to compare the critical behavior of the pure and doped materials.

10:12AM Y16.00012 Redefining the metal/charge-transfer insulator paradigm in transition metal oxides¹, HUNG DANG, XINYUAN AI, Department of Physics, Columbia University, CHRIS MARIANETTI, Department of Applied Physics, Columbia University, ANDREW MILLIS, Department of Physics, Columbia University — The universality of the phase diagram in the variables of interaction strength and d-occupancy, shown for late transition metal oxides in Ref.[1], is examined for two series of early transition metal oxides: (SrVO_3 , SrCrO_3 , SrMnO_3) and (LaTiO_3 , LaVO_3 , LaCrO_3) using density functional theory (DFT), DFT+U and DFT+dynamical mean field theory methods. The interaction required to drive the metal-insulator transition is found to depend sensitively on the d-occupancy N_d , and beyond a threshold value of the d-occupancy an insulating state cannot be achieved for any practical value of the interaction. The critical N_d values are determined and compared to ab initio and experimental estimates where available. Additionally, the minimal model for the transition is determined and the crucial role played by the Hund's coupling is demonstrated.

[1] Xin Wang, M. J. Han, Luca de' Medici, C. A. Marianetti, and Andrew J. Millis (2011). arXiv:1110.2782

¹Supported by the Basic Energy Sciences Program of the US Department of Energy under grant DOE ER 046169.

10:24AM Y16.00013 Implementation of a dynamical cluster approximation within an augmented plane-wave framework, HUNPYO LEE, Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, 60438 Frankfurt, Germany, KATERYNA FOYEVTSOVA, JOHANNES FERBER, Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, 60438 Frankfurt, Germany, MARKUS AICHHORN, Institute of Theoretical and Computational Physics, TU Graz, Graz, Austria, HARALD O. JESCHKE, ROSE VALENTI, Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, 60438 Frankfurt, Germany — Even though the local density approximation in combination with dynamical mean field theory (LDA+DMFT) accounts for various and interesting physics such as Mott insulator and enhancement of effective mass for real compounds, the pseudo-gap and spin density wave behaviors are missed due to the absence of spatial correlations. In order to consider the short-range spatial correlations beyond the LDA+DMFT approach for real compounds, we introduce a combination of LDA with a dynamical cluster approximation (LDA+DCA) in the framework of the full-potential linear augmented plane-wave basis and show results for SrVO₃. We discuss how to implement the LDA+DCA approach in the WIEN2k density functional theory code and analyze the momentum spectral properties on SrVO₃ as a result. We compare our LDA+DCA results with LDA+DMFT as well as with angle-resolved photoemission spectra (ARPES). We find that LDA+DCA results compare better with ARPES than the LDA+DMFT results due to inclusion of spatial correlations.

10:36AM Y16.00014 Pressure induced insulator to metal transition and orbital dynamics in Sr₂VO₄, SUKANTA KARMAKAR¹, Bhabha Atomic Research Centre, Mumbai — The unusual ground states of transition metal oxides with layered perovskite structure (K₂NiF₄ type) are driven by a complex interplay between charge, orbital, spin and lattice degrees of freedom. The S=1/2 and 3d¹ system Sr₂VO₄, a Mott insulator, is of particular interest because of its vicinity to the insulator-metal boundary. The strong two-dimensionality along with a weak Jahn-Teller distortion (slightly elongated VO₆ octahedra along c-axis) causes splitting of t_{2g} orbitals (xy orbital and doubly degenerate yz and zx orbitals), pressure-tuning of which is expected to reveal interesting physical properties. Our recent high pressure Raman spectroscopic investigations at low temperature describe the orbital dynamical changes in this system. The anomalous pressure dependence of the strong magnetic excitations in Raman spectra confirms the unconventional spin-orbital composite nature (magnetic octupolar type order) of the dxy/zy levels [PRL **103**, 067205, (2009)]. The system transforms from high temperature orbital liquid like state to the low temperature orbital ordered state via a short range orbital order precursor at 150K. With increasing pressure the orbital ordering transition temperature decreases, predicting a QCP at ~8 GPa. At this pressure the system undergoes an insulator to metal transition (as observed from mid IR reflectance measurements as well as sharp rise in Raman intensity of phonon modes due to occurrence of intraband transitions).

¹Also at Max Planck Institute for Solid State Research, Stuttgart, Germany

10:48AM Y16.00015 ab-initio calculations of electronic structure and magnetism of O₂MF₆ (M=Sb, Pt) : Coulomb correlation and spin-orbit interaction effects in 2p and 5d electrons, MINJAE KIM, B. I. MIN, Department of Physics, Pohang University of Science and Technology — We have investigated electronic structures and magnetic properties of O₂MF₆ (M=Sb, Pt), which are composed of two building blocks of strongly correlated electrons: O₂⁺ dioxygenyls and MF₆⁻ octahedra, by employing the first-principles electronic structure band method. For O₂SbF₆, as a reference system of O₂PtF₆, we have shown that the Coulomb correlation of O(2p) electrons drives the Mott insulating state. For O₂PtF₆, we have demonstrated that the Mott insulating state is induced by the combined effects of the Coulomb correlation of O(2p) and Pt(5d) electrons and the spin-orbit (SO) interaction of Pt(5d) states. The role of the SO interaction in forming the Mott insulating state of O₂PtF₆ is similar to the case of Sr₂IrO₄ that is a prototype of a SO induced Mott system with J_{eff} = 1/2.

Friday, March 2, 2012 8:00AM - 10:48AM —

Session Y17 DCMP: Nanostructures and Interfaces: Electrons, Phonons, and Plasmons 252A

8:00AM Y17.00001 Transport and Kondo correlations in magnetic break junction devices, GAVIN D. SCOTT, Bell Laboratories, Alcatel-Lucent, 600 Mountain Ave, Murray Hill, NJ 07974, DOUGLAS NATELSON, Department of Physics and Astronomy, 6100 Main St, Rice University, Houston, TX 77005; Department of Computer and Electrical Engineering, Rice University — A single molecule transistor device fabricated with a break junction technique is utilized as a tunable model system for probing transport properties of the highly correlated Kondo state. The emergence of this collective phenomenon occurs due to an antiferromagnetic interaction between conduction electrons and a local magnet moment represented by an unpaired spin on the molecule. Low energy non-equilibrium conductance measured in the Kondo regime has been shown to obey a particular scaling relationship with respect to different perturbations. Devices are now fabricated with ferromagnetic and strongly paramagnetic electrodes, and the applicability of such scaling behavior is investigated in the presence of magnetic interactions and anomalous transport characteristics.

8:12AM Y17.00002 Phonon transmission across Si/Ge interface from first-principles by the Green's function method¹, ZHITING TIAN, KEIVAN ESFAJANI, GANG CHEN, MIT — Modeling phonon transmission as a function of phonon frequency and incidence angle is vital for multiscale modeling of heat transport in nanostructured materials. In this study, we calculate the phonon transmission in three-dimensions via Green's function method. It will be applied to silicon/germanium interface for which the force constants will be calculated from either the Stillinger-Weber semi-empirical potential, or from first-principles density functional methods. Both the perfect interface and the rough interface will be investigated. The transmission as a function of interface roughness will give us more guidance for surface engineering. Results between first-principles and the SW potential will be compared to see how reliable the predictions from SW potential are. The contribution of optical modes is illustrated by comparing the results with the prediction of the acoustic mismatch model (AMM) which is also harmonic and the long-wavelength limit of the general theory. It will now be possible to integrate the information on momentum and frequency-dependent transmission and the bulk mean free paths, both calculated from first-principles DFT, to accurately model heat transport in complex nanostructured materials.

¹This material is based upon work supported as part of the S3TEC, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-FG02-09ER46577

8:24AM Y17.00003 Ultrafast Characterization of Nanostructures in GaAs, STEPHANIE GILBERT, Vanderbilt University, JASON KAWASAKI, University of California Santa Barbara, ANDREW STEIGERWALD, JUSTIN GREGORY, Vanderbilt University, CHRIS PALMSTRØM, University of California Santa Barbara, NORMAN TOLK, Vanderbilt University — We combine ultrafast pump-probe and optoacoustic spectroscopy with magneto-optical Kerr rotation measurements to characterize embedded, self-assembled magnetically active nanostructures in a GaAs host matrix. We observe variations in the pump-probe and optoacoustic signals depending on the composition and growth characteristics of the embedded layers. Further, we observe (a) distinct behaviors in the femtosecond response of the composite structures when the probe photon energy is tuned near the GaAs band edge and (b) strong modulation of the optoacoustic signal inside the embedded layer. These results indicate an effective change in the transient femtosecond response of the composite structure, likely originating in strain effects due to the presence of nanoparticles within the host lattice. We additionally probe ultrafast magneto-optical interactions through time-resolved Kerr measurements. Finally, we present a potential method for high-resolution depth-dependent magnetic characterization by combining the Kerr rotation and optoacoustic experimental techniques.

8:36AM Y17.00004 Position-dependent Diffusion Coefficient as Localization Criterion in Non-Conservative Random Media, BEN PAYNE, ALEXEY YAMILOV, Missouri University of Science and Technology — Characterization of different regimes of electromagnetic wave transport in random media is an important area of research with ramifications in condensed matter physics. For passive systems, transport can be either ballistic, diffusive, or localized. Wave corrections to otherwise classical transport in a finite random media result in position-dependent diffusion coefficient $D(z)$. If media is active or dissipative (contains optical gain or absorption), then $D(z)$ can be used to distinguish a multitude of distinct wave transport regimes. Using a numerical model, we validate the existence of the position-dependent diffusion, including for media with absorption. We have previously developed a phase space enumerating all regimes exhibiting distinct transport behavior. Here we present recent results from our numerical simulations which demonstrate the ability to use $D(z)$ to distinguish between these regimes.

8:48AM Y17.00005 Probing phonon surface scattering in nanostructures, RICHARD ROBINSON, JARED HERTZBERG, OBAFEMI OTELAJA, Cornell University, Department of Materials Science and Engineering — In insulating materials, heat is transmitted by atomic vibrations ("phonons"). In nanostructured materials such as nanowires and nanosheets, the characteristic length scale of a material can be less than the mean free path of a phonon. The phonon transport is then drastically altered and becomes dominated by scattering from surfaces. We demonstrate a method to assess the scattering rate and transmission factor of phonons traversing a silicon nanosheet. Generation and detection of phonons is accomplished by a superconducting tunnel junction attached to the silicon nanostructure and operated at a temperature of 0.3K. Decay of excited states in the superconductor is employed as a tunable narrow-band source of phonons [1,2]. This tunable source enables investigation of the phonon mean free path as a function of phonon frequency and surface roughness, for frequencies from ~ 100 GHz to ~ 500 GHz in nanosheets 100 to 200 nm thick. This work is supported by DOE (DE-SC0001086).

[1] H. Kinder. Phys. Rev. Lett. 28, 1564 (1972)

[2] J. B. Hertzberg et al, Rev. Sci. Instr. 82, 104905 (2011).

9:00AM Y17.00006 Self-assembled, vertically aligned, epitaxial nanoscale $p-n$ heterojunctions for thin film based photovoltaic applications, DANIELA F. BOGORIN, TOLGA AYTUG, PARANS M. PARANTHAMAN, ANDREW A LUPINI, ADAM RONDINONE, KYLE WINTERS, Oak Ridge National Laboratory, Oak Ridge, TN 37831, OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831 TEAM — Using *rf*-sputtering technique we have exploited phase-separated self-assembly and developed epitaxial, nanostructured composite films composed of phase separated, and vertically oriented $p-n$ interfacial nanocolumns of Cu_2O (p type; 2eV bandgap) and TiO_2 (n type; 3.2 eV bandgap). The characteristic band gaps of these phases allow extension of the solar capture from ultraviolet to a visible wavelength. The composite films were grown on perovskite substrates and exhibit single crystalline epitaxy in both phases. We have investigated crystalline structure, interfacial quality and optical properties of the nanopillar arrays using XRD, TEM, SEM, AFM, and optical absorption techniques. Here, we show nearly complete atomic order at Cu_2O - TiO_2 interface (i.e., $p-n$ junction) and an absorption profile that captures a wide range of solar spectrum extending from ultraviolet to visible wavelengths. Compared to layered thin film architectures, the use of such vertically aligned nanostructures in solar cells can promote cost-effective fabrication of high efficiency PV devices by providing low defect concentrations, improved absorption and light trapping capabilities, and increased minority carrier diffusion lengths.

9:12AM Y17.00007 Ab initio calculation of the electron-phonon coupling for transport¹, NATHALIE VAST, JELENA SJAKSTE, PAOLA GAVA, IURII TIMROV, Laboratoire des Solides Irradiés - Ecole Polytechnique - CEA DSM - CNRS UMR7642 - France, VALERY TYUTEREV, Tomsk State Pedagogical University - Russia — We have developed an approach which enables us to compute matrix elements of the electron-phonon coupling within the density functional perturbation theory for the electronic interaction with short-wavelength phonons.² Combining this *ab initio* approach to the Boltzmann transport equation, we have obtained the thermoelectric coefficients of silicon.³ The lifetime of the $2p_0$ shallow impurity state in doped-silicon turns out to be shorter than expected.⁴ The lifetime of the exciton in germanium under pressure⁵ is found to be well described. Effect of the material nanostructuring on the electron-phonon coupling constants will be shown for small semiconducting superlattices. Finally, the calculation of deformation potentials for intravalley scattering will be discussed, and results shown for silicon and for bismuth, which is the prototype material for thermoelectricity.

¹This work was supported by ANR Project PNANO ACCATTONE and by DGA, and computer time was granted by GENCI (project 2210)

²J. Sjakste, N. Vast, V. Tyuterev, Phys. Rev. Lett. 99, 236405 (2007).

³Z. Wang, S. Wang, S. Obukhov, N. Vast, J. Sjakste, V. Tyuterev, and N. Mingo, Phys. Rev. B 83, 205208 (2011).

⁴V. Tyuterev, J. Sjakste, N. Vast, Phys. Rev. B 81, 245212 (2010)

⁵V.G. Tyuterev and S.V. Obukhov N. Vast and J. Sjakste, Phys. Rev. B 84, 035201

9:24AM Y17.00008 ABSTRACT WITHDRAWN —

9:36AM Y17.00009 Effect of Interlayer Interaction on the Structural, Electronic, and Thermal Properties of Layered MS_2 ($M=\text{W}, \text{Mo}$) Structures, SEOUNG-HUN KANG, SORA PARK, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University — Using density functional theory (DFT) supplemented with van der Waals interaction, we investigate the effect of interlayer interaction on the structural, electronic, and thermal properties of transition-metal disulfides MS_2 , such as MoS_2 and WS_2 . We calculate the relative stability of various layer-layer stacking configurations determined by considering relative positions and orientations between neighboring layers. We find that MS_2 layers may slide over each other with a small sliding barrier. We explore the effect of layer stacking on the electronic structure, and find an intriguing coupling effect. We also calculate their thermal properties including thermal expansion behavior especially along the direction normal to the plane. Such thermal expansion behavior is considered for our study of Li-intercalation into layered MS_2 , which may become a fundamental understanding for future development of Li-ion battery. We evaluate thoroughly the diffusion paths and barriers in between layers and compare them with those on the surface. Interestingly we find that the diffusion barrier between layers is ~ 100 meV smaller than that on a single layer, implying layered MS_2 may be a good candidate for Li-ion battery electrodes.

9:48AM Y17.00010 Surface plasmon modes management by Thompson plasmonics¹, NAI JING DENG, CHEUNG WAI CHAU, SAI KIT YUNG, KIN WAH YU, The Chinese University of Hong Kong — We have studied the dispersion and propagation of the surface plasmons in a structure consisting of a metal slab and a dielectric slab, the latter of which contains randomly distributed small metal particles. In our model, the metal material is characterized by the Drude model and the pudding structure is studied with Maxwell-Garnett effective medium theory. This construction of material can bring a new hybridized band in the dispersion relation where light has a relatively small group velocity. The geometric profile of volume fraction of metal balls in pudding structure can effectively change the behaviour of the plasmon propagation. For example, by adding a parabolic confinement, it is shown by the Hamiltonian optics that the light propagation is trapped, i.e., the light experiences an oscillation in a small space. Experimentally, the confinement condition can be achieved with various means, thus it may be useful in development of new mechanism of solar cell.

¹Supported by the General Research Fund of the HKSAR Government

10:00AM Y17.00011 Tunable Propagation and Localization of Hybrid Surface Plasmon Polaritons in Chirped Metal-Dielectric Waveguides¹, CHEUNG WAI CHAU, SAI KIT YUNG, KIN WAH YU, The Chinese University of Hong Kong — We have studied the propagation of coupled surface plasmon polariton (SPP) waves in a metal-dielectric-metal (e.g. Au/MgF₂/Au) waveguide by the transfer matrix method. Due to the evanescent coupling of the SPP waves at the two interfaces in the dielectric layer, three hybridized surface plasmon polariton (HSPP) branches are achieved with a nearly flat branch at intermediate frequencies. The flat HSPP branch is tunable by varying the thickness and/or the permittivity of the dielectric layer. Moreover, by imposing a gradual variation of the permittivity (or thickness) of the dielectric layer along the propagation direction, it is possible to alter the local dispersion relation so that a localization of SPP waves can be realized. Under a parabolic confinement, Hamiltonian optics is used for simulating the propagation and localization of HSPP waves. We demonstrate that HSPP are localized at different locations at different frequencies, which is useful for achieving trapped SPP rainbow. The results of this research can have fruitful applications in optical computing, etc.

¹Supported by the General Research Fund of the HKSAR Government.

10:12AM Y17.00012 Energy concentration in plasmonic nanostructures: Green function formalism¹, SAI KIT YUNG, CHEUNG WAI CHAU, KIN WAH YU, The Chinese University of Hong Kong — We have developed the Green function formalism (GFF), which can be used to study the field distribution and electrostatic resonance of different nanostructures. In the GFF, a surface integral equation is formulated for the scalar potential for an arbitrary number of nanostructures of various shapes. This formalism has the advantage of avoiding matching the complicated boundary conditions on the surfaces of the nanostructure. In particular, we have studied the cases of two approaching metal cylinders and non-touching metal crescent under a uniform applied electric field. It is shown that there is an energy concentration within the air narrow gap and the metal narrow gap in the cases of approaching cylinders and non-touching crescent respectively. The numerical GFF results are compared with the analytic results by conformal transformation. The results are useful in designing plasmonic light-harvesting devices.

¹Supported by the General Research Fund of the HKSAR Government.

10:24AM Y17.00013 Circular Dichroism and Spin Polarization of Rashba Split Surface States on a Bi/Ag Surface Alloy, GUANG BIAN, LONGXIANG ZHANG, YANG LIU, T. MILLER, T.-C. CHIANG, University of Illinois at Urbana-Champaign — The Bi/Ag surface alloy possesses a huge Rashba splitting in its surface bands due to the prominent corrugation in the surface reconstruction and the large atomic spin-orbit coupling of the Bi atom. This system is an intriguing candidate to realize the 2D $p_x + ip_y$ superconductor and further, Majorana states. In this work, we study the electronic structure of the Bi/Ag surface alloy prepared by depositing Bi onto ultrathin Ag films followed by annealing. The electronic structure of the system is measured using circular angle resolved photoemission spectroscopy (CARPES). The results reveal two interesting phenomena: the hybridization of spin polarized surface states with Ag bulk quantum well states and the umklapp scattering by the perturbed surface potential. In addition, our CARPES spectra show clearly a unique dichroism pattern which is closely related to the spin texture of this 2D strongly spin-orbit coupled electron system.

10:36AM Y17.00014 Atomic structure, energetics, and dynamics of topological solitons in indium chains on Si(111) surfaces, HUI ZHANG, Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, USTC, JIN-HO CHOI, JUN-HYUNG CHO, Department of Physics, Hanyang University, CHANGGAN ZENG, ZHENYU ZHANG, JIANGUO HOU, ICQD, Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, USTC — Besides the presence of exotic ground states, potentially more intriguing are the elementary excitations of the One-dimensional charge density waves (1D-CDWs), including the nonlinear topological excitation or soliton. Solitons may possess spin-charge inversion properties, and act as the effective carriers that account for the high conductivity in conducting polymers. However, comprehensive quantitative study of topological solitary excitations at the atomic level remains a challenge. In this talk, I will present our recent work on the quantitative characterization of solitons in In chains grown on Si(111) surfaces at atomic scale. The precise atomic structure of the topological soliton in In/Si(111) is determined based on scanning tunneling microscopy and first-principles calculations. Variable temperature measurements of the soliton population allow us to determine the soliton formation energy to be ~ 60 meV, smaller than one-half of the band gap of ~ 200 meV. Once created, these solitons have very low mobility; the sluggish nature is attributed to the exceptionally low attempt frequency for soliton migration. We further demonstrate local electric field enhanced soliton dynamics, and the feasibility of aggregating solitons into soliton polymers.

Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y18 DMP: Focus Session: Interfaces in Complex Oxides - Functional Interfaces 252B

8:00AM Y18.00001 Tunable ferroelectricity and magnetoelectricity at the interfaces of superlattices of antiferromagnets, CHRISTOS PANAGOPOULOS, Nanyang Technological University — In heterostructures composed of transition metal oxides, the disruption introduced even by an ideal interface can drastically upset the delicate balance of the competing interactions among electronic spins, charges and orbitals, leading to a range of exotic phenomena. These include interfacial conduction, magnetism, superconductivity but also improved ferroelectric properties. Possible incorporation of magnetoelectrics in these structures would further enable electrical control of magnetization as well as magnetic sensing of the polarization state. Naturally occurring magnetoelectrics are however, rare and generally with weak coupling. In this work we report a strategy and evidence for the emergence and control of ferroelectricity and strong magnetoelectric coupling in superlattices *consisting of solely non-ferroelectric antiferromagnetic layers*. By selecting appropriate yet abundant starting materials one may now design a plethora of low dimensional heterostructures with the desired relative arrangement of the oxide layers, of potential utility to miniature valves with electric and magnetic field tunable functions, promising to set new standards in future electronics.

8:36AM Y18.00002 Interfacial Properties of Ultra-thin YBCO/LCMO Superlattices¹, BENJAMIN GRAY, JIAN LIU, E.J. MOON, M. KAREEV, D.J. MEYERS, Physics Department, University of Arkansas, I.C. TUNG, M.J. BEDZYK, Department of Materials Science and Engineering, Northwestern University, M. VEENENDAAL, J.W. FREELAND, Advanced Photon Source, Argonne National Laboratories, J. CHAKHALIAN, Physics Department, University of Arkansas — The rational design of complex oxide heterostructures enables the investigation of novel materials with antagonistic order parameters. Our previous work using resonant x-ray spectroscopies has provided insight into the role of orbital reconstruction and covalent bonding at the interface of such heterostructures. In this talk, we will further address the intriguing interfacial electronic and magnetic properties and possible coupling between layers in superlattices composed of alternating superconductive YBa₂Cu₃O₇ and ferromagnetic La_{2/3}Ca_{1/3}MnO₃ layers upon approaching the ultra-thin limit, where a superconductor to insulator transition with increasing thickness N is observed in [YBCO (1 u.c.)/LCMO (N u.c.)] superlattices.

¹J.C. was supported by DOD-ARO under the Contract No. W911NF-11-1-0200 and NSF Contract No. DMR-0747808.

8:48AM Y18.00003 Scanning tunneling microscope investigation of the interfacial electronic properties of YBCO/LCMO , J.C. WANG, B.C. HUANG, Y.P. CHIU, Department of Physics, National Sun Yat-Sen University, Kaohsiung, 80424, Taiwan, Y.C. HUANG, Y.C. CHEN, Department of Physics, National Cheng Kung University, Tainan, 701, Taiwan, V.T. TRA, J.Y. LIN, Institute of Physics, National Chiao Tung University, Hsinchu, 300, Taiwan, J.C. YANG, Y.H. CHU, Department of Materials Science and Engineering, National Chiao Tung University, Hsinchu, 1001, Taiwan — Direct measurements of the interfacial electronic structures in YBCO/LCMO hetero-structures have been performed using cross-sectional scanning tunneling microscopy (STM) and spectroscopy (STS). Both scanning tunneling spectroscopy and analysis of the local electronic states across the interface of YBCO/LCMO reveal the evolution of the energy-band structures. Closely examining the recognition of the electronic structure by the unique combination of STM and STS reveals the direct information on the local interaction between superconductivity and magnetism in this work.

9:00AM Y18.00004 Quasiparticle dynamics in YBCO and YBCO/LSMO Using Femtosecond Optical Pulses , J. LEE, D. TALBAYEV, J. XIONG, CINT, Los Alamos National Laboratory, J. ZHU, Theoretical Division, Los Alamos National Laboratory, Q. JIA, A.J. TAYLOR, R.P. PRASANKUMAR, CINT, Los Alamos National Laboratory, CENTER FOR INTEGRATED NANOTECHNOLOGIES, LOS ALAMOS NATIONAL LABORATORY TEAM, THEORETICAL DIVISION, LOS ALAMOS NATIONAL LABORATORY TEAM — The properties of various complex oxide systems, such as multiferroics, high- T_c superconductors and colossal magnetoresistance manganites, have been extensively studied for the past ~25 years. In particular, the interplay between superconductivity (SC) and ferromagnetism (FM) is interesting from both academic and applied viewpoints. We have temporally resolved quasiparticle dynamics in multilayered films composed of the high-temperature superconductor YBCO and the ferromagnetic manganite LaSrMnO_3 (LSMO) by performing temperature-dependent UOS experiments. In YBCO alone, we observed two distinct decay relaxation channels that have previously been related to the pseudogap and superconducting gaps and can be explained with the phenomenological Rothwarf-Taylor (RT) model. However, the fast sub-picosecond relaxation related to the pseudogap was not observed in our YBCO/LSMO heterostructures, possibly due to the influence of FM order. These first UOS experiments on SC/FM heterostructures demonstrate the ability of UOS to quantify the influence of ferromagnetism on superconductivity through time domain measurements.

9:12AM Y18.00005 Ba and Sr templates on Ge(001) for epitaxial oxide growth , MIRI CHOI, AGHAM POSADAS, CHIH-KANG SHIH, ALEXANDER A. DEMKOV, The University of Texas at Austin — In the epitaxial growth of oxides on semiconductors, Ba and Sr templates are used as transition layers for perovskite deposition. Furthermore, the interface between complex oxides and semiconductors are relatively unexplored. The ability to control the interface between them can lead to new phenomena and new combinations of oxide-semiconductor heterostructures. In this work, we compare the differences between the Sr template with Ba templates on Ge(001) at various temperatures. The sub-monolayer coverage of Ba and Sr shows different morphology and nucleation behavior depending on the deposition temperature. For example, at higher deposition temperature, the electron diffraction pattern of Sr on Ge shows a 9×1 phase which was not observed at lower deposition temperature. We perform an atomic-scale study of Ba and Sr templates grown on Ge(001) by molecular beam epitaxy as a function of deposition temperature and coverage, using a combination of reflection high energy electron diffraction and *in situ* scanning tunneling microscopy (STM). An understanding of the behavior of Ba and Sr template formation on germanium can potentially be used as a means of better controlling the subsequent oxide growth.

9:24AM Y18.00006 Structure of SrTiO_3 films on Si , C. STEPHEN HELLBERG, Naval Research Lab, KRISTOPHER ANDERSEN, High Performance Technologies, Inc., HAO LI, Shenzhen New Degree Technology Co., PHILIP RYAN, Argonne National Laboratory, JOSEPH WOICIK, National Institute of Standards and Technology — The epitaxial deposition of oxides on silicon opens the possibility of incorporating their diverse properties into silicon-device technology. Deposition of SrTiO_3 on silicon was first reported over a decade ago, but growing the coherent, lattice-matched films that are critical for many applications has been difficult for thicknesses beyond 5 unit cells. Using a combination of density functional calculations and x-ray diffraction measurements, we determine the atomic structure of coherent SrTiO_3 films on silicon, finding that the Sr concentration at the interface varies with the film thickness. The structures with the lowest computed energies best match the x-ray diffraction. During growth, Sr diffuses from the interface to the surface of the film; the increasing difficulty of Sr diffusion with film thickness may cause the disorder seen in thicker films. The identification of this unique thickness-dependent interfacial structure opens the possibility of modifying the interface to improve the thickness and quality of metal oxide films on silicon.

9:36AM Y18.00007 Low kV Atomic Resolution and First Principles Study of the Structure and Bonding at $\text{SrTiO}_3/\text{GaAs}$ Hetero-interfaces¹ , QIAO QIAO, ROBERT KLIE, SERDAR OGUT, University of Illinois at Chicago — Ultrathin transition-metal oxide films on polar substrates have attracted increasing attention in recent years, due to the emergence of novel interfacial phases, not seen in the bulk of either material. In this study, we have combined aberration-corrected atomic-resolution Z-contrast imaging, electron energy loss spectroscopy (EELS) with first-principles density functional theory calculations to examine the atomic and electronic structures of epitaxially grown, ultrathin SrTiO_3 (100) films on GaAs (001). We find that the interface is atomically abrupt and no surface reconstruction of the GaAs (001) surface is observed. Using atomic-column resolved EELS, we show that Ti diffuses into the first few monolayers of GaAs and we will present evidence for the formation of As-oxides at the interface depending on the thin film growth conditions. First-principles DFT calculations will be used to analyze the formation energies of Ti-related impurity defects in the bulk and surface regions of GaAs, as well as the stability of any surface reconstruction at the $\text{SrTiO}_3/\text{GaAs}$ interface. These findings are used to explain transport behavior of the SrTiO_3 films as a function of deposition conditions.

¹Supported by NSF Grant No. DMR-0846748

9:48AM Y18.00008 Ultimate photovoltage in perovskite oxide heterostructures with critical film thickness , KUI-JUAN JIN, CONG WANG, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — One order larger photovoltage is obtained with critical thicknesses of $\text{La}_{0.9}\text{Sr}_{0.1}\text{MnO}_3$ films in both kinds of heterostructures of $\text{La}_{0.9}\text{Sr}_{0.1}\text{MnO}_3/\text{SrTiO}_3$ (0.8 wt % Nb-doped) and $\text{La}_{0.9}\text{Sr}_{0.1}\text{MnO}_3/\text{Si}$ fabricated at various oxygen pressures. Our self-consistent calculation reveals that the critical thickness of the $\text{La}_{0.9}\text{Sr}_{0.1}\text{MnO}_3$ film with the ultimate value of photovoltage is just the thickness of the depletion layer of $\text{La}_{0.9}\text{Sr}_{0.1}\text{MnO}_3$ in the $p-n$ heterostructures of $\text{La}_{0.9}\text{Sr}_{0.1}\text{MnO}_3/\text{SrTiO}_3$ (0.8 wt % Nb-doped) and $\text{La}_{0.9}\text{Sr}_{0.1}\text{MnO}_3/\text{Si}$, respectively.

10:00AM Y18.00009 Topological insulators from complex orbital order in transition-metal oxides heterostructures¹ , GREGORY FIETE, ANDREAS RUEGG, University of Texas at Austin — Topological band insulators which are dynamically generated by electron-electron interactions have been theoretically proposed in two and three dimensional lattice models. We present evidence that the two-dimensional version can be stabilized in digital (111) heterostructures of transition-metal oxides as a result of purely local interactions. The topological phases are accompanied by spontaneous ordering of complex orbitals and we discuss their stability with respect to the Hund's rule coupling, Jahn-Teller interaction and inversion symmetry breaking terms. As main competitors we identify spin-nematic and magnetic phases.

¹We gratefully acknowledge funding from ARO grant W911NF-09-1-0527 and NSF grant DMR- 0955778.

10:12AM Y18.00010 The electronic structure of epitaxially strained iridate thin films and superlattices from first principles, JOHANNES VOSS, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University, Ithaca, NY — Within the Ruddlesden-Popper iridates $\text{Sr}_{n+1}\text{Ir}_n\text{O}_{3n+1}$, strong spin-orbit interactions lead to the formation of a half-filled, narrow $J_{\text{eff}} = 1/2$ band and filled $J_{\text{eff}} = 3/2$ bands. This places the iridates in the vicinity of a Mott transition, which is sensitive to perturbations in crystal structure, despite relatively weak on-site Coulomb interactions [1]. For example, Sr_2IrO_4 ($n = 1$) is an antiferromagnetic Mott insulator that displays an almost rigid coupling between spin canting and IrO_6 octahedron rotations [2], while epitaxially stabilized SrIrO_3 ($n = \infty$) is a correlated metal. In this talk, we will discuss from first-principles within the LDA+SO+ U approach the possibility to engineer the electronic structure of SrIrO_3 and CaIrO_3 thin films using epitaxial strain and by creating superlattices of the form $(\text{AlrO}_3)_m(\text{A}'\text{BO}_3)_{m'}$ with $A, A' = \text{Ca}, \text{Sr}$. [1] S.J. Moon, H. Jin, K.W. Kim, W.S. Choi, Y.S. Lee, J. Yu, G. Cao, A. Sumi, H. Funakubo, C. Bernhard, and T.W. Noh, PRL 101, 226402 (2008). [2] B.J. Kim, H. Jin, S.J. Moon, J.-Y. Kim, B.-G. Park, C.S. Leem, J. Yu, T.W. Noh, C. Kim, S.-J. Oh, J.-H. Park, V. Durairaj, G. Cao, and E. Rotenberg, PRL 101, 076402 (2008).

10:24AM Y18.00011 The Structure of $\text{Y}_2\text{O}_3\text{:ZrO}_2$ / SrTiO_3 Layered Heterostructures, MATTHEW DYER, GEORGE DARLING, JOHN CLARIDGE, MATTHEW ROSSEINSKY, The University of Liverpool — Since the discovery of greatly increased conductivity in layered heterostructures of yttria stabilized zirconia (YSZ) and strontium titanate (STO) there has been considerable study and discussion regarding the origin of the high level of conductivity. The detailed atomic structure of layered YSZ-STO heterostructures is likely to be a crucial source of understanding, and as yet remains undetermined, particularly in the region of the buried interfaces between YSZ and STO. We present the results of density functional theory calculations on YSZ-STO heterostructures layered in the [001] direction, with different structures and compositions. We find that structures built using the terminations of the fluorite crystal structure of YSZ do not produce heterostructures which follow conventional solid state chemistry. These heterostructures contain Ti and Zr ions with unlikely O coordination geometries, reduced Ti^{3+} and Zr^{3+} ions and O-O bonding. In contrast, heterostructures built using a reconstructed YSZ termination, based on a rock-salt ordered ZrO layer, give more stable and more conventional atomic structures and are calculated to be electrically insulating. We describe these structures in detail, and the reasons behind the necessary reconstruction of YSZ at the interface.

10:36AM Y18.00012 Structural Rearrangement of Niobium Oxides from Lamellar Phases to Discrete Nanosheets and Nanoscrolls Probed by DFT Calculations, JHASHANATH ADHIKARI, LUIS J. SMITH, Clark University — Inorganic niobates $\text{ACa}_2\text{Nb}_3\text{O}_{10}$ ($A = \text{H}$ and K) with layered structures are good photocatalytic materials due to their high surface areas accommodating a larger number of active sites and ease of processing through soft chemical techniques like exfoliation and restacking. Alkali metal phases can be ion-exchanged to the acid phase, which in turn can be easily exfoliated to individual nanosheets. The nanosheets can change their form to nanoscrolls with a curled geometry instead of a flat surface. During these morphological transformations, the local structure at the Nb-atom, H-atom and the interface may undergo rearrangement which is responsible for the alteration of properties of the materials. This presentation highlights the preliminary results on these structural modifications (interface variation, stacking of layers, lattice contraction and space group settings) and the possible positions of the proton. Our calculations show that the protons in the acid form are non-bridging and bonded to the same layer oxygen atoms unlike the K-atoms in its parent compound. The Electric field gradient (EFG) is a parameter very sensitive to the electron density around a quadrupolar nucleus ^2H and ^{93}Nb that can be detected using NMR. Changes in its magnitude/sign can be correlated to the change in the local environment (bond lengths and angles) around the sites of interest. EFG values from DFT calculations based on the proposed structural models will be used for the characterization of surface O-H bond lengths, H-bonding and Nb-O bond lengths and can be used to interpret NMR studies.

10:48AM Y18.00013 Study of interface interactions in ZnO /Mesoporous silica nanocomposite, R.C. REDDY A, SOWRI BABU K, SUJATHA CH, V.G. REDDY K, National Inst. of Technology Warangal (A.P) 506004, India — The Photoluminescence (PL) properties of ZnO /Mesoporous silica (MPS) nanocomposite annealed under different temperatures were studied. A broad PL band at 395 nm has been observed in all samples and analysis was made by using Gaussian fitting. As the temperature increased, emission bands were blue shifted and the relative intensity ratio of the oxygen vacancies at ZnO - SiO_2 interface to the oxygen vacancies in inner ZnO crystallites was increased. The emission peaks at 363 nm and 384 nm are attributed to the near band edge emission (NBE) and to the phonon replica emission. At 550C the exciton confinement effect disappears due to the large amount of surface effects. The influence of porosity of host media on Si-O-Zn cross linking bonds was also investigated. ZnO nanoparticles were loaded into nanocrystalline silica (NCS) and silica gel (SG). The surface area increases monotonously from NCS to MPS through SG. Si-O-Zn cross linking bonds were almost absent in the sample prepared with NCS. It exhibits NBE emission at 360 nm which was found to be absent in other samples prepared with SG and MPS. It was also found that the emission intensity of the samples decreases with aging. This is due to diffusion of oxygen atoms from the atmosphere to interior of the sample.

Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y19 DCMP: Invited Session: Novel Mechanisms of Multiferrocity 253AB

8:00AM Y19.00001 Multiferroicity due to Charge Ordering, JEROEN VAN DEN BRINK, IFW Dresden — In this contribution I discuss multiferroicity that is driven by different forms of charge ordering, presenting first the generic mechanisms by which charge ordering can induce ferroelectricity in magnetic systems. In type-I multiferroics [1], ferroelectricity and magnetism have different origins and occur at different temperatures. There is a number of specific classes of materials for which this is relevant. Discussed will be in some detail (i) perovskite manganites of the type $(\text{PrCa})\text{MnO}_3$ [2,3], (ii) the complex and interesting situation in magnetite Fe_3O_4 , (iii) strongly ferroelectric frustrated LuFe_2O_4 and (iv) an example of a quasi-one-dimensional organic system [4]. In type-II multiferroics [1], ferroelectricity is completely due to magnetism, but with charge ordering playing an important role [5], such as (v) multiferroic $\text{Ca}_3\text{CoMnO}_6$, (vi) possible ferroelectricity in rare earth perovskite nickelates of the type RNiO_3 [6,7], (vii) multiferroic properties of manganites of the type RMn_2O_5 [8], (viii) perovskite manganites with magnetic E-type ordering.

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[8] G. Giovannetti and J. van den Brink, Phys. Rev. Lett. 100, 227603 (2008).

8:36AM Y19.00002 Soft X-ray Observation of electronic contribution to ferroelectric polarization, STUART WILKINS, Brookhaven National Laboratory — Multiferroic materials open up new interesting possibilities for devices by enabling the switching of an electric state by magnetic field or *vice-versa*. In addition to this functionality, multiferroics are intriguing from a fundamental physics perspective, raising interesting questions concerning coupling of the electric and magnetic order parameters. To date, most coupling mechanisms are understood to occur due to distortions in the crystal lattice. Here we present experimental evidence that in the multiferroics RMn_2O_5 (where R is a rare earth) there exists a new, purely *electronic* contribution to the ferroelectric polarization, which can exist in the absence of any lattice distortions. This contribution arises due to spin-dependent hybridization of O $2p$ and Mn $3d$ states and was observed through soft x-ray resonant scattering, which has proved to be a very useful tool in the study of the magnetic structure of multiferroics[1]. Through resonant x-ray scattering at the oxygen K-edge, we find that such spin dependent hybridization occurs in both TbMn_2O_5 [2] and YMn_2O_5 [3]. Remarkably, in YMn_2O_5 we find that the temperature dependence of the integrated intensity of the signal at the oxygen K-edge closely follows the macroscopic electric polarization [3], and hence is proportional to the ferroelectric order parameter. This is in contrast with the temperature dependence observed at the Mn L_3 edge, which reflects the Mn magnetic order parameter. Work performed at BNL was supported by the US Department of Energy, Division of Materials Science, under contract No. DE-AC02-98CH10886.

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9:12AM Y19.00003 Dynamic magnetoelectric interaction in multi-orbital Mott insulators¹, MAXIM MOSTOVOY, Zernike Institute for Advanced Materials, University of Groningen — The control of spin textures in magnetic insulators with an applied voltage can be of great importance for dissipationless spintronics. The coupling between spin and charge degrees of freedom in Mott insulators originates from the fluctuations of electron occupancy of strongly correlated orbitals of transition metal ions. Several microscopic mechanisms resulting from the virtual hopping of electrons from a magnetic site to its neighbor, e.g. the “inverse Dzyaloshinskii-Moriya” and the Heisenberg exchange striction mechanisms, are responsible for the electric polarization induced by non-centrosymmetric magnetic orders, the excitation of spin waves with the oscillating electric field of a light wave, and other effects recently observed in multiferroic materials. I will discuss a new dynamic magnetoelectric interaction, which describes the electric polarization induced by time-dependent spin textures [1]. Simple symmetry arguments as well as the explicit derivation from an extended Hubbard model of multi-orbital Mott insulators are used to obtain the form of this interaction, which is the electric analogon of the coupling between the scalar spin chirality and magnetic field. It is closely related to the so-called spinmotive force exerted by spins on electrons in magnetic conductors. This interaction makes possible to displace spin textures in ferromagnetic insulators by applying a voltage. It couples the external electric field to the center-of-mass coordinates of topological spin textures in ferromagnetic thin films, such as Skyrmions and magnetic vortices. The effect of this coupling is dramatically amplified in the resonant absorption of circularly polarized light by spin vortices in nanodiscs.

[1] M. Mostovoy, K. Nomura and N. Nagaosa, Phys. Rev. Lett. 106, 047204 (2011).

¹This work supported by FOM grant 08PR2586.

9:48AM Y19.00004 Multiferroic vortices: arrested Kosterlitz-Thouless order¹, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials — The fascinating concept of topological defects permeates ubiquitously our understanding of the early-stage universe, hurricanes, quantum matters such as superfluids and superconductors, and also technological materials such as liquid crystals and magnets. Large-scale spatial configurations of these topological defects have been investigated only in a limited degree. Exceptions include the cases of supercurrent vortices or liquid crystals, but they tend to exhibit either trivial or rather-irregular configurations. Hexagonal REMnO_3 (RE= rare earths) with RE=Ho-Lu, Y, and Sc, is an improper ferroelectric where the size mismatch between RE and Mn induces a trimerization-type structural phase transition, and this structural transition leads to three structural domains, each of which can support two directions of ferroelectric polarization. We reported that domains in h- REMnO_3 meet in cloverleaf arrangements that cycle through all six domain configurations. Occurring in pairs, the cloverleaves can be viewed as vortices and antivortices, in which the cycle of domain configurations is reversed. Vortices and antivortices are topological defects: even in a strong electric field they won't annihilate. These ferroelectric vortices/antivortices are found to be associated with intriguing magnetism. The seemingly-irregular configurations of a zoo of multiferroic vortices and antivortices in h- REMnO_3 can be neatly analyzed in terms of graph theory and this graph theoretical analysis reflects the nature of self-organized criticality in complexity phenomena as well as the condensation and eventual annihilation processes of topological vortex-antivortex pairs. Furthermore, these numerous multiferroic vortices/antivortices can be understood as an arrested Kosterlitz-Thouless phase.

[1] Insulating Interlocked Ferroelectric and Structural Antiphase Domain Walls in Multiferroic YMnO_3 , T. Choi, - - -, S.-W. Cheong, Nature Materials 9, 253 (2010).

[2] Self-organization, condensation, and annihilation of topological vortices and antivortices in a multiferroic, S. C. Chae, - - -, S.-W. Cheong, PNAS 107, 21366 (2010).

[3] Direct observation of the proliferation of ferroelectric dislocation loops and vortex-antivortex pairs, S. C. Chae, - - -, S.-W. Cheong, Phys. Rev. Lett., submitted.

¹This work is supported by NSF grant DMR-1104484 and DOE grant DE-FG02-07ER46382.

10:24AM Y19.00005 Interplay between trimerization, ferroelectric, and magnetic order in the hexagonal manganites¹, MANFRED FIEBIG, Department of Materials, ETH Zurich — The hexagonal manganites h- RMnO_3 with R = Sc, Y, In, Dy – Lu are a model system for multiferroics with pronounced magnetoelectric effects in which the magnetic and ferroelectric order emerge independently (so-called split-order-parameter or type-I multiferroics). In spite of many years of intense investigations the system never ceases to surprise us with novel, unexpected manifestations of its five-fold long-range order (antiferrodistortive, ferroelectric, antiferromagnetic Mn order, and rare-earth order on the 2a and 4b sites). Here I will discuss several such examples: (i) “Incompatible” magnetic order of the Mn and rare-earth sublattices according to different symmetry representations in combination with triggered ordering at the 4b site. (ii) The absence of ferroelectric order in h- InMnO_3 down to low temperatures in spite of its apparent similarities to, in particular, h- YMnO_3 . (iii) Observation of a direct and rigid coupling of the ferroelectric to the antiferrodistortive order in annealing experiments at 1300 K. In summary, all these experiments allow us to present a comprehensive model for the microscopic origin of the ferroelectric and the multiple magnetic (re-) ordering in this important group of compounds.

¹Support by the SFB 608 of the DFG is appreciated.

Friday, March 2, 2012 8:00AM - 11:00AM –
Session Y20 DCMP GSNP: Invited Session: New Anisotropy-Driven Phenomena in Colloidal Suspensions 253C

8:00AM Y20.00001 Entropically patchy particles: Shape-driven self assembly of hard colloids¹

, SHARON GLOTZER, Department of Chemical Engineering, University of Michigan, Ann Arbor, MI — Although the structural diversity of colloidal fluids and crystals has grown substantially in recent years, it still aspires to that of atomic and molecular systems. Ionic colloidal crystals and binary nanoparticle superlattices, by exploiting electrostatic interactions in mixtures of particles of opposite charge, have substantially broadened the diversity of structures beyond those obtainable in traditional hard sphere systems, but rely on energetic interactions as well as entropy for their stability. Likewise, “traditional” patchy particles with sticky interactions exploit explicit attractive interactions for assembly. Here we explore the role of shape and entropy in phase transitions of hard particle fluids, in the absence of all other interactions. Using computer simulations, we show that particle shape alone can suffice to produce a rich diversity of colloidal crystals, quasicrystals, glasses and mesophases through thermodynamic self-assembly whose complexity rivals that of atomic analogues. We compare self-assembled phases of hard polyhedra with their dense packings obtained from small unit cell compressions, and show the packings tend to be less structurally complex than the assemblies. Based on our findings, we present design rules for anisotropic hard, faceted colloids as “entropically patchy particles” for self assembly.

¹SCG acknowledges financial support from the U.S. Department of Defense, the National Science Foundation, the Department of Energy Office of Science, and the J.S. McDonnell Foundation.

8:36AM Y20.00002 Lock-and-Key Colloids¹

, DAVID PINE, New York University — We have developed a new kind of colloidal particle that is spherical but with one or more spherical dimples in the particle surface. These dimples serve as docking points for colloidal spheres whose radius matches the radius of dimples. The attractive docking force is provided by the depletion interaction and can be controlled by changing the depletant concentration or, in some cases, the temperature. The docking is completely reversible and mimics the classic lock-and-key interaction often used to describe protein binding. The lock-and-key binding is size specific and can be used to assemble a number of interesting colloidal superstructures, including flexible jointed chains, dumbbells, trimers, tetramers, and other assemblies. A new synthetic method for making the dimpled particles can be generalized to make a number of other new structured colloidal particles, with different functionalities analogous to block copolymers.

¹This work is supported by the National Science Foundation, Award number DMR-1105455 and was performed in collaboration with S. Sacanna, W. T. M. Irvine, P. M. Chaikin, and G.R. Yi.

9:12AM Y20.00003 Glass transitions in quasi-two-dimensional suspensions of colloidal ellipsoids

, YILONG HAN, Hong Kong University of Science and Technology — Colloidal glasses constitute of anisotropic particles were mainly studied by simulations in three dimensions with incomplete phase diagrams. Here we report the experiment about glass transitions in a colloidal suspension of micro-ellipsoids at the single-particle level. Video microscopy revealed a two-step glass transition corresponding to inter-domain freezing and inner-domain freezing respectively. The glass transition in the rotational degree of freedom was at a lower density than that in the translational degree of freedom. Between the two transitions, ellipsoids formed an “orientational glass” in the area fraction range $0.72 < \phi < 0.79$ for aspect ratio $p = 6$ ellipsoids and $0.60 < \phi < 0.72$ for $p = 9$. Such orientational glass is expected to be replaced by the rotator phase at small aspect ratios and the nematic phase at large aspect ratios. The observed decoupling between diffusion and relaxation for both of translational and rotational motions reflects the dynamic heterogeneity. Approaching the respective glass transitions, the rotational and translational fastest-moving particles in the supercooled liquid moved cooperatively and formed clusters with power-law size distributions. The mean cluster sizes diverge in power law as approaching the glass transitions. The translational and rotational fastest- and slowest-moving ellipsoids are all spatially anticorrelated: most translational fast-moving ellipsoids and rotational slow-moving ellipsoids formed at different areas within pseudonematic domains, while most rotational fast-moving ellipsoids and translational slow-moving ellipsoids formed at different areas around the domain boundaries.

9:48AM Y20.00004 Suppression of the coffee-ring effect by shape-dependent capillary interactions

, PETER YUNKER, Univ of Pennsylvania — No abstract available.

10:24AM Y20.00005 Glassy dislocation dynamics in colloidal dimer crystals

, SHARON GERBODE, Harvey Mudd College — Dislocation mobility is central to both the mechanical response and the relaxation mechanisms of crystalline materials. Recent experiments have explored the role of novel particle anisotropies in affecting the rules of defect motion in crystals. “Peanut-shaped” colloidal dimer particles consisting of two connected spherical lobes form densely packed crystals in 2D. In these “degenerate crystals,” the particle lobes occupy triangular lattice sites while the particle axes are randomly oriented among the three crystalline directions. One consequence of the random orientations of the dimers is that dislocation glide is severely limited by certain particle arrangements in the degenerate crystals. Using optical tweezers to manipulate single lobe-sized spherical intruder particles, we locally deform the crystal, creating defects. During subsequent relaxation, the dislocations formed during the deformation leave the crystal grain, either via annihilation with other dislocations or by moving to a grain boundary. Interestingly, in large crystalline grains this dislocation relaxation occurs through a two-stage process reminiscent of slow relaxations in glassy systems, suggesting the novel concept that glassy phenomena may be introduced to certain kinds of colloidal crystals via simple anisotropic constituents.

Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y21 DCMP: Bi-based Cuprates – Experiment 254A

8:00AM Y21.00001 Phase Determination for Intra-unit-cell Fourier Transform STM – Picometer Registration of Zn Impurity States in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$

, INES FIRMO, MOHAMMAD HAMIDIAN, KAZUHIRO FUJITA, SOURIN MUKHOPADHYAY, Cornell University; Brookhaven National Lab, JOSEPH ORENSTEIN, University of California, Berkeley, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology, Japan, SHIN-ICHI UCHIDA, University of Tokyo, Japan, MICHAEL LAWLER, EUN-AH KIM, Cornell University, J.C. DAVIS, Cornell University; Brookhaven National Lab; University of St. Andrews, Scotland; Kavli Institute at Cornell — By studying the real and imaginary components of the Bragg peaks in Fourier transforms of electronic structure images, distinct types of intra-unit cell (IUC) symmetry breaking can be studied using SI-STM [Lawler *et al.*, Nature **466** 347 (2010)]. However, establishing the precise r-space symmetry point of each unit cell is crucial in defining the phase for such analysis. Exemplary of this challenge is the high- T_c superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ for which the Bi atoms in the surface BiO layer are observable, while it is the invisible Cu atoms that define the relevant CuO_2 unit-cell symmetry point. We demonstrate, by imaging with pm precision the electronic impurity states at individual Zn atoms substituted at Cu sites, that the phase established using the Bi lattice produces a $\sim 2\%(2\pi)$ error relative to the Cu lattice. In this case, IUC C_{4v} symmetry breaking in the CuO_2 plane can be determined reliably using the phase assignment from the BiO layer. Moreover, impurity atom substitution at the relevant symmetry site can be of general utility in phase determination for Bragg-peak Fourier analysis of IUC symmetry.

8:12AM Y21.00002 Imaging broken symmetry in the electronic structure of Bi-doped cuprates by scanning tunneling microscopy¹, YANG HE, TESS WILLIAMS, ANJAN SOUMYANARAYANAN, MICHAEL YEE, Harvard University, TAKESHI KONDO, HIROSHI IKUTA, Nagoya University, ERIC HUDSON, Pennsylvania State University, JENNIFER HOFFMAN, Harvard University — The relationship between the mysterious pseudogap phase in the cuprate superconductors and the myriad broken symmetries observed by various experimental techniques is a source of much controversy. We use low-temperature scanning tunneling microscopy and spectroscopy to image electronic nematic order in the cuprate superconductor $\text{Bi}_{2-x}\text{Pb}_x\text{Sr}_2\text{CuO}_{6+\delta}$. We determine the robustness of the nematic order parameter to experimental conditions.

¹We acknowledge funding from NSF(DMR-0847433), NDSEG, A*STAR, and NSERC.

8:24AM Y21.00003 Investigating structural distortions in Bi based superconductors by scanning tunneling microscopy¹, MICHAEL M. YEE, ILIJA ZELJKOVIC, Department of Physics, Harvard University, ANJAN SOUMYANARAYANAN, Department of Physics, Massachusetts Institute of Technology, ELIZABETH MAIN, T. WILLIAMS, Department of Physics, Harvard University, TAKESHI KONDO, T. TAKEUCHI, HIROSHI IKUTA, Department of Crystalline Materials Science, Nagoya University, G.D. GU, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, E.W. HUDSON, Department of Physics, Pennsylvania State University, JENNIFER E. HOFFMAN, Department of Physics, Harvard University — We use scanning tunneling microscopy to image symmetry-breaking structural distortions in the bismuth-based high- T_c superconductors, $\text{Bi}_2\text{Sr}_2\text{Ca}_{n-1}\text{Cu}_n\text{O}_{2n+4+x}$ (BSCCO). To elucidate the structure, we have implemented a new algorithm that quantifies atomic distortions with picometer resolution. Using this algorithm, we have observed an in-plane inversion-symmetry-breaking orthorhombic structural distortion in the BiO layer. We have also quantified the lattice distortions resulting from the use of Pb substitution to suppress the supermodulation in BSCCO. Each of these structural distortions break point group symmetries of the CuO_2 plaquette, which may be generally relevant to understanding the broken symmetries of the mysterious pseudogap state in high- T_c cuprates.

¹We acknowledge support from NSERC (DMR-0847433), A*STAR, NDSEG and NSERC.

8:36AM Y21.00004 Exploring the Nature of the Electronic Scatters in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$, EDUARDO CALLEJA, JIXIA DAI, University of Colorado at Boulder, GENDA GU, Brookhaven National Laboratory, KYLE MCELROY, University of Colorado at Boulder — The superconducting cuprates have been one of the most studied classes of materials over the last 20 years. While much progress has been made in understanding the strange electronic properties which govern their rich phase diagram, the interplay between coulomb interactions (which are thought to play a key role in their unconventional superconductivity) and the corresponding quasi particle scattering caused by coulomb interactions, are still the subject of debate among the community. We attempt to explore this issue by using spectroscopic imaging scanning tunneling spectroscopy (SI-STs) at variable temperatures which allows us to probe the Local Density of States (LDOS). The LDOS can be fitted with the theorized Dynes' formula allowing for the extraction of the quasi particle scattering rates. Furthermore, we seek to understand the scattering process by simulating the patterns produced by quasi particle interference (QPI) by either a pair potential impurity or a non-magnetic impurity. Extraction of these rates at various dopings and temperatures in the phase diagram will be presented.

8:48AM Y21.00005 Imaging the impact of single dopant atoms on the electronic order and disorder of $\text{Bi}_{2+y}\text{Sr}_{2-y}\text{CaCu}_2\text{O}_{8+x}$ ¹, ILIJA ZELJKOVIC, Harvard University, GENDA GU, Brookhaven National Laboratory, JENNIFER HOFFMAN, Harvard University — High- T_c cuprate superconductors display startling nanoscale disorder in essential properties such as critical temperature, pseudogap energy, and even band structure. The underlying cause of this disorder has remained mysterious; theoretical explanations have ranged from chemical inhomogeneity to spontaneous electronic phase separation. We extend the energy range of scanning tunneling spectroscopy, allowing the first-ever direct mapping of both types of interstitial oxygen dopants in $\text{Bi}_{2+y}\text{Sr}_{2-y}\text{CaCu}_2\text{O}_{8+x}$, as well as vacancies at the apical oxygen site. We show that a subset of these dopants are indeed the direct cause of the nanoscale disorder. We further explain how the spatial variations in electronic orders, such as the pseudogap and the charge order, are governed by the disorder in the dopant concentrations, particularly vacancies in the apical oxygen site.

¹We acknowledge the support from NSF Career (DMR-0847433).

9:00AM Y21.00006 Imaging Locally Oriented Charge Modulations in a Cuprate Superconductor, JENNIFER HOFFMAN, ELIZABETH MAIN, Harvard University, BENJAMIN PHILLABAUM, Purdue University, HIROSHI IKUTA, Nagoya University, ERIC HUDSON, Penn State University, KARIN DAHMEN, University of Illinois, Urbana-Champaign, ERICA CARLSON, Purdue University — We use scanning tunneling microscopy to image the local orientation of the static charge modulations in $\text{Bi}_{2-y}\text{Pb}_y\text{Sr}_{2-z}\text{La}_z\text{CuO}_{6+x}$, for samples spanning a wide range of doping. For each sample, we compute the size distribution of locally x -oriented and locally y -oriented clusters. We analyze the size distributions within a random field Ising model to obtain the fractal dimension and other critical exponents. We discuss the utility of scaling collapse to extract the critical doping x_c of the smectic charge order in $\text{Bi}_{2-y}\text{Pb}_y\text{Sr}_{2-z}\text{La}_z\text{CuO}_{6+x}$.

9:12AM Y21.00007 Structure of intra-unit cell C_{4v} symmetry breaking domains in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ from SI-STM, MOHAMMAD HAMIDIAN, INES FIRMO, KAZUHIRO FUJITA, Cornell University; Brookhaven National Lab, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology, Japan, SHIN-ICHI UCHIDA, University of Tokyo, Japan, MICHAEL LAWLER, EUN-AH KIM, Cornell University, J.C. DAVIS, Cornell University; Brookhaven National Lab; University of St. Andrews, Scotland; Kavli Institute, Cornell — Mounting evidence from a number of experimental probes supports the idea that the electronic structure of the cuprate pseudogap phase breaks rotational symmetry. Furthermore, ARPES, neutron scattering and spectroscopic imaging scanning tunneling microscopy (SI-STM) data all point to an intra-unit cell origin. We present new findings for near optimally doped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (BSCCO) which elucidate the domains associated with intra-unit cell C_{4v} symmetry breaking in the electronic structure. The analysis method will be motivated by the preceding talk, 'Phase Determination of Intra-Unit Cell Fourier Transform STM – Picometer Registration of Zn Impurity States in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ ' given by I. A. Firmo.

9:24AM Y21.00008 Optical conductivity of exfoliated $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ nanocrystals, LUKE SANDILANDS, VIKTORIYA BAYDINA, ALEXANDER SU, ANJAN REIJNDERS, University of Toronto, Canada, TOR PEDERSEN, FERENC BORONDICS, Canadian Light Source, Canada, GENDA GU, Brookhaven National Laboratory, USA, SHIMPEI ONO, University of Tokyo, Japan, YOICHI ANDO, Osaka University, Japan, KENNETH BURCH, Institute for Optical Sciences, University of Toronto, Canada — We report on infrared spectromicroscopy of mechanically exfoliated under-doped and optimally-doped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ thin crystals on SiO_2/Si substrates. The infrared reflectance and transmission was measured for samples of various thicknesses and the optical conductivity extracted in the frequency range 0.15 eV to 1 eV. Trends in the optical conductivity with thickness are discussed. In particular, we observe that the conductivity of thicker (~ 100 nm) samples is comparable to bulk while that of thinner (~ 20 nm) samples is markedly suppressed.

9:36AM Y21.00009 Evidence of two-dimensional quantum critical behavior in the superfluid density of deeply underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$, JIE YONG, MICHAEL HINTON, ANDY MCCRAY, Dept. of Physics, The Ohio State University, M. NAAMNEH, AMIT KANIGEL, Dept. of Physics, Technion, Israel, MOHIT Randeria, THOMAS LEMBERGER, Dept. of Physics, The Ohio State University — Evidence of two-dimensional (2-D) quantum critical fluctuations is observed in the superfluid density $n_s(T) \propto \lambda^{-2}(T)$ of deeply underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ (Bi-2212). Quantum critical behavior is indicated by the evolution of the T-dependence of $n_s(T)/n_s(0)$, which loses any evidence for thermal critical behavior and becomes quasi-linear when underdoping drops the transition temperature T_c below roughly 48K. Two-dimensionality is indicated by the linear scaling of transition temperature T_c with $n_s(0)$. The 2-D behavior contrasts with that of the less anisotropic $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$, which sustains 3D quantum critical fluctuations.

9:48AM Y21.00010 Coherent THz emission from isosceles-triangular mesas of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$, RICHARD KLEMM, ERICA LABERGE, CANDY REID, DUSTIN MORLEY, University of Central Florida, KAVEL DELFANAZARI, KAZUO KADOWAKI, University of Tsukuba — Using the standard emission patterns predicted for thin, isosceles triangular patch antennae, combined with a spatially uniform ac Josephson current source, we have performed two-parameter least-squares fits to our recently obtained unpublished experimental emission data from isosceles-triangularly-shaped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ mesas. Our results support the notion that such irregular patch antennae shapes may be useful in constructing high-powered, tunable continuous-wave coherent sources of light in the sub-terahertz to terahertz regime.

10:00AM Y21.00011 Tunable sub-terahertz emission from intrinsic Josephson junctions in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ enhanced by the internal cavity resonance¹, MANABU TSUJIMOTO, TAKASHI YAMAMOTO, KAVEH DELFANAZARI, RYO NAKAYAMA, TAKEO KITAMURA, MASASHI SAWAMURA, TAKANARI KASHIWAGI, HIDETOSHI MINAMI, MASASHI TACHIKI, University of Tsukuba, RICHARD KLEMM, University of Central Florida, KAZUO KADOWAKI, University of Tsukuba — Intense, continuous and coherent terahertz electromagnetic wave emission from the intrinsic Josephson junction system in cuprate high- T_c $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ with remarkably higher intensity [L. Ozyuzer *et al.*, Science **318**, 1291 (2007).] than previously generated from single or arrayed Josephson junctions has been understood by the enhancement of the output intensity by the internal cavity resonance. However, we have recently observed emission, which seems to have low enhancement due perhaps to the relatively low- Q factor, in a wide frequency range, covering almost all frequencies continuously as long as the ac Josephson effect is satisfied. This broadly tunable behavior is very different from that with the tunability found in the inner current-voltage branch region [M. Tsujimoto *et al.*, to be published in 2011.] and enables us to design useful and tunable sub-terahertz source devices. In the presentation, we will also discuss the possible high-power devices using the high- Q -electromagnetic cavity.

¹This work was supported in part by CREST-JST, WPI-MANA project (NIMS) and Strategic Initiative category (A) at the University of Tsukuba.

10:12AM Y21.00012 Effect of magnetic field on the coherent THz emission from mesas of single crystal $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$, TAKEO KITAMURA, TAKANARI KASHIWAGI, MANABU TSUJIMOTO, KAVEH DELFANAZARI, RYO NAKAYAMA, MASASHI SAWAMURA, TAKASHI YAMAMOTO, HIDEHIRO ASAI, HIDETOSHI MINAMI, MASASHI TACHIKI, KAZUO KADOWAKI, University of Tsukuba — Coherent and continuous electromagnetic (EM) waves radiation phenomena with a mesa structure of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ single crystal have been investigated precisely in magnetic field up to only 200 Oe where the emission intensity decreases sharply expectedly for the field H parallel to the c -axis. The emission could not be observed above 20 Oe for $H//c$ -axis whereas it persisted up to 160 Oe for $H//ab$ plane [1]. These results indicate that both pancake vortices as well as Josephson vortices suppress the THz emission very strongly. On the other hand, the Josephson plasma resonance phenomena have been observed in both $H//ab$ and $H//c$ even in very high fields ($\sim$ Tesla). The emission processes are considered to be the reverse processes of the absorption. It is interesting to pose a question what happens in high fields in the EM waves emission. We show interesting experimental results of THz emission in high magnetic fields including low field region and will argue the mechanism of emission in high magnetic fields.

[1] K. Yamaki *et al.*, physica C **470** (2010) S804-805.

10:24AM Y21.00013 Quasiparticle dynamics in overdoped $\text{Bi}_{1.4}\text{Pb}_{0.7}\text{Sr}_{1.9}\text{CaCu}_2\text{O}_{8+\delta}$: Coexistence of superconducting gap and pseudogap below T_c , SARITHA K. NAIR, XINGQUAN ZOU, Nanyang Technological University, Singapore, JIAN-XIN ZHU, Los Alamos National Laboratory, CHRISTOS PANAGOPOULOS, Nanyang Technological University, Singapore, SHIGEYUKI ISHIDA, SHIN-ICHI UCHIDA, The University of Tokyo, ELBERT E.M. CHIA, Nanyang Technological University, Singapore — Photoexcited quasiparticle relaxation dynamics in overdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ ($T_c=65$ K, hole doping $p=0.22$) single crystal is investigated as a function of temperature. We provide evidence of a ~ 22 meV pseudogap ($T^*\approx 100$ K) at this doping level. Moreover, this pseudogap vanishes at T^* . Our data support the scenario where both the superconducting gap and pseudogap coexist in the superconducting state. Our results also suggest an increased scattering rate between electrons and spin fluctuations as the sample enters the pseudogap phase. Phys. Rev. B **82**, 212503 (2010)

10:36AM Y21.00014 THz wave radiation from the triangular mesas in layered high- T_c superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ intrinsic Josephson junctions¹, KAVEH DELFANAZARI, MANABU TSUJIMOTO, TAKANARI KASHIWAGI, HIDEHIRO ASAI, TAKASHI YAMAMOTO, MASASHI SAWAMURA, TAKEO KITAMURA, RYO NAKAYAMA, KAZUYA ISHIDA, HIDETOSHI MINAMI, TOSHIAKI HATTORI, KAZUO KADOWAKI, University of Tsukuba — Recently, it has been reported that the mesa structures fabricated from single crystalline high- T_c superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ intrinsic Josephson junctions generate THz waves [1, 2]. However, most of radiations in the previous studies were observed either below the critical current where the junctions switched to the resistive state or around the retrapping region. We present here three types of emission for isosceles triangular mesas in which THz waves were also additionally detected above the critical current where the external current is increasing in the resistive branch structures. Furthermore, intense, coherent, monochromatic, continuous and tunable THz waves were observed in various triangular mesas fabricated by the focus ion beam (FIB) technique [3]. Moreover, elucidating the oscillating modes inside the mesas by precisely studying the IV characteristics, FT-IR spectrum and angular dependence of the emission intensity will be discussed in detail at meeting.

[1] L. Ozyuzer *et al.* Science **318**, 1291 (2007).

[2] K. Kadowaki *et al.* Physica C **468** 634 (2008).

[3] K. Delfanazari *et al.* J. Phys. Conf. Ser. Accepted (2011).

¹This work was supported by CREST-JST and WPI-MANA Project (NIMS).

10:48AM Y21.00015 Particle-hole asymmetric QPI in the pseudogap phase of underdoped Bi-2212, CHUNG KOO KIM, Cornell, BNL, JHINHWAN LEE, KAIST, KAZUHIRO FUJITA, Cornell, HIROSHI EISAKI, AIST, SHINICHI UCHIDA, Tokyo University, J.C. SEAMUS DAVIS, Cornell, BNL, St. Andrews Univ., JINHO LEE, BNL — Quasi-Particle Interference (QPI) measured by STM revealed many interesting phenomena in Correlated Electron Systems. Particle-hole (p-h) symmetric QPI observed in the superconducting $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ disappears around the reduced zone boundary [1], while p-h asymmetric QPI's on non-superconducting $\text{Sr}_3\text{Ru}_2\text{O}_7$ [2] and $\text{Ca}(\text{Fe}_x\text{Co}_{1-x})_2\text{As}_2$ [3] identified dominant band structures, suggesting electronic nature of the nematic phases. In light of these discoveries, here we report the observation of p-h asymmetric QPI of underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ in the pseudogap phase continuously dispersing through E_F . The Fermi velocity measured from this dispersion is $\sim 0.12 \times 10^6$ m/s. We will discuss the possible origin and implications by comparing its symmetry and dispersion using theoretical model and currently available experimental data from other probes.

[1] Y. Kohsaka et al., Nature 454, 1072 (2008)

[2] Jinho Lee et al., Nature Physics 5, 800 (2009)

[3] Chuang et al., Science 327, 181 (2010)

Friday, March 2, 2012 8:00AM - 11:00AM –
Session Y22 DMP DCOMP: Focus Session: Fe-based Superconductors - Crystal Growth and New Materials 254B

8:00AM Y22.00001 Single crystal growth and physical properties of SrCu_2As_2 , SrCu_2Sb_2 and BaCu_2Sb_2 ¹, V.K. ANAND, P.K. PERERA, A. PANDEY, R.J. GOETSCH, A. KREYSSIG, D.C. JOHNSTON, Ames Laboratory and Dept. Phys. Astron., Iowa State Univ., Ames, IA 50011 — We present the physical properties of self-flux-grown single crystals of SrCu_2As_2 , SrCu_2Sb_2 , $\text{SrCu}_2(\text{As}_{0.84}\text{Sb}_{0.16})_2$ and BaCu_2Sb_2 investigated by magnetic susceptibility χ , specific heat C_p and electrical resistivity ρ vs. temperature T measurements. Contrasting structures occur for SrCu_2As_2 (ThCr_2Si_2 -type), SrCu_2Sb_2 (CaBe_2Ge_2 -type) and BaCu_2Sb_2 (a distorted intergrowth of ThCr_2Si_2 -type and CaBe_2Ge_2 -type unit cells). The $\chi(T)$ data for all these compounds exhibit weakly anisotropic diamagnetic behaviors. For $1.8 \leq T \leq 300$ K, the $\rho(T)$ data show metallic character and are well-described by the Bloch-Grüneisen model, and the $C_p(T)$ data are well-fitted by metallic γT plus Debye lattice contributions. From the low- T $C_p(T)$ data, we infer Sommerfeld coefficients $\gamma = 2.2\text{--}3.9$ mJ/mol K² and Debye temperatures $\Theta_D = 204\text{--}246$ K. The electronic properties indicate that these compounds are *sp* metals containing Cu in a nonmagnetic $3d^{10}$ electronic configuration.²

¹Research at Ames Laboratory was supported by the USDOE-Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

²D. J. Singh, Phys. Rev. B **79**, 153102 (2009).

8:12AM Y22.00002 Synthesis of Large Single Crystals Within the Zr - Fe - Si System¹, GREG SMITH, JACOB E. GROSE, J.W. SIMONSON, M.C. ARONSON, Physics and Astronomy Dept., Stony Brook University — The synthesis of large single crystals of intermetallic silicides from a metal flux is challenging, owing to the poor solubility of silicon in many of the traditional fluxes at low temperatures. Accordingly, single crystal syntheses of several compounds within the Zr - Fe - Si system from a gallium flux were investigated. $\text{Zr}_4\text{Fe}_4\text{Si}_7$, a member of the well-known V-phase family of compounds, forms as silver lustrous rods. Successful growths yielded crystals with dimensions up to 12.1 mm by 0.14 mm by 0.14 mm, large enough to perform the first transport measurements of this compound. We grew for the first time single crystals of the hexagonal Laves phase $\text{ZrFe}_{1.5}\text{Si}_{0.5}$, which has previously only been reported in the polycrystalline form. Two previously unreported phases, including the silver lustrous rods $\text{Zr}_{2-x}\text{Fe}_4\text{Si}_{12-y}$, have been discovered as single crystals within this system. The composition of all phases was verified with powder and single crystal x-ray diffraction. Our group is currently investigating the growth of similar compounds using the methods developed for this system.

¹Research supported by a DOD National Security Science and Engineering Fellowship via the AFOSR

8:24AM Y22.00003 Exploration of Superconductivity in Layered Structures¹, ATHENA SEFAT, Oak Ridge National Laboratory — Superconductivity at high temperatures is of great interest in terms of both basic science and applications. Although there are many findings on the chemistry and physics of superconductors, there are a lot of questions that remain unanswered. We will review experimental routes to possibly finding and identifying new superconducting materials.

¹This work is supported by the Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

9:00AM Y22.00004 High T_c electron doped $\text{Ca}_{10}(\text{Pt}_3\text{As}_8)(\text{Fe}_2\text{As}_2)_5$ and $\text{Ca}_{10}(\text{Pt}_4\text{As}_8)(\text{Fe}_2\text{As}_2)_5$ superconductors¹, NI NI, JARED M. ALLRED, Chemistry department, Princeton University, BENNY C. CHAN, Department of Chemistry, The College of New Jersey, ROBERT J. CAVA, Chemistry department, Princeton University, NI NI, J. M. ALLRED, R. J. CAVA TEAM, B. C. CHAN COLLABORATION — In this talk, we will present the crystal structures and physical properties of two new iron arsenide superconductors, $\text{Ca}_{10}(\text{Pt}_3\text{As}_8)(\text{Fe}_2\text{As}_2)_5$ (the “10-3-8 phase”) which crystallizes in the triclinic structure and $\text{Ca}_{10}(\text{Pt}_4\text{As}_8)(\text{Fe}_2\text{As}_2)_5$ (the “10-4-8 phase”) which crystallizes in the tetragonal structure. They are very similar compounds for which the most important differences lie in the structural and electronic characteristics of the intermediary platinum arsenide layers. Electron doping through partial substitution of Pt for Fe in the FeAs layers leads to T_c of 11 K in the 10-3-8 phase and 26 K in the 10-4-8 phase. The anisotropic H_{c2} measurement indicates the multiband superconductivity in these compounds. The often-cited empirical rule in the arsenide superconductor literature relating T_c to As-Fe-As bond angles does not explain the observed differences in T_c of the two phases; rather, comparison suggests the presence of stronger FeAs interlayer coupling in the 10-4-8 phase due to the two-channel interlayer interactions and the metallic nature of its intermediary Pt_4As_8 layer. The interlayer coupling is thus revealed as important in enhancing T_c in the iron pnictide superconductors.

¹This work was supported by the AFOSR MURI on superconductivity. Preliminary XRD data was collected with funds from the NSF Major Research Instrumentation program 0922931.

9:12AM Y22.00005 Influence of Cr-doping on the magnetic structure of the FeAs strip compounds CaFe_4As_3 : a single crystal neutron diffraction study, PASCAL MANUEL, ISIS Facility, STFC Rutherford Appleton Laboratory, Chilton, Didcot OX11 0QX, United Kingdom, LAURENT CHAPON, Institut Laue Langevin, 6 rue Jules Horowitz, BP156, Grenoble Cedex 9, France, ILLIYA TODOROV, DUCK Y. CHUNG, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, BACHIR OULADDIAF, Institut Laue Langevin, 6 rue Jules Horowitz, BP156, Grenoble Cedex 9, France, MERCOURI G. KANATZIDIS, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439 & Department of Chemistry, Northwestern University — CaFe_4As_3 offers the unique opportunity to modify the topology of the Fe_2As_2 layers, key in the understanding of superconductivity in the new iron pnictide superconductors, from infinite layers to strips of finite width linked a rectangular cross pattern. Bulk measurement on CaFe_4As_3 indicate a magnetic ordering at 90K with a second transition seen at about 26K. Neutron diffraction allowed to ascribe the high temperature transition to a Spin Density Wave(SDW) with a propagation vector $\mathbf{k}=(0,\delta,0)$ eventually locking to $\delta=3/8$ at the lower transition. As expected a profound effect on the magnetic properties of CaFe_4As_3 can be obtained by chemically doping or applying pressure. We report here on the consequence of Cr-doping on the magnetic structure of CaFe_4As_3 derived from single crystal neutron diffraction.

9:24AM Y22.00006 Anisotropic H_{c2} curves determined up to 92 T and the signature of two-band superconductivity in the novel superconductor $\text{Ca}_{10}(\text{Pt}_4\text{As}_8)((\text{Fe}_{1-x}\text{Pt}_x)_2\text{As}_2)_5$, EUNDEOK MUN, VIVIEN ZAPF, OSCAR AYALA, ROSS MCDONALD, NEIL HARRISON, National High Magnetic Field Laboratory (NHMFL), Los Alamos National Lab (LANL), Los Alamos, NM, NI NI, JARED ALLRED, ROBERT CAVA, Department of Chemistry, Princeton University, Princeton, NJ 08544, USA — The upper critical fields, $H_{c2}(T)$, of single crystals of the novel superconductor $\text{Ca}_{10}(\text{Pt}_4\text{As}_8)((\text{Fe}_{1-x}\text{Pt}_x)_2\text{As}_2)_5$ with $x=0.02$ were determined over a wide range of temperatures down to $T = 1.42$ K and magnetic fields up to $H = 92$ T. The measurements of anisotropic $H_{c2}(T)$ curves are performed in pulsed magnetic fields using radio-frequency contactless penetration depth measurements for magnetic field applied both parallel and perpendicular to the ab-plane. Whereas a clear upward curvature in $H_{c2}^c(T)$ along $H||c$ is observed with decreasing temperature, the $H_{c2}^{ab}(T)$ along $H||ab$ shows a flattening at low temperatures. The rapid increase of the $H_{c2}^c(T)$ suggests that the superconductivity can be described by two dominating bands. The anisotropy parameter, $H_{c2}^{ab}(T)/H_{c2}^c(T)$, is ~ 7 close to T_c and decreases considerably to ~ 1 with decreasing temperature, showing rather weak anisotropy at low temperatures.

9:36AM Y22.00007 Direct measurement of the absolute value of the magnetic penetration depth in two-dimensional pnictide superconductor $\text{Ca}_{10}(\text{Pt}_3\text{As}_8)[(\text{Fe}_{1-x}\text{Pt}_x)_2\text{As}_2]_5$, JEEHOON KIM, FILIP RONNING, LANL, EVGENY NAZARETSKI, BNL, NI NI, J.M. ALLRED, R.J. CAVA, Princeton University, J.D. THOMPSON, R. MOVSHOVICH, LANL — We have measured the absolute value of the magnetic penetration depth λ in a single crystal of the $\text{Ca}_{10}(\text{Pt}_3\text{As}_8)[(\text{Fe}_{1-x}\text{Pt}_x)_2\text{As}_2]_5$ ("10-3-8") superconductor using low temperature magnetic force microscopy (MFM). We directly probed local values of λ in the "10-3-8" sample using Meissner response measurements and compared Meissner curves to those obtained in a Nb reference sample. The Meissner response measured at different locations on the sample shows similar behavior indicating homogeneity of the superconducting state, in accord with tunnel-diode resonator measurements. We also discuss larger values of λ in 10-3-8 relative to λ values measured in other pnictide systems.

9:48AM Y22.00008 Local Displacements, Magnetoelastic Coupling, and Bonding in Spin-Ladder Iron Selenides, JAMES NEILSON, JOSEPH CARON, DAVID MILLER, Johns Hopkins University, ANNA LLOBET, Los Alamos National Laboratory, TYREL MCQUEEN, Johns Hopkins University — The spin-ladder "1-2-3" compounds BaFe_2Se_3 and KFe_2Se_3 , built of double-chains of edge-sharing $[\text{FeSe}_4]$ tetrahedra, are localized-moment antiferromagnetic semiconductors. Total neutron scattering of BaFe_2Se_3 reveals local iron displacements coupled to long-range ordered antiferromagnetism comprised of ferromagnetic Fe_4 plaquettes. The magnitude of the iron displacements follow the antiferromagnetic order parameter: a manifestation of magnetoelastic coupling. These local displacements are essential for properly understanding the electronic structure of these systems, as local structural modulations necessarily perturb the ground state wavefunctions. Furthermore, while iron displacements from magnetoelastic coupling in FeX_4 -based materials are hypothesized to be important in the emergence of superconductivity, the spin-ladders remain insulating down to 1.8 K, even upon hole doping by substitution of K for Ba. As with the copper oxide superconductors two decades ago, our results highlight the importance of reduced dimensional spin-ladder compounds in the study of the coupling of spin, charge, and atom positions in superconducting materials.

10:00AM Y22.00009 Spin glass and semiconducting behavior of the flux grown $\text{BaFe}_{2-\delta}\text{Se}_3$ crystals¹, BAYRAMMURAD SAPAROV, STUART CALDER, BALAZS SIPOS, HUIBO CAO, SONGXUE CHI, DAVID SINGH, ANDREW CHRISTIANSON, MARK LUMSDEN, ATHENA SEFAT, Oak Ridge National Laboratory — In this talk, physical properties and crystal and electronic structures of $\text{BaFe}_{2-\delta}\text{Se}_3$ crystals, synthesized using tellurium flux, will be discussed. This phase is an iron-deficient derivative of the ThCr_2Si_2 -type and its structure is made of double chains formed from edge-sharing FeSe_4 tetrahedra. The semiconducting $\text{BaFe}_{2-\delta}\text{Se}_3$ with $\delta \approx 0.2$ does not order magnetically, however, there is evidence for short-range magnetic correlations of spin glass type below 50 K in magnetization, heat capacity and neutron diffraction results. The semiconducting behavior of $\text{BaFe}_{2-\delta}\text{Se}_3$ is in line with the detrimental influence of iron deficiency to the superconductivity in $A_x\text{Fe}_{1.8}\text{Se}_2$ (A = alkali metal) superconductors. The electronic structure calculations suggest that this compound can be considered as a low-dimensional (1D) ladder structure with a weak interchain coupling. Based on the survey of available data on BaFe_2Se_3 so far, lower concentrations of iron vacancies may lead to a long range antiferromagnetic order, whereas higher concentrations of iron vacancies may suppress long range order and then lead to a spin glass behavior.

¹This work was supported by the Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division and Scientific User Facilities Division.

10:12AM Y22.00010 $\text{Ba}_{1-x}\text{K}_x\text{Mn}_2\text{As}_2$: An Antiferromagnetic Local Moment Metal¹, ABHISHEK PANDEY, R.S. DHAKA, J. LAMSAL, Y. LEE, V.K. ANAND, A. KREYSSIG, R.J. MCQUEENEY, A. GOLDMAN, B.N. HARMON, A. KAMINSKI, D. C. JOHNSTON, Ames Laboratory and Dept. Phys. Astron., Iowa State Univ., Ames, IA 50011, T.W. HEITMANN, The Missouri Research Reactor, Univ. Missouri, Columbia, MO 65211 — The syntheses of K-doped single crystalline $\text{Ba}_{0.984}\text{K}_{0.016}\text{Mn}_2\text{As}_2$ and polycrystalline $\text{Ba}_{0.95}\text{K}_{0.05}\text{Mn}_2\text{As}_2$ with the tetragonal ThCr_2Si_2 structure are reported. Electrical resistivity, heat capacity, magnetic susceptibility, angle-resolved photoemission spectroscopy and neutron diffraction measurements and spin-polarized electronic structure calculations consistently establish that these hole-doped $\text{Ba}_{1-x}\text{K}_x\text{Mn}_2\text{As}_2$ samples are antiferromagnetic local-moment metals, in contrast to the parent BaMn_2As_2 [1-3] which is an antiferromagnetic local-moment semiconductor. This new class of materials bridges the gap between the iron pnictide and cuprate high T_c materials. Investigations of the phase diagram of the $\text{Ba}_{1-x}\text{K}_x\text{Mn}_2\text{As}_2$ system and other similar systems are underway.

[1] Y. Singh et al., Phys. Rev. B **79**, 094519 (2009).

[2] Y. Singh et al., Phys. Rev. B **80**, 100403 (2009).

[3] D. C. Johnston et al., Phys. Rev. B **84**, 094445 (2011).

¹Research at Ames Laboratory was supported by the USDOE-Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

10:24AM Y22.00011 Role of ruthenium in iron-based superconductors and related materials¹

, MICHAEL MCGUIRE, ATHENA SEFAT, BRAIN SALES, Oak Ridge National Laboratory — Ruthenium and iron share the same valence electron count, and form many isostructural compounds. However, the larger covalent radius and extent of the d-electrons of ruthenium lead to interesting and sometimes unexpected behavior when iron is partially or fully substituted by ruthenium. For example, “doping” layered iron compounds with ruthenium has been shown to produce superconductivity in some cases but not others, and ruthenium analogs of certain layered iron compounds do not form under similar conditions. We have investigated full and partial ruthenium substitution in several iron-based materials, including the superconducting 1111 and 122 families, and studied the effects on formation, crystal structures, and physical properties. Our new experimental findings and results from available literature will be used to discuss the unusual role that ruthenium plays in iron-based superconductors and related materials.

¹Research supported by the US Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division

10:36AM Y22.00012 Neutron Diffraction Studies on $\text{Ba}_{0.95}\text{K}_{0.05}\text{Mn}_2\text{As}_2$, J. LAMSAL, Ames Lab and Dept.

Phys. Astron., Iowa State Univ, Ames, IA 50011, T.W. HEITMANN, The Missouri Research Reactor, Univ. of Missouri, Columbia, MO 65211, A. PANDEY, V.K. ANAND, Y. LEE, R.S. DHAKA, A. KAMINSKI, B.N. HARMON, D.C. JOHNSTON, R.J. MCQUEENEY, A. KREYSSIG, A.I. GOLDMAN, Ames Lab and Dept. Phys. Astron., Iowa State Univ, Ames, IA 50011 — There has been a great deal of interest in compounds, such as BaMn_2As_2 , which are closely related to the iron pnictide superconductors. Although undoped BaMn_2As_2 is an antiferromagnetic (AF) insulator[1, 2], recent studies of lightly doped $\text{Ba}_{1-x}\text{K}_x\text{Mn}_2\text{As}_2$ have shown a striking change to metallic behavior for $x > 0.01$ and, therefore, may offer a bridge between the high T_c cuprates and the iron-pnictide superconductors. We will present neutron diffraction measurements on polycrystalline $\text{Ba}_{0.95}\text{K}_{0.05}\text{Mn}_2\text{As}_2$ performed on the powder diffractometer at the Missouri Research Reactor. Our measurements reveal that the antiferromagnetism in the doped compound remains nearly the same as that found for undoped BaMn_2As_2 , characterized by a G-type collinear AF spin structure below $T_N \sim 607(2)$ K with an ordered moment of $4.21(6) \mu_B/\text{Mn}$ ion at 14 K. Research at Ames Lab was supported by the USDOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

[1] Y. Singh et al., Phys. Rev. B **80**, 100403 (2009).

[2] D. C. Johnston et al., Phys. Rev. B **84**, 094445 (2011).

10:48AM Y22.00013 Growth of parent and electron doped NaFeAs , YU SONG, University of Tennessee —

It has been found hole doping on Fe sites in BaFe_2As_2 does not induce superconductivity with Cr and Mn as dopants, but doping on Ba sites with K induces superconductivity as high as 38K. We have investigated hole doping with Titanium to be compared with other hole doping compounds. Single crystals of Titanium doped BaFe_2As_2 were grown by flux method. Transport and susceptibility measurements were done showing doping Titanium suppresses the Neel temperature but no superconductivity was found up to 4% doping. Susceptibility measurements also showed spin glass behavior. Phase diagrams of temperature vs doping concentration have been constructed from transport and Susceptibility measurements.

Friday, March 2, 2012 8:00AM - 11:00AM —

Session Y23 DCMP: Superconductor-Insulator Transitions 255

8:00AM Y23.00001 Theory of Giant Magnetoresistance Peak in InO Superconducting Films

, ANIRBAN GANGOPADHYAY, JOE MITCHELL, VICTOR GALITSKI, University of Maryland, College Park, MARKUS MUELLER, The Abdus Salam International Centre for Theoretical Physics — It has been suggested that the giant magnetoresistance peak seen on the insulating side of a superconductor-insulator transition in $\text{In}_2\text{O}_{3-x}$ films is a signature of remanent localized pairs which can participate in variable-range-hopping transport. A theory of pair-transport must necessarily take into account the bosonic nature of the pairs, as opposed to the fermionic nature of single-electron carriers. We show that this opposite statistical nature of the carriers alone can lead to opposite variations of the localization length with magnetic field and thus be a possible candidate for explaining the giant magnetoresistance peak. We further provide an explanation of the pairing mechanism in $\text{In}_2\text{O}_{3-x}$ films. We argue that the electron pairing mechanism here is non-BCS-type and is related instead to the local effect of electron pairs occupying Oxygen vacancies (with charge +2e). The neutral state of these defects may be more stable than the singly-charged defect, as supported by an ab initio analysis. This simple phenomenon leads naturally to a negative-U Hubbard model with strong disorder.

8:12AM Y23.00002 Broadband microwave study of 2D superconductor-insulator quantum phase transition , WEI LIU, LIDONG PAN, Johns Hopkins University, MINSOO KIM, SAMBANDAMURTHY GANAPATHY, SUNY-Buffalo, PETER ARMITAGE, Johns Hopkins University —

Using our broadband microwave spectrometer, we investigate the complex AC conductance of disordered InO_x films as a function of magnetic field through the 2D superconductor-insulator quantum phase transition. We have studied the behaviors of the frequency dependent complex response function of a particular InO_x sample near the critical point in the limit of $\hbar\omega < K_B T$ and $\hbar\omega > K_B T$ and compare our results to theoretical models. We discuss the possibility for a novel insulating state on the insulating side of the transition through the frequency dependent conductance.

8:24AM Y23.00003 Superconductor-insulator transition in amorphous indium oxide films: Role of in-plane magnetic field , MINSOO KIM, TAILUNG WU, GANAPATHY SAMBANDAMURTHY, SUNY Buffalo, Buffalo, NY 14260 —

We present experimental results from transport studies on amorphous indium oxide films that are driven through a superconductor-insulator transition by applying a pair-breaking magnetic field. The direction of the magnetic field is varied continuously from being perpendicular to the film plane to parallel to the film plane and we identify characteristically different transport regimes at different magnetic field values when the film is rotated in a magnetic field. We also study the evolution of these transport regimes as a function of disorder in these films. A distinctly clear magnetic field value, in the insulating phase, at which the sample resistance is independent of the angle and very weakly dependent on temperature and disorder is observed. Implications for our current understanding of the 2D superconductor - insulator transition will be presented.

8:36AM Y23.00004 Evolution of magnetoresistance peak on disordered systems¹ , YEONBAE LEE,

University of Minnesota, Minneapolis — Measurements of the electric and magnetic properties of amorphous indium oxide films are reported. The carrier densities of films have been tuned by employing electrostatic gating using electric double layer transistor (EDLT) configurations employing the ionic liquid DEME.TFSI. We have observed the emergence of the magnetoresistance peak as films are tuned from the insulating to the superconducting regimes, and its disappearance as the system is doped further with additional carriers. The result also demonstrates the reversible tuning of the superconductor-insulator transition with low gate voltages

¹This work was supported by the DOE under Grant No. DE-FG02-02ER46004

8:48AM Y23.00005 Superconductor-Insulator transition in long Mo-Ge nanowires, HYUNJEONG KIM, ANDREY ROGACHEV, University of Utah — We have studied transport properties of two series of long (1-25 μ m) and very narrow (9-20nm) homogenous amorphous Mo-Ge wires fabricated by advanced electron beam lithography. We observed that the wires undergo a superconducting-insulator transition that is controlled by the wire cross sectional area, i.e. by local physics. Reduction of mean-field critical temperature can be explained by the fermionic mechanism. We also observed an unusual zero-bias anomaly in the insulating state that has signatures of both Coulomb blockade and perturbative electron-electron interaction correction. In addition, some of our long superconducting wires appear to be localized superconductor, namely in these wires one-electron localization lengths is several times shorter than the length of a wires.

9:00AM Y23.00006 The extent of the Cooper pair insulator phase in amorphous $\text{Pb}_{0.9}\text{Bi}_{0.1}$ nanohoneycomb films¹, S.M. HOLLEN, J.C. JOY, A.H. BERG, Brown University, Department of Physics, G.E. FERNANDES, Brown University, Division of Engineering, J. SHAINLINE, Brown University, Department of Physics, J.M. XU, Brown University, Division of Engineering, J.M. VALLES, JR., Brown University, Department of Physics — Amorphous Bi nanohoneycomb (NHC) thin films, which contain a nanometer-scale array of holes and regular thickness undulations, exhibit an insulating phase made up of localized Cooper pairs (CPs) near their thickness-driven insulator to superconductor transition (IST). This Cooper pair insulator (CPI) phase includes a giant magnetoresistance peak, also observed in InO_x and TiN. We have now produced NHC films of a new material, $\text{Pb}_{0.9}\text{Bi}_{0.1}$, that show a qualitatively similar CPI phase. We will show the evolution of this CPI phase from deep in the insulating state to the IST using transport measurements. Throughout this regime, we will track the appearance, growth, and range of the magnetoresistance oscillations (which indicate CP transport) and giant magnetoresistance peak. Considering these observations, we will discuss the likely extent of CP transport in these insulators.

¹This work is supported by the AAUW, the NSF through Grant No. DMR-0605797 and No. DMR-0907357, by the AFRL, and by the ONR.

9:12AM Y23.00007 Superconductor-to-Insulator Transition in $\text{BaPb}_{1-x}\text{Bi}_x\text{O}_3$, PAULA GIRALDO-GALLO, Geballe Laboratory for Advanced Materials and Department of Physics, Stanford University, HAN-OH LEE, Geballe Laboratory for Advanced Materials, Stanford University and SLAC National Accelerator Laboratory, THEODORE GEBALLE, IAN FISHER, Geballe Laboratory for Advanced Materials and Department of Applied Physics, Stanford University — BaBiO_3 is a charge density wave (CDW) insulator. Hole doping with Pb, i.e. $\text{BaPb}_{1-x}\text{Bi}_x\text{O}_3$, eventually suppresses the CDW, leading to superconductivity, with a maximum critical temperature T_c of 10 to 13K for $x \approx 0.25$. The origin of the CDW state, its doping dependence, the nature of the pairing mechanism and the effects introduced by disorder remain open questions. Here we investigate the normal state properties in the vicinity of the metal-semiconductor transition. Single crystalline samples of the solid solution $\text{BaPb}_{1-x}\text{Bi}_x\text{O}_3$, with $0 < x < 0.35$ were grown using a flux technique, and studied via measurements of resistivity, magnetoresistance, magnetic susceptibility and heat capacity. For compositions near the optimal doping, the material exhibits a magnetic field tuned superconductor-to-insulator transition with a temperature independent crossing point in resistivity, scaling as $\rho(T, H) = \rho_c f(|H - H_{\text{cross}}|T^{-1/0.65})$ for fields around H_{cross} , the crossing point field. These results are discussed in the context of quantum phase transitions and compared to the results obtained in 2D disordered thin films of other novel materials.

9:24AM Y23.00008 Electrostatic doping of high T_c superconductors¹, JOSEPH KINNEY, JAVIER GARCIA-BARRIOCANAL, XIANG LENG, ALEXEY KOBRINSKII, BOYI YANG, STEPHEN SNYDER, ALLEN GOLDMAN, University of Minnesota — The application of field effect transistor concepts to electrostatically doped strongly correlated electron systems has been the focus of intense research during the last years [C. H. Ahn et al., Rev. Mod. Phys. 78, 1185 (2006)]. In this talk we will show our recent results on Electronic Double Layer Transistor (EDLT) techniques applied to high T_c cuprates. The EDLT configuration, which employs ionic liquids as gate dielectrics, has succeeded in achieving unprecedented charge transfers, of the order of 10^{15} carriers/cm². This large accumulation and depletion of carriers allows us to explore the phase diagram of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ and $\text{La}_2\text{CuO}_{4+\delta}$. We will focus on the physics of the superconductor to insulator transition [X. Leng et al., Phys. Rev. Lett. 107, 027001 (2011)] and discuss the magneto-transport properties of the underdoped and overdoped regions of the phase diagram [X. Leng, et al., arXiv:1108.0083v1].

¹NSF/DMR-0709584 and NSF/DMR-0854752

9:36AM Y23.00009 Dynamic charge order and superconductivity in lightly doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ thin films¹, XIAOYAN SHI, D. POPOVIC, Dept. of Phys. & Natl. High Magnetic Field Lab., Florida State Univ., C. PANAGOPOULOS, Dept. of Phys., Univ. of Crete and FORTH & Div. of Phys. and Appl. Phys., Nanyang Tech. Univ., A. BOLLINGER, G. LOGVENOV, I. BOZOVIC, Brookhaven Natl. Lab. — Recent experiments have demonstrated the existence of a charge glass state at very low temperatures deep within the spin glass phase ($T \ll T_{SG}$) in lightly doped, insulating $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) with $x = 0.03$. Here we use magnetotransport measurements in a series of high quality MBE-grown LSCO films ($x = 0.03, 0.05, 0.055$, and 0.06) to investigate the doping dependence of this dynamically inhomogenous, charge ordered state as the superconductor-insulator transition (SIT) is approached. We show that the charge glassiness is suppressed with doping. Nevertheless, close enough to the SIT on the insulating side, it coexists and competes with superconducting fluctuations (SCFs), leading to a suppression of SCFs at low T .

¹Supported by NSF DMR-0905843, NHMFL via NSF DMR-0654118, EURYI, MEXT-CT-2006-039047, the National Research Foundation of Singapore, US DOE, Basic Energy Sciences, Materials Sciences and Engineering Division, and the Center for Emergent Superconductivity.

9:48AM Y23.00010 Two component Coulomb glass in disordered superconducting films, JOE MITCHELL, ANIRBAN GANGOPADHYAY, VICTOR GALITSKI, University of Maryland, College Park, MARKUS MUELLER, The Abdus Salam International Center for Theoretical Physics — We propose a new two component Coulomb glass model which includes strong disorder, Coulomb interaction, and on-site electron pairing to investigate the effects of localized pairing in disordered films on the insulating side of a superconductor-insulator transition. In particular, we show how the density of states (DOS) changes with increasing on-site coupling between electrons, from an Efros-Shklovskii linear DOS for the electrons at weak coupling, to a strongly modified, non-monotonic DOS with nonuniversal Coulomb gap for electrons and on-site pairs at moderate coupling, and finally to an Efros-Shklovskii linear DOS for pairs at strong coupling. We discuss the effects of a spatially random coupling. We use a Miller Abrahams resistor network mapping to numerically calculate resistance for samples of this model, given temperature and localization length. With certain parameter choices, we can obtain a peak in resistance with respect to magnetic field, reminiscent of magnetoresistance peaks reported experimentally.

10:00AM Y23.00011 ABSTRACT WITHDRAWN —

10:12AM Y23.00012 Superconductor-insulator transition in Josephson junction arrays screened by a superconducting ground plane, JOSHUA PARAMANANDAM, MICHAEL GERSHENSON, Rutgers University — We have studied quantum phase transitions in unconventional Josephson arrays with a large number of interacting nearest-neighbour islands (typically, 10). The range of inter-island interactions was controlled by the presence/absence of a superconducting ground plane placed in close proximity to the array. We have found that the superconductor-to-insulator transition occurs in the arrays with both short- and long-range interactions at $E_J/E_C \sim 1$. Here E_J is the effective Josephson energy per island, E_C is its charging energy. However, the critical resistance for the arrays with short-range interactions greatly exceeds the quantum resistance, in contrast to the case of arrays with long-range interactions. These experiments clearly show that the ratio E_J/E_C is the only relevant (for the SIT) parameter, while the critical resistance can vary a great deal depending on the interaction range.

10:24AM Y23.00013 Strong quantum interference in strongly disordered bosonic insulators, SERGEY SYZРАНOV, Institut fuer Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany, ANDREAS MOOR, KONSTANTIN EFETOV, Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany — We study the model of variable-range hopping of bosons in an array of sites with short-range interactions and a large characteristic coordination number, which describes conduction in a broad class of insulators, such as strongly disordered superconductive films, systems close to the Anderson transition, Josephson networks, etc. Large coordination number leads to strong quantum interference phenomena yet allows for their analytical study. We develop a functional renormalization group scheme that repeatedly eliminates high-energy sites properly renormalizing the tunneling between the low-energy ones. Using this approach we determine the temperature and magnetic field dependence of the hopping conductivity and find a large positive magnetoresistance. With increasing magnetic field the behaviour of the conductivity crossovers from the Mott's law to an activation behaviour with the activation gap proportional to the magnetic field.

10:36AM Y23.00014 Numerical identification of three distinct phases in a $(2+1)D$ array of quantum dissipative Josephson junctions, EINAR STIANSEN, IVER BAKKEN SPERSTAD, ASLE SUDBØ, Department of Physics, Norwegian University of Science and Technology, N-7491 Trondheim, Norway — We have performed large-scale Monte-Carlo simulations on a model describing a $(2+1)D$ array of quantum dissipative Josephson junctions. With the superconducting phases as our fundamental degrees of freedom we are able to identify three distinct phases as function of Josephson coupling and dissipation strength. Apart from the fully superconducting state, where fluctuations in both space and time are at bay, and the normal phase, characterized by wild fluctuations, we find an additional phase featuring spatial phase coherence coinciding with temporal disorder.

10:48AM Y23.00015 Metallic state in La-doped $\text{YBa}_2\text{Cu}_3\text{O}_y$ thin films with n-type charge carriers¹, S.W. ZENG, X. WANG, W.M. LV, Z. HUANG, M. MOTAPOTHULA, Z.Q. LIU, Y. L. ZHAO, A. ANNADI, S. DHAR, T. VENKATESAN, - ARIANDO, NUSNNI-Nanocore, National University of Singapore, Singapore — Through substitution of La for Ba and reduction of oxygen, we successfully doped n- and p-type charge carriers into La-doped $\text{YBa}_2\text{Cu}_3\text{O}_y$ thin films synthesized by pulsed laser deposition technique. The n-type samples demonstrated metallic behaviors and in-plane resistivity exhibited a quadratic temperature dependence within the metallic regime, and then evolved into a $\ln T$ -dependence insulating-like state. Furthermore, the doping evolution of temperature with minimum resistivity (T_{min}) and electron-electron rate were investigated and showed asymmetry between p- and n-side. The present results suggest the potential of obtaining n-type superconductivity in La-doped $\text{YBa}_2\text{Cu}_3\text{O}_y$ and investigating n-p asymmetry (symmetry) in cuprates with the same crystallographic structure.

¹We thank National Research Foundation (NRF) Singapore under the Competitive Research Program (CRP) "Tailoring Oxide Electronics by Atomic Control" NRF2008NRF-CRP002-024 and Ministry of Education (MOE) FRC-ARF Grant No. R-144-000-278-112.

Friday, March 2, 2012 8:00AM - 10:48AM – Session Y24 DCOMP: Quantum Many-Particle Systems: DMFT & DMRG 256

8:00AM Y24.00001 A New Lanczos-Based Low Rank Algorithm for Inhomogeneous Dynamical Mean-Field Theory¹, PIERRE CARRIER, YOUSEF SAAD, University of Minnesota, JAMES K. FREERICKS, Georgetown University — Inhomogeneous DMFT is used to approximately solve models of ultracold atoms in optical lattices. The intensive part of the IDMFT algorithm is the solution of the Dyson equation for the local Green's function, which involves the computation of the diagonal of the inverse of a sparse matrix. Our new algorithm for finding the diagonal of the inverse of a large sparse matrix is based on domain decomposition into interior and interface points. Since the number of interface points is much less than the interior points, it is a low-rank matrix. Using this matrix allows for a much smaller number of Lanczos steps to obtain the exact solution of the diagonal of the inverse and hence reduces the need for as many re-orthogonalization steps in Lanczos. We show that the problem of finding the diagonal of the inverse is transformed into a naturally parallel GMRES solver (based on the domain decomposition) solved at each of the Lanczos iterations. We successfully implemented a coarray fortran (CAF) program code of this new algorithm for the 2D Fermionic-Bosonic Falicov-Kimball Hamiltonian (mixture of light and heavy atoms). Results of parallel performance and advantages of using a CAF implementation are discussed, in terms of a 3D implementation which is planned for the Hubbard model.

¹Computations were performed on the Cray XE6 "Hopper", through a 2011 NISE-NERSC award (P. Carrier). This work is supported by NSF grants OCI-0904587 (Y. Saad) and OCI-0904597 (J.K. Freericks).

8:12AM Y24.00002 Continuum Numerical Renormalization Group, NANDAN PAKHIRA, Department of Physics, Georgetown University, Washington, DC 20057, USA, HULLIKEL KRISHNAMURTHY, Department of Physics, Indian Institute of Science, Bangalore 560012, India, JAMES FREERICKS, Department of Physics, Georgetown University, Washington, DC 20057, USA — The numerical renormalization group (NRG) has emerged as one of the most powerful techniques for calculating emergent renormalized low-temperature properties of strongly correlated systems. When applied as an impurity solver within the dynamical mean-field theory (DMFT), it allows one to directly find spectral functions and how they evolve with temperature. In spite of this success, the NRG method has a number of well-known shortcomings. It fails to properly produce the Fermi liquid state down to $T=0$ in DMFT and hence it does not properly calculate transport, and it produces only semiquantitative features of the spectral functions. We believe, this is mainly due to the fact that the spectral representation involves a discrete set of delta function peaks at logarithmically discretized frequency intervals which are broadened to the continuum. The broadening parameters are chosen in an *ad-hoc* basis. Here we formulate this problem as a discrete degree of freedom embedded in a continuum, which involves coupling the original semi-infinite NRG chain to another semi-infinite chain, arising from the neglected continuum degrees of freedom. This residual coupling can be solved perturbatively and provides an *ab initio* approach to constructing spectral functions from the NRG.

8:24AM Y24.00003 Nonequilibrium dynamical mean-field study of correlated electron systems driven by a mono-cycle pulse, NAOTO TSUJI, ETH Zurich, TAKASHI OKA, HIDEO AOKI, Department of Physics, University of Tokyo, PHILIPP WERNER, ETH Zurich — A few-cycle pulse can be generated and has been widely used in recent ultrafast optical experiments, but its potential application to correlated electron systems has remained unexplored in contrast to many-cycle pulses. What is characteristic of the few-cycle pulse is to induce a shift of electron's momentum dynamically. To reveal its effect on the electronic properties of the system, we study the single-band Hubbard model driven by half-cycle and mono-cycle pulses using the nonequilibrium dynamical mean-field theory. As an impurity solver, we employ the continuous-time quantum Monte Carlo method and the iterative perturbation theory. We show that when the momentum shift is nearly π (half of the Brillouin zone) the shifted population relaxes to a negative-temperature state, where the electron-electron interaction is effectively switched from repulsive to attractive. The shift is found to deviate from the dynamical phase $\phi = \int F(t)dt$ due to electron correlation effects, which suggests that one can generate the repulsion-to-attraction transition by a mono-cycle pulse with $\phi = 0$.

8:36AM Y24.00004 PIMC study of spin-polarized 1D trapped fermions with strong attractive contact interaction, CHANGMO YANG, University of Illinois — Spin imbalance in a trapped one-dimensional gas of ^6Li atoms ($F = 1/2$) is studied with continuous-space path-integral Monte Carlo simulation. This follows closely the experiment of Liao et al. [1], which aims to confirm the existence of the FFLO pairing predicted from the Bethe ansatz [2,3] and DMRG [4,5]. Algorithmic improvements [6] to the configuration-space sampling efficiency of a previous work [7] is made in order to explore the conditions where the attractive contact interaction between unlike-spin atoms can be stronger than in the previously accessible. Signatures of FFLO pairing is looked for in the pair momentum distribution.

- [1] Y.-A. Liao et al., *Nature* **467**, 567 (2010).
- [2] X.-W. Guan et al., *Phys. Rev. B* **76**, 085120 (2007).
- [3] E. Zhao et al., *Phys. Rev. Lett.* **103**, 140404 (2009).
- [4] M. Rizzi et al., *Phys. Rev. B* **77**, 245105 (2008).
- [5] F. Heidrich-Meisner et al., *Phys. Rev. A* **81**, 023629 (2010).
- [6] M. Boninsegni et al. *Phys. Rev. E*, **74**, 036701, (2006).
- [7] M. Casula et al. *Phys. Rev. A*, **78**, 033607, (2008).

8:48AM Y24.00005 Stability of Topological Quantum Phases at Zero Temperature, SPYRIDON MICHALAKIS, Caltech, JUSTYNA PYTEL, Oregon State University — We prove stability of the spectral gap for gapped, frustration-free Hamiltonians under general, quasi-local perturbations. We present a necessary and sufficient condition for stability, which we call *Local Topological Quantum Order* and show that this condition implies an area law for the entanglement entropy of the groundstate subspace. This result extends previous work by Bravyi et al, on the stability of topological quantum order for the groundstate subspace of Hamiltonians composed of commuting projections with a common zero-energy subspace. Moreover, our result implies that zero-temperature topological order is robust against quasi-local perturbations, for all topologically ordered subspaces that correspond to the groundstate space of a gapped, frustration-free Hamiltonian. Finally, even in the absence of topological order, we show that symmetry-protected sectors are also stable against perturbations respecting the same symmetries.

9:00AM Y24.00006 Recurrence relations and time evolution in the relativistic electron gas at long wavelengths¹, ERICA SILVA², Instituto de Física, Universidade Federal de Mato Grosso, Cuiabá, MT, Brazil — Some years ago M. Howard Lee developed the recurrence relations method to solve the Heisenberg motion equation in an exact way. The relaxation and memory functions, as other linear-response quantities, e.g., the density-density response function and the dynamic structure factor, were obtained for the two- and three-dimensional non-relativistic electronic systems at long wavelengths. In this work we study the time- and frequency-dependent behavior of the relativistic electron gas. As some applications, one can cite graphene, in two dimensions, and dwarf stars, in the three-dimensional case, since both systems have a relativistic electron gas in their compositions.

¹Work supported by CAPES (Brazilian Agency) under Grant No. 1177/10-9.

²Present address: Department of Physics and Astronomy, University of Georgia, Athens, GA, USA

9:12AM Y24.00007 Combining Tensor Networks with Monte Carlo: Applications to the MERA, ANDY FERRIS, Université de Sherbrooke, GUIFRE VIDAL, Perimeter Institute for Theoretical Physics — Our recent understanding of the entanglement properties of ground states of many-body quantum systems has led to the development of a variety of variational wavefunctions based on tensor networks. The so-called *bond dimension* of the tensor network, χ , sets both the limit to the amount of entanglement allowed in the ansatz as well as the required computational power to contract the tensor network. Because the cost scales very strongly with χ in higher dimensions, these approaches are currently challenging in 2D and currently unusable in 3D. We present our efforts in combining Monte Carlo techniques with tensor networks to ease the computational bottleneck. Classical Monte Carlo sampling can be used to estimate the contracted value of the network, allowing one to sample expectation values and vary parameters to optimize ground states. In particular, we show a perfect sampling scheme can be efficient for tensor networks which are also unitary quantum circuits. We apply this to the Multi-scale Entanglement Renormalization Ansatz (MERA) in 1D, formally reducing the cost from $O(\chi^9)$ to $O(\chi^5)$ per sample, and demonstrate that we can optimize wavefunctions. We expect the advantages from Monte Carlo sampling will be stronger in 2D and 3D systems.

9:24AM Y24.00008 Recent Progress In Exactly Solvable Discrete Models for Topological Phases in Two Dimensions¹, YONG-SHI WU², YUTING HU, SPENCER D. STIRLING³, Department of Physics and Astronomy, University of Utah — The study of two-dimensional topological phases in condensed matter systems is a frontier in the field of condensed matter theory as well as topological quantum computation. Discrete or lattice models, which are exactly solvable have been proposed by Kitaev and by Levin and Wen, respectively, some years ago. Here we present a summary of recent progress in studying these models and their generalizations. The topics to be covered include 1) Duality between the Kitaev and Levin-Wen models in certain special cases; 2) General procedure for computing ground state degeneracy when the models are put on a topologically non-trivial surface; 3) More detailed study of the properties (exchange and exclusion statistics etc) of topological excitations (e.g. fluxons); 4) General framework for studying constraints of topological invariance on a wide class of discrete models on more general fluctuating graphs; 5) Generalization of these models to general graphs that incorporates more general degrees of freedom. Our approach, though closely related to topological field theory and tensor category theory, could be understood by physicists.

¹YSW is supported in part by US NSF grant No, 1068558

²Key State Laboratory of Surface Physics, and Department of Physics, Fudan University, Shanghai, China

³Department of Mathematics, University of Utah

9:36AM Y24.00009 Time Evolution of Density Matrices Using BBGKY Hierarchy, ALI AKBARI, Nano-Bio Spectroscopy Group, Departamento de Física de Materiales, Universidad del País Vasco, San Sebastián, Spain, JAVAD HASHEMI, RISTO NIEMINEN, Department of Applied Physics, Aalto University, P.O. Box 11100, FI-00076 AALTO, Finland, ROBERT VAN LEEUWEN, Department of Physics, Nanoscience Center, FIN 40014, University of Jyväskylä, Jyväskylä, Finland, ANGEL RUBIO, Nano-Bio Spectroscopy Group, Departamento de Física de Materiales, Universidad del País Vasco, San Sebastián, Spain — Our work starts with the BBGKY hierarchy equations which can be straightforwardly derived from the time-dependent Schrödinger equation for each n -body reduced density matrices (n -RDM). The equations of the BBGKY hierarchy in each level, couple an n -RDM to the $(n + 1)$ -RDM. In order to make this set of equations tractable we need to truncate the hierarchy. While people usually truncate the hierarchy at the first level, one can also truncate it at the level of second equation by approximating 3-RDM in terms of 2-RDM and 1-RDM. Regardless of approximations that we choose, the total energy and momentum will be conserved if we solve the first and second equation together. However, we will show that most of the existing approximations are unstable and even diverging in time and ponder the reasons behind it.

9:48AM Y24.00010 Optimizing Matrix- and Tensor-Product Algorithms for Momentum-Space Hamiltonians using Quantum Entropy, REINHARD NOACK, Philipps-University Marburg, ÖRS LEGEZA, JENŐ SÓLYOM, Research Institute for Solid State Physics, Budapest — Momentum-space formulations of local models such as the Hubbard model are hard to treat using matrix- and tensor-product-based algorithms because they contain non-local interactions. Quantum entropy-based measures such as the single-site and block entropies and the mutual information can be used to map the entanglement structure in order to gain physical information and to optimize algorithms. In this contribution, we will discuss the optimization of density-matrix-renormalization-group and tree-tensor-network algorithms and their application to the two-dimensional Hubbard model.

10:00AM Y24.00011 Topological liquid nucleation induced by vortex-vortex interactions in Kitaev's honeycomb model, VILLE LAHTINEN, Nordita, ANDREAS LUDWIG, University of Santa Barbara, JIANNIS PACHOS, University of Leeds, SIMON TREBST, Station Q — We provide a microscopic understanding of the nucleation of topological quantum liquids for interacting non-Abelian anyons by making an explicit connection between the microscopics of the pairwise interactions - typically showing oscillations in sign, but decaying exponentially with distance - and the nature of the collective many-anyon state. We investigate this issue in the context of Kitaev's honeycomb lattice model, where non-Abelian vortex excitations can be arranged on superlattices. Depending on microscopic parameters such as the vortex-spacing, we observe the nucleation of several distinct Abelian topological phases. By reformulating the collective behavior of the interacting vortex superlattice in terms of an effective lattice model of tunneling Majorana fermion zero modes, we show that the pairwise interactions fully determine the phase diagram of the nucleated phases. We find that due to the oscillations longer-range interactions beyond nearest neighbor can influence the nature of the collective state and thus need to be included for a comprehensive microscopic picture. Corresponding results should hold for vortices forming an Abrikosov lattice in a p-wave superconductor or quasiholes forming a Wigner crystal in non-Abelian quantum Hall states.

10:12AM Y24.00012 Optimizing the Hartree-Fock orbitals by the DMRG, MINGPU QIN, Institute of Physics, The Chinese Academy of Sciences, HONGGANG LUO, Lanzhou University, P.R. China, TAO XIANG, Institute of Physics, The Chinese Academy of Sciences — We have proposed a density matrix renormalization group (DMRG) scheme to optimize the one-electron basis states of molecules. It improves significantly the accuracy and efficiency of the DMRG in the study of quantum chemistry or other many-fermion system with nonlocal interactions. For a water molecule, we find that the ground state energy obtained by the DMRG with only 61 optimized orbitals already reaches the accuracy of best quantum Monte Carlo calculation with 92 orbitals.

10:24AM Y24.00013 Determination of Boundary Scattering, Intermagnon Scattering, and the Haldane Gap in Heisenberg Chains¹, HIROSHI UEDA, KOICHI KUSAKABE, Graduate School of Engineering Science, Osaka University — Low-lying magnon dispersion in a $S = 1$ Heisenberg antiferromagnetic (AF) chain with boundary $S/2$ spins coupling antiferromagnetically ($J_{\text{end}} > 0$) is analyzed by use of the non-Abelian DMRG method. The Haldane gap Δ , the magnon velocity v , the inter-magnon scattering length a , and the scattering length a_b of the boundary coupling are evaluated. The length a_b , which represents the contribution of boundary effects, depends on J_{end} drastically, while Δ , v , and a are constant irrespective of J_{end} . Our method estimates the gap of the $S = 2$ AF chain as $\Delta = 0.0891623(9)$ using a chain length up to 2048, which is longer than the correlation length.

¹This work was supported in part by a Grant-in-Aid for JSPS Fellows, Grant-in-Aids (No. 19051016), and Global COE Program (Core Research and Engineering of Advanced Materials Interdisciplinary Education Center for Materials Science) from MEXT of Japan.

10:36AM Y24.00014 Fractional exclusion statistics: the paradigm to describe interacting particle systems¹, ANGHEL DRAGOS-VICTOR, Horia Hulubei National Institute of Physics and Nuclear Engineering — The thermodynamics and statistical mechanics calculations for systems of interacting particles represent in general a difficult task. Even in relatively simple cases, like systems described in the Fermi liquid theory or in the Hartree or Hartree-Fock approximations, the dependence of the quasiparticle energies on the population of all the quasiparticle energy levels makes it impossible to apply the standard formalism. This is because either the sum of quasiparticle energies is different from the total energy of the system or the typical Bose and Fermi populations do not maximize the partition function. The solution to this problem is provided by the application of the fractional exclusion statistics. In this presentation I will compare the standard treatment of systems of interacting particles, given in terms of the Bose or Fermi populations of the quasiparticle energy levels, with a method based on the fractional exclusion statistics. This method is the only paradigm for describing rigorously the interacting particle systems in terms of quasiparticles.

¹Financial support from the ANCS grant 114/05.10.2011 and JINR-IFIN grants N4063 and Titeica-Markov

Friday, March 2, 2012 8:00AM - 11:00AM – Session Y25 DCOMP DMP: Focus Session: Multiscale Modeling 257A

8:00AM Y25.00001 The heterogeneous multiscale method: A ten-year review, WEINAN E, Peking University, Princeton University — The heterogeneous multiscale method (HMM) was proposed 10 years ago, as a unified framework for designing multiscale algorithms in different applications. It is a top-down strategy in the sense that it relies on a preconceived form of macroscale model. Missing data in the macroscale model are estimated on the fly using a reliable microscale model. In this talk, we will take a critical look at HMM. We will discuss applications to various problems, including dynamic fracture, complex fluids, transition pathways in complex systems and stochastic simulation algorithms. We will also examine areas where improvement are needed in order to make HMM more successful.

8:36AM Y25.00002 Progress Towards Atomistic Simulations that Reach Anthropological Timescale and Beyond¹

JU LI, MIT — Atomistic and first-principles modeling, which describe the world as assembly of atoms and electrons, provide the most fundamental answer to problems of materials. However, they also suffer the most severe timescale limitations. For instance, in molecular dynamics (MD) simulations, in order to resolve atomic vibrations, the integration time step is limited to hundredth of a picosecond, and therefore the simulation duration is limited to sub-microsecond due to computational cost. Although a nanosecond simulation is often enough (surprisingly) for many physical and chemical properties, it is usually insufficient for predicting microstructural evolution and thermo-mechanical properties of materials. In this invited talk I will discuss recent attempts at overcoming the timescale challenges of atomic-resolution simulations: (a) strain-boost hyperdynamics [Phys. Rev. B 82 (2010) 184114] for simulating primarily displacive events and associated issues of activation entropy and the Meyer-Neldel compensation rule, (b) diffusive molecular dynamics (DMD) [Phys. Rev. B 84 (2011) 054103] for microstructural evolution driven by repetitive diffusion events and coupled displacive-diffusive processes, and (c) a Markovian network statistical mechanical treatment of the energy-landscape basin connectivity and a formula for the viscosity of supercooled liquid and glass [PLoS ONE 6 (2011) e17909]. Challenges and future directions are discussed.

9:12AM Y25.00003 Adaptation of multiscale thermal modeling methods to general crystalline solids

BRENT KRACZEK, PETER CHUNG, Computational and Informational Science Directorate, US Army Research Laboratory — From the nano- to micro-scale, phonons act as the primary mechanism for energy transport and storage in most non-metallic, crystalline materials. While phonon properties are determined by interatomic interactions on the scale of the atomistic unit cell, phenomena and microstructures of interest are often at length and time scales that are too large for atomistic simulations. The phonon Boltzmann transport equation (pBTE) enables continuum-scale calculations that capture both atomistic- and continuum-scale thermal behavior, though so far pBTE-based methods have been limited primarily to silicon [1]. We have developed a pBTE-based method for general crystalline materials with up to hundreds of atoms per unit cell. We demonstrate its applicability in silica (9-atom unit cell) and RDX (168-atom unit cell), though presently limited to one dimension in k-space. We discuss the main challenges when moving to larger unit cells, including the automated untangling of phonon dispersion data, discretization of phonon modes and the treatment of high energy modes, including the omission and/or lumping of modes and the use of reservoir modes.

[1] Chunjian Ni and J. Murthy, in *11th Intersociety Conference on Thermal and Thermomechanical Phenomena in Electronic Systems, ITherm*, 2008, 1097

9:24AM Y25.00004 Extended Lagrangian Born-Oppenheimer Molecular Dynamics: quantum mechanical molecular dynamics for extended time and length scales¹

ANDERS NIKLASSON, MARC CAWKWELL, Los Alamos National Laboratory — Born-Oppenheimer molecular dynamics (BOMD) based on density functional theory offers a very accurate quantum mechanical approach to atomistic simulations that is more reliable and general compared to classical MD. Unfortunately, BOMD simulations are often limited by a high computational cost or by problems such as unbalanced phase space trajectories, numerical instabilities and a systematic long-term energy drift. These problems become particularly severe in combination with reduced complexity or linear scaling algorithms that are necessary for the study of large systems. We have recently taken some steps toward a new generation of first principles MD, which combines some of the best features of regular BOMD and Car-Parrinello MD, while avoiding their most serious shortcomings. The new dynamics is given in terms of an extended Lagrangian (XL), where auxiliary extended electronic degrees of freedom are added to the nuclear part. Our framework enables accurate geometric integration of both the nuclear and electronic degrees of freedom that provide a time-reversible and energy conserving dynamics on the ground state BO potential energy surface that is stable also under approximate SCF convergence. XL-BOMD provides a surprisingly simple and general framework for atomistic simulations

¹DOE, BES Office of Science and LDRD-DR

9:36AM Y25.00005 Multi scale modeling of atomic layer deposition¹

MAHDI SHIRAZI, SIMON D. ELLIOTT, Tyndall National Institute — Atomic layer deposition (ALD) is one of the techniques now used to grow conformal nanometer thin films with the quality required for electronic devices. ALD is a type of chemical vapor deposition that depends on self-limiting surface chemistry. Many aspects of chemical reactions and their effect on the stoichiometry of the film remain unclear. We have used therefore density functional theory (DFT) to explore those reactions. The growth of HfO₂ from H₂O and Hf(N(CH₃)₂)₄ was regarded as a sample ALD system. The process of densification was explained accurately. A new mechanism of multiple proton diffusion was propounded and DFT energetics showed it to be the most favourable path way. We also found that reaction rates are strongly coupled with the coordination number of Hf atoms at the surface. Then this complex chemistry was implemented in kinetic Monte-Carlo (KMC). The KMC calculation showed the effect of intermediate reactions on the growth rate. Furthermore the morphology of the film and the growth rate under different reaction conditions were compared with experimental data.

¹The authors wish to acknowledge the SFI-funded strategic research cluster 'Functional Oxides and Related Materials for Electronics' (FORME) for their funding. www.tyndall.ie/forme

9:48AM Y25.00006 A unified approach to preserve structure and thermodynamics in a coarse-grained model of aqueous mixtures

PRITAM GANGULY, Center of Smart Interfaces, TU Darmstadt, Germany, DEBASHISH MUKHERJI, CHRISTOPH JUNGHANS, Max Planck Institute for Polymer Research, Mainz, Germany, NICO VAN DER VEGT, Center of Smart Interfaces, TU Darmstadt, Germany — Biological organizations depend on a sensitive balance of noncovalent interactions, in particular also those involving interactions of small molecules, including inorganic salts and urea, with biomolecules in aqueous solution. Computer simulations of these types of systems require simple-yet-specific models in order to cover all relevant time and length scales. We present a method to systematically coarse-grain liquid mixtures using Kirkwood-Buff theory of solution combined with an iterative Boltzmann inversion technique that infers single-site interaction potentials for the solution components from the pair correlation functions. Our method preserves both the solution structure at pair level and variations of solution components' chemical potentials with compositions within a unified coarse-graining framework. To test the robustness of our approach, we simulated urea-water and benzene-water systems over a wide-range of concentrations. We also observe the coarse-grained potentials to be reasonably transferable with varying concentrations.

10:00AM Y25.00007 Novel mesoscopic approach for modeling Carbon Nanotube System, IGOR OSTANIN¹, ROBERTO BALLARINI², TRAIAN DUMITRICA³, University of Minnesota, DAVID POTYONDY⁴, Itasca Consulting Group Inc, UNIVERSITY OF MINNESOTA/ITASCA CG COLLABORATION — We present a distinct spherical element concept for simulating morphologies and mechanical properties of carbon nanotube systems. The important interactions present at the microscopic level are encapsulated into two types of contact models that act simultaneously. Each individual nanotube is coarse-grained into a chain of spherical elements interacting by parallel contact bonds, representing the microscopic covalent bonding. An anisotropic model with aligning moments acts at the contact between elements located in different tubes to represent the van der Waals long-ranged interactions. The accuracy, computational efficiency, and capabilities of the created mesoscopic model are discussed along with illustrative examples, including self-folding of individual nanotubes, mechanical testing of nanotube ropes, self-assembly of a high-porosity nanotube paper, and mechanical testing of a low-porosity nanotube paper.

¹PhD student at the Department of Civil Engineering department, University of Minnesota.

²PhD, Professor at the Department of Civil Engineering, University of Minnesota

³PhD, Professor at the Department of Mechanical Engineering, University of Minnesota.

⁴PhD, Software engineer at Itasca Consulting Group Inc.

10:12AM Y25.00008 Structure formation of toluene around C60: Application of the Adaptive Resolution Scheme, CHRISTOPH JUNGHANS¹, Los Alamos National Laboratory, SEBASTIAN FRITSCH, KURT KREMER, Max Planck Institute for Polymer Research — In the adaptive resolutions scheme (AdResS) a local, typically all-atom cavity is coupled to a surrounding medium of coarse grained, simplified molecules. This methodology cannot only be used to reduce the CPU time demand of atomistic simulations but also to systematically investigate the relative influence of different interactions on structure formation. For this, we vary the thickness of the all atom layer of toluene around a C60, analyze the first toluene layers and compare the result to a full resolution simulation. With this system, we also introduce the implementation of AdResS for molecular simulations into GroMaCS.

¹Work was performed at the Max Planck Institute for Polymer Research

10:24AM Y25.00009 Characterization of phase behavior in assemblies of colloidal nanoparticles, RAY SEHGAL, Chemical Engineering, University of Massachusetts Amherst, DANIEL BELTRAN-VILLEGAS, MICHAEL BEVAN, Chemical and Biomolecular Engineering, Johns Hopkins University, DIMITRIOS MAROUDAS, DAVID FORD, Chemical Engineering, University of Massachusetts Amherst — We report results of a systematic investigation of the phase behavior of clusters of colloidal nanoparticles, which interact via a hard core and depletion attraction potential, as a function of system size and inter-particle interaction strength. To describe the various phases that may be present in such nanoparticle assemblies, we carry out a set of windowed Monte Carlo umbrella sampling (MC-US) simulations to generate free energy landscapes (FELs). For the MC-US generation of the FELs, we use the diffusion mapping method to identify the system's underlying dimensionality and define the dynamically relevant coarse variables. The resulting set of FELs samples broad ranges of the system size and interaction potential strength. These computed FELs describe the phase behavior of the nanoparticle assemblies and allow us to analyze the effects of interaction strength and system size as these assemblies approach the bulk thermodynamic limit. In very small clusters, only a single stable liquid-like phase exists. However, as the number of nanoparticles in the cluster increases, a second crystalline phase emerges in coexistence with the liquid-like phase. The corresponding critical cluster size marks the onset of nucleation of crystalline assemblies of colloidal nanoparticles.

10:36AM Y25.00010 New algorithms for field-theoretic block copolymer simulations: Progress on using adaptive-mesh refinement and sparse matrix solvers in SCFT calculations, SCOTT SIDES, BEN JAMROZ, ROBERT CROCKETT, ALEXANDER PLETZER, Tech-X Research — Self-consistent field theory (SCFT) for dense polymer melts has been highly successful in describing complex morphologies in block copolymers. Field-theoretic simulations such as these are able to access large length and time scales that are difficult or impossible for particle-based simulations such as molecular dynamics. The modified diffusion equations that arise as a consequence of the coarse-graining procedure in the SCF theory can be efficiently solved with a pseudo-spectral (PS) method that uses fast-Fourier transforms on uniform Cartesian grids. However, PS methods can be difficult to apply in many block copolymer SCFT simulations (eg. confinement, interface adsorption) in which small spatial regions might require finer resolution than most of the simulation grid. Progress on using new solver algorithms to address these problems will be presented. The Tech-X Chompst project aims at marrying the best of adaptive mesh refinement with linear matrix solver algorithms. The Tech-X code PolySwift++ is an SCFT simulation platform that leverages ongoing development in coupling Chombo, a package for solving PDEs via block-structured AMR calculations and embedded boundaries, with PETSc, a toolkit that includes a large assortment of sparse linear solvers.

10:48AM Y25.00011 Concurrent multiscale modeling of 3D granular systems, HOLGER MEIER, STEVEN MEIER, FUSHEN LIU, PETER GORDON, ExxonMobil Research and Engineering, TUAN TRAN, ExxonMobil Technical Computing — Large-scale granular mechanics simulations are often based on continuum approaches such as the finite element method (FEM). However, these approaches require continuum descriptions of the constitutive relationship between stresses and strains. As a result, grain-scale dynamics are not explicitly considered. Therefore, modeling of large-scale history dependent phenomena due to grain-scale rearrangement and strain localization remains a long-standing challenge. For small-scale studies, discrete element method (DEM) simulations model grain-scale interactions and thus capture history dependent phenomena. However, the application of this approach to large-scale systems is computationally expensive and impractical. We demonstrate a scalable multiscale approach where large-scale granular systems are discretized with the classical FEM simulation, while the necessary constitutive relation is calculated concurrently from DEM simulations of representative volume elements of grains subject to the loading and deformation prescribed by each finite element.

Friday, March 2, 2012 8:00AM - 11:00AM —
Session Y26 DCOMP: General Theory / Computational Physics I 257B

8:00AM Y26.00001 Computation of Collision-Induced Absorption by dense Hydrogen-Helium gas mixtures up to Thousands of Kelvin, for Astrophysical Applications¹, MARTIN ABEL, LOTHAR FROMMHOLD, The University of Texas at Austin, XIAOPING LI, KATHARINE L.C. HUNT, Michigan State University — The interaction-induced absorption by collisional pairs of H₂ molecules is an important opacity source in the atmospheres of the outer planets and cool stars. The emission spectra of cool white dwarf stars differ significantly in the infrared from the expected blackbody spectra of their cores, which is largely due to absorption by collisional H₂-H₂, H₂-He, and H₂-H complexes in the stellar atmospheres. Using quantum-chemical methods we compute the atmospheric absorption from hundreds to thousands of kelvin, as required, for example, in astrophysical analyses of objects, including cool white dwarf stars, brown dwarf stars, M dwarfs, cool main sequence stars, solar and extra-solar planets, and the formation of so-called first stars [1]. Comparisons of our calculations with laboratory measurements, which exist only at room temperature and below, show close agreement.

[1] Martin Abel, Lothar Frommhold, Xiaoping Li, and Katharine L. C. Hunt, "Collision-Induced Absorption by H₂ pairs: From Hundreds to Thousands of Kelvin," J. Phys. A, 2011, 115 (25), pp 6805-6812

¹This work was supported in part by the National Science Foundation, grants AST 0709106 (L.F.) and AST 0708496 (K.L.C.H.).

8:12AM Y26.00002 Microcanonical entropy inflection points and their relationship to cooperative behavior, MICHAEL BACHMANN, Center for Simulation Physics, The University of Georgia, Athens, GA 30602 — We discuss a method for the systematic classification of the analogs of phase transitions in finite systems. This completely general analysis, which is applicable to any physical system, is based on the microcanonical entropy and its energetic derivative, the inverse caloric temperature. Inflection points of this quantity signal cooperative activity and thus serve as distinct indicators of transitions. The microcanonical entropy as the logarithm of the density of states is the fundamental quantity of statistical mechanics and can directly be obtained by means of contemporary generalized-ensemble computer simulation methodologies. Nowadays, the statistics achieved by employing these methods is sufficiently high such that the accuracy of the data allows for a very precise microcanonical analysis of "phase" transitions, even in mesoscopic systems, where finite-size and surface effects are significant. This can hardly be achieved by the far more prevalent conventional canonical approach. We demonstrate the power of this method in exemplified applications to long-standing problems of polymer and protein nucleation transitions.

8:24AM Y26.00003 Improving Event Identification in the HF Calorimeter of CMS, CHRISTOPHER FRYE, University of Central Florida, JEREMIAH MANS, University of Minnesota, COMPACT MUON SOLENOID COLLABORATION — The Forward Hadron Calorimeter (HF) of the Compact Muon Solenoid (CMS) at the Large Hadron Collider (LHC) lies in a region not covered by an inner tracking system, and we can rely only on the shapes of showers that hit the HF to determine whether or not they are due to electromagnetic particles. We review the current method of distinguishing shower types in the HF, and we bring attention to a drawback that will become present as the luminosity of the LHC increases and creates a need for tighter shower-shape cuts. We provide a method to correct this drawback, and we analyze the effectiveness of various tight cuts at isolating signal from background.

8:36AM Y26.00004 The Effect of White Nonstationary and Colored Nonstationary Noise on Signal Detection¹, MAURICIO FLORES, MATTHEW BENACQUISTA, ALEXANDER STROEER, University of Texas at Brownsville — We analyze the effect of non-stationary noise on the detection of signals on unevenly sampled data. Initial frequency estimation is obtained from a Lomb-Scargle periodogram; which is followed by a global multi-start optimization, as working on a dense local Nelder-Mead iterator for parameter estimates. It has been found that a varying white noise level has no effect on the required relative signal-to-noise ratio for detection in the proposed algorithm, though affecting the absolute amplitude strength of the signal recording. Further analysis has been done on realistic colored noise. Different whitening routines have been incorporated to the proposed algorithm. Detection efficiency is compared for these different routines.

¹This work was funded by NASA URC Grant NASA NNX09AV06A, ARCC grant NSF AST0750913 and CREST grant NSF HRD0734800

8:48AM Y26.00005 Deteriorated Quality of Phase Distorted Gaussian Beams, SERGIY MOKHOV, LEONID GLEBOV, BORIS ZELDOVICH, CREOL - the College of Optics and Photonics, Univ. of Central Florida — The divergence of coherent optical beam is often characterized by the parameter M^2 . For one transverse axis, this beam quality parameter is proportional to the product of the minimal observed beam size divided by the wavelength and multiplied by the divergence angle. Furthermore, M^2 is normalized such that its minimum value equals unity, which is achievable only by a Gaussian beam. An arbitrary phase distortion of a Gaussian beam increases M^2 . Self-phase modulation is a common distortion in which the phase difference across the beam aperture is proportional to the beam intensity profile. For self-phase modulation, the deterioration of the beam quality parameter will depend on only one parameter, the phase at the center of the beam. We have found this dependence analytically. A general phase distortion profile can be represented by higher-order radial phase modes. We have also found the analytical dependence of M^2 in this generalized case. In addition, we derived expressions for beam quality deterioration of super-Gaussian beams due to phase distortions. If the waists of Gaussian and super-Gaussian beams are defined by a residual power criterion, which means both beams outside the same radius have the same amount of residual power, then a super-Gaussian beam will better tolerate phase distortions. It is important that all of our results cannot be efficiently reproduced by the traditional approach, based on the polynomial representation of aberrations, due to the poor convergence of power series for Gaussian profiles.

9:00AM Y26.00006 Exponential tails near the band edges of a one-dimensional disordered exciton system in the Coherent Potential Approximation, ABDELKRIM BOUKAHIL¹, Physics Department, University of Wisconsin-Whitewater, NOUREDINE ZETTILI, Deptment of Physical and Earth Sciences, Jacksonville State University, 700 Pelham Road North, Jacksonville, AL 36265, USA, DAVID HUBER, Physics Department, University of Wisconsin-Madison, Madison, WI 53706, USA — We report the results of studies of the tails near the band edges of a one-dimensional Frenkel exciton system in the Coherent Potential Approximation (CPA). A Gaussian distribution of the transition frequencies with rms width σ ($0.1 \leq \sigma \leq 2.0$) is used. We found that the tails obey two different exponential power laws depending on the value of σ . In the weak disorder limit $0.1 \leq \sigma < 0.5$, the tails of the absorption line shape and the density of states behave like $\exp(-k|E|^{3/2}/\sigma^2)$, and in the strong disorder limit, $0.5 < \sigma \leq 2.0$, the tails behave like $\exp(-|E|^2/\sigma^2)$. In the weak disorder limit, our CPA results are in excellent agreement with previous investigations.

¹Speaker

9:12AM Y26.00007 Elastic impurity scattering and relaxation in electronic lattice under finite electric-field¹, JONG HAN, SUNY Buffalo, WOO-RAM LEE, KWON PARK, Korean Institute for Advanced Study — From the birth of solid state physics, understanding electron transport in solids has been one of the central questions. Recently, rigorous quantum mechanical treatments of solid nonequilibrium have been sought by many groups. Here, we discuss electron transport in tight-binding lattice with disordered potential scatterers when driven by a finite electric field. Based on Floquet formalism with non-perturbative treatment of the electric field, we investigate how the spectral properties evolve when the system is non-dissipative, governed by a *closed* Hamiltonian. As the disorder becomes stronger, the spectra evolve from δ -peaks representing Bloch oscillations to a continuous spectral distribution which is distinctly different from the non-interacting limit. We investigate the fate of electric current in the steady-state nonequilibrium. Finally, we discuss an implementation of energy dissipation channels and the way that the conventional Drude picture is recovered within the Floquet method as a function of Bloch oscillation frequency and electron relaxation-time.

¹Supported by NSF DMR-0907150

9:24AM Y26.00008 Universal resistance quantum in multichannel transport and dissipative field theory, PRASENJIT DUTT, Yale University, THOMAS SCHMIDT, Yale University, Basel University, KARYN LE HUR, Yale University, Ecole Polytechnique — The Landauer formula for coherent DC transport lies at the heart of nanoelectronics and embodies a startling prediction: the quantization of the conductance in one-dimensional metallic wires for ballistic transport, in steps of $R_q^{-1} = e^2/h$ for each channel. Scattering processes undergone by the electrons cause a deviation from this result. The resistance then depends on the transparency of the channel and assumes a nonuniversal value. Recently, the unit of resistance R_q has been shown to be a universal feature for AC transport through a single-channel quantum RC circuit with a large cavity. This result can be understood by mapping the system to the one-channel Kondo model and the emergent low-energy Fermi-liquid theory. In a different context R_q arises in a certain nonequilibrium setting for the multichannel quantum RC circuit. In this work, we study AC transport in the many-channel quantum RC circuit. Under certain well-defined conditions the charge relaxation resistance remains universal and equals R_q . We study the emergence of this universal resistance in the multi-channel limit by using the mapping with a dissipative particle on a ring and making an analogy with the Kondo model.

9:36AM Y26.00009 Holon-Doublon Dynamics in Hubbard Ladders¹, LUIS DIAS DA SILVA, University of Sao Paulo, GONZALO ALVAREZ, Oak Ridge National Laboratory (ORNL), ELBIO DAGOTTO, University of Tennessee/ORNL — Studies of the dynamics of holon-doublon pairs in Mott insulators have unveiled interesting and contrasting results with their band-insulator counterparts [1,2]. In the 1D Hubbard model, a paradigm for a Mott insulator, numerical evidence suggests that the mechanism for exciton decay into magnetic excitations is inefficient [1]. However, transition metal oxides are usually grown in layered superlattices and a real-time study of the holon-doublon propagation on ladders and other layered structures is therefore needed. In this talk, we present results for the real-time dynamics of holon-doublon pairs propagating in a *two-leg* Hubbard ladder, a more realistic model for several SCMs. We use the time-dependent density matrix renormalization group (tDMRG) algorithm with a time-step-targeting Krylov method. We find that the ladder geometry changes the dynamics of the holon-doublon pair. A “transfer” of the excitation between the ladder legs is seen, depending on the ratio between the couplings in the two leg directions. Furthermore, the time decay of the total double occupation is modified in the ladder as compared to the 1D case.

[1] K.A. Al-Hassanieh et al., PRL **100** 166403 (2008).

[2] L. Dias da Silva et al., PRB **81** 125113 (2010).

¹This work was supported in part by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division and by Brazilian agencies CNPq and FAPESP.

9:48AM Y26.00010 First principles study of the spin-orbit coupling effect on the Tl-Pb superconducting alloy¹, OMAR DE LA PEÑA-SEAMAN, Institute of Physics (IFUAP), Benemerita Universidad Autonoma de Puebla (BUAP), ROLF HEID, KLAUS-PETER BÖHNEN, Institute of Solid State Physics (IFP), Karlsruhe Institute of Technology (KIT) — We have studied the influence of spin-orbit coupling (SOC) on the phonon dispersion, the electron-phonon (e-ph) coupling and on the superconducting properties for the Pb-Tl alloy in the stable fcc-phase doping regime. This system have been studied within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation (VCA) for modeling the alloy. The Eliashberg spectral function ($\alpha^2F(\omega)$) and the electron-phonon coupling parameter (λ) have been calculated with and without SOC. The observed effects of SOC in the full phonon dispersion and $\alpha^2F(\omega)$ consist in a softening of the phonon frequencies and an increase of the e-ph coupling matrix elements, which become weaker on the Tl-rich side. SOC enhances λ by as much as 48% in some cases and improves its overall behavior as a function of the concentration for the alloy, leading to a very nice agreement with experimental data from tunneling measurements.

¹This research was supported by Consejo Nacional de Ciencia y Tecnologia (CONACYT) Mexico.

10:00AM Y26.00011 Critical point of phase transitions of fractional order at Superconductors, VLADIMIR UDODOV, Katanov Khakas State University, KATANOV KHAKAS STATE UNIVERSITY TEAM — This paper describes the behavior of thermodynamic values superconducting transition at temperature, tending to absolute zero. Using the thermodynamic arguments we demonstrate that superconductors can undergo third, fourth-, fifth- and higher (including fractional) order phase transitions (PT's) within the meaning of Baxter [1] (or Ehrenfest) as the temperature tending to zero. It is proved that the order of PT can be any real (fractional) number at some interval (from 2 to 8). It is established relation between critical exponent of specific heat and critical magnetic field for superconductor as the temperature tending to zero. It is proved that Ehrenfest classification of phase transitions does not work with a zero critical temperature. Note that the results are valid only in the case of thermodynamic equilibrium, making it difficult to reach experimentally at very low temperatures.

[1] Baxter R.J. Exactly Solved Models In Statistical Mechanics. – London, New York, Sydney, Tokyo, Toronto. – Academic press. – 1982.

10:12AM Y26.00012 Numerical simulation of dynamical response in superconducting quantum detectors, YUKIHIRO OTA, Advanced Science Institute, RIKEN, KEITA KOBAYASHI, MASAHIKO MACHIDA, CCSE, Japan Atomic Energy Agency, TOMIO KOYAMA, Institute for Materials Research, Tohoku University, FRANCO NORI, Advanced Science Institute, RIKEN — We numerically study the dynamical response of superconducting quantum detectors such as a single-photon detector, using the time-dependent Ginzburg-Landau equation coupled with heat diffusion and Maxwell equations. Our simulation shows a dynamical transition to a resistive state via an incident particle with energy higher than T_c . We find that such a transition is associated with the generation of vortex-antivortex pairs and the occurrence of a normal-state region within the superconductor. We also discuss the applicability of this approach to a superconducting single-photon detector.

10:24AM Y26.00013 Quantitative examination of out-of-phase mixed holographic gratings¹

KAY-MICHAEL VOIT, HAUKE BRUENING, MIRCO IMLAU, Department of Physics, University of Osnabrueck, Osnabrueck, Germany — Modern holographic applications require advanced photosensitive materials that particularly obey alterations of the complex permittivity with pronounced amplitudes of both real and imaginary parts on the sub-ps-time scale. Promising candidates such as amorphous and crystalline materials remarkably show a mutual phase-shift between phase and absorption gratings that complicates the analysis of the underlying wave-coupling mechanisms. Hence, theoretical descriptions that are simply based on Kogelnik's coupled-wave theory can not be applied, i.e., a formal approach to systematically derive the full parameter space of the gratings from diffraction efficiency measurements is missing in literature. We revised the analysis of the wave-coupling theory omitting former approximations or applying them later. As a result we derived a formal description for mixed gratings allowing for a full description of beam-coupling experiments. Both the modulations of the refractive index and the absorption coefficient as well as the phase shift between these gratings can be determined through measurements of the angular dependent diffraction efficiency around the positive and the negative Bragg angle. Our approach and results are demonstrated along a mixed grating with a most common parameter set.

¹Financial support by the DFG (projects IM 37/5-1, INST 109/137) is gratefully acknowledged.

10:36AM Y26.00014 Extended phase diagram of ASEP with two types of particles¹

AYSE YESIL, M. CEMAL YALABIK, Bilkent University — First introduced by Evans et al. (PR E, 74 208, (1995)), the Asymmetric Simple Exclusion Process (ASEP) has become an important model in the field. The model is simple in structure, however it offers an opportunity to study some of the basic characteristics of nonequilibrium systems. We use mean field, Monte Carlo, and RG methods to present a detailed phase diagram of the ASEP with two types of particles moving in opposite directions. The nature of the spontaneous symmetry broken phases will also be discussed.

¹Turkish Academy of Sciences

10:48AM Y26.00015 Non-Equilibrium Phase Transitions in the Baxter Model

BASAK RENKLIOGLU, M. CEMAL YALABIK, Department of Physics, Bilkent University — The Baxter model in equilibrium is an exactly solved model for which the universality of the static critical phenomena does not hold [1]. The free energy has a branch-point singularity at a phase transition. The exponent of this singularity can range continuously from one to infinity. That is to say, this model has non-universal equilibrium critical exponents [2]. In our study, the non-equilibrium critical dynamics of the Baxter model which is in contact with two thermal baths is analyzed. Monte Carlo methods are applied to the system in which one of the bath is fixed at infinite temperature. The Baxter model is formulated as two interlacing spin-1/2 Ising models on a square lattice, interacting through a four spin coupling. The dynamics of the system is taken to be driven by "spin exchanges" of the neighbor spins in each lattice. We focus on the phase transitions of the system under this spin exchange dynamics. Preliminary results on the universality class properties of the non equilibrium phase transitions is presented.

[1] R.J. Baxter, Phys. Rev. Lett., **26**, 14 (1971).

[2] R.J. Baxter, J. Stat. Phys., **8**, 25 (1973).

Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y27 DCMP: Invited Session: Topological Phases in Magnets 258AB

8:00AM Y27.00001 Formation and dynamics of Skyrmions in B20-type chiral magnets

NAOYA KANAZAWA, Department of Applied Physics, University of Tokyo — The topological stable spin texture called a Skyrmion, in which the directions of the spins wrap a sphere, has been attracting much attention as an arena for unconventional magneto-transport effects. Small angle neutron scattering (SANS) studies identify the formation of two-dimensional triangular Skyrmion lattice in B20-type transition-metal monosilicides, such as MnSi¹ and Fe_{1-x}Co_xSi.² In addition, novel transport properties due to its topological spin arrangement, namely the topological Hall effect³ and the current-induced rotation of the Skyrmion lattice⁴ are observed in MnSi. We have provided crucial evidence of the existence of Skyrmions in B20-type compounds by direct real-space observation using Lorentz transmission electron microscopy (TEM)^{5,6} and also found a large topological Hall effect in much wider temperature region in MnGe than other B20-type magnets.⁷ TEM observation reveals the detailed information on nucleation and fusion processes and topological defects besides the perfect hexagonal arrangement of Skyrmions. Furthermore, we have found that the Skyrmion lattice state is quite stabilized in a thin-plate formed sample with its thickness smaller than the skyrmion lattice constant. The orders of magnitude larger topological Hall effect in MnGe indicates the high-density Skyrmion crystal formation and distinguishable large responses in some novel electromagnetic phenomena. In addition, we have fabricated B20-type thin films where Skyrmions are more stabilized and applied electric current is more easily controlled than in bulk samples. This work was done in collaboration with X. Z. Yu, Y. Onose, J. H. Park, J. H. Han, N. Nagaosa, K. Kimoto, W. Z. Zhang, S. Ishiwata, Y. Matsui, T. Arima, D. Okuyama, K. Ohoyama, S. Wakimoto, K. Kakurai, A. Tsukazaki, M. Ichikawa, Y. Li, Y. Shiomi, K. Shibata, D. Inosov, J. H. Kim, J. White, N. Egetenmeyer, J. Gavilano, B. Keimer, and Y. Tokura.

¹S. Mühlbauer *et al.*, Science **323**, 915 (2009).

²W. Münzer *et al.*, Phys. Rev. B **81**, 041203 (2010).

³A. Neubauer *et al.*, Phys. Rev. Lett. **102**, 186602 (2009).

⁴F. Joneitz *et al.*, Science **330**, 1648 (2010).

⁵X. Z. Yu *et al.*, Nature **465**, 901 (2010).

⁶X. Z. Yu *et al.*, Nature Materials **10**, 106 (2011).

⁷N. Kanazawa *et al.*, Phys. Rev. Lett. **106**, 156603 (2011).

8:36AM Y27.00002 Magnetic Blue Phase in the Chiral Itinerant Magnet MnSi

DMITRY REZNIK, University of Colorado-Boulder — In MnSi with the cubic crystal structure B20, the lack of inversion symmetry induces a chiral Dzyaloshinsky-Moriya interaction between magnetic moments. It locally favors helical magnetic order. In addition to a long-range helical order with the well-defined propagation vector, other locally helical phases such as skyrmions and partial order appear in its phase diagram. These enigmatic phases are suspected to be behind many unusual properties of MnSi. I will report results of model calculations, which show that such phases should arise naturally as a result of the basic Dzyaloshinsky-Moriya Hamiltonian. Specifically, in the absence of an applied magnetic field, the free energy in MnSi should be minimized by the magnetic analogue of blue phases, which have previously been observed in chiral liquid crystals. This result is consistent with our recent neutron scattering measurements as well as those of others. The properties of this blue phase explain a number of previously reported puzzling features of MnSi such as partial magnetic order and a two-component specific-heat as well as, possibly, non-Fermi-liquid resistivity at high pressure.

9:12AM Y27.00003 Quasi-two-dimensional Skyrmion lattices and other exotic structures in confined chiral nematic liquid crystals¹, SLOBODAN ZUMER, University of Ljubljana and Jozef Stefan Institute — Skyrmions are localized particle-like topological entities in a number of continuous fields that play important roles in various condensed matter systems, including two-dimensional electron gases exhibiting the quantum Hall effect, Bose–Einstein condensates, and chiral ferromagnets [1, 2]. Here we are using Landau - de Gennes theoretical approach and numerical techniques to show that in a highly chiral nematic liquid crystal confined to a thin film between two parallel surfaces imposing normal alignment nematic director can exhibit thermodynamically stable states characterized by quasi-two-dimensional Skyrmion lattices of disclinations [3]. By confining a chiral nematic, that in bulk forms blue phases characterized by cubic lattices of nematic defect lines, to a layer with thickness comparable to the lattice constant of the blue phase [3-5], various quasi 2D defect lattices can be stable. Depending on the anchoring direction of the nematic director on confining surfaces, temperature, and layer thickness, beside skyrmion structures, lattices of double helical half-integer disclinations running along the layer [4], and lattices of ring defects [5] are the most interesting. A chiral nematic liquid crystal film can thus serve as a model system, allowing direct investigation of numerous defect lattices by a variety of optical techniques at conditions that are less demanding than used for other condensed matter Skyrmion systems.

[1] U.K. Röbler, A. N. Bogdanov, & C. Pfleiderer, Spontaneous skyrmion ground states in magnetic metals. *Nature* 442, 797 (2006).

[2] A. Hamann, D. Lamago, Th. Wolf, H. v. Löhneysen, and D. Reznik, Magnetic Blue Phase in the Chiral Itinerant Magnet MnSi, *Phys. Rev. Lett.* 107, 037207 (2011).

[3] J. Fukuda and S. Zumer, Quasi-two-dimensional Skyrmion lattices in a chiral nematic liquid crystal, *Nature Communications* 2, 246 (2011).

[4] J. Fukuda and S. Zumer, Novel defect structures in a strongly confined liquid-crystalline blue phase. *Phys. Rev. Lett.* 104, 017801 (2010).

[5] J. Fukuda and S. Zumer, Ring Defects in a Strongly Confined Chiral Liquid Crystal, *Phys. Rev. Lett.* 106, 097801 (2011).

¹Work done with Jun-ichi Fukuda, Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1 Umezono, Tsukuba 305-8568, Japan

9:48AM Y27.00004 Unusual Hall effect Anomaly in MnSi under pressure¹, MINHUEA LEE, University of Colorado at Boulder — Recent works in B20 type transition metal compounds have revealed a new topological object in spin systems – the skyrmion, a particle-like object in which spins point all directions to wrap around the sphere. While neutron scattering and scanning probe experiments^{2,3} confirmed the existence of individual skyrmions and skyrmion lattices in a particular part of the phase diagram, the interaction between skyrmions and electronic degrees of freedom remains to be unveiled. In this talk, we report the observation of a highly unusual Hall current in the helical magnet MnSi under pressure.⁴ In addition to the normal Hall effect and the anomalous part that arises from spontaneous magnetization, the Hall conductivity displays a distinctive stepwise field profile quite unlike any other Hall response observed in solids. This additional contribution was observed in a much larger range of temperature and applied field than the so-called *A*-phase, where the skyrmion lattice was observed in ambient pressure. It suggests that fluctuating, *i.e.* non-static, skyrmions might be present over a broad range of the phase diagram under pressure when the magnetic ordering becomes weakened.

¹This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0006888

²S. Mühlbauer *et al.*, *Science* **323**, 915 (2009).

³X. Z. Yu, *et al.*, *Nature*, **465**, 901 (2010).

⁴M. Lee *et al.*, *Phys. Rev. Lett.* **102**, 186601 (2009).

10:24AM Y27.00005 Cosmic Strings Meet Multerroics: Understanding topological defects in spontaneous symmetry breaking phase transitions, SINEAD GRIFFIN, ETH Zurich — Jumping from the expanse of galactic scales to land in the laboratory might seem a gargantuan task. Common to both, however, is the concept of symmetry breaking and in particular the formation of topological defects. Here I discuss the formation of topological defects in multiferroic YMnO₃ whose ferroelectric behavior enables the direct imaging of these defects. I also show how this material can be used to study the Kibble-Zurek model of topological defect formation in the early universe and give quantitative insights on the number of domains formed during the spontaneous symmetry breaking phase transition.

Friday, March 2, 2012 8:00AM - 11:00AM –
Session Y29 GQI: Focus Session: Quantum Optics with Superconducting Circuits: Nonlinearity and Itinerant Microwave Photons 259A

8:00AM Y29.00001 Microwave Photon Counter Based on Josephson Junctions, GUILHEM RIBEILL, DAVID HOVER, UMESHKUMAR PATEL, University of Wisconsin-Madison Department of Physics, YUNG-FU CHEN, Department of Physics, National Central University, ROBERT MCDERMOTT, University of Wisconsin-Madison Department of Physics — We describe progress in the development of a microwave photon counter based on current biased Josephson junctions; absorption of a single photon causes the junction to switch to the voltage state, producing a large and easily measured classical signal. We have combined multiple junctions with a broad-band, on-chip microwave beam splitter to realize a multiplexed microwave photon detector. We discuss application of the Josephson microwave counter to the study of full counting statistics of the microwave emission from various mesoscopic conductors, and we describe alternative biasing schemes to enable operation in more traditional photon counting modes.

8:12AM Y29.00002 Quantum efficiency of a single microwave photon detector based on a current-biased Josephson junction¹, AMRIT POUDEL, ROBERT MCDERMOTT, MAXIM VAVILOV, University of Wisconsin-Madison — We analyze the quantum efficiency of a single microwave photon detector based on a current-biased Josephson junction. We consider the Jaynes-Cummings Hamiltonian to describe coupling between the photon field and the junction. We then take into account coupling of the junction and the resonator to the environment. Numerically solving the equation of motion of the density matrix of the resonator-junction system, we compute the quantum efficiency of the photon detector as a function of detection time, bias current and the junction's decay time. For current-biased Josephson junctions, the efficiency to detect a single photon with frequency in the microwave regime is around 50%. Our results also indicate that a highly efficient single microwave photon detector is feasible for a moderate improvement in the junction's decay time.

¹This work was supported by NSF and DOD

8:24AM Y29.00003 Backaction of Microwave Photon Detection by a Strongly Coupled Josephson Junction¹, EMILY PRITCHETT, Saarland University, LUKE GOVIA, University of Waterloo, SETH MERKEL, IBM T. J. Watson Research Center, FRANK WILHELM, Saarland University — We analyze the functionality of on-chip Josephson junctions as single microwave photon detectors, as has been demonstrated recently in Chen, *et al.*, arXiv:1011.4329. The Josephson junction device, which we refer to as a Josephson Photomultiplier (JPM), acts as a nearly perfect binary detectors of microwave photons by undergoing an observable switching event when there are one or more photons in an incident cavity. We analyze the backaction of this switching event on the state of incident light, including the energy dissipation and dephasing affecting an imperfect JPM. This analysis improves the efficiency and fidelity with which a JPM reconstructs the state of light in an incident transmission line 'cavity', which are commonly used to store and transfer quantum states in implementations of circuit-QED.

¹This work was supported by DARPA-QuEST.

8:36AM Y29.00004 Cooperative effects for Qubits in a Transmission Line: Theory, K. LALUMIÈRE, A. BLAIS, Université de Sherbrooke, B.C. SANDERS, University of Calgary, A.F. VAN LOO, A. FEDOROV, A. WALLRAFF, ETH Zurich — Strong extinction of the transmitted power in a 1D transmission line coupled to an artificial atom has recently been achieved [1]. In contrast to the 3D case, large extinctions are made possible by the strong light-matter coupling occurring because of reduced dimensionality. Motivated by this, here we consider the situation where multiple artificial atoms (ie transmon qubits) are coupled to the 1D line. Following the work of Lehmberg for the 3D case [2], we obtain a master equation describing the dynamics of an arbitrary number of qubits coupled to the line. This master equation reveals interaction between the qubits mediated by the line. Using the input-output formalism, the model is compared to experimental results for multiple qubits coupled to the 1D line. [1] O. Astafiev *et al.*, Science 327, 840 (2010) [2] R. H. Lehmberg. Phys. Rev. A 2, 883 (1970).

8:48AM Y29.00005 Cooperative Effects for Qubits in a Transmission Line: Experiment, A.F. VAN LOO, A. FEDOROV, ETH Zurich, K. LALUMIÈRE, Université de Sherbrooke, B.C. SANDERS, University of Calgary, A. BLAIS, Université de Sherbrooke, A. WALLRAFF, ETH Zurich — The interaction probability between freely propagating photons and atoms or atom-like systems is greatly enhanced in one dimension. Thus a system of many atoms coupled to a one-dimensional continuum of electromagnetic modes is expected to reveal many interesting phenomena - the photons emitted by an atom can be absorbed by other atoms and coherently interact with propagating modes of the continuum. We implement three superconducting qubits coupled strongly to an open transmission line to investigate such light-matter interactions in one dimension. We characterize our system by scattering radiation off the qubits and measuring the transmitted and reflected field. For low driving powers, a single qubit reflects nearly all incident radiation resonant with its transition frequency [1]. When two qubits are tuned such that their emitted radiation has a wavelength close to twice the distance between the qubits we observe interference effects in the reflection and transmission spectra. At high driving powers resonance fluorescence is measured for single qubits and multiple qubits in resonance. These results present first steps towards investigating cooperative effects for multiple qubits in open one-dimensional space. [1] O. Astafiev *et al.*, Science, **327**, 840 (2010)

9:00AM Y29.00006 Hong-Ou-Mandel Interference in Circuit QED Experiments, MATTHEW WOOLLEY, Université de Sherbrooke, CHRISTIAN LANG, CHRISTOPHER EICHLER, ANDREAS WALLRAFF, ETH Zurich, ALEXANDRE BLAIS, Université de Sherbrooke — The Hong-Ou-Mandel (HOM) effect is a quantum interference effect whereby two indistinguishable photons incident at either side of a balanced beam splitter will be detected together at one output port or the other, but never with one photon at each output port. Such experiments have long been performed in the optical domain, but recent developments have raised the possibility of performing such experiments in the microwave domain, using linear amplifiers and quadrature amplitude detectors instead of photon counting [Bozyigit *et al.*, Nat. Phys. **7**, 154-158 (2010)]. Here we determine the signature of HOM interference in a system consisting of two independent circuit QED systems out-coupled into an on-chip microwave beam splitter. We have calculated the beam splitter output intensity auto- and cross-correlations for both trains of pulsed Lorentzian photons, and continuously-driven sources based on photon blockade. The HOM interference is manifest as antibunching in the output intensity cross-correlation. Controllable distinguishability may be introduced via a time delay in the pulsed case, or via a frequency offset in the continuously-driven case. The frequency offset leads to a quantum beat effect. Preliminary experimental results will be discussed.

9:12AM Y29.00007 Generating distributable and unconditional entanglement on-chip at microwave frequencies, W.F. KINDEL, H.S. KU, JILA and the University of Colorado, S. GLANCY, G.C. HILTON, K.D. IRWIN, E. KNILL, L.R. VALE, NIST, K.W. LEHNERT, JILA and the University of Colorado — Entanglement is a critical requirement for quantum teleportation protocols. In a strategy to generate entanglement between two separate microwave lines, we integrate two Josephson Parametric Amplifiers (JPAs) and a quadrature hybrid onto a single chip making the entangler circuit. When two squeezed states created by the JPAs are combined on the hybrid (microwave beam splitter), the two output modes are entangled. We observe entanglement using a quantum efficient two channel quadrature measurement device. In our initial tests, the degree of entanglement has been limited by undesirable coupling among the elements of our entangler circuit. We present our investigation of the undesired coupling along with design strategies to reduce it.

9:24AM Y29.00008 Quantifying distributable and unconditional entanglement at microwave frequencies, H.S. KU, W.F. KINDEL, JILA and University of Colorado at Boulder, S.C. GLANCY, E. KNILL, L.R. VALE, G.C. HILTON, K.D. IRWIN, NIST, K.W. LEHNERT, JILA, NIST and University of Colorado at Boulder — Unconditional and distributable entanglement can be created by combining a squeezed state and a vacuum state at a beam splitter. We create a single integrated circuit designed to pursue this strategy at microwave frequencies. The squeezed state is created with a Josephson Parametric Amplifier and then combined with a vacuum state in a hybrid (microwave beam splitter) producing entanglement of the output modes. In this talk, we will present the measurement and quantification of entanglement between separate microwave transmission lines. We quantify the entanglement and estimate the fidelity when applying this entangled state as a quantum teleportation channel.

9:36AM Y29.00009 Microwave photonics and Josephson junction arrays, JUAN J. MAZO, DAVID ZUECO, Instituto de Ciencia de Materiales de Aragon (CSIC-Universidad de Zaragoza), ENRIQUE SOLANO, IKERBASQUE and Universidad del Pais Vasco, JUAN J. GARCIA-RIPOLL, Instituto de Fisica Fundamental (CSIC) — We present an architecture for a photonic crystal in the microwave regime based on superconducting transmission lines interrupted by Josephson junctions. A study of the scattering properties of a single junction in the line shows that the junction behaves as a perfect mirror when the photon frequency matches the Josephson plasma frequency. We generalize our calculations to periodic arrangements of junctions, demonstrating that they can be used for tunable band engineering, forming what we call a quantum circuit crystal. As a relevant application, we discuss the creation of stationary entanglement between two superconducting qubits interacting through a disordered media.

9:48AM Y29.00010 Modeling of a Flying Microwave Qubit, KYLE KEANE, University of California, Riverside, Department of Physics and Astronomy, ALEXANDER N. KOROTKOV, University of California, Riverside, Department of Electrical Engineering — We investigate the transfer efficiency of sending a flying microwave qubit through a transmission line from one resonator to another resonator. Our model is based on the current technology of coupling superconducting phase qubits to microwave resonators and transmission lines. Analytical as well as numerical results are presented. Procedural imperfections have been modeled, including weak detuning, imperfect timing, and deviations from the ideal time dependence of the coupling modulation. The effects of multiple reflections within the transmission line and energy dissipation in the system are also considered.

10:00AM Y29.00011 A Four-wave Mixing Toolbox For Photon State Manipulation in Superconducting Resonators¹ , A.V. SHARYPOV, XIUHAO DENG, LIN TIAN, University of California, Merced — We present a circuit scheme to generate quantum operations on superconducting resonators by engineering effective interaction Hamiltonians. We show that both the linear Bogoliubov transformations, including the beam-splitter operation, the squeezing operation, and the phase shifter, and the nonlinear interactions such as the cross-Kerr interaction can be realized with one single circuit. Our circuit is composed of two superconducting qubits coupled with each other to form a quantum four-level system. Each qubit interacts directly with one superconducting resonator. We exploit the four-wave mixing (FWM) approach and use the circuit as a toolbox to generate the above-mentioned quantum operations by controlling circuit parameters with external sources. Using numerical simulations to study the error rates, we show that the transformations can be realized with high fidelity. Arbitrary quantum operations on the microwave photons can be realized by combining these effective interactions.

¹This work is supported by NSF-DMR-0956064 and NSF-CCF-0916303.

10:12AM Y29.00012 Dephasing and Kerr type interaction effects in circuit quantum electrodynamics , ERAN GINOSSAR, Advanced Technology Institute and Department of Physics, University of Surrey, STEVEN GIRVIN, Department of Physics, Yale University — There has been recently a significant advance in obtaining high quality factor resonators in superconducting circuit architectures. The reduction of the resonator line width motivates us to consider subtle Kerr type interaction effects in small clusters of cavities and transmon type qubits. The Kerr interaction leads to entanglement of cavities, which in the transient regime is manifested in collapse-revival dynamics. For longer time scales, the interaction of the system with its environment becomes important and we discuss how the entangled states are modified. The signal of this steady-state Kerr interaction is a multi-photon port-to-port scattering process which can be observed in homodyne measurements or in a spectral analysis (correlations). We discuss the relevance of these effects to the challenge of building quantum memories.

10:24AM Y29.00013 Dynamic quantum Kerr effect in circuit quantum electrodynamics , YI YIN, HAOHUA WANG, MATTEO MARIANTONI, RAMI BARENDTS, RADOSLAW C. BIALCZAK, YU CHEN, MIKE LENANDER, JULIAN KELLY, ERIK LUCERO, ANTHONY MEGRANT, PETER O'MALLEY, DANIEL SANK, JIM WENNER, TED WHITE, ANDREW CLELAND, JOHN MARTINIS, University of California, Santa Barbara — In the dispersive regime of circuit quantum electrodynamics (QED), where the qubit and resonator frequencies differ slightly, photons in the resonator exhibit induced frequency and phase shifts. The qubit-state dependent phase shift is usually measured by monitoring the resonator transmission spectrum at fixed qubit-resonator detuning. In this static scheme, the phase shift can only be monitored in the far-detuned, linear dispersion regime, in order to avoid measurement-induced demolition of the quantum state. By using a dynamic procedure to adiabatically drive the qubit frequency, here we are able to explore the dispersive interaction over a much broader range, and we further monitor the interaction using resonator Wigner tomography. Exotic non-linear effects on different photon states, e.g., Fock states, coherent states and Schrodinger cat states, are thereby directly revealed. Correspondingly, we demonstrate a quantum Kerr effect in the dynamic framework in circuit QED.

10:36AM Y29.00014 Shaping an Itinerant Quantum Field into a Multimode Squeezed Vacuum by Dissipation¹ , JUAN JOSE GARCIA-RIPOLL², Instituto de Fisica Fundamental, CSIC, DIEGO PORRAS³, Facultad de Ciencias Fisicas, Universidad Complutense de Madrid — This work shows how to create tunable continuous sources of single and multimode squeezed light by controlling single emitters coupled to propagating modes of the EM field. Our work builds on recent experiments that implement the main tools of cavity Quantum Electrodynamics (QED) using superconducting qubits coupled to microwave transmission lines, as well as quantum dots coupled to microcavity photons, or plasmons. The main results of this letter, presented in sequential order are: A multicolor driving of an artificial atom modifies its coupling to the EM field, inducing sidebands. Combining the sidebands with an auxiliary bath, a single qubit may cool a quantum field in a single mode cavity to a squeezed vacuum. If instead of a cavity, the driven qubit is placed in a waveguide, the high energy modes play the role of a dissipative bath and the result is tunable multimode squeezing of the propagating quantum field. Through the manuscript we will also discuss implementations, measurement schemes and further outlook.

¹Research projects QUITEMAD S2009-ESP-1594, MICINN FIS2009-10061 and CAM-UCM/910758, and RyC Contract Y200200074

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10:48AM Y29.00015 Effects of nonlinearity in the emission spectrum of the driven nonlinear oscillator , MICHAEL MARTHALER, STEPHAN ANDRE, LINGZHEN GUO, Institut für Theoretische Festkörperphysik, Karlsruhe, VITTORIO PEANO, Department of Physics and Astronomy, Michigan State University, East Lansing, GERD SCHÖN, Institut für Theoretische Festkörperphysik, Karlsruhe — Motivated by many experiments on nonlinear driven systems realized using superconducting circuits we investigate the properties of a coherently driven nonlinear resonator. By using Josephson junctions in superconducting circuits, strong nonlinearities can be engineered, which lead to a relatively low number of photons in the resonator and the appearance of pronounced nonlinear effects. Based on a master equation approach, which takes into account the quantum nature of noise, we determine the emission spectrum and observe for typical circuit QED parameters, in addition to the primary side-peaks, second-order peaks not predicted by a linearized theory.

Friday, March 2, 2012 8:00AM - 11:00AM —

Session Y30 GQI: Quantum Computing, Quantum Algorithms, and Quantum Simulation 259B

8:00AM Y30.00001 Phase Slips in Topological Superconductor Wire Devices , SAMUEL GOLDBERG, DORON BERGMAN, DAVID PEKKER, GIL REFAEL, California Institute of Technology — We make a detailed study of phase slips in topological superconducting wires and devices based on topological wires. We begin by investigating a device composed of a topological superconducting wire connected to a non-topological wire (T-S). In the T-segment only slips of the phase by multiples of 4π are allowed, while in the S-segment slips by 2π are also allowed. We show that near the interface, 2π phase slips are also allowed and we comment on the consequences of such phase slips for the Aharonov-Casher effect. We also consider an implementation of a q-bit consisting of a T-S-T device, where the quantum information is stored in the parity of the two topological segments via the four Majorana modes. We show that the central S-segment of this type of device can support 2π phase-slips which result in the decoherence of the q-bit.

8:12AM Y30.00002 ABSTRACT WITHDRAWN —

8:24AM Y30.00003 String localization and delocalization in the disordered toric code¹, PEJMAN JOUZDANI, EDUARDO R. MUCCIOLO, Department of Physics, University of Central Florida — Topological quantum memories based on the toric code model have the ability to protect quantum information by self correcting a large class of errors. However, excitations such as a string of spin flips, when allowed to perform a quantum walk, can change the logical state encoded in the system every time they wind around the torus. It has been proposed that by adding randomness to the local spin exchange couplings, one can localize these string excitations and avoid logical errors. In our work, we investigate this proposal numerically through the use of an efficient time-dependent numerical quantum evolution method. We determine the dependence of the winding time on the torus size and on the amount of randomness. We study the effect of dephasing in the quantum evolution of the string excitations and show that a transition to delocalization can occur.

¹Financial support by the ONR and by NSF CCF-1117241

8:36AM Y30.00004 Implementing quantum gates through scattering between an electron and a magnetic impurity in a graphene nanoribbon, GUILLERMO CORDOURIER-MARURI, ROMEO DE COSS, Departamento de Física Aplicada, Cinvestav-Mérida, SOUGATO BOSE, Department of Physics and Astronomy, University College London — We study the feasibility of implementing quantum logic gates and generate entanglement when a ballistic electron is scattered by a magnetic impurity fixed in a graphene nanoribbon. Because electrons in graphene behaves like massless Dirac Fermions, we use the Dirac equation to describe the system. In our model we consider the ballistic electron spin as a relativistic flying qubit and the impurity spin as a static qubit. The interaction between spins is described by a Heisenberg - like operator. The interaction by electron scattering shows the advantage of a low control in the interaction, and the operation success can be measured by means the electron transmission probability. We show that is possible to implement quantum logic gates of the type SWAP, and partial SWAP with a physically feasible coupling strenght between spins. We also present the condition to generate states of maximum entanglement. The possible use of the graphene pseudospin as an additional degree of freedom is discussed.

8:48AM Y30.00005 Long-lived qubit constructed from three identical atoms, RUI HAN, Centre for Quantum Technologies, Singapore, HUI KHOON NG, Centre for Quantum Technologies, Singapore and DSO, National Laboratories, applied physics lab, Singapore, NIELS LÖRCH, Centre for Quantum Technologies, Singapore and Universitt Heidelberg, Philosophenweg 16-19, 69120 Heidelberg, Germany, JUN SUZUKI, National Institute of Informatics, 2-1-2 Hitotsubashi, Chiyoda ku, Tokyo 101-8430, Japan, BERGE ENGLERT, Centre for Quantum Technologies, National University of Singapore, Singapore — In this talk, I will present a scheme for constructing logical qubits from clusters of three identical atoms that are long-lived against decoherence from fluctuating magnetic fields, a limiting source of noise in many experiments. Each qubit is stored in a rotationally invariant subsystem of the total angular momentum states of the three atoms, and can persist with high fidelity for time-scales on the order of hours. This is to be compared with a fraction of a millisecond for an unprotected atomic qubit. I will first present the scheme of rotationally invariant subsystems in atomic systems and show that the information stored in the system is robust against decoherence. Then I will move on to discuss a proposal for an experiment to demonstrate the feasibility of the scheme. In our proposal, the state preparation is done with the help of Rydberg blockade for three atoms, where the atoms are localized in space and addressed by a sequence of laser pulses simultaneously. By carefully selecting the atomic levels addressed and tuning the parameters of the applied lasers, an arbitrary logical qubit state can be prepared. Lastly, the fidelity of state preparation will be discussed. Ref: R. Han, N. Lörch, J. Suzuki and B. G. Englert, Phys. Rev. A 84, 012322 (2011)

9:00AM Y30.00006 Deterministic and Cascadable Conditional Phase Gate for Photonic Qubits, CHRISTOPHER CHUDZICKI, ISAAC CHUANG, JEFFREY SHAPIRO, MIT — Cross-phase modulation (XPM) at the single-photon level, if strong enough, would enable a simple conditional π -phase gate for photonic qubits. Together with easily realized single-qubit rotations for such qubits, this would provide a universal gate set for quantum computation. However, previous analyses of photonic conditional ϕ -phase gates that treat XPM in a causal, multimode, quantum field setting suggest that a large ($\sim\pi$ rad) nonlinear phase shift is always accompanied by fidelity-degrading noise. We present a conditional phase gate that, for sufficiently small nonzero ϕ , has high fidelity. Moreover, our gate is cascable, in that it preserves the structure of the principal modes used to encode qubit information, and can therefore be cascaded to realize a high-fidelity conditional π -phase gate. The key components of our gate are: (1) an atomic $\mathcal{V}$ -system to create XPM; (2) a principal-mode restorer that compensates the evolution a principal-mode incurs when the $\mathcal{V}$ -system is driven by a single photon; and (3) a principal-mode projector that exploits the quantum Zeno effect to preclude the accumulation of fidelity-degrading departures from the principal-mode Hilbert space when both control and target photons illuminate the gate.

9:12AM Y30.00007 Dynamic Phases and Robust Quantum Gates¹, YASUSHI KONDO, TSUBASA ICHIKAWA, MASAMITSU BANDO, MIKIO NAKAHARA, Kinki University — We are interested in composite pulses widely employed in Nuclear Magnetic Resonance (NMR) and geometric phase gates (GQGs) with vanishing dynamic phases in Quantum Information Processing (QIP). A composite pulse in NMR is constructed with poor quality pulses but becomes more reliable than its components. We found: a composite pulse robust against pulse length error in NMR is always a GQG [1]. We then extended this observation to two-qubit operations. Let us consider the interaction $e^{-i\theta\sigma_z\otimes\sigma_z}$ and assume that there is a systematic error in θ . When we construct a “composite pulse” robust against this error, we obtain a two-qubit GQG [2]. We clarified that geometric phase gates are really useful in QIT.

[1]Y. Kondo & M. Bando, *J. Phys. Soc. Jpn.* **80**, 054002.

[2] T. Ichikawa, M. Bando, Y. Kondo & M. Nakahara, submitted to *philosophical transaction A*.

¹Open Research Center Project for Private Universities; matching fund subsidy, MEXT, Japan

9:24AM Y30.00008 Non-Adiabatic Holonomic Quantum Gates in an atomic system, VAHID AZIMI MOUSOLOU, CARLO M. CANALI, School of Computer Science, Physics and Mathematics, Linnaeus University, Kalmar, Sweden, ERIK SJOQVIST, Department of Quantum Chemistry, Uppsala University, Uppsala, Sweden — Quantum computation is essentially the implementation of a universal set of quantum gate operations on a set of qubits, which is reliable in the presence of noise. We propose a scheme to perform robust gates in an atomic four-level system using the idea of non-adiabatic holonomic quantum computation proposed in [1]. The gates are realized by applying sequences of short laser pulses that drive transitions between the four energy levels in such a way that the dynamical phases vanish.

[1] E. Sjoqvist, D.M. Tong, B. Hessmo, M. Johansson, K. Singh, arXiv:1107.5127v2 [quant-ph]

9:36AM Y30.00009 Single-qubit gates by graph scattering¹, MICHAEL S. UNDERWOOD, BENJAMIN A. BLUMER, DAVID L. FEDER, IQIS, University of Calgary — Continuous-time quantum walkers with tightly peaked momenta can simulate quantum computations by scattering off finite graphs. We enumerate all single-qubit gates that can be enacted by scattering off a single graph on up to $n = 9$ vertices at certain momentum values, and provide numerical evidence that the number of such gates grows exponentially with n . The single-qubit rotations are about axes distributed roughly uniformly on the Bloch sphere, and rotations by both rational and irrational multiples of π are found.

¹This work was supported by Alberta Innovates – Technology Futures (MSU), and the Natural Sciences and Engineering Research Council of Canada.

9:48AM Y30.00010 Recent Results in Photonic Quantum Computations, Simulations and Quantum Networks, PHILIP WALTHER, University of Vienna — The applications of photonic entanglement manifold and reach from quantum communication [1] to quantum metrology [2] and optical quantum computing [3]. The advantage of the photon's mobility makes optical quantum computing unprecedented in speed, including feed-forward operations with high fidelity [4]. During the last few years the degree of control over photonic multi-particle entanglement has improved substantially and allows for not only overcoming the random nature of spontaneous emission sources [5], but also for the quantum simulation of other quantum systems. Here, I will also present the simulation of four spin-1/2 particles interacting via any Heisenberg-type Hamiltonian [6]. Moreover, recent experimental and theoretical progress, using the concepts of measurement-based quantum computation, indicates that photons are best suited for quantum networks. I will also present results for the realization for such a client-server environment, where quantum information is communicated and computed using the same physical system [7]. References: [1] PRL 103, 020503 (2009); [2] Nature 429, 158 (2004); [3] Nature 434, 169 (2005); [4] Nature 445, 65 (2007); [5] Nature Photon 4, 553 (2010); [6] Nature Physics 7, 399 (2011); [7] in press.

10:00AM Y30.00011 Physics of an isolated electron puddle revealed via dephasing in thermal equilibrium, EMIL WEISZ, HYUNGKOOK CHOI, OKTAY GÖKTAŞ, MOTY HEIBLUM, YUVAL GEFEN, VLADIMIR UMANSKY, DIANA MAHALU, Weizmann Institute of Science — Low dimensional electron systems serve as a good setup for studying interactions among quantum systems. In our study, we examined a system comprised of an electron puddle, confined in a quantum dot, coupled to an electronic Mach-Zehnder interferometer via Coulomb interactions. Surprisingly, even when the electron puddle was in thermal equilibrium and nearly isolated, it induced full and robust dephasing in the nearby interferometer when the average puddle's occupation was $N+1/2$. We attribute this unexpected behavior to a unique manifestation of the Friedel Sum Rule, which connects the occupation of a system with its scattering phase. Furthermore, this phenomena allowed accessing various properties of the isolated electron puddle, such as its average occupation, in thermal equilibrium and under bias, and decoherence rate of the confined electrons.

10:12AM Y30.00012 Quantum trajectories for systems probed by fields in multimode Fock and Schrodinger cat states¹, JOSHUA COMBES, BEN Q. BARAGIOLA, Center for Quantum Information and Control, University of New Mexico, Albuquerque, NM 87131-0001, USA, AGATA M. BRANCZYK, Department of Physics and Centre for Quantum Information and Quantum Control, University of Toronto, Toronto ON M5S 1A7, Canada, ROBERT L. COOK, Center for Quantum Information and Control, University of New Mexico, Albuquerque, NM 87131-0001, USA, JOHN E. GOUGH, Institute for Mathematics and Physics, Aberystwyth University, SY23 3BZ, Wales, United Kingdom, MATTHEW R. JAMES, HENDRA I. NURDIN, Research School of Engineering, Australian National University, Canberra, ACT 0200, Australia — Using Gardiner and Collet's input-output theory we derive system and output field master equations for an arbitrary quantum system probed by a field in a non-classical state of light. Specifically the field states we study are arbitrary combinations (superpositions and / or mixtures) of continuous-mode Fock states or continuous mode-coherent states. We also unravel the master equations for the system state to get the conditional evolution (the stochastic master equation) for homodyne and photon counting measurements.

¹JC acknowledges support from National Science Foundation Grant No. PHY-0903953 and PHY-1005540 and Office of Naval Research Grant No. N00014-11-1-008

10:24AM Y30.00013 Optimal Experimental Detection and Characterization of SU(2) Decoherence, LEE A. ROZEMA, ARDAVAN DARABI, DYLAN H. MAHLER, AEPHRAIM M. STEINBERG, Centre for Quantum Information and Quantum Control, and Institute for Optical Sciences, Department of Physics, University of Toronto, ROBIN BLUME-KOHOUT, Theoretical Division, Los Alamos National Lab & CQULC, University of New Mexico — Quantum metrology is the art of measuring tiny forces by preparing quantum states, then measuring how much they get displaced by the force. The resulting precision often exceeds classical limits. The best state depends on what we want to detect. N00N states [1] are optimal for U(1) phase shifts. Measuring arbitrary dynamical shifts requires quantum process tomography (QPT)[3], in which the process is applied to a complete set of input states. In this work, we experimentally study the important intermediate case of SU(2) decoherence (SD), fluctuating SU(2) rotations, by probing it with biphotons [2]. We show that N00N states are optimal for detecting SD. Then, we turn to QPT, and examine how accurately SU(2)-covariant sets of states can identify SD. The set of spin-coherent states (generated by SU(2)-displacements of a "highest-weight" state) are sufficient for QPT [4], but exponentially insensitive to some parameters. We show that N00N states (though optimal at detecting SD) generate even less effective input sets, with zero sensitivity to some parameters. Finally, we show evidence that optimal input sets are 2-designs, which can be generated from a fiducial state and SU(2) rotations.

[1] PRL 85,2733(2000) [2] Nature 457,67(2009) [3] PRL 91,120402(2003) [4] Science 322,563(2008)

10:36AM Y30.00014 Complete characterization of linear amplifiers including the quantum limits for nongaussian noise¹, SHASHANK PANDEY, ZHANG JIANG, JOSHUA COMBES, CARLTON CAVES, Center for Quantum Information and Control, University of New Mexico — We characterize the quantum limitations on the entire probability distribution of added noise in a phase-preserving linear amplifier. Previously the quantum limits have been given entirely in terms of second moments, i.e., noise power or noise temperature [1]. As Josephson parametric amplifiers approach fundamental quantum limits on noise temperature [2,3,4], it becomes important to investigate the limits on higher moments of the amplifier noise. We prove that all phase-preserving linear amplifiers with arbitrary noise are formally equivalent to a parametric amplifier: $\rho_{out} = \text{tr}[S(r) \rho_{in} \otimes \sigma S^\dagger(r)]$, where the gain is $g^2 = \cosh^2(r)$, S is a two-mode squeeze operator, and σ is a physical state of an ancillary mode whose quantum noise determines the noise properties of the amplifier. We discuss generalization of these limits to the nondeterministic linear amplifiers proposed by Ralph and Lund [5]. [1] C. M. Caves, Phys. Rev. D **26**, 1817 (1982). [2] A. A. Clerk et al., Rev. Mod. Phys. **82**, 1155-1208 (2010). [3] N. Bergeal et al., Nature 465, 64–68 (2010). [4] D. Kinion and John Clarke Appl. Phys. Lett. **98**, 202503 (2011). [5] T. C. Ralph and A. P. Lund, in QCMC Vol. 1110 of AIP Conf. Proc. (2009).

¹we acknowledge support from National Science Foundation Grant No. PHY-0903953 and PHY-1005540 and Office of Naval Research Grant No. N00014-11-1-008

10:48AM Y30.00015 Playing the Aharon-Vaidman quantum game with a Young type photonic qutrit, PIOTR KOLENDESKI, URBASI SINHA, Institute for Quantum Computing, University of Waterloo, 200 University Ave. West, Waterloo, Ontario, Canada, YOUNING LI, Department of Physics, Tsinghua University, Beijing 100084, China, TONG ZHAO, MATTHEW VOLPINI, Institute for Quantum Computing, University of Waterloo, 200 University Ave. West, Waterloo, Ontario, Canada, ADAN CABELLO, Departamento de Fisica Aplicada II, Universidad de Sevilla, E-41012 Sevilla, Spain ; Department of Physics, Stockholm University, S-10691 Stockholm, RAYMOND LAFALMME, Institute for Quantum Computing, University of Waterloo, 200 University Ave. West, Waterloo, Ontario, Canada, THOMAS JENNEWEIN, Institute for Quantum Computing, University of Waterloo, 200 University Ave. West, Waterloo, Ontario, CA — The Aharon-Vaidman (AV) game exemplifies the advantage of using simple quantum systems to outperform classical strategies. We present an experimental test of this quantum advantage by using a three-state quantum system (qutrit) encoded in a spatial mode of a single photon passing through a system of three slits. The preparation of a particular state is controlled as the photon propagates through the slits by varying the number of open slits and their respective phases. The measurements are achieved by placing detectors in the specific positions in the near and far-field after the slits. This set of tools allowed us to perform tomographic reconstructions of generalized qutrit states, and implement the quantum version of the AV game with compelling evidence of the quantum advantage.

Friday, March 2, 2012 8:00AM - 10:36AM –

Session Y31 DMP: Focus Session: Topological Insulators: Synthesis & Characterization - Optical & THz Spectroscopy 260

8:00AM Y31.00001 Topological surface state dispersion measured using THz magneto-ellipsometry, JASON N. HANCOCK, J.L.M. VAN MECHELEN, ALEXEY KUZMENKO, DIRK VAN DER MAREL, University of Geneva, CHRISTOPHE BRUNE, ELENA NOVIK, GEORGY ASTAKHOV, HARTMUT BUHMANN, LAURENS MOLENKAMP, Universität Würzburg — We present a magneto-optical study of the three-dimensional topological insulator, strained HgTe. Using polarization-sensitive time-domain THz spectroscopy in a magnetic field, reliable information on the Drude weight and cyclotron resonance frequency severely constrain the details of surface state dispersion within 1meV of the Fermi level. Details of the technique and its prospect for future observation of axion electrodynamics using THz spectroscopy will also be discussed.

8:12AM Y31.00002 Terahertz Kerr Measurements of the Surface States on n- and p-type Bi₂Se₃ Topological Insulators¹, G.S. JENKINS, A.B. SUSHKOV, D.C. SCHMADEL, M.-H. KIM, K.M. BHAMIDIPATI, P. SYERS, J. PAGLIONE, H.D. DREW, CNAM, University of Maryland, College Park, N.P. BUTCH, Cond. Mat. and Matls. Div., Lawrence Livermore National Lab, J.G. ANALYTIS, I.R. FISHER, Dept. of Physics, Stanford University — We report terahertz magneto-optical characterization of a single surface state on bulk crystals of n-type Bi₂Se₃ and p-type Bi₂Se₃ doped with Mg as well as Sm, breaking time reversal symmetry and opening a gap at the Dirac point. A gate is used to apply an electric field which creates and modulates a small depletion layer. The modulated Fermi energy of the surface state produces differential optical signals with no contribution arising from bulk carriers. The real and imaginary parts of the differential Kerr angle yield the transport scattering rate, spectral weight, and mass of the surface state carriers. Comparison with ARPES and other transport measurements will be discussed.

¹This work supported by DOE grant #DESC0005436.

8:24AM Y31.00003 Nonlinear optical responses to circularly polarized lights of the surface state of a topological insulator, TETSURO MISAWA, TAKEHITO YOKOYAMA, SHUICHI MURAKAMI, Tokyo Institute of Technology — Recent photoelectron spectroscopy experiments have revealed the presence of the Dirac cone on the surface of the topological insulator and its spin-splitting due to the spin-orbit interaction. In general, on spin-orbit coupled systems, electric fields induce spin polarizations as linear and nonlinear responses. Here we investigate the inverse Faraday effect on the surface of the topological insulator. The inverse Faraday effect is a non-linear optical effect where a circularly polarized light induces a dc spin polarization. We employ the Keldysh Green's function method to calculate the induced spin polarization and discuss its frequency dependence. In particular, in the low frequency limit, our analytical result gives the spin polarization proportional to the frequency and the square of the lifetime. As for the finite frequency regime, we employ numerical methods to discuss the resonance due to interband transitions. We also discuss the photogalvanic effect, where an illumination of a circular polarized light generates the dc charge current. Lastly, we evaluate those quantities with realistic parameters.

[1] T. Misawa, T. Yokoyama, S. Murakami, Phys. Rev. B84, 165407 (2011).

8:36AM Y31.00004 Optical properties of highly resistive Bi₂Te₂Se, ANJAN REIJNDERS, S. Y. F. ZHAO, LOUISE NIEMEYER, RAPHAEL BOUSKILA, H. J. CHO, SEYEDYARA MOHAJERANI, LUKE J. SANDILANDS, University of Toronto, ROBERT J. CAVA, Princeton University, KENNETH S. BURCH, University of Toronto — Topological insulators are characterized by strong spin-orbit coupling, producing metallic surface states while the bulk remains insulating. Experimental observations of surface states in transport and optical measurements have been obstructed by bulk contributions due to sample defects, placing the Fermi level in the bulk energy gap. Bi₂Te₂Se (BTS), a three-dimensional topological insulator, has recently been shown to exhibit a bulk resistivity larger than any other topological insulator measured to date. However, quantum oscillations are still observed, and attributed to the surface states. In this talk I will present the optical properties of BTS, obtained by broadband FTIR spectroscopy combined with ellipsometry, over a range of 20 - 45,000 cm⁻¹, as well as the Raman spectrum of BTS.

8:48AM Y31.00005 Quasiparticle dynamics of topological insulator Bi₂Se₃ studied by time and angle-resolved photoemission spectroscopy, YIHUA WANG, DAVID HSIEH, EDBERT SIE, DILLON GARDNER, HADAR STEINBERG, YOUNG LEE, PABLO JARILLO-HERRERO, NUH GEDIK, MIT — Topological insulator is a new state of matter that hosts spin helical surface states that may be important for future spintronic applications. Even though the conical bandstructure of the helical Dirac fermions is well established, elastic and inelastic scattering rates of their excitations are less well known because conventional transport or optical techniques can not easily separate surface contribution from bulk effects. Here we use time and angle-resolved photoemission spectroscopy to study the surface electron time-domain dynamics of a prototypical topological insulator Bi₂Se₃. We observe non-Fermi liquid behavior of quasiparticles both above and below the Fermi level. Our result suggests that surface-bulk scattering can play an important role in the transport properties of topological insulator.

9:00AM Y31.00006 Ultrafast Bulk and Surface Dynamics of Bi₂Se₃ Measured by Time-Resolved ARPES, JONATHAN SOBOTA, SHUOLONG YANG, JAMES ANALYTIS, YULIN CHEN, Stanford University, IAN FISHER, Stanford University, PATRICK KIRCHMANN, Fritz Haber Institute of the Max Planck Society, ZHI-XUN SHEN, Stanford University — We investigated the nonequilibrium carrier dynamics of the topological insulator Bi₂Se₃ using femtosecond time- and angle- resolved photoemission spectroscopy. Optical excitation leads to a metastable population of bulk carriers due to the presence of the bandgap. We discuss the coupling of these carriers to the Dirac surface state, which results in a long-lived nonequilibrium surface carrier distribution. We will comment on the implications for topological insulator device applications.

9:12AM Y31.00007 Optical and magneto-optical spectra of Bi_{1-x}Sb_x with x = 0.015, M.S. WOLF, S.V. DORDEVIC, The University of Akron, N. STOJILOVIC, University of Wisconsin Oshkosh, S.S. VUJATOVIC, M.V. NIKOLIC, P.M. NIKOLIC, Serbian Academy of Arts and Sciences, L.C. TUNG, National High Magnetic Field Laboratory — Bismuth and its alloys with antimony have attracted attention in recent years due to possible realization of topological insulating state. In this study we have used infrared and magneto-optical spectroscopies to probe the electrodynamic response of bismuth doped with 1.5 % of antimony. The spectra will be presented for temperatures down to 5 K, and in magnetic fields as high as 18 Tesla. The results reveal strong magneto-optical activity, especially around the plasma minimum in reflectance. These findings will be compared and contrasted with magneto-optical results on pure bismuth.

9:24AM Y31.00008 Magneto-reflectance of Bi₂Se₃ in 18 Tesla fields, S.V. DORDEVIC, M.S. WOLF, The University of Akron, N. STOJILOVIC, University of Wisconsin Oshkosh, H. LEI, C. PETROVIC, Brookhaven National Laboratory, L.C. TUNG, National High Magnetic Field Laboratory — Magneto-optical measurements can provide valuable information in studies of topological insulators. We will report magneto-reflectance spectra of Bi₂Se₃ in magnetic fields up to 18 Tesla. Magnetic-field induced changes in reflectance are most pronounced around the plasma minimum and around the 60 cm⁻¹ mode. Such large magneto-optical activity is unusual for a phonon, and might indicate coupling to collective modes of magnetic origin. Model fits will provide deeper insight into evolution of optical functions with magnetic field.

9:36AM Y31.00009 Photo-induced Chiral Edge Current in the 3D Topological Insulator Bi_2Se_3 , RICKY ROY, University of Washington, MAO LI, Washington State University, GRANT AIVAZIAN, University of Washington, WANG YAO, University of Hong Kong, DAVID COBDEN, University of Washington, CHUANWEI ZHANG, Washington State University, XIAODONG XU, University of Washington — We perform scanning photocurrent (PC) microscopy measurements on the 3D topological insulator Bi_2Se_3 , and observe spatially separated PC peaks of opposite sign, localized along the sample edges. The physics origin of this experimentally observed two-way PC is attributed to the chiral nature of the TI surface states. We show that the coupling between the optical field and the topological surface states yields a spin population imbalance along the edges of the surface, leading to the first order chiral edge charge current observed in the experiment. Further experimental observations of the weak polarization and strong temperature dependence of the PC agree with the theoretical predictions. The PC fades away at a low temperature indicating a mean-free path of $\sim 3 \mu\text{m}$ for topologically protected surface spins.

9:48AM Y31.00010 Terahertz studies and colossal Kerr rotation in the topological insulator Bi_2Se_3 ¹, ROLANDO VALDÉS AGUILAR, A.V. STIER, L. WU, L.S. BILBRO, W. LIU, N.P. ARMITAGE, Department of Physics & Astronomy, Johns Hopkins University, Baltimore, MD 21218, N. BANSAL, M. BRAHLEK, S. OH, Department of Physics & Astronomy, Rutgers University, Piscataway, NJ 08854, D.K. GEORGE, J. CERNE, A.G. MARKELZ, Department of Physics, SUNY Buffalo, Buffalo, NY 14260 — We report a study of high quality MBE grown Bi_2Se_3 topological insulator thin films using time domain terahertz spectroscopy (TDS). We explicitly demonstrate the 2D character of the response by studying films of different thicknesses. In addition, we take advantage of a unique feature of TDS that allows to measure the time structure of the THz pulses. In this way we measure the Faraday and Kerr rotation angles in a single experiment. We find an unprecedentedly large value of the Kerr rotation that is due to the cyclotron resonance of the 2D Dirac fermions². We will also show results on the effect of exposure of the thin films to atmospheric conditions for prolonged periods of time.

¹Work supported by The Institute of Quantum Matter under DOE grant DE-FG02-08ER46544 and by the Gordon and Betty Moore Foundation.

²R. Valdés Aguilar, *et al.* Arxiv:1105.0237.

10:00AM Y31.00011 Size effect in Bi_2Se_3 Topological Insulator micro and nanoparticles, FANGZE LIU, EUGEN PANAITESCU, SWASTIK KAR, Northeastern University — 3D Topological insulators are electronic materials that have a semiconducting bulk interior but a metal-like (zero-gap) surface. We present the investigations of optical transitions in bulk and nanoscale structures of the Topological Insulator Bi_2Se_3 , using optical absorption spectroscopy over a range of energies between 1.1 eV and 6.5 eV. Bi_2Se_3 micro and nanoparticles were obtained by a sequence of ultrasonication steps developed by our group for this purpose. Investigations were performed on particles of different size scales ranging from 10 microns to sub-25 nanometers. While the bulk samples demonstrated expected absorption properties, the smallest (sub-25 nm) particles showed the appearance of a number of new high-energy absorption edges. The fabrication, detailed characterization, and possible reasons for the appearance of the high-energy excitation states will be discussed within the framework of its electronic band-structure description

10:12AM Y31.00012 Temperature-Dependence in Optical Properties of Topological Insulator $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.8}\text{Se}_{1.2}$, CHI SIN TANG, XING QUAN ZOU, BIN XIA, MINGYI LIAO, LAN WANG, ELBERT E.M. CHIA, Nanyang Technological University — Topological Insulators are materials with insulating bulk states and conducting states on their edge or surface. Using Terahertz Time-Domain Spectroscopy (THz-TDS), we studied the temperature-dependence of the optical properties of $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.8}\text{Se}_{1.2}$ single-crystals from 5 K to 300 K in the terahertz regime (0.4 THz to 3.0 THz). We observed a spectral weight shift from low frequencies to frequencies above 1.0 THz in the real conductivity at temperatures below ~ 100 K.

10:24AM Y31.00013 Efficient THz emission from a topological insulator surface, LI-GUO ZHU, Case Western Reserve University; Tsinghua University, Beijing 100084, China, BRIAN KUBERA, Case Western Reserve University, KIN FAI MAK, Columbia University, JIE SHAN, Case Western Reserve University — Bi_2Se_3 is a 3D topological insulator (TI) recently confirmed by the ARPES.¹ Direct optical probe of its metallic surface states is, however, hindered by the remnant Drude response of the bulk material. Second-order nonlinear optical techniques with their surface specificity provide unique opportunities for studying surface electronic transitions in TIs such as Bi_2Se_3 with bulk inversion symmetry.² Here we demonstrate efficient THz emission from the surface of Bi_2Se_3 under the excitation of a femtosecond optical pulse. The emission arises from optical rectification of the optical pulse at the TI surface and the transient current within the surface depletion region. By spectrally resolving the emission under different pump and emission polarizations, we separate the different contributions. Effects arising from just a few atomic layers of the sample surface due to resonance enhancement of the quasi-real optical transitions between the surface electronic states will be discussed.

¹Hsieh et al. Nature 460, 1101 (2009).

²Hsieh et al. Phys. Rev. Lett. 106, 057401 (2011).

Friday, March 2, 2012 8:00AM - 10:36AM – Session Y32 DCOMP: Topological Insulators: General Theory 261

8:00AM Y32.00001 Z_Q topological invariants for identification of short range entangled states, ISAO MARUYAMA, Osaka University, SHO TANAYA, YASUHIRO HATSUGAI, Tsukuba University — Since the Berry phase is quantized as Z_2 value, i.e., 0 or π , due to the time-reversal, or lattice-inversion symmetry in any dimension, the quantized Berry phase[1] is useful for characterization of a topological or quantum order in various models including strongly correlated electron systems[2] and spin systems[3]. Recently, we have proved Z_Q quantization of Berry phases for the general lattice symmetry, where Z_Q ($Q = d+1$) Berry phases are defined for d -dimensional lattices: Polyacetylene, Kagome and Pyrochlore lattice respectively for $d = 1, 2$ and 3.[4]. We have also characterized the dimer-plaquette transition of the orthogonal dimer model in two dimension[5]. [1]Y.Hatsugai, J. Phys. Soc. Jpn, **75**, 123601 (2006). [2]IM, Y. Hatsugai, J. Phys. Soc. Jpn, **76**, 113601 (2007). [3]IM, T.Hirano, Y.Hatsugai, Phys. Rev. B, **79**, 115107 (2009)[4]Y.Hatsugai, IM, Euro. Phys. Lett., **95**, 20003 (2011) [5] I.Maruyama, S.Tanaya, M.Arikawa, Y.Hatsugai, J. Phys.:Conf. Ser., **320**, 01219 (2011)

8:12AM Y32.00002 Trace index and spectral flow in the entanglement spectrum of topological insulators, ARIS ALEXANDRADINATA, Princeton Physics Dept, TAYLOR HUGHES, UIUC Physics Dept, ANDREI BERNEVIG, Princeton Physics Dept — We investigate the entanglement spectra of topological insulators, which manifest edge states on a lattice with spatial boundaries. In the physical energy spectrum, a subset of the edge states that intersect the Fermi level translates to discontinuities in the trace of the single-particle entanglement spectrum, which we call a “trace index.” We find that any free-fermion topological insulator that exhibits spectral flow has a nonvanishing trace index, which provides us with a new description of topological invariants. In addition, we identify the signatures of spectral flow in the single-particle and many-body entanglement spectrum; in the process we present new methods to extract topological invariants and establish a connection between entanglement and quantum Hall physics.

8:24AM Y32.00003 Axions strings and Goldstone-Wilczek currents in quantum spin systems and topological insulators, AKIHIRO TANAKA, National Institute for Materials Science — Axion, originally a high-energy physics entity, has in recent years come into focus in the condensed matter community due to its incarnation in the physics of topological insulators. Much of the discussion so far has concentrated on the physics at the interface/junction of these insulators, which can be viewed as axion domain walls. Here we look into a slightly different situation: axion strings, which are vortex configurations of the axion fields. We discuss how these objects can arise in quantum spin systems and topological insulators, along with their electrodynamic and elastic implications. We also point to some novel Goldstone-Wilczek fermionic currents which can be relevant to the systems considered.

8:36AM Y32.00004 Casimir Interaction Between Topological Insulator Thin Films and Graphene Sheets¹, WANG-KONG TSE, A.H. MACDONALD, University of Texas at Austin — The Casimir effect is a peculiar manifestation of quantum vacuum fluctuations of the electromagnetic field, resulting in an attractive force between closely-spaced conductors. Because of the advent of new materials like graphene and topological insulators, it is of fundamental and potentially also of practical interest to investigate the Casimir effect between conductors described by two-dimensional Dirac models. In this work we study the Casimir effect between topological insulator thin films and graphene planes in the presence of a time-reversal breaking perturbation, most practically an external magnetic field, that gives rise to a half-quantized quantum Hall effect. We evaluate the Casimir energies and forces from the reflection properties of the double layer system. We demonstrate the essential role that is normally played by the Dirac system's dissipative longitudinal conductivity which is neglected in topological field theory descriptions of the Casimir effect. We also show that repulsive Casimir forces are possible in the presence of a magnetic field.

¹This work is supported by the Welch Foundation under 790 Grant No. F1473 and NSI-SWAN.

8:48AM Y32.00005 Exact duality between symmetry protected topological order and intrinsic topological order, ZHENGCHENG GU, MICHAEL LEVIN, Kavli Institute for Theoretical Physics — The discovery of topological insulator (TI) motivates the intensive study of symmetry protected topological (SPT) order. Different from the intrinsic topological order, SPT order is only distinguishable from a trivial disorder phase when certain symmetry is preserved. Indeed, SPT order has a long history in 1D, it has been shown the well known Haldane phase of $S=1$ Heisenberg chain belongs to this class. However, in higher dimensions, most of the previous studies focus on free electron systems with a time reversal symmetry. Until very recently, it was realized that SPT order also exists in interacting boson/spin systems in higher dimensions. In this talk, I will show in 2D boson/spin systems, there exists an interesting duality map between the intrinsic topological order and the SPT order. The duality map implies the SPT orders are stable and distinguishable against arbitrary perturbations if the symmetry is preserved. I will focus on a simplest exact solvable model with an Ising symmetry and discuss the nature of its symmetry protected low-lying edge excitations. The duality map can of course be generalized into arbitrary symmetry group G in any dimension. In principle, the duality map is also applicable for interacting fermion/electron systems.

9:00AM Y32.00006 Asymmetric spatial structure of zero modes for birefringent Dirac fermions¹, MALCOLM P. KENNETT, Simon Fraser University, BITAN ROY, NHMFL, Florida State University, PETER M. SMITH, Simon Fraser University — We study the zero energy modes that arise in an unusual vortex configuration involving both the kinetic energy and an appropriate mass term in a model which exhibits birefringent Dirac fermions as its low energy excitations. We find the surprising feature that the ratio of the length scales associated with states centered on vortex and anti-vortex topological defects can be arbitrarily varied but that fractionalization of quantum numbers such as charge is unaffected. We discuss this situation from a symmetry point of view and present numerical results for a specific lattice model realization of this scenario.

¹Support from NSERC

9:12AM Y32.00007 Location of Singularities in tight-binding wave function of loop-ordered states with Chern numbers, YAN HE, CHANDRA VARMA, University of California Riverside — As a pedagogic exercise, we consider time-reversal violating tight-binding wave-functions for Haldane states in the Graphene model and in a Copper-Oxide model. We locate the singularities in the wave-functions and derive the movement in their location as well as the change in the Berry phase with the choice of Gauge.

9:24AM Y32.00008 Effects of spin-orbit interaction on a triangular lattice potential patterned two-dimensional electron gas, CHON-SAAR CHU, WIE-LIN SU, RONGSING CHANG, Department of Electrophysics, National Chiao Tung University, Hsinchu 30010, Taiwan — We have studied theoretically the electronic states of a two-dimensional electron gas (2DEG) in the presence of a triangular lattice of muffin-tin potentials. In particular, spin-orbit interaction due to the in-plane potential gradient is included. At the K and K' points in the Brillouin zone, the Dirac cones open up a gap and their respective Berry curvatures are of the same sign which, in turn, depends on the electron spin. This contrasting feature, from that of graphene, is related to the fact that inversion symmetry is preserved in our case. The system thus exhibits Z_2 physics.

9:36AM Y32.00009 Smooth gauge for topological insulators, ALEXEY SOLUYANOV, DAVID VANDERBILT, Rutgers University — We develop a technique for constructing Bloch functions for Z_2 quantum spin-Hall insulators that are smooth functions of $\mathbf{k}$ on the whole Brillouin-zone torus. As the initial step, the occupied subspace of the insulator is decomposed into a direct sum of two "Chern bands," i.e., topologically non-trivial subspaces with opposite Chern numbers. This decomposition remains robust independently of underlying symmetries or specific model features. Starting with the Chern bands obtained in this way, we construct a topologically non-trivial unitary transformation that rotates the occupied subspace into a direct sum of topologically trivial subspaces. The possibility of using such a transformation is validated, and the entire procedure is illustrated, by applying it to the Kane-Mele model.

9:48AM Y32.00010 Stable nontrivial Z_2 topology in ultrathin Bi (111) films: a first-principles study¹, ZHENG LIU, Tsinghua University & University of Utah, CHAO-XING LIU, Wuerzburg Universitat, YONG-SHI WU, University of Utah, WEN-HUI DUAN, Tsinghua University, FENG LIU, University of Utah, JIAN WU, Tsinghua University — Recently, there have been intense efforts in searching for new topological insulator (TI) materials. Based on first-principles calculations, we find that all the ultrathin Bi (111) films are characterized by a nontrivial Z_2 number independent of the film thickness, without the odd-even oscillation of topological triviality as commonly perceived. The stable nontrivial Z_2 topology is retained by the concurrent band gap inversions at multiple time-reversal-invariant $\mathbf{k}$ -points and associated with the intermediate inter-bilayer coupling of the multi-bilayer Bi film. Our calculations further indicate that the presence of metallic surface states in thick Bi(111) films can be effectively removed by surface adsorption.

¹This work is supported by MST and NSF of China, DOE-BES, US-NSF and Humboldt foundation

10:00AM Y32.00011 Breakdown of Landau-Ginzburg-Wilson Scheme by Spontaneous Orbital Currents in Zero-gap Semiconductors¹

, MOYURU KURITA, YOUHEI YAMAJI, Department of Applied Physics, University of Tokyo, MASATOSHI IMADA, Department of Applied Physics, University of Tokyo and JST CREST — Critical phenomena of phase transitions are classified into a small number of universality classes. For understanding such symmetry-breaking transitions, a Landau-Ginzburg-Wilson (LGW) scheme greatly helps us. Here, we study the critical phenomena of topological Mott insulator (TMI)[1] where spontaneous orbital currents induced by electron correlation bring the system to topological insulator by formally following the spirit of LGW. Then an unconventional criticality surprisingly emerges around the quantum critical point of TMI: It is governed not only by the symmetry as in the LGW framework but also by topology through electron dispersions and spatial dimension. We demonstrate it by studying an extended Hubbard model on several lattices such as honeycomb and pyrochlore lattice[2] within the Hartree-Fock mean-field level. Both fully numerical calculations and analytical calculations using effective band dispersions are performed.

[1] S. Raghu *et al.*, Phys. Rev. Lett. **100** 156401 (2008)

[2] M. Kurita *et al.*, J. Phys. Soc. Jpn **80** 044708 (2011)

¹This work is financially supported by HPCI Strategic Programs for Innovative Research (SPIRE)

10:12AM Y32.00012 Transition in topological phase of Ge-Sb-Te and Ge-Bi-Te heterostructures

, JEONGWOO KIM, JINWOONG KIM, Department of Physics, Pohang University of Science and Technology, KI-SEOK KIM, Asia Pacific Center for Theoretical Physics, Pohang University of Science and Technology, SEUNG-HOON JHI, Department of Physics, Pohang University of Science and Technology — We studied the transition of topological phase of ternary chalcogenide compounds using first-principles methods. Our calculations show that they undergo a transition between band insulator and topological insulator phases upon the variation of atomic composition and layer thickness. In order to understand the transition, we developed a model Hamiltonian of 1D Dirac fermionic superlattice. We introduced to the Hamiltonian an effective interaction between Dirac fermions that is mediated by the electrons from the band insulating layers. We obtained the phase diagram of the transition as a function of materials parameters including layer thickness, band gap, and Dirac fermionic mass gap. We also discussed the implication of our results to the conducting properties of chalcogenide compounds

10:24AM Y32.00013 Nontrivial topological effects on the surface of strong and weak topological insulators and superconductors

, CHING-KAI CHIU, MICHAEL STONE, University of Illinois at Urbana-Champaign — We investigate states on the surface of strong or weak topological insulators and superconductors that have been gapped by a magnetic material or by a charge density wave. The surface of a strong 3D topological insulator gapped by a magnetic material is well known to possess a half quantum Hall effect. Furthermore, a recent paper (arXiv:1110.3420) showed that the surface of a weak 3D topological insulator gapped by charge density wave has a half quantum spin Hall effect. We generalize these results to all classes of topological insulator and superconductors. We find that if, in d-1 dimension and that symmetry class, there is a Z or Z_2 topological invariant, then the resulting surface state may have a nontrivial topological phase.

Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y40 DBIO DPOLY: Focus Session: Cytoskeleton and Biomechanics - Role of Motors
(Including DBIO Best Thesis Award Lecture) 156A

8:00AM Y40.00001 Forces driving three-dimensional tissue patterning during morphogenesis

, HENG LU, ADAM SOKOLOW, U. SERDAR TULU, DANIEL KIEHART, GLENN EDWARDS, Duke University — Dorsal closure is an essential stage of *Drosophila* embryogenesis and is a model system for *in-vivo* investigations of cell sheet morphogenesis. During closure a system of four biological processes work collectively to close a gap in the epithelium, which initially is filled with a transient tissue. The geometry of the dorsal opening is similar to that of two intersecting circular arcs being pulled apart at a nearly constant rate. Substantial progress in understanding the dynamics has been made in the past by largely viewing closure as a two-dimensional process. However, tissue and cell dynamics are not confined to the embryo surface. We have been investigating the three-dimensional kinematics of dorsal closure by imaging the actomyosin purse strings at the periphery of the dorsal opening and by imaging the apical belts of DE-cadherin in each cell within the opening. We have analyzed the results with the methods of analytic geometry. In addition, in the past we have determined the relative magnitudes of the forces that drive dorsal closure. We have been using magnetic tweezers, time-resolved *in-vivo* microscopy, and biophysical modeling to measure the net force and to determine the magnitude of each force.

8:12AM Y40.00002 Cell Autonomous Shape Changes in Germband Retraction

, HOLLEY LYNCH, ELLIOTT KIM, ROBERT GISH, M. SHANE HUTSON, Vanderbilt University — Germband retraction involves the cohesive movement and regulated cellular mechanics of two tissues on the surface of fruit fly embryos, the germband and the amnioserosa. The germband initially forms a 'U' shape, curling from the ventral surface, around the posterior of the embryo, and onto the dorsal surface; the amnioserosa lies between the arms of this 'U'. Retraction straightens the germband and leaves it only on the ventral side. During retraction, the germband becomes clearly segmented with deep furrows between segments, and its cells elongate towards the amnioserosa, along what becomes the dorsal-ventral axis. To determine the importance of these changes for the overall movement of the tissues, we observed embryos that did not complete germband retraction due to targeted laser ablation of half the amnioserosa. Without the chemical and mechanical influence of the amnioserosa, germband furrows still formed and germband cells still elongated; however, this elongation was misaligned compared to unablated embryos. Thus, furrow formation and cell elongation in the germband are autonomous, but insufficient to drive proper tissue motion. These results suggest that part of the necessary role of the amnioserosa is proper orientation of germband cell elongation.

8:24AM Y40.00003 Wavefronts and mechanical signaling in early *Drosophila* embryos

, TIMON IDEMA, University of Pennsylvania, JULIEN DUBUIS, Princeton University, LISA MANNING, Syracuse University, PHILIP NELSON, ANDREA LIU, University of Pennsylvania — Mitosis in the early syncytial *Drosophila* embryo has a high degree of spatial and temporal correlations, visible as mitotic wavefronts that travel across the embryo. This mitosis wavefront is preceded by another wavefront which corresponds to chromosome condensation. The two wavefronts are separated by a time interval that is independent of cell cycle and propagate at the same speed for a given embryo in a given cycle. We study the wavefronts in the context of excitable medium theory, using two different models, one with biochemical signaling and one with mechanical signaling. We find that the dependence of wavefront speed on cell cycle number is most naturally explained via a mechanical signaling, and that the entire process suggests a scenario in which biochemical and mechanical signaling are coupled.

8:36AM Y40.00004 Passive cellular microrheology in developing fruit fly embryos , SARAH CREWS, XIAOYAN MA, STACEY LAWRENCE, M. SHANE HUTSON, Vanderbilt University — The development of fruit fly (*Drosophila*) embryos involves spatial and temporal regulation of cellular mechanical properties. These properties can be probed *in vivo* using laser hole drilling experiments; however, this technique only infers relative forces. Conversion to absolute forces requires measurement of cellular viscoelastic properties. Here, we use passive microrheology of fluorescently labeled cell membranes to measure the viscoelastic properties of amnioserosa cells. These dynamic epithelial cells play an important mechanical role during two developmental stages: germ band retraction and dorsal closure. Passive microrheology in this system is confounded by active contractions in the cytoskeleton. Thus, the fruit fly embryos are transiently anesthetized with CO₂, halting active cellular movements, leaving only passive Brownian motion. The power spectra of these fluctuations are well fit by a Lorentzian – as expected for Brownian motion – and allow us to extract cellular viscoelastic parameters at different developmental stages. These measured parameters inform previous hole-drilling experiments and provide inputs for quantitative computational models of fruit fly embryonic development.

8:48AM Y40.00005 Remodeling of cellular cytoskeleton drives tissue level morphogenesis , MADHAV MANI, KITP and UCSB Physics, THOMAS LECUIT, IBDML, BORIS SHRAIMAN, KITP and UCSB Physics — Mechanical stresses are central to morphogenesis, both as a cause that generates geometric and topological change, and as regulatory signals that couple cells. Live imaging of fluorescently tagged tissues gives us insight into the cellular processes underlying tissue dynamics during morphogenesis. Amongst these is the remodeling of the cytoskeleton and cellular adhesion. Here, following observations from *drosophila* germ band extension and ventral furrow formation, we a) investigate the mechanical state of the tissue b) perform a quantitative analysis and verification of the cell and tissue level stresses and c) determine how conserved cellular processes are regulated to generate tissue level stresses that drive morphogenesis.

9:00AM Y40.00006 Investigation of autonomous cell dynamics using holographic laser microsurgery , AROSHAN JAYASINGHE, M. SHANE HUTSON, Dept. of Physics & Astronomy, Vanderbilt University, Nashville, TN — Laser-microsurgery has emerged as a powerful technique for evaluating *in vivo* tissue mechanics. We extend this technique by using a spatial light modulator (SLM) to diffract a single UV laser pulse to simultaneously ablate multiple points in living tissue. Using this method, we can quickly and cleanly isolate a single cell by destroying all its nearest neighbors. The post-ablation dynamics of such an isolated cell are then largely dependent on autonomous intracellular forces. Here, we use this technique to investigate cell shape pulsations in amnioserosa cells in *Drosophila* embryos during dorsal closure – specifically to address the degree to which these pulsations are cell autonomous or driven by the contractions of neighboring cells. When cells are isolated at different points in the pulsation cycle, we find that the post-isolation dynamics are strongly dependent on the pre-isolation pulsation phase: cells in a contractile phase collapse immediately, but cells in an expansionary phase continue to expand – at least for 20-60 s before collapsing. These results are in conflict with previous pulsation models that place expanding cells under large extensional strain, and instead suggest that even the expansion phase has a significant cell autonomous component.

9:12AM Y40.00007 DBIO Best Thesis Award: Mechanics, Dynamics, and Organization of the Bacterial Cytoskeleton and Cell Wall , SIYUAN WANG, Harvard University — Bacteria come in a variety of shapes. While the peptidoglycan (PG) cell wall serves as an exoskeleton that defines the static cell shape, the internal bacterial cytoskeleton mediates cell shape by recruiting PG synthesis machinery and thus defining the pattern of cell-wall synthesis. While much is known about the chemistry and biology of the cytoskeleton and cell wall, much of their biophysics, including essential aspects of the functionality, dynamics, and organization, remain unknown. This dissertation aims to elucidate the detailed biophysical mechanisms of cytoskeleton guided wall synthesis. First, I find that the bacterial cytoskeleton MreB contributes nearly as much to the rigidity of an *Escherichia coli* cell as the cell wall. This conclusion implies that the cytoskeletal polymer MreB applies meaningful force to the cell wall, an idea favored by theoretical modeling of wall growth, and suggests an evolutionary origin of cytoskeleton-governed cell rigidity. Second, I observe that MreB rotates around the long axis of *E. coli*, and the motion depends on wall synthesis. This is the first discovery of a cell-wall assembly driven molecular motor in bacteria. Third, I prove that both cell-wall synthesis and the PG network have chiral ordering, which is established by the spatial pattern of MreB. This work links the molecular structure of the cytoskeleton and of the cell wall with organismal-scale behavior. Finally, I develop a mathematical model of cytoskeleton-cell membrane interactions, which explains the preferential orientation of different cytoskeleton components in bacteria.

9:48AM Y40.00008 Coupling of Active Motion and Advection Shapes Intracellular Cargo Transport , PHILIPP KHUC TRONG, Department of Physics, and Department of Applied Mathematics and Theoretical Physics, University of Cambridge, JOCHEN GUCK, Department of Physics, University of Cambridge, RAYMOND GOLDSTEIN, Department of Applied Mathematics and Theoretical Physics, University of Cambridge — Three different mechanisms can contribute to intracellular cargo transport: (1) passive diffusion, (2) active motor-driven transport along cytoskeletal filament networks and (3) passive advection by fluid flows. Active and advective transport are coupled because cytoplasmic flows can arise through entrainment of the fluid that surrounds actively moving cargo on cytoskeletal networks. Here, we report a reaction-advection-diffusion model for transport of a passive mass-conserved scalar that can cycle between a bound state, where advection represents active transport on a cytoskeletal network, and an unbound state, where the advecting fluid flow field is driven by forces from the cytoskeletal network. Cargo transport and localization patterns are explored for different cytoskeletal network topologies and for varying reaction kinetics. We find that for sufficiently low diffusion, localization of cargo to a target area is optimized either by low reaction kinetics and decoupling of bound and unbound state, or by a mostly disordered cytoskeletal network with only weak directional bias. The principles exemplified by this model likely have implications for our understanding and interpretation of transport patterns and cytoskeletal network structures.

10:00AM Y40.00009 Motion in partially and fully cross-linked F-actin networks , ELIZA MORRIS, ALLEN EHRLICHER, DAVID WEITZ, Harvard University — Single molecule experiments have measured stall forces and procession rates of molecular motors on isolated cytoskeletal fibers in Newtonian fluids. But in the cell, these motors are transporting cargo through a highly complex cytoskeletal network. To compare these single molecule results to the forces exerted by motors within the cell, an evaluation of the response of the cytoskeletal network is needed. Using magnetic tweezers and fluorescence confocal microscopy we observe and quantify the relationship between bead motion and filament response in F-actin networks both partially and fully cross-linked with filamin. We find that when the transition from full to partial cross-linking is brought about by a decrease in cross-linker concentration there is a simultaneous decline in the elasticity of the network, but the response of the bead remains qualitatively similar. However, when the cross-linking is reduced through a shortening of the F-actin filaments the bead response is completely altered. The characteristics of the altered bead response will be discussed here.

10:12AM Y40.00010 Measurements of the constituent contributions to the physical properties of fibroblast populated collagen microtissues with magnetic micro-tissue stretchers¹, RUOGANG ZHAO, ALAN LIU, Johns Hopkins University, THOMAS BOUDOU, CHRISTOPHER CHEN, University of Pennsylvania, DANIEL REICH, Johns Hopkins University — The mechanical properties of fibroblast populated collagen matrix (FPCM) provide important physical cues to regulate physiological and pathological processes of encapsulated cells. The mechanical strength of FPCM is arises from both of its constituents: the collagen matrix and the fibroblasts. Existing methods to separate the contribution of individual constituents by treating cm-scale tissue samples with decellularization drugs for prolonged periods have been shown to adversely affect the properties of the collagen matrix. To minimize such matrix damage, we have developed a magnetic microtissue stretching system that allows us to grow arrays of sub-mm scale microtissues that can be rapidly decellularized. This consists of arrays of paired micro-cantilevers that support the 3D FPCM and can be driven by incorporated magnetic material via externally applied magnetic fields. By measuring the tensile force applied to the FPCM and the tissue strain, we found the stiffness of the matured FPCM is 28.1 $\pm$ 1.8 kPa and that of the decellularized collagen matrix is 23.1 $\pm$ 3.1 kPa. These measurements of the stiffness of the intact collagen matrix in a remodeled FPCM can provide important clues on the mechanical environment that regulates the biological function of encapsulated cells.

¹Supported in part by NIH grant HL090747

10:24AM Y40.00011 Crowding of molecular motors determines microtubule depolymerization, LOUIS REESE, ANNA MELBINGER, ERWIN FREY, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universitaet Muenchen — Assembly and disassembly dynamics of microtubules (MTs) is tightly controlled by MT associated proteins. Here, it is investigated how plus-end-directed depolymerases of the kinesin-8 family regulate MT depolymerization dynamics. We reproduce experimental findings within the framework of a totally asymmetric simple exclusion process with Langmuir kinetics (TASEP/LK). Thereby, crowding is identified as the key regulatory mechanism of depolymerization dynamics. The analysis gives two qualitatively distinct phases. For motor densities above a particular threshold, a macroscopic traffic jam emerges at the plus-end and the MT dynamics become independent of the motor concentration. Below this threshold, microscopic traffic jams at the tip arise which cancel out the effect of the depolymerization kinetics such that the depolymerization speed is determined by the motor density. Because this density varies over the MT length, length-dependent regulation is possible. The critical length at which MTs start to depolymerize in a length-dependent way is discussed. Reference: Louis Reese, Anna Melbinger and Erwin Frey. Biophys. J. 101, 2190 (2011)

10:36AM Y40.00012 Physics of the actin cortex in shape oscillations of dividing cells, GUILLAUME SALBREUX, Max Planck Institute for the Physics of Complex Systems, Dresden, EWA PALUCH LAB COLLABORATION¹ — During cytokinesis, a contractile actomyosin cortex is present at the poles of the dividing cell. For a large enough tension of the polar cortex, a physical symmetry-breaking instability of the cell shape can occur where one pole transfers its volume to the other. Such a shape instability can indeed be observed in control and treated dividing cultured cells where it results in cell shape oscillations and in some cases leads to cytokinesis failure. The cell oscillation properties can be accurately described with a theoretical model based on a competition between cortex turnover and contraction dynamics. Interestingly, our results indicate that a sufficiently large cell elasticity is needed to ensure successful cytokinesis.

¹Max Planck Institute for Cell Biology and Genetics, Dresden

10:48AM Y40.00013 Geometrical Reorganisation of the Cytoskeleton and Changes in Cellular Stiffness Following Stretch, HARIKRISHNAN PARAMESWARAN, BELA SUKI, Boston University — Cells in the lung and the vasculature are under a highly dynamic mechanical environment where they are constantly exposed to stretch. Cells adapt to these fluctuations in stretch by remodeling their cytoskeleton. However, the influence of these geometrical changes on cell stiffness is not well understood. We developed a computational model to simulate the geometrical reorganization of the actin by non-muscle myosin-II under conditions of monotonous cyclic stretch, where amplitude and frequency is constant from cycle to cycle and variable stretch, where the amplitude is varied from cycle-to-cycle and the frequency is inversely proportional to amplitude. With the monotonous cyclic-stretch, the network exhibited significant hysteresis in geometry, it reorganized itself into a more stable configuration and the internal prestress decreased after each cycle. In contrast, the more realistic variability in stretch amplitude prevented these stable configurations from forming and preserved the prestress. This behavior was dependent on the variability in stretch amplitude and the timing of the large amplitude stretches. We conclude that prestress is a consequence of cytoskeletal reorganization which exhibits structural hysteresis and is dependent on the nature of the stretch pattern.

Friday, March 2, 2012 8:00AM - 10:12AM –
Session Y41 DBIO: Focus Session: Physics of Cancer III – Imaging 156B

8:00AM Y41.00001 Cancer Imaging, CHENGHANG ZONG, —

8:36AM Y41.00002 Optimality in the Development of Intestinal Crypts, ALEXANDER VAN OUDENAAR-DEN, MIT — Intestinal crypts in mammals are comprised of long-lived stem cells and shorter-lived progenies, maintained under tight proportions during adult life. Here we ask what are the design principles that govern the dynamics of these proportions during crypt morphogenesis. We use optimal control theory to show that a stem cell proliferation strategy known as a 'bang-bang' control minimizes the time to obtain a mature crypt. This strategy consists of a surge of symmetric stem cell divisions, establishing the entire stem cell pool first, followed by a sharp transition to strictly asymmetric stem cell divisions, producing non-stem cells with a delay. We validate these predictions using lineage tracing and single molecule fluorescent in-situ hybridization of intestinal crypts in newborn mice and find that small crypts are entirely composed of Lgr5 stem cells, which become a minority as crypts further grow. Our approach can be used to uncover similar design principles in other developmental systems.

9:12AM Y41.00003 Molecular Imaging System for Monitoring Tumor Angiogenesis, ESRA AYTAC, MEHMET BURCIN UNLU, None — In cancer, non-invasive imaging techniques that monitor molecular processes associated with the tumor angiogenesis could have a central role in the evaluation of novel antiangiogenic and proangiogenic therapies as well as early detection of the disease. Matrix metalloproteinases (MMP) can serve as specific biological targets for imaging of angiogenesis since expression of MMPs is required for angiogenesis and has been found to be upregulated in every type of human cancer and correlates with stage, invasive, metastatic properties and poor prognosis. However, for most cancers it is still unknown when, where and how MMPs are involved in the tumor angiogenesis [1]. Development of high-resolution, high sensitivity imaging techniques in parallel with the tumor models could prove invaluable for assessing the physical location and the time frame of MMP enzymatic activity. The goal of this study is to understand where, when and how MMPs are involved in the tumor angiogenesis. We will accomplish this goal by following two objectives: to develop a high sensitivity, high resolution molecular imaging system, to develop a virtual tumor simulator that can predict the physical location and the time frame of the MMP activity. In order to achieve our objectives, we will first develop a PAM system and develop a mathematical tumor model in which the quantitative data obtained from the PAM can be integrated. So, this work will develop a virtual tumor simulator and a molecular imaging system for monitoring tumor angiogenesis. 1.Kessenbrock, K., V. Plaks, and Z. Werb, MMP:regulators of the tumor microenvironment. Cell, 2010. 141(1)

9:24AM Y41.00004 Characterizing Spatial Organization of Cell Surface Receptors in Human Breast Cancer with STORM, EVAN LYALL, Department of Bioengineering, University of California, Berkeley, MATTHEW R. CHAPMAN, Biophysics Graduate Group, University of California, Berkeley, LYDIA L. SOHN, Department of Mechanical Engineering, University of California, Berkeley — Regulation and control of complex biological functions are dependent upon spatial organization of biological structures at many different length scales. For instance Eph receptors and their ephrin ligands bind when opposing cells come into contact during development, resulting in spatial organizational changes on the nanometer scale that lead to changes on the macro scale, in a process known as organ morphogenesis. One technique able to probe this important spatial organization at both the nanometer and micrometer length scales, including at cell-cell junctions, is stochastic optical reconstruction microscopy (STORM). STORM is a technique that localizes individual fluorophores based on the centroids of their point spread functions and then reconstructs a composite image to produce super resolved structure. We have applied STORM to study spatial organization of the cell surface of human breast cancer cells, specifically the organization of tyrosine kinase receptors and chemokine receptors. A better characterization of spatial organization of breast cancer cell surface proteins is necessary to fully understand the tumorigenesis pathways in the most common malignancy in United States women.

9:36AM Y41.00005 In Vivo Fluorescence Resonance Energy Transfer Imaging for Targeted Anti-Cancer Drug Delivery Kinetics¹, KEVIN WEBB, VAIBHAV GAIND, HSIAORHO TSAI, BRIAN BENTZ, VENKATESH CHELVAM, PHILIP LOW, Purdue University — We describe an approach for the evaluation of targeted anti-cancer drug delivery *in vivo*. The method emulates the drug release and activation process through acceptor release from a targeted donor-acceptor pair that exhibits fluorescence resonance energy transfer (FRET). In this case, folate targeting of the cancer cells is used - 40 % of all human cancers, including ovarian, lung, breast, kidney, brain and colon cancer, over-express folate receptors. We demonstrate the reconstruction of the spatially-dependent FRET parameters in a mouse model and in tissue phantoms. The FRET parameterization is incorporated into a source for a diffusion equation model for photon transport in tissue, in a variant of optical diffusion tomography (ODT) called FRET-ODT. In addition to the spatially-dependent tissue parameters in the diffusion model (absorption and diffusion coefficients), the FRET parameters (donor-acceptor distance and yield) are imaged as a function of position. Modulated light measurements are made with various laser excitation positions and a gated camera. More generally, our method provides a new vehicle for studying disease at the molecular level by imaging FRET parameters in deep tissue, and allows the nanometer FRET ruler to be utilized in deep tissue.

¹Supported by NSF

9:48AM Y41.00006 Exploring X-Ray Phase-Contrast Imaging using Photon Counting Detectors for Early Breast Cancer Detection¹, MINI DAS, Department of Physics, University of Houston, Houston, TX — X-ray attenuation-contrast (AC) imaging in the form of digital mammography (DM) is the current gold standard of screening for deep-set cancers like breast cancer. DM creates images based on the attenuation differences between normal and malignant breast tissue, but the extremely low attenuation contrast poses severe challenges for early cancer detection. In order to overcome these limitations posed by AC imaging, there is a growing interest in exploring phase changes in x-rays as they propagate through the tissue. Theoretical estimations show that the x-ray phase difference between normal and malignant breast tissue is three orders of magnitude higher than the corresponding absorption contrast. While x-ray attenuation is determined by the atomic number of the elements forming the tissue, the phase change is determined by the density or refractive index. Due to high energy of x-rays, absolute measurement of phase change is challenging. We will present our efforts to understand x-ray phase contrast in biological tissue using a photon counting detector (TIMEPIX), which is capable of energy and time resolved measurements with very high spatial resolution (about 50 microns). We are exploring novel methods, which will also be clinically feasible to extract phase information using a combination of PCDs and phase retrieval techniques. Phase changes and contrast details of various breast cancer types will also be investigated using the energy resolved measurements obtained using PCDs.

¹Funding support from NIH/NCI (K25CA140858).

10:00AM Y41.00007 Uncovering cancer cell behavioral phenotype in 3-D *in vitro* metastatic landscapes, LIYU LIU, Physics, Princeton University, BO SUN, Mechanical & Aerospace Engineering, GUILLAUME DUCLOS, Physics, Princeton University, YOONSEOK KAM, ROBERT GATENBY, Moffitt Cancer Institute, HOWARD STONE, Mechanical & Aerospace Engineering, ROBERT AUSTIN, Physics, Princeton University, PHYSICS-MECHANICAL & AEROSPACE ENGINEERING, PRINCETON TEAM, PHYSICS, PRINCETON-MOFFITT CANCER INSTITUTE COLLABORATION — One well-known fact is that cancer cell genetics determines cell metastatic potentials. However, from a physics point of view, genetics as cell properties cannot directly act on metastasis. An agent is needed to unscramble the genetics first before generating dynamics for metastasis. Exactly this agent is cell behavioral phenotype, which is rarely studied due to the difficulties of real-time cell tracking in *in vivo* tissue. Here we have successfully constructed a micro *in vitro* environment with collagen based Extracellular Matrix (ECM) structures for cell 3-D metastasis. With stable nutrition (glucose) gradient inside, breast cancer cell MDA-MB-231 is able to invade inside the collagen from the nutrition poor site towards the nutrition rich site. Continuous confocal microscopy captures images of the cells every 12 hours and tracks their positions in 3-D space. The micro fluorescent beads pre-mixed inside the ECM demonstrate that invasive cells have altered the structures through mechanics. With the observation and the analysis of cell collective behaviors, we argue that game theory may exist between the pioneering cells and their followers in the metastatic cell group. The cell collaboration may explain the high efficiency of metastasis.

Friday, March 2, 2012 8:00AM - 11:00AM —
Session Y42 DBIO: Physics of Bacteria and Viruses 156C

8:00AM Y42.00001 Membrane-mediated interaction between retroviral capsids, RUI ZHANG, North-eastern State University, TOAN NGUYEN, Georgia Institute of Technology — A retrovirus is an RNA virus that is replicated through a unique strategy of reverse transcription. Unlike regular enveloped viruses which are assembled inside the host cells, the assembly of retroviral capsids happens right on the cell membrane. During the assembly process, the partially formed capsids deform the membrane, giving rise to an elastic energy. When two such partial capsids approach each other, this elastic energy changes. Or in other words, the two partial capsids interact with each other via the membrane. This membrane mediated interaction between partial capsids plays an important role in the kinetics of the assembly process. In this work, this membrane mediated interaction is calculated both analytically and numerically. It is worth noting that the differential equation determining the membrane shape in general nonlinear and cannot be solved analytically, except in the linear region of small deformations. And it is exactly the nonlinear regime that is important for the assembly kinetics of retroviruses as it provides a large energy barrier. The theory developed here is applicable to more generic cases of membrane mediated interactions between two membrane-embedded proteins.

8:12AM Y42.00002 Discrete fracture patterns of virus shells reveal mechanical building blocks

, IRENA L. IVANOVSKA, Biophysical Engineering Laboratory, University of Pennsylvania, Philadelphia, PA, ROBERTO MIRANDA, JOSÉ L. CARRASCOSA, Dept. Struct. Macromol., Centro Nacional de Biotecnología, Campus Universidad Autónoma de Madrid, GJIS J.L. WUITE, Dept. Physics and Astronomy, Vrije Universiteit Amsterdam, CHRISTOPH F. SCHMIDT, Third Institute of Physics, Georg-August-Universität Göttingen — Viral shells are self-assembled protein nanocontainers with remarkable material properties. They combine simplicity of construction with toughness and complex functionality. To date we know little about how virus structure determines assembly pathways and shell mechanics. We have used atomic force microscopy to study structural failure of the shells of the bacteriophage $\Phi 29$. We observed rigidity patterns following the symmetry of the capsid proteins and under prolonged force exertion, we see fractures along well-defined lines of the 2D crystal lattice. We found the mechanically most stable building block of the shells was a trimer. Our approach of “reverse engineering” the virus shells thus made it possible to identify stable structural intermediates. Such stable intermediates point to a hierarchy of interactions among equal building blocks correlated with distinct next-neighbor interactions. The results also demonstrate that concepts from macroscopic materials science, such as fracture, can be usefully employed in molecular engineering.

8:24AM Y42.00003 Pili-driven surface motility of *Myxococcus xanthus*

, MAXSIM GIBIANSKY, UCLA Bioengineering, WEI HU, UCLA School of Dentistry, KUN ZHAO, UCLA Bioengineering, HONGWEI PAN, WENYUAN SHI, UCLA School of Dentistry, KARIN DAHMEN, UIUC Physics, GERARD WONG, UCLA Bioengineering — *Myxococcus xanthus* is a common, rod-shaped soil-dwelling bacterium with complex motility characteristics. In groups, *M. xanthus* bacteria can move via social “S” motility, in which the Type IV Pili (TFP) attach to secreted exopolysaccharides (EPS). We examine this motility mechanism using high-frame-rate video acquisition, taking data on individual bacteria at 400 frames per second; using particle tracking algorithms, we algorithmically reconstruct the bacterial trajectories. The motion of a single bacterium as it is pulled by its TFP through the EPS layer on the surface is not smooth, but instead displays distinct plateaus and slips, with a wide range of plateau and slip lengths. The distribution of slips exhibits power law scaling, consistent with a crackling noise model; crackling noise has previously been used to model nonbiological systems such as earthquake dynamics and Barkhausen noise. We show quantitative agreement between mean field friction models and observed bacterial dynamics. We demonstrate that the crackling noise behavior of *M. xanthus* is strongly dependent on the presence of EPS, but is unaffected by the chemotactic behavior of the bacterium; we also demonstrate velocity coupling between pairs of bacteria in the early stages of social motility.

8:36AM Y42.00004 Pili-taxis: Clustering of *Neisseria gonorrhoeae* bacteria

, JOHANNES TAKTIKOS, Technical University Berlin, Germany, VASILY ZABURDAEV, Harvard University, NICOLAS BIAIS, Columbia University, HOLGER STARK, Technical University Berlin, DAVID A. WEITZ, Harvard University — The first step of colonization of *Neisseria gonorrhoeae* bacteria, the etiological agent of gonorrhea, is the attachment to human epithelial cells. The attachment of *N. gonorrhoeae* bacteria to surfaces or other cells is primarily mediated by filamentous appendages, called type IV pili (Tfp). Cycles of elongation and retraction of Tfp are responsible for a common bacterial motility called twitching motility which allows the bacteria to crawl over surfaces. Experimentally, *N. gonorrhoeae* cells initially dispersed over a surface agglomerate into round microcolonies within hours. It is so far not known whether this clustering is driven entirely by the Tfp dynamics or if chemotactic interactions are needed. Thus, we investigate whether the agglomeration may stem solely from the pili-mediated attraction between cells. By developing a statistical model for pili-taxis, we try to explain the experimental measurements of the time evolution of the mean cluster size, number of clusters, and area fraction covered by the cells.

8:48AM Y42.00005 The Psl economy in early *P. aeruginosa* biofilm development

, KUN ZHAO, University of California, Los Angeles, BOO SHAN TSENG, University of Washington, FAN JIN, MAX GIBIANSKY, University of California, Los Angeles, JOE HARRISON, MATTHEW PARSEK, University of Washington, GERARD WONG, University of California, Los Angeles — Psl from *P. aeruginosa* (PAO1) is a mannose- and galactose-rich exopolysaccharide (EPS). It has been shown that Psl plays an important role in bacterial surface adhesion. Here, we examine role of Psl in controlling motility and microcolony formation during early biofilm development, by translating video microscopy movies into searchable databases of bacterial trajectories. We use a massively-parallel cell tracking algorithm to extract the full motility history of every cell in a large community. We find that at early stages of growth, *P. aeruginosa* motility is guided by Psl and self-organize in a manner analogous to a capitalist economic system, resulting in a power law bacterial distribution where a small number of bacteria are extremely “rich” in communally produced Psl. By comparing overproducers and underproducers of Psl, we find that local Psl levels determine post-division cell fates: High local Psl levels drive the formation of sessile microcolonies that grow exponentially.

9:00AM Y42.00006 Roles of Pel and Psl in very early biofilm development

, B.J. COOLEY, TRAVIS THATCHER, GUILLAUME L'HER, ERIN REED, JAMIE STUART, APRIL KISSINGER, VERNITA GORDON, Center for Nonlinear Dynamics and Department of Physics, University of Texas at Austin — Biofilms are dynamic, multicellular communities of unicellular organisms. Biofilms cause many chronic infections; an important case is the opportunistic human pathogen *Pseudomonas aeruginosa*. Bacteria in biofilms produce an extracellular matrix that binds bacteria to each other and to a surface. The two primary extracellular matrix components produced by *P. aeruginosa* are the polysaccharides Pel and Psl. Here we examine the roles of Pel and Psl in the very early stages of biofilm development, just after initial surface attachment. We use high-throughput automated tracking and analysis to compare wild-type bacteria with mutants incapable of producing Pel, Psl, or both. We examine motion on a surface as well as inter-bacterial interactions. These results quantify the unique roles played by Pel and Psl and show an unexpected relationship between Pel expression and adhesion to a surface.

9:12AM Y42.00007 Quorum activation at a distance: spatiotemporal patterns of gene regulation from diffusion of an autoinducer signal

, GABRIEL DILANJI¹, JESSICA LANGEBAKE², PATRICK DELEENHEER³, STEPHEN J. HAGEN⁴, University of Florida — Bacteria in colonies coordinate gene regulation through the exchange of diffusible signal molecules known as autoinducers (AI). This “quorum signaling” often occurs in physically heterogeneous and spatially extended environments such as biofilms. Under these conditions the space and time scales for diffusion of the signal limit the range and timing of effective gene regulation. We expect that spatial and temporal patterns of gene expression will reflect physical environmental constraints as well as nonlinear transcriptional activation and feedback within the gene regulatory system. We have combined experiments and modeling to investigate how these spatiotemporal patterns develop. We embed engineered plasmid/GFP quorum sensor strains or wild type strains in a long narrow agar lane, and then introduce AI signal at one terminus of the lane. Diffusion of the AI initiates reporter expression along the length of the lane, extending to macroscopic distances of mm-cm. Resulting patterns are captured quantitatively by a mathematical model that incorporates logistic growth of the population, diffusion of AI, and nonlinear transcriptional activation. Our results show that a diffusing quorum signal can coordinate gene expression over distances of order 1cm on time scales of order 10 hrs.

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²Department of Mathematics

³Department of Mathematics

⁴Department of Physics

9:24AM Y42.00008 Biofilm Formation in Microscopic Double Emulsion Droplets, CONNIE CHANG, DAVID WEITZ, Harvard University — In natural, medical, and industrial settings, there exist surface-associated communities of bacteria known as biofilms. These highly structured films are composed of bacterial cells embedded within self-produced extracellular matrix, usually composed of exopolysaccharides, proteins, and nucleic acids; this matrix serves to protect the bacterial community from antibiotics and environmental stressors. Here, we form biofilms encapsulated within monodisperse, microscopically-sized double emulsion droplets using microfluidics. The bacteria self-organize at the inner liquid-liquid droplet interfaces, multiply, and differentiate into extracellular matrix-producing cells, forming manifold three-dimensional shell-within-a-shell structures of biofilms, templated upon the inner core of spherical liquid droplets. By using microfluidics to encapsulate bacterial cells, we have the ability to view individual cells multiplying in microscopically-sized droplets, which allows for high-throughput analysis in studying the genetic program leading to biofilm development, or cell signaling that induces differentiation.

9:36AM Y42.00009 Atomic Force Microscope Investigations of Bacterial Biofilms Treated with Gas Discharge Plasmas¹, KURT VANDERVOORT, Physics Department, California State Polytechnic University, Pomona, CA, ANNA ZELAYA, Biological Sciences Department, California State Polytechnic University, Pomona, CA, GRACIELA BRELLES-MARINO, Biological Sciences Department, California State Polytechnic University, Pomona, CA and CINDEFI, Universidad Nacional de La Plata, Argentina — We present investigations of bacterial biofilms before and after treatment with gas discharge plasmas. Gas discharge plasmas represent a way to inactivate bacteria under conditions where conventional disinfection methods are often ineffective. These conditions involve biofilm communities, where bacteria grow embedded in an exopolysaccharide matrix, and cooperative interactions between cells make organisms less susceptible to standard inactivation methods. In this study, biofilms formed by the opportunistic bacterium *Pseudomonas aeruginosa* were imaged before and after plasma treatment using an atomic force microscope (AFM). Through AFM images and micromechanical measurements we observed bacterial morphological damage and reduced AFM tip-sample surface adhesion following plasma treatment.

¹Funding was provided by an NSF-NUE grant 0406533 and by an NIH-SCORE grant 1SC3GM088070-01. In addition, Anna Zelaya acknowledges support from the NIH MBRS Research Initiative for Scientific Enhancement (RISE) Program, grant 2R25GM061190-05A2.

9:48AM Y42.00010 High speed dynamic characterization of an *E. coli* population using advanced optical methods (DDM and DFM), RONGJING ZHANG, LAURENCE WILSON, Rowland Institute at Harvard University — The motility of microbes/bacteria in a complex environment, especially the average motility of the whole group of microorganisms, is directly related to behavior such as virulence, biofilm formation, etc. It is challenging to use traditional tracking methods to quantify the average motility of a large population. It is even more challenging when the environment is constantly changing. Two optical methods were developed to solve the problem: differential dynamic microscopy (DDM) and dark field flickering microscopy (DFM). The key features of bacteria motility were quantified automatically: average swimming speed, motile fraction, diffusion coefficient, cell body rotation speed and flagellar bundle rotation speed. This method is able to measure $\sim 10^4$ cells simultaneously. With the help of a high speed camera, the timescale of the dynamic measurement can be in a wide range from 10^{-4} s to 10^5 s. Using this tool, temperature effects on *E. coli* motility were studied. Potential biomedically-relevant applications will also be discussed.

10:00AM Y42.00011 Bacterial Swimming at Air/Water and Oil/Water Interfaces, MICHAEL MORSE, ATHENA HUANG, GUANGLAI LI, JAY TANG, Brown University, JAY TANG'S BIOPHYSICS GROUP TEAM — The microbes inhabiting the planet over billions of years have adapted to diverse physical environments of water, soil, and interfaces between water and either solid or air. Following recent studies on bacterial swimming and accumulation near solid surfaces, we turn our attention to the behavior of *Caulobacter crescentus*, a singly flagellated bacterium, at water/air and water/oil interfaces. The latter is motivated by relevance to microbial degradation of crude oil in light of the recent oil spill in the Gulf of Mexico. Our ongoing study suggests that *Caulobacter* swarmer cells tend to get physically trapped at both water/air and water/oil interfaces, accumulating at the surface to a greater degree than boundary confinement properties like that of solid surfaces would predict. At the water/air interface, swimmers move in tight circles at half the speed of swimmers in the bulk fluid. At the water/oil interface, swimming circles are even tighter with further reduced swimming speed. We report experimental data and present preliminary analysis of the findings based on low Reynolds number hydrodynamics, the known surface tension, and surface viscosity at the interface. The analysis will help determine properties of the bacterium such as their surface charge and hydrophobicity.

10:12AM Y42.00012 Bacterial thermotaxis by modulation of the swimming speed, MAHMUT DEMIR, HANNA SALMAN, Department of Physics and Astronomy, University of Pittsburgh, SALMAN LAB TEAM — It has been long established that random walkers such as bacteria can migrate in inhomogeneous environments, even without actively responding to changes they sense around them, by modulating their swimming speed and/or run time. We will show that *E. coli* bacteria migrate in shallow temperature gradients due to their speed dependence on temperature even without the presence of sensing receptors. Interestingly however, we find that the direction of their migration in the gradient depends on the serine concentration in the medium. This results from the fact that the bacterial swimming speed exhibits a two-state function of serine concentration and the difference between the two states increases with temperature. Our results show that the swimming speed of the bacteria increases monotonically with temperature when serine is present at high concentration, while it decreases for temperatures above 30 °C at low serine concentration. This observed difference in the speed dependence on temperature is found to be due to a change in the intracellular pH of the bacteria when serine is added to their surroundings, which occurs only in the presence of the serine receptor Tsr. We will discuss some details of the mechanism underlying this effect and its consequences for the bacterial behavior.

10:24AM Y42.00013 Role of cell bending and slime navigation in swarms of *M. xanthus*¹, CAMERON HARVEY, University of Notre Dame, DALE KAISER, Stanford University, MARK ALBER, University of Notre Dame — Many bacteria use motility described as swarming to colonize surfaces that allows them to optimize their access to nutrients. The swarming of the bacterium *M. xanthus* on surfaces is a remarkable interplay between motility mechanisms, cell flexibility, cell-cell adhesive interactions and directional reversals. The properties of individual cells from different mutant strains and density regimes will be demonstrated in this talk. Then, a computational model based on subcellular elements for cell representation and implemented on graphical processing units (GPUs) will be presented. High-quality high magnification movies of bacterial motility together with biologically justified computational simulations will be used for investigation of collective motion and order in swarming populations of bacteria. Collective motion will be shown to include the dynamical formation of cell clusters as well as streams of cells moving over networks of cell-generated slime tracks.

¹Research was partially supported by NIH grant 1R01GM100470-01.

10:36AM Y42.00014 Effect of Antimicrobial Agents on MinD Protein Oscillations in *E. coli* Bacterial Cells, COREY KELLY, MAXIMILIANO GIULIANI, JOHN DUTCHER, University of Guelph — The pole-to-pole oscillation of MinD proteins in *E. coli* cells determines the location of the division septum, and is integral to healthy cell division. It has been shown previously that the MinD oscillation period is approximately 40 s for healthy cells [1] but is strongly dependant on environmental factors such as temperature, which may place stress on the cell [2,3]. We use a strain of *E. coli* in which the MinD proteins are tagged with green fluorescent protein (GFP), allowing fluorescence visualization of the MinD oscillation. We use high-resolution total internal reflection fluorescence (TIRF) microscopy and a custom, temperature controlled flow cell to observe the effect of exposure to antimicrobial agents on the MinD oscillation period and, more generally, to analyze the time variation of the spatial distribution of the MinD proteins within the cells. These measurements provide insight into the mechanism of antimicrobial action. [1] Raskin, D.M.; de Boer, P. (1999) Proc. Natl. Acad. Sci. 96: 4971-4976. [2] Touhami, A.; Jericho, M; Rutenberg, A. (2006) J. Bacteriol. 188: 7661-7667. [3] Downing, B.; Rutenberg, A.; Touhami, A.; Jericho, M. (2009) PLoS ONE 4: e7285.

10:48AM Y42.00015 Residence and transit times of MinD in *E. coli* bacterial cells, MAXIMILIANO GIULIANI, COREY KELLY, JOHN DUTCHER, University of Guelph — A key step in the life of a bacterial cell is its division into two daughter cells of equal size. This process is carefully controlled and regulated so that an equal partitioning of the main cell components is obtained, which is critical for the viability of the daughter cells. In *E. coli* this regulation is accomplished in part by the Min protein system, that determines the localization of the division machinery. Of particular interest is the MinD protein that exhibits an oscillation between the poles in the rod shaped bacteria. The oscillation relies on a ATP mediated dimerization of the MinD protein that allows its insertion into the inner membrane at one of the poles of the cell, followed by an interaction with the MinE protein, which releases the MinD from the membrane, allowing it to travel to the other pole of the cell where the cycle is repeated. We have studied the spatio-temporal characteristics of the MinD oscillation from which we extract the average times for the two main processes that determine the oscillation period: the residence time in the membrane and the transit time to travel the length of the cell. Additionally, we explore how these two timescales are affected by stresses on the bacterial cells due to unfavorable physiological conditions.

Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y43 DBIO: Invited Session: Physical Organizing Principles for Amyloid Matter: Prediction, Structure, Function 157AB

8:00AM Y43.00001 Prions, From Structure to Epigenetics and Neuronal Functions¹, SUSAN LINDQUIST, Whitehead Institute for Biomedical Research, Howard Hughes Medical Institute, Department of Biology, MIT — Prions are a unique type of protein that can misfold and convert other proteins to the same shape. The well-characterized yeast prion [PSI⁺] is formed from an inactive amyloid fiber conformation of the translation-termination factor, Sup35. This altered conformation is passed from mother cells to daughters, acting as a template to perpetuate the prion state and providing a mechanism of protein-based inheritance. We employed a variety of methods to determine the structure of Sup35 amyloid fibrils. First, using fluorescent tags and cross-linking we identified specific segments of the protein monomer that form intermolecular contacts in a "Head-to-Head," "Tail-to-Tail" fashion while a central region forms intramolecular contacts. Then, using peptide arrays we mapped the region responsible for the prion transmission barrier between two different yeast species. We have also used optical tweezers to reveal that the non-covalent intermolecular contacts between monomers are unusually strong, and maintain fibril integrity even under forces that partially unfold individual monomers and extend fibril length. Based on the handful of known yeast prion proteins we predicted sequences that could be responsible for prion-like amyloid folding. Our screen identified 19 new candidate prions, whose protein-folding properties and diverse cellular functions we have characterized using a combination of genetic and biochemical techniques. Prion-driven phenotypic diversity increases under stress, and can be amplified by the dynamic maturation of prion-initiating states. These qualities allow prions to act as "bet-hedging" devices that facilitate the adaptation of yeast to stressful environments, and might speed the evolution of new traits. Together with Kandel and Si, we have also found that a regulatory protein that plays an important role in synaptic plasticity behaves as a prion in yeast. Cytoplasmic polyAdenylation element binding protein, CPEB, maintains synapses by promoting the local translation of mRNAs. We postulate that the self-perpetuating folding of the prion domain acts as a molecular memory. Thus yeast prions have provided evidence for the surprising possibility that amyloid protein folds can serve as the basis for memory and inheritance.

¹Supported by the Mathers Foundation, the HHMI, and NIH.

8:36AM Y43.00002 Exploring the Amylome: Predicting Amyloidogenic proteins & mapping their roles, functional or not, ROLAND RIEK, ETH Zurich — No abstract available.

9:12AM Y43.00003 Toxic β -Amyloid ($A\beta$) Alzheimer's Ion Channels: From Structure to Function and Design, RUTH NUSSINOV, NCI-Frederick, SAIC-Frederick, Inc. — Full-length amyloid beta peptides ($A\beta_{1-40/42}$) form neuritic amyloid plaques in Alzheimer's disease (AD) patients and are implicated in AD pathology. Recent biophysical and cell biological studies suggest a direct mechanism of amyloid beta toxicity – ion channel mediated loss of calcium homeostasis. Truncated amyloid beta fragments ($A\beta_{11-42}$ and $A\beta_{17-42}$), commonly termed as non-amyloidogenic are also found in amyloid plaques of Alzheimer's disease (AD) and in the preamyloid lesions of Down's syndrome (DS), a model system for early onset AD study. Very little is known about the structure and activity of these smaller peptides although they could be key AD and DS pathological agents. Using complementary techniques of explicit solvent molecular dynamics (MD) simulations, atomic force microscopy (AFM), channel conductance measurements, cell calcium uptake assays, neurite degeneration and cell death assays, we have shown that non-amyloidogenic $A\beta_{9-42}$ and $A\beta_{17-42}$ peptides form ion channels with loosely attached subunits and elicit single channel conductances. The subunits appear mobile suggesting insertion of small oligomers, followed by dynamic channel assembly and dissociation. These channels allow calcium uptake in APP-deficient cells and cause neurite degeneration in human cortical neurons. Channel conductance, calcium uptake and neurite degeneration are selectively inhibited by zinc, a blocker of amyloid ion channel activity. Thus truncated $A\beta$ fragments could account for undefined roles played by full length $A\beta$ s and provide a novel mechanism of AD and DS pathology. The emerging picture from our large-scale simulations is that toxic ion channels formed by β -sheets are highly polymorphic, and spontaneously break into loosely interacting dynamic units (though still maintaining ion channel structures as imaged with AFM), that associate and dissociate leading to toxic ion flux. This sharply contrasts intact conventional gated ion channels that consist of tightly interacting α -helices that robustly prevent ion leakage, rather than hydrogen-bonded β -strands. Moreover, in comparison with β -rich antimicrobial peptide (AMP) such as a protegrin-1 (PG-1), both $A\beta$ and PG-1 are cytotoxic, and capable of forming fibrils and dynamic channels which consist of subunits with similar dimensions. These combined properties support a functional relationship between amyloidogenic peptides and β -sheet-rich cytolytic AMPs, suggesting that PG-1 is amyloidogenic and amyloids may have an antimicrobial function.

9:48AM Y43.00004 Predicting Amyloid Structure Without Bioinformatic Support: Threading the Left Handed Beta Helix, ALEXANDER KLUBER, UC-Davis — No abstract available.

10:24AM Y43.00005 Functional Hydrogel Materials Inspired by Amyloid, JOEL SCHNEIDER, National Cancer Institute — Protein assembly resulting in the formation of amyloid fibrils, assemblies rich in cross beta-sheet structure, is normally thought of as a deleterious event associated with disease. However, amyloid formation is also involved in a diverse array of normal biological functions such as cell adhesion, melanin synthesis, insect defense mechanism and modulation of water surface tension by fungi and bacteria. These findings indicate that Nature has evolved to take advantage of large, proteinaceous fibrillar assemblies to elicit function. We are designing functional materials, namely hydrogels, from peptides that self-assembled into fibrillar networks, rich in cross beta-sheet structure. These gels can be used for the direct encapsulation and delivery of small molecule-, protein- and cell-based therapeutics. Loaded gels exhibit shear-thinning/self-healing mechanical properties enabling their delivery via syringe. In addition to their use for delivery, we have found that some of these gels display antibacterial activity. Although cytocompatible towards mammalian cells, the hydrogels can kill a broad spectrum of bacteria on contact.

Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y44 DPOLY: Focus Session: Directed Assembly of Hybrid Materials - Particle Organization and Arrays 157C

8:00AM Y44.00001 Simulations of nanoparticle ionic and organic hybrid materials¹, ATHANASSIOS

Z. PANAGIOTOPOULOS, Princeton University — We have used molecular dynamics simulations over microsecond time scales to study the structure and dynamics of coarse-grained models for nanoparticle-based ionic and organic hybrid materials [1]. The systems of interest consist of particles with charged surface groups and linear or three-arm counterions, which also act as the solvent. A comparable uncharged model of nanoparticles with tethered chains is also studied. The pair correlation functions display a rich structure resulting from the packing of cores and chains, as well as electrostatic effects. Even though electrostatic interactions between oppositely charged ions at contact are much greater than the thermal energy, we find that chain dynamics at intermediate time scales are dominated by chain hopping between core particles. We have also used molecular dynamics simulations and density functional theory to investigate the structure of solvent-free oligomer-grafted nanoparticles [2,3]. At low temperatures and moderate to high oligomer lengths, the qualitative features of the core particle pair probability, structure factor, and the oligomer brush configuration obtained from the simulations can be explained by a density-functional theory that incorporates the configurational entropy of the space-filling oligomers. In particular, the structure factor at small wave numbers attains a value much smaller than the corresponding hard-sphere suspension, the first peak of the pair distribution function is enhanced due to entropic attractions among the particles, and the oligomer brush expands with decreasing particle volume fraction to fill the interstitial space. At higher temperatures, the simulations reveal effects that differ from the theory and are likely caused by steric repulsions of the expanded corona chains.

[1] B. Hong, A. Chremos, and A. Z. Panagiotopoulos; Faraday Disc., DOI: 10.1039/c1fd00076d (2012).

[2] A. Chremos, A. Z. Panagiotopoulos, H.-Y. Yu, and D. L. Koch; J. Chem. Phys., 135:114901, 12pp (2011).

[3] A. Chremos and A. Z. Panagiotopoulos; Phys. Rev. Lett., 107:105503, 5pp (2011).

¹Supported by KUS-C1-018-02 (KAUST), DE-SC-0002128 (DOE) and CBET-1033155 (NSF)

8:36AM Y44.00002 Reverse-engineering the anisotropic assembly of grafted nano-particles ,

BEHNAZ BOZORGUI, SANAT KUMAR, Columbia University — We use computer simulations to study the self assembly and directed phase separation of nanoparticles grafted with polymeric chains in an implicit solvent. The formation of anisotropic clusters from building blocks that are symmetric (both in shape and interactions) has been the subject of recent studies. This anisotropy has roots in many body physics, which manifests itself as a directional assembly. Here we apply both full and coarse-grained simulations to get a better insight of the physics behind the assembly of such systems.

8:48AM Y44.00003 Crystalline assembly of hard polyhedra via directional entropic forces¹ ,

PABLO F. DAMASCENO, MICHAEL ENGEL, SHARON C. GLOTZER, University of Michigan — Entropic forces are effective forces that result from a system's statistical tendency to increase its entropy. Hard rods and disks spontaneously align and can assemble into layers and columns if those structures increase the configurational space available to the particles. Hard spheres, cubes and even tetrahedra order for the same reason. Here we extend those findings by showing that hard polyhedra can self-assemble into a variety of complex phases, most of them never before reported in systems of single-component hard particles. The role of shape and directional entropic forces in stabilizing these structures will be discussed. Our results suggest new possibilities for self-assembling complex target structures from colloidal building blocks.

[1] Damasceno, PF; Engel, M; Glotzer, SC. arXiv:1109.1323v1

¹Supported by AFOSR (FA9550-06-1-0337) and DOD-DDRE (N00244-09-1-0062)

9:00AM Y44.00004 Facile Fabrication of 3-D Nanoparticle Arrays in Thin Films toward Photonic Materials ,

JOSEPH KAO, SEONG-JUN JEONG, VIVIAN PENG-WEI CHUANG, PETER JIN BAI, UC Berkeley, ZHEN ZHANG, CHENG SUN, Northwestern University, TING XU, UC Berkeley — 3-D hierarchical assemblies of nanoparticles in thin films enable one to exploit their collective properties to generate functional electronic, magnetic, and photonic materials. Among many templates, block copolymer-based supramolecules is one of the most promising candidates since they combine solution processibility and high precision in nanoparticle spatial distribution. Herein, we report a facile way of fabricating 3-D nanoparticle arrays in thin films of diblock copolymer-based supramolecules exhibiting bandgap in the visible regime. The entropy-dominant assembly drives the formation of 3-D lattice of nanoparticle arrays with precise inter-array spacings in thin films. The coupling effect between the precisely positioned nanoparticle arrays with adjustable lattice spacings in the hierarchically-structured nanocomposites allows potentially interesting optical properties.

9:12AM Y44.00005 Creating Opal Templated Continuous Conducting Polymer Films with Ultralow Percolation Thresholds Using Thermally Stable Nanoparticles ,

D.J. KANG, T. KWON, M.P. KIM, B.J. KIM, KAIST, H. JUNG, J. BANG, Korea Univ. — We propose a novel and robust strategy for creating continuous conducting polymer films with ultralow percolation thresholds using polymer-coated gold nanoparticles (Au NPs) as surfactant. Continuous poly(triphenylamine) (PTPA) films of high internal phase polymeric emulsions were fabricated using an assembly of crosslinked polystyrene (PS) colloidal particles as template. Polymer-coated Au NPs localize at the PS/PTPA interface and function as surfactant to efficiently produce a continuous conducting PTPA polymer film with very low percolation thresholds. The volume fraction threshold for percolation of the PTPA phase with insulating PS colloids was found to be 0.20. In contrast, with the addition of an extremely low volume fraction of surfactant Au NPs, the volume fraction threshold for percolation of the PTPA phase was dramatically reduced to 0.05. The SEM and TEM measurements clearly demonstrated the formation of a continuous PTPA phase within the polyhedral phase of PS colloids. To elucidate the influence of the nanoparticle surfactant on the blend films, the morphology and conductivity of the blends at different PS colloid/PTPA volume ratios were carefully characterized as a function of the Au NP concentration.

9:24AM Y44.00006 Magnetic fields in long-range alignment of functional hybrid soft materials¹

, PAWEŁ MAJEWSKI, MANESH GOPINADHAN, CANDICE PELLIGRA, Yale University, SHANJU ZHANG, California Polytechnic State University, LISA PFEFFERLE, CHINEDUM OSUJI, Yale University — We present a magnetic field-based method to impose long range order in self-assembled soft materials including polymer-nanowire composites, block copolymers and surfactant mesophases. We discuss the broad utility of this approach, indicating its advantages and limitations. Our method yields highly anisotropic materials with quality of alignment in many cases comparable to that of single crystals as assessed by X-ray scattering techniques. We take advantage of the high fidelity of alignment to systematically explore and characterize the anisotropic properties of these materials. We present a perspective for improving electron and hole transport, as well as exciton utilization in magnetically doped ZnO nanowire-polythiophene composites for photovoltaic applications by global alignment of the nanowires. For block copolymers, we focus on enhancing Li-ion transport in membranes with self-assembled cylindrical and lamellar morphology by alignment of the Li-conducting PEO domains.

¹NSF support (DMR-0847534 and DMR-0934520) is gratefully acknowledged.

9:36AM Y44.00007 ²H NMR study of the Assembly of Gold Nanoparticles Dispersed in Nematic Liquid Crystal¹, LINDA REVEN, J MILETTE, R. BRUCE LENNOX, ALEJANDRO REY, McGill University, Montreal, Qc, Canada, EZEQUIEL SOULE, Institute of Materials Science and Technology (INTEMA), University of Mar del Plata, Argentina — Gold nanoparticles (AuNP) with mesogenic ligands, tailored to be highly miscible in the liquid phase of 4-n-pentyl-4'-cyanobiphenyl (5CB) liquid crystal (LC), form reversible, micron-scale cellular networks upon cooling to the nematic phase. The network topology and LC director field orientation are controlled by the cooling rate, film thickness, ligand shell composition and AuNP concentration. Isotopically labeled samples allow selective probing of the orientational order of the NP ligands and host LC by ²H NMR. The ²H NMR spectra of AuNPs dispersed in nematic 5CB display isotropic and doublet peaks assigned to disordered and field aligned ligands respectively. The intensity of the ligand doublet signal increases relative to the isotropic peak with decreasing temperature and NP concentration. Conversely an isotropic peak along with the expected doublet is observed for the host 5CB in the nematic phase. The intensity of the host 5CB isotropic peak, which persists far into the nematic phase and decreases with NP concentration, shows the coexistence of isotropic and nematic phases. The NP ligand and host LC orientational orders are related the formation of the cellular network and theoretical phase diagrams of NP-LC dispersions.

¹Centre for Self-Assembled Chemical Structures (CSACS-CRMAA)

9:48AM Y44.00008 Organization of Gold Nanorods in Cylinder-Forming Block Copolymer Films¹, GUOQUAN JIAN, ROBERT RIGGLEMAN, RUSSELL COMPOSTO, University of Pennsylvania — The addition of gold nanorods (AuNRs) to copolymer films can impart unique optical and electrical properties. To take full advantage of this system, the AuNRs must be dispersed in a self-organizing copolymer that directs the orientation of the anisotropic particle. In the present work, AuNRs with aspect ratio 3.6 (8 nm x 29 nm) are grafted with poly(2-vinyl pyridine) (P2VP) brushes and dispersed in a cylindrical forming diblock copolymer of polystyrene-b-P2VP (180K-b-77K, 29.6 wt% P2VP). Films are spun cast and solvent annealed in chloroform to produce a perpendicular cylindrical morphology at the surface. Using TEM and UV-ozone etching combined with AFM, the AuNRs are well dispersed and co-locate (top down view) with the P2VP cylinders, ~50nm diameter. However, the AuNRs mainly lie parallel to the surface indicating that they likely locate at the junction created at the intersection between P2VP cylinders and P2VP brush layer adjacent to the silicon oxide surface. Self-consistent field calculations of the Au:PS-b-P2VP morphology as well as the effect of adding P2VP homopolymer to the nanocomposite will be discussed.

¹NSF Polymer and MRSEC programs

10:00AM Y44.00009 Nanopatterned poly(ethylene glycol) brushes: A route for highly tunable assembly of Au nanoparticles, M. SERDAR ONSER, PAUL F. NEALEY, University of Wisconsin-Madison — Assembly of metallic nanoparticles (NPs) on surfaces offers many interesting opportunities for scientific studies as macroscopic properties of the assemblies depend on organization of the particles at the nanometer length scale. On the other hand, new/improved functionalities of the assemblies are promising in the potential technological applications such as chemical sensing and metamaterials. Chemical patterning of surfaces for directed assembly of ex-situ synthesized NPs is advantageous due to controllable substrate-particle interaction and applicability to a range of different size and type of particles. Here we present assembly of Au NPs (15-50 nm) on lithographically patterned poly(ethylene glycol) (PEG) brushes. The density of NPs on the patterns can be controlled with the molecular weight of PEG brush and the size of particles. The ability to pattern PEG brushes with high chemical contrast and resolution (sub 50 nm) with the interesting particle brush interaction provides routes for highly controllable assembly of NPs. For example, number of particles per spot can be precisely controlled with high yields (single 95% and dimer 70% for 30 nm Au NP) and NPs of two different sizes (heterostructures) can be assembled on patterned spots.

10:12AM Y44.00010 Distribution of POSS Nanoparticles in Symmetric Diblock Copolymer Thin Films, UMESH SHRESTHA, DILRU RATNAWEERA, Clemson University, STEPHEN CLARSON, University of Cincinnati, DVORA PERAHIA, Clemson University — The distribution of Polyhedral Oligomeric Silsesquioxanes (POSS) nanoparticles in thin films of symmetric diblock copolymer polystyrene-b-poly dimethyl siloxane (PS-b-PDMS) was studied by neutron reflectometry. Blending of nanoparticles (NPs) with polymers provide a pathway to tune properties of the polymer such as conductivity, mechanical strength, optical activity as well as dewetting, where the properties depend on the distribution of the NPs. Controlling the distribution of NPs in polymers thin films however, remains a challenge where entropic contributions drive segregation of the NPs to the interface. Different approaches were taken including modifying the interfacial interactions of the NP. The current study investigates effects of the relative size of the NP with respect to that of the polymer layers following distribution of POSS cages which consist of a silicon cage in a symmetric PS-PDMS. The temperature was varied from room temperature to 150°C, investigating the distribution above and below the glass transition temperature of the styrene blocks. The distribution of the NPs as well as structural changes for two molecular weights of the diblock 10kg/mol and 50kg/mol within the films will be discussed.

10:24AM Y44.00011 Long-range Ordering of Symmetric Block-copolymers by Chaining of Superparamagnetic Nanoparticles in External Magnetic Fields, V. RAMAN, M.I.T, A. BOSE, University of Rhode Island, B.D. OLSEN, T.A. HATTON, M.I.T — Chaining of superparamagnetic nanoparticles is numerically investigated as a new method to align the block copolymer without additional lithographic processing. The method relies on the chaining of superparamagnetic nanoparticles, sequestered preferentially in one of the blocks, in the direction of in-plane external magnetic fields to achieve long-range order in the block copolymer. Effects of nanoparticle size, concentration, and magnetization strength are explored using Hybrid-Particle-Field technique (Sides et al, 2006). The 2D simulations reveal that, for the same nanoparticle loading, the nanoparticle sizes commensurate with the domain sizes yield defect-free alignment. While small sizes lead to jamming and kinetic trapping of defects, larger sizes lead to swelling of domains and break the symmetry of the lamellar phase. A window of optimal nanoparticle concentrations exists over which orientational order is achieved. For low concentrations, only local alignment is observed, while high concentrations lead to order-order phase transition from lamellae to cylindrical phase. Scaling calculations corroborate the effect of high magnetization strengths in lowering the equilibrium defect density for such nematic-isotropic phase transitions observed in monolayers.

10:36AM Y44.00012 Highly Ordered Superstructures of Single-Walled Carbon Nanotubes in Polymeric Systems, SUNG-MIN CHOI, HYOUNG-SIK JANG, CHANGWOO DOE, TAE-HWAN KIM, Department of Nuclear and Quantum Engineering, KAIST, Daejeon, Republic of Korea — Fabrication of highly ordered arrays of single-walled carbon nanotubes (SWNTs) has been of great interest for a wide range of potential applications. Block copolymers exhibit rich phase behavior and have been extensively used as excellent templates for highly ordered nanostructure materials with various architectures. Therefore, utilization of the rich phase behavior of block copolymers may provide a general and inexpensive way for fabricating a large variety of self-assembled and highly ordered arrays of SWNTs without going through complicated preparative procedures. Here, we investigated the cooperative self-assembling behavior of functionalized isolated SWNTs in Pluronic block copolymer systems using small angle neutron and x-ray scattering techniques, which show highly ordered superstructures of SWNTs with different symmetries.

10:48AM Y44.00013 Block copolymer modified epoxies: Role of localized network damage¹

CARMELO DECLET-PEREZ, ERICA REDLINE², LORRAINE FRANCIS, FRANK BATES³, Department of Chemical Engineering and Materials Science, University of Minnesota — Adding block copolymers to epoxy resins has proven to be an effective approach to toughening these materials while retaining commercially relevant properties such as high modulus and glass transition temperature. When properly designed, block copolymers self-assemble into spherical micelles that disperse in the monomer resin. These structures survive curing into a dense network. At this point, a complete description of the toughening mechanism for block copolymer modified epoxies is still lacking. Here we present new experimental evidence that challenges the current understanding in this area. We compared the toughening effect of spherical micelle forming block copolymers with rubbery and glassy cores. Consistent with previous reports rubbery cores produced significant toughening, but surprisingly the glassy core micelles also imparted some toughness. These results suggest that the block copolymer/epoxy interface plays a significant role during deformation. We propose that the micelles compromise the integrity of the glassy matrix by damaging or plasticizing the crosslinked network in contact with the corona blocks, thereby facilitating shear yielding.

¹Support was provided by the NSF sponsored MRSEC at the University of Minnesota

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Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y45 DPOLY: Focus Session: Soft Matter Physics of Drops, Bubbles, Foams and Emulsions - Bubbles, Films, Foams 159

8:00AM Y45.00001 Mechanical properties of surface modified microbubbles by Atomic Force Microscopy (AFM), JONATHAN MCKENDRY, COLIN GRANT, STEPHEN EVANS, None — Atomic force microscopy has been used to investigate the mechanical properties of phospholipid coated microbubbles and to quantify their stiffness. The mechanical properties were investigated using tipless AFM cantilevers to compress microbubbles attached to a gold surface in aqueous conditions. The phospholipid microbubbles were produced by microfluidic flow focusing and were found to have a stiffness of 25 mN/m. The attachment of a streptavidin coating increased the microbubble stiffness by a factor of 30 to around 750 mN/m. Further, the effect of temperature on the mechanical and time dependent properties of bubbles has been studied, the results of which have demonstrated that increasing temperature leads to a decrease in microbubble stiffness and an increase creep-displacement. The standard linear model was used to extract the visco-elastic parameters at different temperatures, this allowed the first determination of the activation energy for creep for a microbubble.

8:12AM Y45.00002 Cylindrical bubbles and blobs from a Class II Hydrophobin¹, PAUL RUSSO, MICHAEL PHAM, BRAD BLALOCK, Louisiana State University, HYDROPHOBIN COLLABORATION — *Cerato ulmin* is a class II hydrophobin. In aqueous suspensions, it easily forms cylindrical air bubbles and cylindrical oil blobs. The conditions for formation of these unusual structures will be discussed, along with scattering and microscopic investigations of their remarkable stability. Possible applications in diverse fields including polymer synthesis and oil spill remediation will be considered. Acknowledgment is made to Dr. Wayne C. Richards of the Canadian Forest Service for the gift of *Cerato ulmin*.

¹Supported by Gulf Coast Research Initiative

8:24AM Y45.00003 The collapse and the folding of a particle rafts under compression¹, CHIN-CHANG KUO, MICHAEL DENNIN, Department of Physics & Astronomy, University of California, Irvine — Compressing a single-layer of particles or bubbles that are confined to the air-water interface results in a range of interesting collapse dynamics. We report on the collapse modes of two systems: (1) a single layer of gas bubbles at the surface and (2) a single layer of polypropylene beads. Under compression, both systems exhibit a critical areal density beyond which there is a transition to a multi-layered structure. Generally speaking, the transformation is characterized by localized submergence into the subphase of bubbles or beads. For both systems, we observe single bubbles/beads being pushed underneath surrounding particles. However, for sufficiently small beads, we observe a folding mode, which corresponds to the long-ranged one dimensional wrinkling of the monolayer surface. In this talk, we will report on the transition between single particle submergence and folding, as well as general characterization of the collapse as a function of compression speed and initial structure of the particle raft.

¹We acknowledge the support of NSF-DMR-0907212 and Research Corporation.

8:36AM Y45.00004 Falling drops skating on a film of air, SHMUEL RUBINSTEIN, Dept. of Physics of Complex Systems, Weizmann Institute of Science — When a raindrop hits a window, the surface immediately becomes wet as the water spreads. Indeed, this common observation of a drop impacting a surface is ubiquitous in our everyday experience. I will show that the impact of a drop on a surface is a much richer, more complex phenomenon than our simple experience may suggest: To completely wet the surface the drop must first expel all the air beneath it; however, this does not happen instantaneously. Instead, a very thin film of air, only a few tens of nanometers thick, remains trapped between the falling drop and the surface as the fluid spreads. The thin film of air serves to lubricate the drop enabling the fluid to skate laterally outward at strikingly high velocities. Simultaneously, the wetting fluid spreads inward at a much slower velocity, trapping a bubble of air within the drop. However, these events occur at diminutive length scales and fleeting time scales; therefore, to visualize them we develop new imaging modalities that are sensitive to the behavior right at the surface and that have time resolution superior to even the very fastest cameras. These imaging techniques reveal that the ultimate wetting of the surface occurs through a completely new mechanism, the breakup of the thin film of air through a spinodal like dewetting process that breaks the cylindrical symmetry of the impact and drives an anomalously rapid spreading of a wetting front. These results are in accord with recent theoretical predictions and challenge the prevailing paradigm in which contact between the liquid and solid occurs immediately, and spreading is dominated by the dynamics of a single contact line.

9:12AM Y45.00005 Compression of multiwall microbubbles, NATALIA LEBEDEVA, SAM MOORE, University of North Carolina at Chapel Hill, ANDREY DOBRYNIN, University of Connecticut, MICHAEL RUBINSTEIN, SERGEI SHEIKO, University of North Carolina at Chapel Hill — Optical monitoring of structural transformations and transport processes is prohibited if the objects to be studied are bulky and/or non-transparent. This paper is focused on the development of a microbubble platform for acoustic imaging of heterogeneous media under harsh environmental conditions including high pressure (<500 atm), temperature (<100 °C), and salinity (<10 wt%). We have studied the compression behavior of gas-filled microbubbles composed of multiple layers of surfactants and stabilizers. Upon hydrostatic compression, these bubbles undergo significant (up to 100×) changes in volume, which are completely reversible. Under repeated compression/expansion cycles, the pressure-volume P(V) characteristic of these microbubbles deviate from ideal-gas-law predictions. A theoretical model was developed to explain the observed deviations through contributions of shell elasticity and gas effusion. In addition, some of the microbubbles undergo peculiar buckling/smoothing transitions exhibiting intermittent formation of faceted structures, which suggest a solid-like nature of the pressurized shell. Preliminary studies illustrate that these pressure-resistant microbubbles maintain their mechanical stability and acoustic response at pressures greater than 1000 psi.

9:24AM Y45.00006 The life cycle of individual boiling bubbles: Insights from beyond optical imaging, SCOTT PARKER, SUNG CHUL BAE, DAVID CAHILL, STEVE GRANICK, University of Illinois — With a high-speed camera, we have investigated the dynamics of individual vapor bubbles boiling on a laser-heated surface. Their sizes and shapes as they grow and depart from a surface are correlated with simultaneous thermal imaging measurements of the boiling surface using thermoreflectance-based microscopy to measure temperatures of individual stochastic events. Analysis of both the thermal profiles and the bubble shapes suggests the presence of an evaporating liquid microlayer under the developing bubble. Tuning surface and heating properties, we control the shapes of bubbles, ranging from regular periodic growth and departure to stochastic bubbles which exhibit rapid cavitation-like expansion and collapse. Unlike typical cavitation bubbles which collapse and form jets pointed towards the surface, jets from bubbles observed during boiling were observed to be directed away from the surface. By tuning the wettability of the substrate, we will report on how wettability affects the strength and direction of these jets.

9:36AM Y45.00007 Nonclassical Thermomigration of an Air Bubble, DOMINIK MICHLER, RUDOLF SPRIK, PETER SCHALL, DANIEL BONN, Soft Matter, Van der Waals-Zeeman Instituut, Universiteit van Amsterdam, SHELL COLLABORATION — We study air bubbles confined in capillaries with a temperature gradient. Classically, air bubbles move in a temperature gradient due to decreased surface tension at higher temperatures, creating a net surface traction towards the cold pole, pushing the bubble towards the hot pole for mass conservation. Here we report non-classical thermo-migration of confined air bubbles: in the presence of surfactant the bubbles can go the other way.

9:48AM Y45.00008 Two-Dimensional Microfluidics: Stable Island Emulsions in Freely Suspended Smectic Liquid Crystal Films¹, CHEOL PARK, ZOOM NGUYEN, CHANEY CRANFILL, SARAH RADZIHOVSKY, JOE MACLENNAN, MATT GLASER, NOEL CLARK, University of Colorado at Boulder, LCMRC TEAM — Islands (circular regions of greater thickness) in smectic films are easily created and manipulated, but are generally unstable, tending to grow or shrink over time. We have recently created stable emulsions of smectic islands by “work hardening” of the smectic film using shear and extensional flow to form a dense, mechanically stable network of edge dislocations. In this talk, we discuss this novel type of two-dimensional colloidal system, in particular the island size distribution, network of edge dislocations and topological defects that form stable two-dimensional emulsions.

¹Work supported by NSF MRSEC Grant DMR- 0820579 and NASA Grant NAG No. NNX07AE48G

10:00AM Y45.00009 Spherical and Non-Spherical Double Emulsions with Multiple Components, LAURA ADAMS, THOMAS KODGER, Harvard University, JACY BIRD, MIT, SHIN-HYUN KIM, LOUISE JAWERTH, VINOTHAN MANOHARAN, DAVID WEITZ, Harvard University — Monodispersed double emulsions, drops inside of drops, with multiple and tunable components are generated using microfluidics. A fluid dynamic model based on fast camera images of the single step emulsification technique is being developed to determine the critical separation between channels in the injection capillary; this model addresses the maximum number of distinct drops that can be controllably loaded inside a double emulsion for a given diameter capillary. New stable, non-spherical emulsions with two and three different components, Janus and Cerberus emulsions, are also reported.

10:12AM Y45.00010 Stability of thin liquid films: Influence of interfacial viscoelasticity¹, GERALD FULLER, LIAT ROSENFELD, Stanford University — Lipid layer spreading and liquid film dewetting are important variables influencing numerous processes, including the stability of the tear film. The viscoelasticity of insoluble monolayers may govern thin liquid film dewetting phenomena. The purpose of this work is to gain insight into the effects of surface viscoelasticity elasticity by insoluble monolayers on dewetting of thin films of water with a particular attention paid to materials, such as meibum, that stabilize the tear film. For this purpose an experiment has been devised wherein monolayers of known surface pressure and surface rheology are introduced atop thin, liquid films that would normally spontaneously dewet. The results reveal that monolayers of viscoelastic surfactants are able to stabilize thin films against spontaneous dewetting. As the surface pressure and surface rheology of these layers is increased, their effectiveness is enhanced. Meibum is particularly effective in stabilizing thin films. These results suggest that the role of the meibum is to offer the tear film enhanced stability and not only to suppress evaporation.

¹Alcon Corporation

10:24AM Y45.00011 Light-controlled air-water interfaces and thin liquid films using photosurfactants, ELOISE CHEVALLIER, ESPCI, CHRISTOPHE TRIBET, ENS Paris, FRANCOIS LEQUEUX, CECILE MONTEUX, ESPCI — We study the interfacial behavior of photosurfactants containing an azobenzene moiety in the apolar tail –which switch from cis to trans conformation depending on the wavelength of light. We present here results on the effect of stimulation on the interfacial dynamics of such photosurfactants upon illumination. First, without light stimulus, the trans isomers is found to desorb more slowly than the cis, this leads to a fast enrichment of the interface with trans. Under light, adsorbed trans convert to their cis form which quickly desorb resulting in an important decrease of the surface excess and an increase of the surface tension. Besides, we stimulate thin-liquid films stabilized by such surfactants. Several types of hydrodynamical instabilities in the thin-liquid films are generated. We show that these instabilities are due to a strong rise of concentration in-situ but also a light-induced variation of DLVO interactions that usually stabilize the films.

10:36AM Y45.00012 Supercritical Carbon Dioxide Assisted Processing of Silica/PMMA Nanocomposite Foams¹, DENIZ RENDE, LINDA S. SCHADLER, RAHMI OZISIK, Rensselaer Polytechnic Institute — Polymer nanocomposite foams receive considerable attention in both scientific and industrial communities. These structures are defined as closed or open cells (pores) surrounded by bulk material and are widely observed in nature in the form of bone structure, sponge, corals and natural cork. Inspired by these materials, polymer nanocomposite foams are widely used in advanced applications, such as bone scaffolds, food packaging and transportation materials due to their lightweight and enhanced mechanical, thermal, and electrical properties compared to bulk polymer foams. The presence of the nanosized fillers facilitates heterogeneous bubble nucleation as a result, the number of bubbles increases while the average bubble size decreases. Therefore, the foam morphology can be controlled by the size, concentration, and surface chemistry of the nanofiller. In the current study, we used supercritical carbon dioxide as a foaming agent for silica/poly(methyl methacrylate), PMMA, foams. The silica nanoparticles were chemically modified by fluoroalkane chains to make them CO₂-philic. The surface coverage was controlled via tethering density, and the effect of silica surface coverage and concentration on foam morphology was investigated through scanning electron microscopy and image processing. Results indicated that nanofiller concentration and filler surface chemistry (CO₂-philicity) had tremendous effect on foam morphology but surface coverage did not have any effect.

¹Partial support was provided by NSF Grant No. 1003574 and RPI. DR is also supported by TUBITAK 2219 program.

10:48AM Y45.00013 Drainage dynamics of aqueous foams generated by sparging and turbulent mixing, MATTHEW J. KENNEDY¹, MICHAEL W. CONROY, RAMAGOPAL ANANTH, JAMES W. FLEMING, Naval Research Laboratory — We investigate the effect of bubble size on the drainage dynamics of aqueous fire-suppression foams using laboratory-scale foam generators and theoretical modeling. We generate foams over a wide range of bubble sizes using two foam generation methods—sparging using fritted sheets of steel, and turbulent mixing using high-pressure T-junctions. The sparged foams comprise bubbles of mean diameter 0.5 mm or larger and begin draining immediately whereas the turbulently mixed foams comprise bubbles of mean diameter 0.15 mm or smaller and begin draining after induction times of 5-15 minutes. We study two proprietary fire-suppression foam solutions: a non-fluorinated surfactant solution containing viscous additives intended for use as a wet foam, *i.e.* liquid fraction > 0.1, and a sodium dodecyl sulfate surfactant solution intended for use as a dry foam, *i.e.* liquid fraction < 0.005. The change in liquid retention time due to change in mean bubble size differs between these two solutions. We compare our experimental results with theoretical models to examine the reasons for the difference in liquid retention time.

¹National Research Council Postdoctoral Research Associate

Friday, March 2, 2012 8:00AM - 10:48AM —
Session Y47 DPOLY: Soft Matter Physics of Biological Systems 160C

8:00AM Y47.00001 Antiviral activity of squalamine: Role of electrostatic membrane binding, BERNARD BECKERMAN, WEI QU, Northwestern University, ABHIJIT MISHRA, UCLA, MICHAEL ZASLOFF, Georgetown University, GERARD WONG, UCLA, ERIK LUIJTEN, Northwestern University — Recent work¹ has demonstrated that squalamine, a molecule found in the liver of sharks, exhibits broad-spectrum antiviral properties. It has been proposed that this activity results from the charge-density matching of squalamine and phospholipid membranes, causing squalamine to bind to membranes and displace proteins such as Rac1 that are crucial for the viral replication cycle. Here we investigate this hypothesis by numerical simulation of a coarse-grained model for the competition between Rac1 and squalamine in binding affinity to a flat lipid bilayer. We perform free-energy calculations to test the ability of squalamine to condense stacked bilayer systems and thereby displace bulkier Rac1 molecules. We directly compare our findings to small-angle x-ray scattering results for the same setup.

¹M. Zasloff *et al.*, Proc. Nat. Acad. Sci. (USA) **108**, 15978 (2011).

8:12AM Y47.00002 Simulating ligand receptor binding at a membrane interface with graphics processing accelerated coarse-grained molecular dynamics, SHARON M. LOVERDE, Department of Chemical and Biomolecular Engineering, University of Pennsylvania, DAVID N. LEBARD, Department of Chemistry, Temple University, ZHENGYU MA, Penn Institute for Immunology, University of Pennsylvania, MICHAEL L. KLEIN, Department of Chemistry, Temple University, DENNIS E. DISCHER, Department of Chemical and Biomolecular Engineering, University of Pennsylvania — Motivated by a deeper understanding of the immunological synapse, we develop a molecular-based model to understand receptor-polymer/ligand binding at a membrane interface. We examine the case of weak ligand binding in the limit of confined polymer chains as a function of chain length, binding constant, and system size. We utilize a coarse-grained (CG) model of poly(ethylene oxide) and dimyristoylphosphatidylcholine (DMPC) previously developed by the Klein group and mimic weak binding with a sticky potential. This work employs graphics processing units (GPU) to accelerate the CG-MD simulations, where each simulation is run with multiple random-walker replicas to enhance sampling and facilitate statistical convergence of physical observables. Our results demonstrate that such an aggressive combination of GPU acceleration with CG modeling can yield accurate and precise data on polymer-DMPC binding, and, more importantly, hints at the mechanism behind empirical data of polymer binding to a T-cell receptor protein.

8:24AM Y47.00003 Stabilization of concentration fluctuations in mixed membranes by hybrid lipids, BENOIT PALMIERI, SAMUEL SAFRAN, Weizmann Institute of Science — Finite-size domains have been observed at the surface of cells. These lipids “rafts” are stable nanodomains enriched in saturated lipids and cholesterol. While line tension favors macrodomains, one explanation for raft stabilization suggests that the membrane composition is tuned close to a spinodal temperature. From this point of view, rafts are long-lived concentration fluctuations in the mixed phase. We propose a ternary mixture model for the cell membrane that includes hybrid lipids which have one saturated and one unsaturated hydrocarbon chain. Finite amount of hybrid lipids reduces the packing incompatibility at the saturated/unsaturated lipid interface and stabilizes the concentration fluctuations. Hybrid-Hybrid interactions are included in the model and further increase the life-time of the rafts and decrease their length-scales. Moreover, the hybrid has extra orientational degrees of freedom that may lead to modulated phases.

8:36AM Y47.00004 Cooperativity in cholesterol-induced demixing of saturated and unsaturated lipids, JAMES KINDT, Emory University — The ternary DPPC/DOPC/cholesterol system exhibits a phase separation between liquid-ordered and liquid-disordered domains that may capture some features of demixing believed to occur in biomembranes. Using semi-grand canonical ensemble Monte Carlo approaches on a model with atomistic detail, we have investigated the degree of non-ideality of mixing of DPPC and DOPC as influenced by cholesterol. While the signature of phase separation is observed, more surprising is that in the region of composition space characterized by low DPPC and low cholesterol content, the mixing is approximately ideal. Through simple models we have shown that this behavior is inconsistent with a simple nearest-neighbor description of the interactions between these membrane components.

8:48AM Y47.00005 Steric Repulsion and Compressibility of Protein Resistant Brushes, MARIA SANTORE, Department of Polymer Science and Engineering University of Massachusetts — End-grafted polymer brushes, such as polyethylene glycol, have become commonplace as biocompatibilizers for medical devices and diagnostic surfaces. Key to their non-fouling character is the brush's steric repulsion towards biomolecules and cells. By functionalizing the substrate with small (order 10 nm) bioadhesive features around which the brush is placed, we gain insight into the repulsion between biomolecules and cells with the brush itself. While approximately exponential compression profiles are to be expected, some features of protein interactions with these brushes are unexpected, especially for small proteins whose dimensions are within a factor of 2 or 3 of the brush persistence length. The scaling of the compressive force, for example inferred from series of studies that vary the amounts and spacings of the adhesive elements, is weakly dependent on protein size, while one might expect a proportionality between this force and the effective protein footprint. These results are consistent with entropically inexpensive chain reconfigurations around the smaller proteins and the penetration of these proteins at least partially into the brush.

9:00AM Y47.00006 Topological defects induced by the retina's curvature improve vision , JOHNNATAN ALJADEFF, TATYANA SHARPEE, Computational Neurobiology Laboratory, The Salk Institute; Center for Theoretical Biological Physics and Department of Physics, UCSD — The theory of disclinations and dislocations on curved surfaces predicts the length and density of grain boundary scars on a sphere. These predictions were successfully tested with colloids on droplets for systems satisfying $5 \leq R/a \leq 20$ (R - sphere radius, a - lattice constant). The foveal cone mosaic is another realization of this problem, for which $R/a \sim 10^4$. New theories are needed to extend current predictions for scar length and density to this regime. We present a method of introducing the effect of irregularities that changes the prediction in the relevant regime. We do so by deriving a noise induced disclination density which truncates the scars: the cone density is mapped to an effective displacement h_{eff} from the sphere; then the deviation from the constant curvature is computed to first order in h_{eff} ; and finally the effective curvature is compared to a threshold above which noise induced disclinations appear. We compare stimuli projected on mosaics and on jittered lattices and show that the curvature induced correlations in the mosaics reduce aliasing by a factor of up to 50. This reduction increases with spatial frequencies, meaning that anti-aliasing is maximal in the visual acuity limit.

9:12AM Y47.00007 Exploring the low temperature thermodynamics of lattice proteins and polymers with chain lengths > 1000 , THOMAS WUEST, Swiss Federal Institute for Forest, Snow and Landscape Research WSL — Coarse-grained (lattice-) models have a long tradition in aiding to decipher the physical or biological complexity of polymers and proteins. Despite their simplicity however, numerical simulations of such models are often computationally very demanding and the quest for efficient algorithms is as old as the models themselves. I present a computational method based on Wang-Landau sampling in combination with suitable trial move sets which is particularly effective to study models such as the hydrophobic-polar (HP) lattice model of protein folding or its counterpart in polymer physics, the interactive self-avoiding walk (ISAW) at low temperatures. The approach provides a versatile and powerful mean for both the ground state search and the determination of the entire energy density of states (DOS) yielding reliable estimates of thermodynamic quantities for chain lengths > 4000 (ISAW) even in the very dense collapsed phase. The appearance of multiple low temperature pseudo-transitions for ISAWs will be elucidated. Further methodological improvements will be discussed.

9:24AM Y47.00008 Long-range mechanical force in epithelial tubule self assembly , CHIN-LIN GUO, None — In vivo, epithelial cells can respond to extracellular matrix (ECM) molecules, type I collagen (COL), and switch their morphology from a lobular lumen (100-200 micron) to a tubular lumen (1mm-1cm). However, the mechanism is unclear. Using a temporal control of cell-ECM interaction, we find that epithelial cells, in response to a fine-tuned percentage of COL in ECM, develop various linear patterns. Remarkably, these patterns allow cells to self-assemble into a tubule of length ~ 1 cm and diameter ~ 400 micron in the liquid phase. In contrast with conventional thought, the linear patterns arise through bi-directional transmission of traction force, but not through diffusible biochemical factors secreted by cells. In turn, the transmission of force evokes a long-range (~ 600 micron) intercellular mechanical interaction. A feedback effect is encountered when the mechanical interaction modifies cell positioning and COL alignment. Micro-patterning experiments further reveal that such a feedback is a novel cell-number-dependent, rich-get-richer process, which allows cells to integrate mechanical interactions into long-range (> 1 mm) linear coordination.

9:36AM Y47.00009 Bottom-up study of flaw tolerance properties of protein networks¹ , ZHAO QIN, MARKUS BUEHLER, Massachusetts Institute of Technology, LAMM TEAM — We study the material properties of an intermediate filament protein network by computational modeling using a bottom-up approach. We start with an atomic model of each filament's and obtain the mechanical behavior of them. We then use these parameters in setting up a mesoscale model of the network material at scales of micrometers. Using this multi-scale method, we report a detailed analysis of the associated deformation and failure mechanisms of this hierarchical material. Our modeling reveals that a structure transition that occurs at the proteins' secondary structure level is crucial for the networks' flaw tolerance property, which implies that the material retains its mechanical function despite the existence of large defects. We also examine the effect of crosslink strength on the failure properties. We discover that relatively weaker crosslinks lead to a more flaw tolerant network that is 23% stronger. This unexpected behavior is caused by that the crosslink strength functions as a switch to alter the failure mechanism. Weak crosslinks are able to efficiently diffuse the stress around the crack tip, making the crack more difficult to propagate. We compare our results to that of elastic and softening materials and find that the effect of crosslink strength is much smaller in those systems. These findings imply that the mechanical properties of both the filaments and interfaces among filaments are critical for bioinspired material designs, challenging the conventional paradigm in engineering design.

¹We acknowledge support from AFOSR, ONR-PECASE.

9:48AM Y47.00010 From Nano to Micro: Importance of Structure and Architecture in Spider Silk Adhesives¹ , VASAV SAHNI, ALI DHINOJWALA, The University of Akron — Spiders have developed outstanding adhesives over millions of years of evolution for prey capture and locomotion. We show that the structure and architecture of these adhesives play an important role in the adhesion. The adhesive produced by orb-weaving spiders to capture prey (viscid glue) is laid on a pair of silk fibers as micron-size glue drops composed of salts and glycoproteins. By stretching single drops, we show that viscid glue behaves like a viscoelastic solid and that elasticity is critical in enhancing adhesion caused by specific adhesive ligands by over 100 times. Comparing viscid glue with gumfoot glue, the glue produced by cob-weavers, the evolutionary descendants of orb-weavers, showed that, in spite of being produced in homologous aggregate glands, gumfoot glue behaves like a viscoelastic liquid. Moreover, gumfoot glue is humidity-resistant and viscid glue is humidity-sensitive. We use a synthetic strategy to spin beads-on-a-string (BOAS) architecture to mimic the adhesive properties of spider silk. Using these mimic threads, we show that the BOAS structure adheres more than a cylindrical structure during contact (collision of prey) and during separation (escape attempt of prey). These results inspire design of novel tunable adhesives.

¹Funded by National Science Foundation

10:00AM Y47.00011 Light scattering studies of human crystallin proteins and loss of transparency in cataracts , BENJAMIN MOHR, MURUGAPPAN MUTHUKUMAR, University of Massachusetts Amherst — The human lens derives its transparency and refractive index from the interactions between crystallin proteins (α -, β -, γ -crystallin). When the ordering of these crystallins is perturbed, insoluble macromolecular aggregates of crystalline proteins can occur resulting in cataracts. Using dynamic light scattering (DLS) and fast protein liquid chromatography (FPLC), we have conducted a detailed study of the formation of these aggregates. Our DLS results on γ -crystallin solutions exhibit the occurrence of slow and fast modes demonstrating the spontaneous formation of aggregates (hydrodynamic radius, $R_h \sim 200$ nm) in equilibrium with monomeric proteins ($R_h \sim 3$ nm). On the other hand, DLS results on α -crystallin solutions clearly demonstrate that α -crystallin molecules exist as a single population ($R_h \sim 18$ nm). Our results on mixtures of α - and γ -crystallin solutions show that the α -crystallin tends to demolish the clumps of γ -crystallin. Our exploration of environmental effects (temperature, pH, salt concentration) has revealed the macromolecular mechanism of dissolution of crystallin aggregates, providing a strategy for cataract prevention and insight into protein-protein interactions.

10:12AM Y47.00012 Quantifying the abnormal hemodynamics of sickle cell anemia¹ , HUAN LEI, GEORGE KARNIADAKIS, Brown University — Sickle red blood cells (SS-RBC) exhibit heterogeneous morphologies and abnormal hemodynamics in deoxygenated states. A multi-scale model for SS-RBC is developed based on the Dissipative Particle Dynamics (DPD) method. Different cell morphologies (sickle, granular, elongated shapes) typically observed in deoxygenated states are constructed and quantified by the Asphericity and Elliptical shape factors. The hemodynamics of SS-RBC suspensions is studied in both shear and pipe flow systems. The flow resistance obtained from both systems exhibits a larger value than the healthy blood flow due to the abnormal cell properties. Moreover, SS-RBCs exhibit abnormal adhesive interactions with both the vessel endothelium cells and the leukocytes. The effect of the abnormal adhesive interactions on the hemodynamics of sickle blood is investigated using the current model. It is found that both the SS-RBC - endothelium and the SS-RBC - leukocytes interactions, can potentially trigger the vicious “sickling and entrapment” cycles, resulting in vaso-occlusion phenomena widely observed in micro-circulation experiments.

¹This work was supported by the NSF grant CBET-0852948 and the NIH grant R01HL094270

10:24AM Y47.00013 The energetics of tightly bent DNA: a composite elastica model including local melting , ARTHUR EVANS, ALEX LEVINE, UCLA Department of Chemistry and Biochemistry — Melting transitions are well-known to be affected by the application of mechanical stress. Motivated by the experiments of Zocchi and collaborators (Qu and Zocchi 2011, EPL **94** 18003), we explore the effect of the application of mechanical stress on DNA melting in a particular composite of a stiff double stranded piece of DNA (dsDNA), shorter than its own persistence length, whose ends are linked by a flexible single stranded piece of DNA (ssDNA). The flexible ssDNA acts as a Gaussian polymer coil bending the stiff dsDNA through an elastic force that is controllable by the length of the ssDNA chain. In this talk we present theoretical predictions for two experimentally accessible features: the degree of local dsDNA melting and the local elastic energy of the dsDNA/ssDNA construct both as a function of the length of the attached ssDNA. We also address the effect of introducing a nick (broken covalent bond) in the dsDNA backbone on these results and discuss the implications of such data on the relative importance of backbone elasticity versus base stacking and base pairing interactions in determining the elasticity of dsDNA. This work also addresses open questions in the nonlinear elasticity of DNA in tightly bent curves.

10:36AM Y47.00014 Dispersion-relation phase spectroscopy of neuron transport , RU WANG, ZHUO WANG, Beckman Institute, University of Illinois at Urbana and Champaign, LARRY MILLET, MARTHA GILLETTE, Cell and Developmental Biology, University of Illinois at Urbana and Champaign, JOSEPH ROBERT LEIGH, NAHIL SOBH, National Center for Supercomputing Applications, University of Illinois at Urbana and Champaign, ALEX LEVINE, Department of Chemistry and Biochemistry, UCLA, GABREIL POPESCU, Beckman Institute, University of Illinois at Urbana and Champaign — Molecular motors move materials along prescribed biopolymer tracks. This sort of active transport is required to rapidly move products over large distances within the cell, where passive diffusion is too slow. We examine intracellular traffic patterns using a new application of spatial light interference microscopy (SLIM) and measure the dispersion relation, i.e. decay rate vs. spatial mode, associated with mass transport in live cells. This approach applies equally well to both discrete and continuous mass distributions without the need for particle tracking. From the quadratic experimental curve specific to diffusion, we extracted the diffusion coefficient as the only fitting parameter. The linear portion of the dispersion relation reveals the deterministic component of the intracellular transport. Our data show a universal behavior where the intracellular transport is diffusive at small scales and deterministic at large scales. We further applied this method to studying transport in neurons and are able to use SLIM to map the changes in index of refraction across the neuron and its extended processes. We found that in dendrites and axons, the transport is mostly active, i.e., diffusion is subdominant.

Friday, March 2, 2012 8:00AM - 10:48AM –
Session Y48 DPOLY DBIO: Focus Session: Statistical Physics of Active Systems Away From Detailed Balance: Swimmers and All That 161

8:00AM Y48.00001 Flow-controlled densification of E. Coli through a constriction , GASTÓN MIÑO, PMMH, UMR 7636 CNRS-ESPCI-Universités Paris 6 and 7, ERNESTO ALTSHULER, CARLOS PÉREZ-PENICHET, LENIN DEL RÍO, Henri Poincaré Group of Complex Systems and Superconductivity Laboratory, University of Havana, ANKE LINDNER, ANNIE ROUSSELET, ERIC CLÉMENT, PMMH, UMR 7636 CNRS-ESPCI-Universités Paris 6 and 7 — Bacterial suspensions are examples of “active matter.” Each bacteria can be regarded as a self-propelled particle that interacts hydrodynamically with its environment, including the surrounding “passive” fluid, the boundaries and other bacteria. In this presentation, we show a new phenomenon concerning E. Coli suspensions flowing through a funnel-like constrictions in micro-fluidic channels. The dynamics of bacterial suspensions flowing in confined spaces is relevant to understand their behavior in scenarios such as porous materials, soil, microbiology, water purification, and biomedical research. The applied flow induces a counter-intuitive symmetry breaking in the bulk bacteria concentration, which is found to increase past the funnel. The concentration enhancement persists over large distances and its amplitude increases linearly with the flow rate and disappears at large flow values. We show that the effect is reversible when the flow direction is reversed. We explain the observed effects on the interactions between the active bacteria and the channel boundaries. This experiment opens the possibility to control the concentration bacterial suspensions in microfluidic channels by simply tuning the flow of liquid.

8:12AM Y48.00002 Bidirectional sorting of flocking particles in the presence of asymmetric barriers , JEFFREY DROCCO, CHARLES REICHHARDT, CYNTHIA REICHHARDT, Los Alamos National Laboratory — We numerically demonstrate bidirectional sorting of flocking particles interacting with an array of funnel-shaped barriers. The particles choose a swimming direction by averaging the headings of their neighbors according to the Vicsek model, and experience additional steric interactions as well as repulsion from the fixed barriers. We show that particles preferentially localize to one side of the barrier array over time, and that the direction of this rectification can be reversed by adjusting the particle-particle exclusion radius or the noise term in the equations of motion. These results provide a conceptual basis for isolation and sorting of single- and multi-cellular organisms which move collectively according to flocking-type interaction rules.

8:24AM Y48.00003 Microfluidic one-way streets for algae , JORN DUNKEL, VASILY KANTSLE, MARCO POLIN, RAYMOND E. GOLDSTEIN, DAMTP, University of Cambridge — Controlling locomotion and transport of microorganisms is a key challenge in the development of future biotechnological applications. Here, we demonstrate the use of optimized microfluidic ratchets to rectify the mean swimming direction in suspensions of the unicellular green alga *Chlamydomonas reinhardtii*, which is a promising candidate for the photosynthetic production of hydrogen. To assess the potential of microfluidic barriers for the manipulation of algal swimming, we studied first the scattering of individual *C. reinhardtii* from solid boundaries. High-speed imaging reveals the surprising result that these quasi-spherical “puller”-type microswimmers primarily interact with surfaces via direct flagellar contact, whereas hydrodynamic effects play a subordinate role. A minimal theoretical model, based on run-and-turn motion and the experimentally measured surface-scattering law, predicts the existence of optimal wedge-shaped ratchets that maximize rectification of initially uniform suspensions. We confirm this prediction in experimental measurements with different geometries. Since the mechano-elastic properties of eukaryotic flagella are conserved across many genera, we expect that our results and methods are applicable to a broad class of biflagellate microorganisms.

8:36AM Y48.00004 Concentrating bacterial cells using a ratchet system: a lattice Monte Carlo simulation study, YUGUO TAO, GARY SLATER, Department of Physics, University of Ottawa — Rectification of motile *E. coli* bacteria has been observed in the presence of funnel-like channels. We present a lattice Monte Carlo model which takes into account both the size and the mechanical and thermodynamic properties of autonomous bacterial cells. The motion of the cells is composed of alternating run and tumble periods. We show that the rectification effect of the funnels is strongly dependent upon the effective random walk step length of the run/tumble cycle as well as the size of the funnel's aperture. Our results agree with experimental observations, and also confirm some conclusions from a previous simulation model of point-like bacteria. We also explore series of funnels as a means to pump and concentrate cells. We observe deviations from theoretical predictions when the size of the cells is comparable to that of the aperture of the funnel. The current model can be extended to study cells with different shapes, e.g. cigar-shape bacteria.

8:48AM Y48.00005 Spontaneous Segregation of Self-Propelled Particles with Different Motilities¹, SAMUEL MCCANDLISH, APARNA BASKARAN, MICHAEL HAGAN, Brandeis University — We study mixtures of self-propelled and passive rod-like particles in two dimensions using Brownian dynamics simulations. The simulations demonstrate that the two species spontaneously segregate to generate a rich array of dynamical domain structures whose properties depend on the propulsion velocity, density, and composition. In addition to presenting phase diagrams as a function of the system parameters, we investigate the mechanisms driving segregation. We show that the difference in collision frequencies between self-propelled and passive rods provides a driving force for segregation, which is amplified by the tendency of the self-propelled rods to swarm or cluster. Finally, both self-propelled and passive rods exhibit giant number fluctuations for sufficient propulsion velocities.

¹We gratefully acknowledge support from the NSF Brandeis MRSEC DMR-0820492. Computational support was provided by Brandeis HPC.

9:00AM Y48.00006 Active Brownian Particles with Active Fluctuations, PAWEŁ ROMANCZUK, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, ROBERT GROSSMANN, LUTZ SCHIMANSKY-GEIER, Department of Physics, Humboldt University Berlin, Germany — We study the effect of different types of noise on the dynamics of self-propelled particles with variable speed (active Brownian particles). We distinguish between passive and active fluctuations. Passive fluctuations are considered independent of the direction of particle's motion (e.g., thermal fluctuations). In contrast, active ones are assumed to be intrinsically connected with the propulsion mechanism of the active particle and, as a result, correlated with its time-dependent orientation. We calculate the stationary speed and velocity probability density functions of non-interacting active Brownian particles in the presence of both fluctuation types and discuss the generic signature of active fluctuations [1]. Furthermore, we discuss a model of active Brownian particles interacting via a velocity-alignment force [2]. We show, based on the results of a corresponding mean-field theory, how the type of fluctuations has a strong impact on the onset and stability of collective motion.

[1] P. Romanczuk and L. Schimansky-Geier, *Phys Rev Lett*, **106**, 230601 (2011)

[2] P. Romanczuk and L. Schimansky-Geier, *Ecol Compl*, in press, doi:10.1016/j.ecocom.2011.07.008 (2011)

9:12AM Y48.00007 Run and tumble, run and reverse, or run reverse and flick - who wins the chemotaxis race?, VASILY ZABURDAEV¹, School of Engineering and Applied Sciences, Harvard University, SERGEY DENISOV², Institute of Physics, Augsburg University, DAVID WEITZ³, School of Engineering and Applied Sciences, Harvard University — Run and tumble of *E. coli* bacteria is a well understood example of the stochastic cell motion that is alternated in the presence of signaling chemicals. By regulating the tumbling frequency bacteria are able to navigate toward the food sources. Another bacteria that use twitching to move on a surface, *M. xanthus*, utilize a different strategy - at the end of the run they completely reverse the direction of motion and continue moving in the opposite direction. The frequency of reversals was shown to be connected to the chemotactic response of the cell. Recently yet another pattern was discovered in marine bacteria *V. alginolyticus* which alternate sharp reversals with flicks - making a turn to an angle with a broad distribution and centered around 90 degrees. In this work we are presenting a theoretical framework that describes all above motion patterns. As a highlight of the developed approach we find the exact analytical expressions for the mean squared displacement of moving cells for arbitrary distribution of run times. That allows us to quantitatively compare the performance of bacteria exploring the environment with and without signaling chemicals and, therefore, to find the winner of the chemotactic race.

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9:24AM Y48.00008 Kinetic theory for systems of self-propelled particles, YEN-LIANG CHOU, THOMAS IHLE, North Dakota State University — Models of self-driven particles similar to the Vicsek model [Phys. Rev. Lett. 75 (1995) 1226] are studied by means of kinetic theory. In these non-equilibrium models, particles try to align their travel directions with the average direction of their neighbors. At strong alignment a global flocking state forms. The alignment is defined by a stochastic rule, not by a Hamiltonian. The corresponding interactions are non-additive and are typically of genuine multi-body nature. The theory [1] is based on a Master equation in 3N-dimensional phase space, which is made tractable by means of the molecular chaos approximation. The phase diagram for the transition to collective motion is calculated and compared to direct numerical simulations. A stability analysis of a homogeneous ordered state is performed, which reveals a long wave length instability for some of the considered models. The mean-field calculations of one of the models show a tricritical point where the flocking transition changes its character from continuous to discontinuous.

[1] T. Ihle, Phys. Rev. E 83 (2011) 030901

9:36AM Y48.00009 Diffusional Variation in Autonomously Motile Catalytic Janus Particles¹, R. LLOYD CARROLL, SHENGRONG YE, ZACHARY JONES, West Virginia University Department of Chemistry — Recently, we and others have studied the motion of Janus particles that undergo catalytically-induced motion in an appropriate chemical environment. Published studies indicate particles move with reduced rotational diffusion, resulting in enhanced effective diffusion coefficient - motile particles move longer distances between each random rotation, resulting in much greater overall motion. We undertook to study the effective diffusion coefficient of janus particles with various structural designs (symmetric and asymmetric anisotropy, angular dislocation of catalytic regimes) and under environmental stresses (external fields, imposed gradients). We find that structural features have a strong effect on the characteristics of observed motion and effective diffusion, and that environmental stresses can change particle dynamics, suppressing rotational diffusion and enhancing correlated motion. These results are consistent, with some caveats, as particles grow smaller, and the effects of Brownian motion become more pronounced. Deeper understanding of the statistical behavior of the systems results in particles with practical applications in transport on a microfluidic scale.

¹We acknowledge the support of WVnano and the use of WVNano Shared Research Facilities

9:48AM Y48.00010 Emergent Collective Behavior of Microscopic Swimmers¹, GUILLAUME LAMBERT, New York University — The individual components of a biological system often express simple behaviors that lead to the spontaneous emergence of order and high levels of complexity; the whole is greater than the sum of its parts. Emergent complexity may arise spontaneously or, more interestingly, in response to external forces present in the surrounding environment. Here, we study the emergence of the emergent collective behavior of swimming *Escherichia coli* bacteria inside microfabricated environments. We first demonstrate how the swimming dynamics of single bacterium cells inside jagged, funnel-shaped geometries leads to the emergence of complex migratory patterns. In particular, by creating ratchet-like barriers that redirect the motion of single *E. coli* cells, we demonstrate that while a single bacterium is unable to “escape” an array of ratchets, a *population* of cells are able to collectively navigate against these motion-rectifying barriers. We then investigate the collective behavior of cells at increasing densities and witness the emergence of multicellularity in bacteria. As the local density of cell increases to reach physiologically relevant concentrations, individual swimming cells respond to the cell-cell interactions and collectively assemble into biofilms. We describe the physiological development of such biofilms inside microfluidics devices and, using in situ measurements, study the physical properties of various biofilms from their motion and deformation.

¹Partially supported by and performance at NCI U54CA143803, CNF ECS-0335765, NSF PHY-0750323, and NSERC.

10:24AM Y48.00011 Active crystallization of Artificial Microswimmers, JEREMIE PALACCI, STEFANO SACANNA, JOYCE LAINE, CSMR, NYU, USA, ASHER PRESKA STEINBERG, Brandeis University, USA, DAVID PINE, PAUL CHAIKIN, CSMR, NYU, USA, CSMR, NYU, USA TEAM — A novel type of light activated microswimmers is used to drive the system far from equilibrium. For sufficient concentrations they spontaneously assemble in crystalline clusters of particles. These clusters are mobile, with complex dynamics –explosion, self healing...– and can reversibly melt down if the activity is shut down. The origin of the attraction between the active particles as well as the crystallization mechanism and the complex dynamics will be presented and rationalized quantitatively.

10:36AM Y48.00012 Collective motility of cells on deformable substrates¹, ARVIND GOPINATH, MICHAEL HAGAN, BULBUL CHAKRABORTY, APARNA BASKARAN, Martin Fisher School of Physics, Brandeis University, BRANDEIS UNIVERSITY TEAM — We consider a simple model for motile cells on deformable substrates. The cells interact through contact interactions and medium-mediated elastic interactions arising due to the adhesion of the cells to the substrate. Using Brownian dynamics simulations and systematic coarse graining of the microscopic model, we characterize the collective velocity field of such a collection of cells by calculating the velocity autocorrelation function and identify the role of elastic interactions in the emergent motility of cell sheets. Our findings include suppression of diffusivity due to the attractive part of the elastic interaction and a growing length scale in the velocity correlations.

¹We acknowledge funding from MRSEC Brandeis.

Friday, March 2, 2012 8:00AM - 10:48AM –
Session Y49 DMP DPOLY: Focus Session: Organic Electronics and Photonics - Small Molecules and General Advances 162A

8:00AM Y49.00001 Charge transport calculations of organic semiconductors by the time-dependent wave-packet diffusion method¹, HIROYUKI ISHII, NOBUHIKO KOBAYASHI, University of Tsukuba, KENJI HIROSE, NEC corporation — Organic materials form crystals by relatively weak Van der Waals attraction between molecules, and thus differ fundamentally from covalently bonded semiconductors. Carriers in the organic semiconductors induce the drastic lattice deformation, which is called as polaron state. The polaron effect on the transport is a serious problem. Exactly what conduction mechanism applies to organic semiconductors has not been established. Therefore, we have investigated the transport properties using the Time-Dependent Wave-Packet Diffusion (TD-WPD) method [1]. To consider the polaron effect on the transport, in the methodology, we combine the wave-packet dynamics based on the quantum mechanics theory with the molecular dynamics. As the results, we can describe the electron motion modified by (electron-phonon mediated) time-dependent structural change. We investigate the transport property from an atomistic viewpoint and evaluate the mobility of organic semiconductors. We clarify the temperature dependence of mobility from the thermal activated behavior to the power law behavior. I will talk about these results in my presentation. [1] H. Ishii, N. Kobayashi, K. Hirose, Phys. Rev. B, 82 085435 (2010).

¹This work was supported by a Grant-in-Aid for Scientific Research from the MEXT of Japan.

8:12AM Y49.00002 Investigation of Interfaces between Sub-Phthalocyanine and C60 using First-Principles Calculations¹, HOSSEIN HASHEMI, XIAO MA, JOHN KIEFFER, STEVEN E. MORRIS, MAX SHTEIN, Materials Science and Engineering Department, University of Michigan, Ann Arbor, Michigan 48109, USA, SHAOHUI ZHENG, EITAN GEVA, BARRY DUNIETZ, Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109, USA — The structure and electronic properties of a boron subphthalocyanine (SubPc) adsorbed on buckminsterfullerene (C60) and of C60 on SubPc surfaces, mimicking reverse orders of deposition, have been studied using density-functional theory (DFT) including long-van der Waals. Total-energy calculations are used to elucidate the initial adsorption of SubPc on C60 low index surfaces and also C60 on SubPc surfaces. The energetics of crystalline substrates with different surface terminations were mapped out using a single molecule of the partnering species. Accordingly, the interfacial structure and properties are different depending on whether the substrate is SubPc or C60, due to the incongruity between lattices and the disorder that develops in the contact layers of C60 and SubPc, respectively. The dependence of the charge transfer energies on the interface morphology is studied using range separated hybrid functionals. The stabilization of charge transfer states to below the absorbing state, needed to optimize the fill factor, also depends on the order of layer deposition. These results are discussed in the context of experiments performed on organic solar cells, showing trade-offs in the short circuit current and open circuit voltage with varying deposition order of the organic layers.

¹DoE-BES Award # DE-SC0000957

8:24AM Y49.00003 First principles study of the electrical and optical properties of SubPc single crystal¹, XIAO MA, HOSSEIN HASHEMI, JOHN KIEFFER, Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, 48109 — We studied the electrical and optical properties of the single crystal of boron subphthalocyanine chloride (SubPc), a popular donor material used in organic photovoltaic (OPV) devices within the framework of density-functional theory (DFT) with added van der Waals long range interactions to deepen our understanding of its performance in light absorption and charge transport. We calculated the frequency-dependent dielectric response, refractive index, extinction coefficient, and intrinsic charge mobility. The complex dielectric constant was computed using first-order perturbation theory, using the electronic wave functions and eigenvalues obtained from supercell DFT calculations. This was done for wave propagation in the (001), (010), (100) directions of optimized SubPc crystal with DFT calculations, revealing significant anisotropy in both electrical and optical properties. Comparison with experimental results allows us to draw conclusions regarding the structural organization of SubPc molecules deposited on a variety of substrates, as well as the conditions for thin film growth and property optimization.

¹DoE-BES Award # DE-SC0000957

8:36AM Y49.00004 Density-functional Theory and Beyond for Donor-Acceptor Complexes: The Example of TTF/TCNQ¹, VIKTOR ATALLA, Fritz-Haber-Institut der MPG, MINA YOON, Oak Ridge National Laboratory, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG — We study the performance of density-functional theory (DFT) with various exchange-correlation (XC) functionals in describing electronic and structural properties of the prototypical donor/acceptor complex TTF/TCNQ. We find that the binding energetics and the amount of electron transfer between TTF and TCNQ depends strongly on the functional. In particular, all semilocal functionals give rise to significant, artificial electron transfer due to a wrong ordering of Kohn-Sham (KS) levels. We consider the HSE [1] "family" of XC functionals using the fraction of exact exchange (α) as adjustable parameter. The optimum XC functional is then identified as that for which the G_0W_0 quasiparticle correction to the energy gap of the KS LUMO of the acceptor and the HOMO of the donor is minimized. We obtain $\alpha \sim 0.8$ which gives an electronic level alignment that is consistent with experiment and free from spurious asymptotic charge transfer. We conclude that the proposed scheme improves the KS spectrum, and that the investigated TTF-TCNQ dimer exhibits intra-molecular electron-density rearrangement rather than electron transfer.

[1] A.V. Krukau, et al., J. Chem. Phys. **125**, 224106 (2006)

¹Research sponsored by the Max Planck Society and the US Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

8:48AM Y49.00005 Understanding the high device efficiency of a class of solution-processed small-molecule solar cells, ANDRIY ZHUGAYEVYCH, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, OLENA POSTUPNA, Department of Chemistry, University of Rochester, Rochester, NY 14627, USA, SERGEI TRETIKOV, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, GUILLERMO BAZAN, Department of Chemistry and Biochemistry, University of California, Santa Barbara, CA 93106, USA — We perform a first principles study of light absorption, exciton and charge carrier transport for two recently synthesized molecular crystals which in bulk heterojunction solar cells with PC70BM acceptor show up to 6.7% power conversion efficiency. Our results distinguish the following factors important for this high efficiency. The large conjugation length facilitates strong light absorption with low-energy absorption edge. The crystalline ordering of properly oriented molecules leads to exciton delocalization over the typical size of the crystallites. The tightly packed pi-stacks allow for fast disorder-resistant hole transport along these stacks. Nevertheless the microscopic characteristics of the considered crystals are typical and comparable with other materials used in photovoltaics. Therefore we conclude that the main factors of the high device efficiency should be searched at the mesoscale including interfaces and grain boundaries.

9:00AM Y49.00006 Relating Molecular-Scale Structure to Spectroscopy in Pentacene-Perfluoropentacene Donor-Acceptor Assemblies from First-Principles, SAHAR SHARIFZADEH, Molecular Foundry, LBNL, LEEOR KRONIK, Weizmann Institute of Science, JEFFREY NEATON, Molecular Foundry, LBNL — Using van der Waals-corrected density functional theory and many-body perturbation theory, we compute the spectroscopic properties of the archetypal organic semiconductors pentacene (PEN), perfluoropentacene (PFP), and their composite donor-acceptor blends. Band structures, bulk crystal densities of states, and low-energy optical excitations are computed for the isolated bulk crystals and their composite assemblies. For the individual crystals, transport and optical gaps are in good agreement with experiment, and the nature and orientation of the excitonic wavefunctions is found to be sensitive to the degree of co-facial packing. For the PEN-PFP systems, different molecular arrangements and compositions are considered in an effort to connect to thin film measurements. The relationship between packing in these structures, the transport gap, and the nature and binding energies of low-lying excitons are explored. We acknowledge DOE-BES, NSF, and US-Israel BSF for support, and NERSC for computational resources.

9:12AM Y49.00007 Quantitative structural analysis of organic thin film deposition: a real time synchrotron X-ray scattering study, ISHVIENE COUR, Materials Science Program, Department of Physics, University of Vermont, Burlington, VT-05405, CHRISTIAN SCHLEPUETZ, YONGSOO YANG, Department of Physics, University of Michigan, Ann Arbor, MI- 48109, SONGTAO WO, Materials Science Program, Department of Physics, University of Vermont, Burlington, VT-05405, RON PINDAK, National Synchrotron light source, Brookhaven National Laboratory, Upton, NY-11973, RANDALL HEADRICK, Materials Science Program, Department of Physics, University of Vermont, Burlington, VT-05405 — Direct writing gives us the ability to deposit films from solution with controlled thickness, grain structure and orientation. We have investigated TIPS-Pentacene films deposited from toluene solution at various speeds via a combination of real time synchrotron x-ray scattering and polarized-light video microscopy. Through video microscopy we observe a well-defined crystallization front that becomes less defined as the writing speed is increased. In synchrotron x-ray scattering we observe that the ordering process is an order of magnitude slower than what is seen under the optical microscope. This discrepancy in the apparent crystallization rate raises questions such as, which part of the film actually rotates the polarized light and becomes visible under crossed polarizers? Observation with varying speeds and substrate temperatures suggest that the crystallization first occurs near the top surface of the drying film, while subsurface regions remain in a disordered state for up to several seconds.

9:24AM Y49.00008 Diindenoperylene as donor and acceptor for organic photovoltaic cells, ANDREAS WILKE, BEN BRÖKER, JOHANNES FRISCH, PATRICK AMSALEM, JENS NIEDERHAUSEN, Humboldt Universität zu Berlin, ANTJE VOLLMER, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, NORBERT KOCH, Humboldt Universität zu Berlin, HUMBOLDT UNIVERSITÄT ZU BERLIN TEAM, HELMHOLTZ-ZENTRUM BERLIN FÜR MATERIALIEN UND ENERGIE GMBH TEAM — In organic photovoltaic cells (OPVCs) typically two organic materials with electron acceptor and donor character are sandwiched between anode and cathode, forming heterojunctions where charge separation occurs. To improve the efficiency of charge separation, understanding the mechanisms of the energy level alignment at these heterojunctions is crucial. We report on ultraviolet photoelectron spectroscopy (UPS) measurements on three different organic-diindenoperylene (DIP) heterojunctions formed on PEDT:PSS electrodes. The measurement reveal that the energy level alignment of C₆₀ on DIP/PEDT:PSS corresponds to a type II heterojunction, with DIP acting as donor. The offset between the highest occupied molecular orbital (HOMO) of DIP and the lowest unoccupied molecular orbital (LUMO) of the acceptor C₆₀, an estimate for the maximum achievable open circuit voltage, is 1.35 eV. In contrast, the energy level alignment of DIP on sexithiophene (6T) and poly(3-hexylthiophene) (P3HT) is of type II as well, but DIP acting as acceptor. The offset between the HOMO of the donors 6T and P3HT and the LUMO of DIP is found to be 1.75 eV and 1.6 eV, respectively.

9:36AM Y49.00009 Gradual thickness change of CuPc on MoO_x on Oxygen Plasma Treated ITO¹, CHENGGONG WANG, IRFAN IRFAN, YONGLI GAO², Department of Physics and Astronomy, University of Rochester — The thickness dependence of copper phthalocyanine (CuPc) interlayer on molybdenum trioxide (MoO₃) and conducting indium tin oxide (ITO) has been investigated with ultraviolet photoemission spectroscopy (UPS). We also investigated the air exposure effect on the CuPc/MoO₃/ITO interlayers. It was found that the MoO₃ interlayer substantially increased the substrate work function (WF). With the deposition of CuPc the WF decreased and saturated at the thickness of 80 Å. We also found that 3x10⁶ Langmuir (L) air exposure decreased both the MoO₃ WF and the interface dipole between CuPc/MoO₃ interface.

¹The authors would like to acknowledge the support of the National Science Foundation under Grant No. DMR-1006098.

²Also affiliate to: Institute for Super Microstructure and Ultrafast Process, the Central South University, Changsha, Hunan 410083, The People's Republic of China.

9:48AM Y49.00010 Voltage dependence of the electric double layer structure at an ionic liquid/Au interface, YUSUKE WAKABAYASHI, RYOSUKE YAMAMOTO, HAZUKI MORISAKI, Grad. Sc. of Eng. Sci., Osaka University, OSAMI SAKATA, National Institute for Materials Science, HIDEKAZU SHIMOTANI, Dept. of Phys., Tohoku University, HONGTAO YUAN, YOSHIHIRO IWASA, Dept. of Appl. Phys., Tokyo University, TSUYOSHI KIMURA, Grad. Sc. of Eng. Sci., Osaka University — Ionic liquids (ILs) have been studied extensively because of their unique characteristics. One of the utilization of them is applying a strong electric field to solids through the electric double layer. Using this field, one can reduce the gate voltage for an organic field effect transistors (FETs) to operate [1]. In order to clarify the microscopic structure of such IL-gated organic FETs, we have performed synchrotron x-ray scattering experiments at BL-13XU of the SPring-8, Japan. While the electric double layer structures at IL-solid interfaces have been studied by x-ray reflectometry [2], the electric double layer is stabilized by the natural polarity of the surface of the solid. In order to observe the electric field effect, we measured an electric double layer formed at the interface between an IL and a Au(111) single crystal under external electric field. The reflectivity profile was found to depend on the applied electric field, which reflects the formation of the electric double layer.

[1] T. Uemura *et al.*, Appl. Phys. Lett., **95**, 103301 (2009).

[2] M. Mezger *et al.*, Science **322**, 424 (2008).

10:00AM Y49.00011 A critical assessment of thiolate self-assembled monolayers (SAMs) on platinum.¹, YENNY CARDONA QUINTERO, HONG ZHU, RAMPI RAMPRASAD, University of Connecticut — Thiolate SAMs have been successfully anchored on metal surfaces, but a critical assessment of the impact on the structural and electronic properties of the metal surfaces has remained elusive. CH₃S and CF₃S were selected as model systems in this work, because of their simple structures which can provide insights about how the composition and electronegativity of SAMs affect the properties of metal-SAM systems. Density functional theory calculations have been used in this work to study the adsorption of CH₃S and CF₃S molecules on the Pt (111) surface at different coverage (1/3, 1/4, 1/6, 1/9 and 1/12) and adsorption sites (fcc and hcp). The geometry, adsorption energy and the work function of the Pt-SAM systems have been determined. Several interesting observations could be made: (1) the optimized SAM is tilted with respect to the Pt surface and the tilted angle decreases with the molecular coverage on the Pt surface; (2) the adsorption energy of both systems are almost always lower at the fcc site compared to the hcp one and shows a coverage-dependence; (3) the work function of Pt-SAM also shows a dependence on coverage and hence controlling the molecular coverage is probably an effective technique to tune the work function.

¹ Financial support of this work by the National Science Foundation (NSF) and computational support through allocations at the NSF Teragrid

10:12AM Y49.00012 Nonlinear light propagation in photopolymers: from self-trapped beams to 3-D optical lattices, KALAICHELVI SARAVANAMUTTU, McMaster University — While liquid crystals, surfactants and colloidal crystal systems assemble into ordered phases to attain free energy minima, strikingly complex patterns can also emerge when condensed matter systems are perturbed away from equilibria. This talk will be an overview of research in our group into the dynamics of light beams that propagate while simultaneously initiating free-radical polymerisation in photopolymers. The consequent nonlinear and reciprocal interactions between the optical field and self-induced refractive index changes in the medium elicit a rich assortment of three-dimensional spatial patterns. These include self-trapping bright and dark beams, beam filamentation due to modulation instability, diffraction rings due to self-phase modulation and the formation of 2-D and 3-D bright and dark optical lattices. The potential of these optical phenomena to spontaneously inscribe complex 3-D polymer architectures that are inaccessible through conventional lithographic techniques and that would have advanced optical applications such as nonlinear photonic crystals will also be described.

10:24AM Y49.00013 Enhancing sensing of nitroaromatic vapors by thiophene-based polymer films, G. NAGARJUNA, University of Massachusetts Amherst, ABHISHEK KUMAR, AKSHAY KOKIL, University of Massachusetts Lowell, KEDAR JADHAV, SERKAN YURT, University of Massachusetts Amherst, JAYANT KUMAR, University of Massachusetts Lowell, D. VENKATARAMAN, University of Massachusetts Amherst — Sensing of nitroaromatic-based explosives is important for homeland security and for the detection of landmines in war zones. These compounds are detected using fluorescence quenching of poly(phenyleneethynylene) (PPE). When compared with PPE, polythiophenes have several features that make them excellent candidates for sensing. However, due to strong $\pi - \pi$ aggregation in polythiophenes, the permeation of the analyte in the thin film is poor. Therefore polythiophenes have poor quenching efficiencies. We have addressed this problem by tuning the side chains on these polymers to disrupt the polymer aggregation, thereby enhancing the analyte diffusion into the polymer thin film. We have now developed a materials platform for next generation sensory materials based on polythiophenes. This talk will discuss our approach and the studies that showed enhanced sensing of nitroaromatics in polythiophene thin films.

10:36AM Y49.00014 Giant Electrocaloric Effect in Ferroelectric Polymers with Great Impact on Energy and Environment, XINYU LI, XIAOSHI QIAN, HAIMING GU, SHENGGUO LU, QIMING ZHANG, Electrical Engineering Department and Materials Research Institute, The Pennsylvania State University — Refrigeration and air conditioning overall consume around 20% of the energy budget in developed countries which necessitates a search for new approaches to increase the energy efficiency of these cooling technologies. Cooling technologies based on the electrocaloric effect (ECE) hold great potential and promise in realizing these goals. The electrocaloric effect (ECE) refers to the change in temperature and/or entropy of a dielectric material by an applied voltage. Recently, a class of P(VDF-TrFE) based ferroelectric polymers have been discovered that provide a giant electrocaloric effect with an adiabatic temperature change of $\Delta T \sim 20$ K and an isothermal entropy change $\Delta S > 90$ J/kgK at room temperature. This talk will review the earlier works in the ECE, as well as present the basic materials considerations and experimental results of the ECE in both normal and relaxor ferroelectric polymers. It will be shown he relaxor ferroelectric polymer displays a nearly flat ECE response over a broad temperature range, which is very attractive for practical cooling device applications. Furthermore, we will present our recent investigation, exploiting the giant ECE in these polymers for cooling devices with compact size, high cooling power and efficiency.

Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y50 DPOLY DFD: Focus Session: Micro and Nano Fluidics III: Microtransport and Thermophysical Properties 162B

8:00AM Y50.00001 Cavitation in confined water: ultra-fast bubble dynamics, OLIVIER VINCENT, PHILIPPE MARMOTTANT, CNRS and University of Grenoble, Lab. Interdisciplinaire de Physique, France — In the hydraulic vessels of trees, water can be found at negative pressure. This metastable state, corresponding to mechanical tension, is achieved by evaporation through a porous medium. It can be relaxed by cavitation, i.e. the sudden nucleation of vapor bubbles. Harmful for the tree due to the subsequent emboli of sap vessels, cavitation is on the contrary used by ferns to eject spores very swiftly. We will focus here on the dynamics of the cavitation bubble, which is of primary importance to explain the previously cited natural phenomena. We use the recently developed method of artificial tress, using transparent hydrogels as the porous medium. Our experiments, on water confined in micrometric hydrogel cavities, show an extremely fast dynamics: bubbles are nucleated at the microsecond timescale. For cavities larger than 100 microns, the bubble “rings” with damped oscillations at MHz frequencies, whereas for smaller cavities the oscillations become overdamped. This rich dynamics can be accounted for by a model we developed, leading to a modified Rayleigh-Plesset equation. Interestingly, this model predicts the impossibility to nucleate bubbles above a critical confinement that depends on liquid negative pressure and corresponds to approximately 100 nm for 20 MPa tensions.

8:12AM Y50.00002 Multiphase flow within 3D porous media , SUJIT DATTA, DAVID WEITZ, Department of Physics, Harvard University — Multiphase flow through porous media is important for a diverse range of processes including aquifer remediation, CO₂ sequestration, and oil recovery. Despite its enormous importance, exactly how flow proceeds within a porous medium is unknown; the opacity of the medium typically precludes direct imaging of the flow. Here, we present an experimental technique to directly visualize multiphase flow within porous media. Using this approach, we show how heterogeneity strongly affects flow behavior during the drainage of porous media.

8:24AM Y50.00003 Modeling capillary filling of micropores with nanoparticle-filled binary fluid , YONGTING MA, AMITABH BHATTACHARYA, OLGA KUKSENOK, University of Pittsburgh, Pittsburgh, PA 15261, DENNIS PERCHAK, Kodak Research Laboratories, Rochester, NY 14650, ANNA C. BALAZS, University of Pittsburgh, Pittsburgh, PA 15261 — We examine the behavior of binary fluids containing nanoparticles that are driven by capillary forces to fill well-defined pores of microchannels. To carry out these studies, we use a hybrid computational approach that combines the lattice Boltzmann model for binary fluids and a Brownian dynamics model for the nanoparticles. The hybrid model allows us to capture the interactions between the binary fluids and the nanoparticles, as well as model the interactions among the fluid, the nanoparticles and the pore walls. We show that the nanoparticles dynamically alter both the interfacial tension between the two fluids and the contact angle on the pore walls; this, in turn, strongly affects the dynamics of the capillary filling. We demonstrate that by tailoring the properties of the nanoparticles, such as their affinity to the fluid components and their interaction with the pore walls, one can effectively control both the filling velocities and the deposition of nanoparticles on the pore walls. Our findings provide fundamental insights into the dynamics of this complex system, as well as potential guidelines for technological processes involving capillary filling with nanoparticles in microchannels with differing geometries.

8:36AM Y50.00004 Label-free Screening of Multiple Cell-surface Antigens Using a Single Pore , KARTHIK BALAKRISHNAN, UC Berkeley Department of Mechanical Engineering, MATTHEW CHAPMAN, UC Berkeley Biophysics Graduate Group, ANAND KESAVARAJU, UC Berkeley Department of Bioengineering, LYDIA SOHN, UC Berkeley Department of Mechanical Engineering — Microfluidic pores have emerged as versatile tools for performing highly sensitive measurements. Pore functionalization can result in slower particle transit rates, thereby providing insight into the properties of particles that travel through a pore. While enhancing utility, functionalizing with only one species limits the broader applicability of pores for biosensing by restricting the insight gained in a single run. We have developed a method of using variable cross-section pores to create unique electronic signatures for reliable detection and automated data analysis. By defining a single pore into sections using common lithography techniques, we can detect when a cell passes through a given pore segment using resistive-pulse sensing. This offers such advantages as 1) the ability to functionalize each portion of a pore with a different antibody that corresponds to different cell surface receptors, enabling label-free multianalyte detection in a single run; and 2) a unique electronic signature that allows for both an accelerated real-time analysis and an additional level of precision to testing. This is particularly critical for clinical diagnostics where accuracy and reliability of results are crucial for healthcare professionals upon which to act.

8:48AM Y50.00005 Tracking rotation and translation simultaneously in confined liquids , SUBHALAKSHMI KUMAR, SUNGCHUL BAE, STEVE GRANICK, University of Illinois, Urbana Champaign — At the same spatially-resolved spots when fluid is confined to molecularly-thin spacings between atomically-smooth mica crystals, we track simultaneously, using fluorescence correlation spectroscopy and time correlated single photon counting, the translational and rotational diffusion of small dyes suspended in octamethylcyclotetrasiloxane (OMCTS). The spatially-resolved quantification of both dynamical quantities gives insight, as it does in bulk glasses, into the origins of dynamical heterogeneity in confined fluids.

9:00AM Y50.00006 Neutron Scattering Applications for Characterizing Phase Behavior and Dynamics of Confined Fluids in Nanoporous Materials , YURI MELNICHENKO, Biology and Soft Matter Division, Oak Ridge National Laboratory — Fluid-solid interactions in natural and engineered porous solids underlie variety of technological processes, including sequestration of anthropogenic greenhouse gases, hydrogen storage, membrane separation, and catalysis. The size, distribution and interconnectivity of pores, the chemical and physical properties of the solid and fluid phases collectively dictate how fluid molecules migrate into and through the micro- and mesoporous media, adsorb and ultimately react with the solid surfaces. Due to the high penetration power and relatively short wavelength of neutrons, small-angle neutron scattering (SANS) as well as quasi elastic neutron scattering (QENS) techniques are ideally suited for *in situ* studies of the structure and phase behavior of confined fluids under pressure as well as for evaluating structure of pores in engineered and natural porous systems. It has been demonstrated recently that SANS and USANS can also be used for evaluating the volume of closed pores as a function of pore sizes in the range from micrometer to sub-nanometer pores. In this talk I will overview some recent developments in the SANS and QENS methodology and give several examples of how it can be used for in-situ studies of the adsorption and dynamics of carbon dioxide and methane in porous fractal silica and carbon aerogels as well as characterizing the abnormal densification of hydrogen in activated carbons at ambient temperatures.

9:12AM Y50.00007 A mathematical model for the transport of a solute through a porous-walled tube , IAN GRIFFITHS, REBECCA SHIPLEY, Mathematical Institute, University of Oxford — Predicting the distribution of solutes or particles in flows within porous-walled tubes is essential to inform the design of cross-flow filtration devices. Here we use Taylor-dispersion theory to derive a radially averaged model for solute transport in a tube with porous walls, where the wall Darcy permeability may vary both spatially and in time. Crucially, this model includes solute advection via both radial and axial flow components, as well as diffusion, and the advection, diffusion and uptake coefficients in the averaged equation are explicitly derived. The model is used to explore the specific example of a hollow-fibre membrane bioreactor for tissue engineering applications - here membrane fouling and cell population expansion mean that the effective membrane permeability is intrinsically coupled to both fluid flow and nutrient transport. We conclude by presenting design considerations that promote spatially uniform cell population growth.

9:24AM Y50.00008 Biased and flow driven Brownian motion in periodic channels¹ , S. MARTENS, A. STRAUBE, Humboldt-University Berlin, G. SCHMID, University Augsburg, L. SCHIMANSKY-GEIER, Humboldt-University Berlin, P. HÄNGGI, University Augsburg — In this talk we will present an expansion of the common Fick-Jacobs approximation to hydrodynamically as well as by external forces driven Brownian transport in two-dimensional channels exhibiting smoothly varying periodic cross-section. We employ an asymptotic analysis to the components of the flow field and to stationary probability density for finding the particles within the channel in a geometric parameter. We demonstrate that the problem of biased Brownian dynamics in a confined 2D geometry can be replaced by Brownian motion in an effective periodic one-dimensional potential $\Psi(x)$ which takes the external bias, the change of the local channel width, and the flow velocity component in longitudinal direction into account. In addition, we study the influence of the external force magnitude, respectively, the pressure drop of the fluid on the particle transport quantities like the averaged velocity and the effective diffusion coefficient. The critical ratio between the external force and pressure drop where the average velocity equals zero is identified and the dependence of the latter on the channel geometry is derived. Analytic findings are confirmed by numerical simulations of the particle dynamics in a reflection symmetric sinusoidal channel.

¹This work has been supported by the VW Foundation via project I/83903 (L.S.-G., S.M.) and I/83902 (P.H., G.S.). P.H. acknowledges the support the excellence cluster “Nanosystems Initiative Munich” (NIM).

9:36AM Y50.00009 ABSTRACT WITHDRAWN —

9:48AM Y50.00010 Crossover from the Hydrodynamic to the Kinetic Regime in Confined Nanoflows¹, CHARLES LISSANDRELLO, VICTOR YAKHOT, KAMIL L. EKINCI, Department of Mechanical Engineering, Boston University — We present an experimental study of a confined nanoflow. The nanoflow is generated in a simple fluid by a sphere oscillating in the proximity of a flat solid wall. Varying the oscillation frequency, the confining length scale and the fluid mean free path over a broad range provides a detailed map of the flow. We use this experimental map to construct a scaling form, which seamlessly describes the nanoflow in both the hydrodynamic and the kinetic regimes. Furthermore, our scaling form unifies previous theories based on the slip boundary condition and the effective viscosity.

¹Support from the US NSF (through grants ECCS-0643178, CMMI-0970071, and DGE-0741448) is acknowledged.

10:00AM Y50.00011 Viscosity of ultrathin water films confined between oxide surfaces – ab initio and classical molecular dynamics simulations¹, PETER J. FEIBELMAN, GARY S. GREEST, Sandia National Laboratories, NEIL HARIA, CHRISTIAN D. LORENZ, King's College London — We compare estimates based on ab initio (DFT/PBE) and on classical molecular dynamics simulations of the viscosity of 2, 3 and 5-layer water films confined between hydrophilic kaolinite surfaces. Results were obtained by constraining the confining surfaces to move in +x and -x directions at equal speeds of 1-200 m/sec and loads up to 1 GPa. In neither simulation approach did the calculated viscosity of the confined water exceed that of bulk water by more than an order of magnitude. Thus neither supports the idea that nano-confinement dramatically enhances water's viscosity.

¹Supported by the DOE Office of Basic Energy Sciences, Division of Materials Science and Engineering. Sandia is operated by the Lockheed Martin Co. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL8500

10:12AM Y50.00012 Submicron flows of polymer solutions, HUGUES BODIGUEL, AMANDINE CUENCA, Université de Bordeaux - LOF — We study flow properties of high molecular weight polymer solutions below the micron scale. Fluorescence photobleaching is used as a non-invasive technique to evaluate the velocity of pressure-driven flows in channels from 100 to 4000 nm height. We observe a striking reduction of the effective viscosity of polyacrylamide solutions in the semi-dilute regime. This effect increases with molecular weight and concentration. Using a Rabinovitch-like approach, we correlate the data at different thicknesses to obtain the wall slip velocity and the flow curve at sub-microscale. Those properties are also evaluated using particle imaging velocimetry close to similar surfaces and standard rheometry. Comparing the measurements in bulk and in confined geometries, we conclude that the observed viscosity reduction can not be solely explained by slippage. We discuss the possible reasons of this effect that are size-dependant filtration and shear-thinning enhancement due to the confinement.

10:24AM Y50.00013 Nanomechanics and dynamics of confined water and other liquids¹, PETER HOFFMANN, Wayne State University, SHAH KHAN, Wayne State University/ University of Peshawar — From oil recovery to molecular biology, nanoconfined water plays an important role in many areas of research. However, the mechanics and dynamics of nanoconfined water are not well understood. Over the last ten years, a number of groups have measured the mechanics of confined water using atomic force microscopy (AFM) or surface force apparatus (SFA) - often with contradictory results. At Wayne State University, we have developed high resolution AFMs for ultra-small amplitude, linear measurements of the mechanics and dynamics of confined liquids. We have shown that water shows a distinct slow-down in dynamics under confinement (PRB 2004), co-discovered a dynamic "solidification" in a model liquid (Langmuir 2006), and showed that normal and shear stiffness are closely related in confined liquids (Rev. Sci. Instr. 2008). Recently, we found dynamic solidification also in water layers (PRL 2010), a finding that explains the contradictory findings in earlier measurements and points to surprisingly complex behavior in this seemingly simple system. Here we will review these findings, as well as present new findings that show the profound effects of ion concentration on these dynamical effects, as well as measurements of colloidal systems, which illustrate that some findings at the molecular scale can be understood from purely geometric considerations and are not dependent on molecular-scale interactions.

¹P. M. H. acknowledges funding through the National Science Foundation, Grant No. DMR-0804283.

10:36AM Y50.00014 Investigation of Nanoscale Structure Using Spin-Echo Small-Angle Neutron Scattering (SESANS), XIN LI, ROGER PYNN, ADAM WASHINGTON, Indiana University, WEI-REN CHEN, KUNLUN HONG, GREGORY SMITH, Oak Ridge National Laboratory, YUN LIU, National Institute of Standards and Technology — Spin-Echo Small-Angle Neutron Scattering (SESANS) is a new technique for probing structural correlations in real space over distances ranging from ~20 nm to several microns. The measured SESANS correlation function is a projection of the normal Patterson correlation function on to a particular spatial direction. A framework to theoretically calculate this correlation function is laid out, followed by a general discussion of the features of the SESANS correlation function for colloidal systems with different interaction potentials. Our calculations for a system of monodisperse spherical particles, show that SESANS is much more sensitive to the intercolloid potential than conventional Small Angle Neutron Scattering. We have used SESANS to study the correlations between 300-nm-diameter surfactant-stabilized poly(methyl methacrylate) (PMMA) spheres suspended in a good solvent, with and without an added polymeric depletant. Below a PMMA volume fraction of ~30% we find good agreement between the experimental data and theoretical prediction based on the Percus-Yevick approximation. With a small amount of polymer added to the suspension (less than 0.2% by weight of 110 kD polymer), the short-range correlations between PMMA spheres are enhanced because of the presence of polymer depletant. The magnitude of the change is roughly as expected on the basis of calculations of a mixture of spherical particles of different sizes.

10:48AM Y50.00015 Non local rheology and near wall fluctuations in microgel jammed suspensions, PATRICK TABELING, CHOONGYEOP LEE, FABRICE MONTI, MICHEL CLOITRE, ESPCI — We study flows of concentrated suspensions of soft nanoparticles in microchannels, over smooth hydrophilic and hydrophobic surfaces, using nano-PTV and μ PIV techniques. With hydrophobic walls, the flow curves are in good agreement with bulk rheology. With hydrophilic walls, substantial deviations from bulk rheology are observed. In the meantime, large velocity oscillations close to the wall are detected. We couple these observations by introducing a local rheology based on an energy barrier. As a whole, our work confirms the existence of non local rheological behavior in glassy systems.

Friday, March 2, 2012 8:00AM - 11:00AM –

Session Y52 GSNP: Focus Session: Spin Glasses: Advances, Algorithms, and Applications 153C

8:00AM Y52.00001 How the Edwards-Anderson Model reaches its Mean-Field Limit; Simulations in $d=3,\dots,7$ ¹, STEFAN BOETTCHER, STEFAN FALKNER, Physics Department, Emory University — Extensive computations of ground state energies of the Edwards-Anderson spin glass on bond-diluted, hypercubic lattices are conducted in dimensions $d = 3, \dots, 7$. Results are presented for bond-densities exactly at the percolation threshold, $p = p_c$, and deep within the glassy regime, $p > p_c$, where finding ground-states becomes a hard combinatorial problem. The “stiffness” exponent y that controls the formation of domain wall excitations at low temperatures is determined in all dimensions. Finite-size corrections of the form $1/N^\omega$ are shown to be consistent throughout with the prediction $\omega = 1 - y/d$. At $p = p_c$, an extrapolation for $d \rightarrow \infty$ appears to match our mean-field results for these corrections. In the glassy phase, ω does not approach the value of $2/3$ for large d predicted from simulations of the Sherrington-Kirkpatrick spin glass. However, the value of ω reached at the upper critical dimension *does* match certain mean-field spin glass models on sparse random networks of regular degree called Bethe lattices.

[1] S. Boettcher and S. Falkner, arXiv:1110.6242;

[2] S. Boettcher and E. Marchetti, PRB77, 100405 (2008);

[3] S. Boettcher, PRL95, 197205 (2005).

¹This work has been supported by grant DMR-0812204 from the National Science Foundation.

8:12AM Y52.00002 Ensemble Inequivalence in Spin Glasses, ZSOLT BERTALAN, HIDETOSHI NISHIMORI, KAZUTAKA TAKAHASHI, Tokyo Institute of Technology — We report on the ensemble inequivalence in many-body spin-glass models with Ising and integer spins. In the Ising case, for many-body interactions the transition between the ferromagnetic and paramagnetic phases is of first order, and the microcanonical and canonical ensembles give different results. The spin-glass transition is of first order for certain values of the crystal field strength in the integer-spin model and is dependent whether it was derived in the microcanonical or the canonical ensemble. We also discuss the ensemble inequivalence of random energy models, corresponding to the limit infinitely many-body interactions. This is the first systematic treatment of spin glasses with long-range interactions in the microcanonical ensemble using the replica approach, which shows how the two ensembles give different results.

8:24AM Y52.00003 Algorithms and long-range order in the two-dimensional $\pm J$ spin glass¹, A. ALAN MIDDLETON, Syracuse University, CREIGHTON K. THOMAS, Northwestern University, DAVID A. HUSE, Princeton University — Numerical methods and results of their application to the two-dimensional Ising spin glasses will be described. For a random mix of ferromagnetic and antiferromagnetic bonds of equal strength, long range correlations at zero-temperature are derived from scaling relations between computed exponents and are confirmed in numerical simulations. This long range order is stabilized by large entropy differences, as large domain walls often have zero energy cost. The order resembles that in higher-dimensional models at finite temperature. A publicly distributed implementation of the algorithms has been developed for computing partition functions and exactly sampling configurations according to their Boltzmann weight for the general spin-glass and related two-dimensional models.

¹NSF DMR-1106731, DMR-0819860

8:36AM Y52.00004 Replica theory of partition-function zeros in spin-glass systems, KAZUTAKA TAKAHASHI, Tokyo Institute of Technology, TOMOYUKI OBUCHI, Osaka University — We study the phase transitions in spin-glass systems by analysing the partition-function zeros (Lee-Yang zeros) with respect to the complex temperature/field. For several models as the random energy and spherical models with many-body interactions, we extend the replica method and the procedure of the replica symmetry breaking ansatz to be applicable in the complex-parameter case. We derive the phase diagrams in the complex plane and calculate the density of zeros in each phase. We find that there is a replica symmetric phase having a large density near the imaginary axis away from the origin. In the spin-glass phase, the density is finite only when the chaos effect is present. This result indicates that the density of zeros is more closely connected to the chaos effect than the replica symmetry breaking. We also investigate the relevance of our result to the finite-dimensional systems by studying the renormalization group flow in the complex plane.

8:48AM Y52.00005 Aging behavior in disordered and frustrated spin systems¹, HYUNHANG PARK, MICHEL PLEIMLING, Virginia Tech — Using Monte Carlo simulations we investigate aging in three-dimensional Ising spin glasses as well as in two-dimensional Ising models with disorder quenched to low temperatures. The time-dependent dynamical correlation length $L(t)$ is determined numerically and the scaling behavior of various two-time quantities as a function of $L(t)/L(s)$ is discussed. For disordered Ising models deviations of $L(t)$ from the algebraic growth law show up. The generalized scaling forms as a function of $L(t)/L(s)$ reveal a generic simple aging scenario for Ising spin glasses as well as for disordered Ising ferromagnets.

¹This work was supported by the US Department of Energy through grant DE-FG02-09ER46613.

9:00AM Y52.00006 Critical behavior of the 1D Lévy lattice spin-glass: from mean-field threshold to the effective lower critical dimension¹, LUCA LEUZZI, IPCF-CNR, Italy, GIORGIO PARISI, FEDERICO RICCI-TERSENGHI, Dept. Physics, Sapienza University of Rome, Italy, JUAN-JOSÉ RUIZ-LORENZO, Dept. Physics, University of Extremadura, Badajoz, Spain — By means of Monte Carlo numerical simulations we analyze the critical behavior of a one dimensional spin-glass model with diluted interactions decaying, in probability, as an inverse power of the distance: the Lévy lattice spin-glass. Varying the power ρ , corresponds to change the effective dimension from mean-field-like (small power $\rho < 4/3$) to finite dimensional-like short-range models ($4/3 < \rho < 2$) and, eventually, to 1D short-range models ($\rho > 2$), where no phase transition occurs. The bond diluteness drastically reduces the computational time and large sizes can be approached. The one dimensionality allows for studying long systems, e.g., long correlation lengths in the critical region. The spin-glass critical behavior can, therefore, be studied in and out of the range of validity of the mean-field approximation. After reviewing the main results in the Lévy lattice model about the spin-glass transition and the nature of the spin-glass phase for different values of the effective dimension, we will present new results on the critical behavior at $\rho = 2$, corresponding to the lower critical dimension, and compare them with old and recent renormalization group approaches in this limit.

¹FIRB/2008 Grant Code RBFR08M3P4, Ministry of Education, University and Research, Italy. Grant No. FIS2010-16587, Ministerio de Ciencia y Tecnología, Spain

9:12AM Y52.00007 Spin glasses: Still frustrating after all these years?, HELMUT G. KATZGRABER, Department of Physics and Astronomy, Texas A&M University and ETH Zurich — Spin glasses are archetypal model systems to study the effects of frustration and disorder. Despite ongoing research spanning several decades, there remain many fundamental open questions, such as the existence of a spin-glass state in a field or the low-temperature structure of phase space for short-range systems. Novel applications across disciplines, as well as progress in algorithms and the advent of fast and cost-effective computers, have recently revived interest in the study of spin glasses. First, an overview of spin glasses will be given, followed by recent novel applications to fields as diverse as structural glasses and quantum computing.

9:48AM Y52.00008 The de Almeida-Thouless line of the four-dimensional Ising spin glass, VICTOR MARTIN-MAYOR, Universidad Complutense de Madrid, JANUS COLLABORATION — We present the results of a large scale numerical simulation of the four dimensional Edwards-Anderson model in an external field. Using the Janus computer, as well as standard CPU clusters, we simulate lattices of size up to $L=16$ at several values of the external field. Our analysis method departs from the standard one. In fact, it has been previously noticed that the spin-glass susceptibility (i.e. the spin-glass propagator at zero external momentum) behaves anomalously. Instead, one should focus on the propagator at small but non-vanishing wave-vector. Starting from this observation, we obtain a simple and powerful finite-size scaling method. Clear evidence for a de Almeida-Thouless line is found. We compute critical exponents, widely differing from the zero field case, with an accuracy of five percent. The shape of the de Almeida-Thouless line in the (T, h) plane follows the Fisher-Sompolinsky scaling. Discrepancies with previous work are explained in terms of very strong scaling corrections.

10:00AM Y52.00009 Reentrance and ultrametricity in three-dimensional Ising spin glasses, HELMUT G. KATZGRABER, Department of Physics and Astronomy, Texas A&M University and ETH Zurich, CREIGHTON K. THOMAS, Department of Materials Science and Engineering, Northwestern University, ALEXANDER K. HARTMANN, Department of Physics, Oldenburg University, Germany — We study the three-dimensional Edwards-Anderson Ising spin glass with bimodal disorder with a fraction of 22.8% antiferromagnetic bonds. Parallel tempering Monte Carlo simulations down to very low temperatures show that for this fraction of antiferromagnetic bonds the phase diagram of the system is reentrant, in agreement with previous results. Furthermore, using a clustering analysis, we analyze the ultrametric properties of phase space for this model.

10:12AM Y52.00010 Replica exchange simulations of the three-dimensional Ising spin glass: static and dynamic properties¹, BURCU YUCESAY, JONATHAN MACHTA, Department of Physics, University of Massachusetts Amherst, HELMUT G. KATZGRABER, Department of Physics, Texas A&M University & ETH Zurich — We present the results of a large-scale numerical study of the equilibrium three-dimensional Ising spin glass with Gaussian disorder. Using replica exchange (parallel tempering) Monte Carlo, we measure various static, as well as dynamical quantities, such as the autocorrelation times and round-trip times for the replica exchange Monte Carlo method. The correlation between static and dynamic observables for 5000 disorder realizations ($N \leq 10^3$ spins) down to very low temperatures ($T \approx 0.2T_c$) is examined. Our results show that autocorrelation times are directly correlated with the roughness of the free energy landscape. We also discuss the size dependence of several static quantities.

¹Supported in part by NSF DMR-0907235

10:24AM Y52.00011 Monte Carlo Simulations of Random Frustrated Systems on Graphics Processing Units, SHENG FENG, YE FANG, SEAN HALL, Louisiana State University, ARIANE PAPKE, University of Gottingen, CADE THOMAS-SON, KA-MING TAM, JUANA MORENO, MARK JARRELL, Louisiana State University — We study the implementation of the classical Monte Carlo simulation for random frustrated models using the multithreaded computing environment provided by the Compute Unified Device Architecture (CUDA) on modern Graphics Processing Units (GPU) with hundreds of cores and high memory bandwidth. The key for optimizing the performance of the GPU computing is in the proper handling of the data structure. Utilizing the multi-spin coding, we obtain an efficient GPU implementation of the parallel tempering Monte Carlo simulation for the Edwards-Anderson spin glass model. In the typical simulations, we find over two thousand times of speed-up over the single threaded CPU implementation.

10:36AM Y52.00012 Monte Carlo simulations of the $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$ diluted dipolar magnet, JUAN CARLOS ANDRESEN, Department of Physics, ETH Zurich, MOSHE SCHECHTER, Department of Physics, Ben Gurion University, HELMUT G. KATZGRABER, Department of Physics and Astronomy, Texas A&M University and ETH Zurich — Recent intriguing experimental results on $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$, a diluted dipolar magnet, along with new analytical insights, suggest that neither a mean-field treatment nor simulations using simplified versions of the underlying Hamiltonian adequately describe these materials. Not only does this imply that novel disordering mechanism might be present, it requires a detailed numerical analysis that incorporates all terms in the Hamiltonian. We present large-scale Monte Carlo simulations of the diluted dipolar magnet with competing interactions on a LiHo lattice with the inclusion of a random field term. For low concentrations of Ho atoms we reproduce the peculiar linear dependence of the transition temperature as a function of the random-field strength found in recent experimental results by Silevich *et al.* [Nature 448, 567 (2007)]. We then find a zero-temperature phase transition between the ferromagnetic and quasi-spin-glass phases, suggesting that it is the underlying spin-glass phase that dictates the above linear dependence of T_c on the random field. For large concentrations we recover the quadratic dependence of the critical temperature as a function of the random field strength.

10:48AM Y52.00013 Novel disordering mechanisms in dipolar spin glasses and ferromagnets, MOSHE SCHECHTER, Physics Department, Ben Gurion University of the Negev, JUAN CARLOS ANDERSEN, Department of Physics, ETH Zurich, HELMUT KATZGRABER, Department of Physics and Astronomy, Texas A&M University and ETH Zurich — At and below the critical dimension the disordering of an ordered phase by a random field occurs via a collective effect of large domains at infinitesimal random field [Imry & Ma, Phys. Rev. Lett. 35, 1399 (1975)]. At larger space dimensions the disordering requires a large random field, of the order of the interaction energy. In a random field, the lower critical dimension is 2 for Ising ferromagnets, whereas it is infinity for spin glasses. We have generalized the Imry-Ma argument for ferromagnets with competing interactions and an underlying spin-glass phase, and for dilute dipolar spin glasses. For dilute dipolar spin glasses we have found [EPL 88, 66002 (2009)] that the broad distribution of random fields dictates more efficient disordering of the glass phase, and domain sizes which depend explicitly on the concentration, i.e., do not obey simple scaling. Here we show that as a result of a competing spin-glass phase, the disordering of the ferromagnet occurs at a finite random field, which is yet much smaller than the interactions. Our results are verified numerically, explain the recently-observed peculiar linear dependence of T_c on the random field strength [Nature 448, 567 (2007)], and predict a zero-temperature random-field driven transition between a ferromagnetic and a quasi spin glass phase.

Friday, March 2, 2012 8:00AM - 10:48AM –
Session Y53 GSNP: Nonlinear Dynamics of Coupled Systems 153B

8:00AM Y53.00001 Frequency Enhancement in Coupled Noisy Excitable Elements¹, WEI-YIN CHIANG, PIK-YIN LAI, Dept. of Physics and Center for Complex Systems, National Central University, Chungli, Taiwan 320, R.O.C., C.K. CHAN, Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan 115, R.O.C. — The oscillatory dynamics of coupled noisy excitable FitzHugh-Nagumo elements is investigated as a function of the coupling strength g . For two such coupled elements, it is found that their frequencies are enhanced by the coupling and will synchronize at a frequency higher than the uncoupled frequencies of each element. As g increases, there is an unexpected peak in the mean of frequency distribution before reaching synchronization at the optimal coupling strength. This phenomenon can be understood with a simplified analytic model based on the excitation across a potential barrier whose height is controlled by g as well as the formation of temporary coherent cluster.

¹National Science Council of Taiwan under grant nos. 98-2112-M-008-023-MY3, 97-2112-M-001-003

8:12AM Y53.00002 Ramification of stream networks, HANSJOERG SEYBOLD, OLIVIER DEVAUCHELLE, ALEXANDER PETROFF, ROBERT YI, DANIEL ROTHMAN, MIT — The geometric complexity of channel networks arises from their successive ramifications — the splitting of a single tip into two branches. Here we show that streams incised by groundwater seepage split at a characteristic angle of $\alpha = 2\pi/5 = 72^\circ$. Our theory represents streams as a collection of paths growing and bifurcating in a diffusing field, which can be described by Loewner dynamics. Analysis of thousands of bifurcations in a $\sim 100 \text{ km}^2$ stream network reveals that the mean branching angle is $72.5^\circ \pm 1.5^\circ$ (95% C.I.) and that the five fold symmetry induced by the branching of the tips is observed on all scales in the network. This consistency between theory and observation suggests that the network geometry is determined by the external flow field rather than flow within the streams themselves, contrary to assumptions made by models that relate geometry to internal dissipation.

8:24AM Y53.00003 Dynamical phyllotaxis: transition modes and Sine-Gorden-like solitons, YUANXI WANG, Penn State University, CRISTIANO NISOLI, T- Division, CNLS Los Alamos National Laboratory, VINCENT CRESPI, Penn State University — Repulsive particles constrained to a cylindrical surface generate a rich set of static spiral patterns known as phyllotaxis. The ground states and quasi-static transitions of phyllotaxis has been well understood based on the conventional hypothesis that particles always form a cylindrical lattice. We investigate inhomogeneous transition modes which break this helical symmetry to connect monojugate and multijugate patterns. Furthermore, traveling Sine-Gordon-like solitons in dynamical phyllotaxis are observed in numerical simulations and explained using a modified Frenkel-Kontorova model. We show that kinks propagate spirally along selected parastichies and carry an intrinsic dipole. Applications in different areas of physics are discussed.

8:36AM Y53.00004 Cascade of bifurcation type trajectories as a general type of attractors in fractional dynamical systems¹, MARK EDELMAN, Stern College at Yeshiva University, Courant Institute at NYU — Based on the results of computer simulations and analytical investigation of fractional maps, we present our latest results related to the existence and stability of the new type of attractors in the fractional dynamical systems: cascade of bifurcation type trajectories (CBTT). We show that in fractional Standard Map (FSM) this type of attractors appears in the area of parameters, where in the corresponding integer system (regular Standard Map) series of period doubling bifurcations and corresponding splitting of islands of stability leads to the disappearance of stability and transition to chaos.

¹ Author thanks Stern College and Courant Institute

8:48AM Y53.00005 Scale-free avalanches in disordered systems of localized charges with long-range Coulomb interaction¹, MATTEO PALASSINI, MARTIN GOETHE, Faculty of Physics, University of Barcelona, Spain — We study theoretically and numerically the charge avalanches created by a perturbation in disordered systems of localized charges with unscreened Coulomb interaction (the so-called electron glass model), in two and three dimensions. Starting from a low-lying local energy minimum, we perturb the system by inserting an extra charge or an extra dipole, and let it relax via one-particle hops until a new minimum is reached. We find that the size distribution of the avalanches created in this process displays generically a power-law tail with an exponent close to the mean-field value 3/2 both in 2D and 3D, without requiring any parameter tuning. We provide a qualitative explanation of these results in terms of the density of states of elementary charge and dipole excitations and the associated Coulomb gap, which shows that the power-law tail arises from arbitrarily long hops, without requiring to assume the existence of a glass phase. Finally, we discuss the experimental relevance of these results and compare our picture to similar scale-free avalanches observed in mean field spin glasses, in which they are associated to a marginal glass phase.

¹Work supported by the Ministerio de Ciencia e Innovación (FIS2009-13730-C02-01, AP2007-01005) and the Spanish Supercomputing Network (BSC-RES)

9:00AM Y53.00006 Cooperation-induced temporal complexity in networks of pulse-coupled units, ELVIS GENESTON, La Sierra University, PAOLO GRIGOLINI, University of North Texas — We study a network of stochastic pulse-coupled units generating bursts with the same size distribution as the neuronal avalanches in mature cultured neurons, recently revealed by the experimental observation. We prove that in addition to this form of complexity this model yields a form of phase transition generating also temporal complexity. This means that the distance from two consecutive bursts fits the prescription of a Mittag-Leffler (ML) function renewal theory. There exists a critical value of the cooperation parameter at which this description applies to the whole time regime. By increasing the cooperation parameter the ML theory breaks down and the sequence of bursts tend to become periodic with the same intensity. We make the conjecture that the analysis of this model may shed light into the theoretical foundation of neuronal burst leaders and that the recently discovered principle of complexity management may be conveniently applied to the neuro-physiological processes that are properly described by this model.

9:12AM Y53.00007 Time dependence of reprecipitation rates in heterogeneous media, DANIEL REEVES, DANIEL ROTHMAN, MIT — The analysis of spatial and temporal variations of the chemical and isotopic compositions of minerals in sedimentary systems provides a powerful tool for calculating dissolution and reprecipitation rates, and has previously been applied to find time-dependent rates in marine sediments. Dissolution and precipitation processes tend to shift the composition of the pore fluids toward that of the solid phase, and vice-versa. Current theory treats both the fluid and solid phases as well-mixed reservoirs, relying on mean-field theory that is inconsistent with the physical structure of the solid, as dissolution and precipitation occur only on the reactive surface of the solid. We present a model that accounts for the heterogeneity of the solid phase by adding and removing material only at the reactive surface. We therefore model the location of the surface with a 1-D random walk, in which the buried bulk of the solid phase can only be modified through repeated dissolution events. We approximate this physical scenario with a three-reservoir kinetic model and more detailed numerical simulations. We develop an understanding of two power-law scaling regimes, the second of which demonstrates 1/time aging in the rate constant, similar to those observed in marine sediment studies.

9:24AM Y53.00008 Properties of compacton-anticompacton collisions, BOGDAN MIHAILA, Los Alamos National Laboratory, ANDRES CARDENAS, New York University, FRED COOPER, ANDRÉS SAXENA, Los Alamos National Laboratory — We study the properties of compacton-anticompacton collision processes. We compare and contrast results for the case of compacton-anticompacton solutions of the $K(l,p)$ Rosenau-Hyman (RH) equation for $l=p=2$, with compacton-anticompacton solutions of the $L(l,p)$ Cooper-Shepard-Sodano (CSS) equation for $p=1$ and $l=3$. This study is performed using a Padé discretization of the RH and CSS equations. We find a significant difference in the behavior of compacton-anticompacton scattering. For the CSS equation, the scattering can be interpreted as “annihilation” as the wake left behind dissolves over time. In the RH equation, the numerical evidence is that multiple shocks form after the collision, which eventually lead to “blowup” of the resulting wave form.

9:36AM Y53.00009 Cardiac arrhythmias and degradation into chaotic behavior prevention using feedback control¹, ILIJA UZELAC, VENIAMIN SIDOROV, Vanderbilt University, Nashville TN, USA, MARC HOLCOMB, Hampden-Sydney College, Hampden-Sydney, VA, USA, JOHN WIKSWO, Vanderbilt University, Nashville TN, USA, RICHARD GRAY, Food and Drug Administration, MD, USA — During normal heart rhythm, cardiac cells behave as a set of oscillators with a distribution of phases but with the same frequency. The heart as a dynamical system in a phase space representation can be modeled as a set of oscillators that have closed overlapping orbits with the same period. These orbits are not stable and in the case of disruption of the cardiac rhythm, such as due to premature beats, the system will have a tendency to leave its periodic unstable orbits. If these orbits become attracted to phase singularities, their disruption may lead to chaotic behavior, which appears as a life-threatening ventricular fibrillation. By using closed-loop feedback in the form of an adjustable defibrillation shock, any drift from orbits corresponding to the normal rhythm can be corrected by forcing the system to maintain its orbits. The delay through the feedback network coincides with the period of normal heart beats. To implement this approach we developed a 1 kW arbitrary waveform voltage-to-current converter with a 1 kHz bandwidth driven by a photodiode system that records an optical electrocardiogram and provides a feedback signal in real time. Our goal is to determine whether our novel method to defibrillate the heart will require much lower energies than are currently utilized in single shock defibrillators.

¹Supported in part by NIH R01 HL58241-11 through ARRA 2009

9:48AM Y53.00010 Experiments on oscillator ensemble with global nonlinear coupling, MICHAEL ROSENBLUM, Potsdam University, AMIRKHAN TEMIRBAYEV, ZEINULLA ZHANABAEV, STANISLAV TARASOV, Kazakh National University, VLADIMIR PONOMARENKO, Institute of RadioEngineering and Electronics of Russian Academy of Sciences, Saratov Department — We experimentally analyze collective dynamics of a population of 20 electronic Wien-bridge limit-cycle oscillators with a linear or nonlinear phase-shifting unit in the global feedback loop. With linear unit we observe, with increase of the coupling strength, a standard Kuramoto-like transition to a fully synchronous state; the threshold of the transition depends on the phase shift. In case of nonlinear global coupling we first observe a transition to a state when approximately half of the population forms a synchronous cluster. With further increase of the coupling strength we observe destruction of this cluster and formation of a self-organized quasiperiodic state, predicted in [M. Rosenblum and A. Pikovsky, PRL, 98, 064101 (2007)]. In this state, frequencies of all oscillators are smaller than the frequency of the mean field, so that the oscillators are not locked to the mean field they create and their dynamics is quasiperiodic. The transition is characterized by a non-monotonic dependence of the order parameter on the coupling strength. We demonstrate a good correspondence between theory and experiment.

10:00AM Y53.00011 Dynamics of Confident Voting, DANIEL VOLOVIK, SIDNEY REDNER, Boston University — In the classical voter model, a voter has no intrinsic confidence in its current opinion. We introduce the confident voter model in which each voter can be in one of two opinions, and can additionally have two levels of commitment to an opinion — confident and vacillating. Upon interacting with an agent of a different opinion, a confident voter becomes less committed, or vacillating, but does not immediately change opinion. However, a vacillating agent changes opinion upon interacting with an agent of a different opinion. In the mean-field limit, a population of size N is quickly driven to a mixed state before consensus is eventually achieved in a time of order $\ln N$. In two dimensions, the distribution of consensus times is characterized by two distinct times — one that scales linearly with N and another that scales as $N^{3/2}$. The longer time arises from configurations that fall into long-lived stripe states, which are caused by an effective surface tension between domains of different opinion states, before consensus is finally reached.

10:12AM Y53.00012 Nonuniversal Effects in Mixing Correlation-Growth Processes with Randomness, ALICE KOLAKOWSKA, Valdosta State University, GA — In mixed-growth dynamical process $P = Y \vee X$ there are two dynamical processes: Y (in one universality class) and X (in another universality class). They *alternate* with each other: "*exclusively either Y (is active with probability q) or X (is active with probability p), $p + q = 1$.* When P models surface growth via deposition/desorption/adsorption with X building universal correlations and Y representing randomness (e. g., thermal effects), in order to correctly construct a continuum growth equation for P a distinction must be made *within a single universality class* of X between processes that do and do not create voids in the bulk of deposited material. Then, model-dependent prefactors in universal scaling of the surface roughness can be linked with the bulk morphology and determined from the bulk structures. This connection is essential to finding correct dynamical scaling and to interpretation of scaling laws for mixed-growth dynamical processes.

10:24AM Y53.00013 Non-equilibrium modulated phases in a system with local energy input¹, LINJUN LI, MICHEL PLEIMLING, Virginia Tech — The equilibrium phase diagram of the two-dimensional Ising model in contact with a single heat bath is well understood. We here study the properties of the two-dimensional Ising model with conserved dynamics where the two halves of the system are in contact with different heat baths. Using Monte Carlo simulations, we identify three different phases for this non-equilibrium system, as a function of the aspect ratio of the lattice and of the temperatures. The first phase is characterized by the complete disorder of the particles, while the second phase is characterized by the complete order of the particles. The third phase is the most interesting one as it displays stripes with widths that depend on the system parameters. The full phase diagram of our non-equilibrium system is determined through the study of the structure factor.

¹Supported in part by the US National Science Foundation through Grant DMR-0904999.

10:36AM Y53.00014 Nonequilibrium relaxation and critical aging for driven Ising lattice gases¹, GEORGE DAQUILA, UWE C. TAUBER, Department of Physics, Virginia Tech — We employ Monte Carlo simulations to study the non-equilibrium relaxation of driven Ising lattice gases in two dimensions. Whereas the temporal scaling of the density auto-correlation function in the non-equilibrium steady state does not allow a precise measurement of the critical exponents, these can be accurately determined from the aging scaling of the two-time auto-correlations and the order parameter evolution following a quench to the critical point. We obtain excellent agreement with renormalization group predictions based on the standard Langevin representation of driven Ising lattice gases, valid to all orders in the dimensional expansion.

¹Research supported by DOE-BES, Grant No. DE-FG02-09ER46613.

Friday, March 2, 2012 11:15AM - 1:51PM –
Session Z1 DAMOP: General Atomic, Molecular and Optical Physics 203

11:15AM Z1.00001 The Timing of Sonoluminescence¹, THOMAS BRENNAN, West Virginia Weleyn College, GUSTAVE FRALICK, NASA Glenn Research Center — We measured the timing of the sonoluminescence flash by scattering laser light from the bubble. We performed this measurement on 17.8 kHz, 13.28 kHz and 7920 Hz systems and found that the flash typically occurs 100 nanoseconds before the minimum radius, contrary to previous claims that the flash always occurs within a nanosecond of the minimum radius. These results are important because they imply that previous *hot* models of sonoluminescence are wrong. We propose a new model: that the flash results from the discharge of an excited cold condensate, formed during the adiabatic expansion of the bubble.

¹We thank the Instrumentation Division at the NASA Glenn research center in Cleveland, Ohio for supproting this research.

11:27AM Z1.00002 Coherence Enhanced Transient Lasing, PANKAJ JHA, ANATOLY SVIDZINSKY, Texas A&M University, MARLAN SCULLY, Texas A&M University and Princeton University — We study the effect of a coherent drive on transient lasing with inversion in three-level Λ and Ξ configurations ($c \leftrightarrow a \leftrightarrow b$). We show that the presence of a resonant coherent drive on the $a \leftrightarrow c$ optical transition can yield substantial enhancement of the output laser energy on a $a \rightarrow b$ XUV or X-ray transition. We demonstrate the crucial role of coherence ϱ_{ac} for this laser power enhancement. Contrary to the forward direction, where forward gain can be enhanced for some choice of Ω_c , coherent drive on the ac transition always suppresses the backward gain. Thus, the use of a coherent drive at optical frequency could be a useful tool for increasing power of lasers in XUV and X-ray regions.

11:39AM Z1.00003 Variable Atomic Radius of Hydrogen Due to Vibrating Nucleus, STEWART BREKKE, Northeastern Illinois University (former grad student) — The H-atomic radius is variable because the H-nucleus is vibrating and the electric force field upon the electron is repeatedly changing due to the changing distance from the positive nucleus to the negatively charged electron. If the the distance from the nucleus to the electron is $d = r + A \cos 2\pi f t$ where $r = 5.29 \times 10^{-11} m$, the calculated Bohr radius, and $d = 2.5 \times 10^{-11} m$, the measured atomic radius of the H-atom, then the equation for the variable atomic radius of the H-atom is $5.29 \times 10^{-11} m + A \cos 2\pi f t = 2.5 \times 10^{-11} m$. If the RMS value for the average cosine is 0.707, solving for A, the average amplitude of nuclear vibration, $A = 3.95 \times 10^{-11} m$. Therefore, the oscillating orbit of the electron in an H-atom has an average amplitude of $A = 3.95 \times 10^{-11}$.

11:51AM Z1.00004 Strong Field Control of Atomic and Molecular Dynamics: An Attosecond Resolved Study, NIRANJAN SHIVARAM, HENRY TIMMERS, University of Arizona, XIAO-MIN TONG, University of Tsukuba, ARVINDER SANDHU, University of Arizona — Strong laser fields are routinely used in attosecond pump-probe studies of atomic and molecular phenomena. However, even a moderately strong field ($\sim 10^{12}$ W/cm²) can significantly alter the electronic structure. By understanding and quantifying the effect of strong fields, one can obtain a high degree of control over the photo-absorption and photo-fragmentation processes. Here, we study the atomic and molecular response to the simultaneous presence of XUV attosecond pulse trains and strong IR fields. We describe an IR laser-dressed atom using Floquet picture. We observe quantum interference between XUV excitation paths to the Fourier components of a given Floquet state, which leads to oscillations in the ion-yield. By measuring the phase of the ion-yield oscillations, we extract the quantum phase difference between the Fourier components of that Floquet state. We obtain a quantitative understanding of how Floquet ionization channels change with intensity and what is the phase associated with each channel. We also extend our studies to molecular fragmentation processes. Our work represents real-time measurement and control of dynamics using strong-field modification of the atomic and molecular structure. This work was support by NSF grant PHY-0955274.

12:03PM Z1.00005 Steady State Ab Initio Laser Theory: Generalizations, ALEXANDER CERJAN, YIDONG CHONG, Yale University, LI GE, Princeton University, A. DOUGLAS STONE, Yale University — We show that Steady-state Ab initio Laser Theory (SALT)¹ can be generalized to find the stationary multimode lasing properties of gain systems with N levels, and to include carrier diffusion. The former result is achieved by mapping the N -level rate equations to an effective two-level inversion equation of the type typically quoted in the Maxwell-Bloch equations.² The latter result is found by rewriting the SALT algorithm to non-linearly solve two coupled non-linear equations in the steady state, with one equation determining the modal field intensities, given the inversion and the other equation determining the inversion given the field intensities. In both cases we find excellent agreement with more computationally demanding Finite-Difference Time-Domain (FDTD) simulations for the steady state. These results generalize the SALT algorithm to handle more realistic lasing systems, including semiconductor lasers.

¹L. Ge, Y. D. Chong, and A. D. Stone, Phys. Rev. A **82**, 063824 (2010).

²A. Cerjan, Y. D. Chong, L. Ge, and A. D. Stone, Opt. Express *in press*, arXiv: 1111.2279v1 [physics.optics]

12:15PM Z1.00006 Dynamical mean-field theory for transition metal dioxide molecules¹, NAN LIN, DOMINIKA ZGID, Columbia University, Department of Physics, CHRIS MARIANETTI, Columbia University, Department of Applied Physics, DAVID REICHMAN, Columbia University, Department of Chemistry, ANDREW MILLIS, Columbia University, Department of Physics — The utility of the dynamical mean-field approximation in quantum chemistry is investigated in the context of transition metal dioxide molecules including TiO_2 and CrO_2 . The choice of correlated orbitals and correlations to treat dynamically is discussed. The dynamical mean field solutions are compared to state of the art quantum chemical calculations. The dynamical mean-field method is found to capture about 50% of the total correlation energy, and to produce very good results for the d-level occupancies and magnetic moments. We also present the excitation spectrum in these molecules which is inaccessible in many wave-function based methods. Conceptual and technical difficulties will be outlined and discussed.

¹This work was supported by the CMCSN program of the US Department of energy.

12:27PM Z1.00007 Disalignment of the $Ne^*(2p_{10} [J=1])$ atoms induced by Helium atom collisions from 10K to 3000K, CRISTIAN BAHRIM, Department of Physics, Lamar University, VAIBHAV KHADILKAR, Department of Computer Science, UT Dallas — Quantum close-coupling many-channel calculations using the new model potential for the interaction between $Ne^*(2p_i [J=1])$ and He atoms proposed in [1] are performed in order to analyze the depolarization of $Ne^*(2p_i [J=1])$ atoms in a gaseous mixture at thermal equilibrium. For temperatures above 77 K we successfully explain measurements of disalignment done with a laser-induced fluorescence spectroscopy method and destruction of alignment using a technique based on the Hanle effect for all four $2p_i [J=1]$ states of the $2p^5 3p$ configuration of neon [1, 2]. Our interpretation of the experimental data is based on the anisotropy between collisional channels which asymptotically converge toward the same $2p_i [J=1]$ state [2]. Below 77 K our disalignment rate coefficients for the $Ne^*(2p_{10} [J=1])$ atoms are much larger than the experimental data [3] after the radiation re-absorption is subtracted from the disalignment rates. The calculations indicate that for the $2p_{10}$ state, at low collision energies, the nuclear rotation has a strong influence in the overall long-range interaction, while the experimental data suggests that below 16 meV, the intramultiplet transitions within the $(2p_i [J=1])$ state of neon are completely negligible. The discrepancy between theory and experiment is carefully analyzed.

[1] Bahrim C and Khadilkar V 2009 *Phys Rev A* **79** 042715.

[2] Khadilkar V and Bahrim C 2010 *J Phys B* **43**235209.

[3] Matsukuma H, Shikama T, and Hasuo M 2011 *J Phys B* **44** 075206.

12:39PM Z1.00008 Cold collisions of complex polyatomic molecules, ZHIYING LI, ERIC HELLER, Department of Physics, Harvard University — We introduce a method for classical trajectory calculations to simulate collisions between atoms and large rigid asymmetric-top molecules. Using this method, we investigate the formation of molecule-helium complexes in buffer-gas cooling experiments at the temperature of 6.5 K for molecules as large as naphthalene. Our calculations show that the mean lifetime of the quasi-bound collision complex is not long enough for the formation of stable clusters under the experimental conditions. Our results suggest that it may be possible to improve the efficiency of the production of cold molecules in buffer-gas cooling experiments by increasing the density of helium. In addition, we find that the shape of molecules is important for the collision dynamics where molecular vibrational motions are frozen. For some molecules, it is even more crucial than the number of accessible degrees of freedom. This indicates that by selecting molecules with suitable shape for buffer-gas cooling, one could cool molecules with a very large number of degrees of freedom.

12:51PM Z1.00009 Spin-boson models for periodic N -site systems, VICTOR V. ALBERT, Department of Physics, Yale University — The single/multi-mode spin-boson model provides a description for numerous two-level exciton-phonon and atom-cavity systems. Existing many-level extensions conserve symmetries but quickly become intractable due to the inclusion of multiple interacting modes. Other ad-hoc single-mode extensions contain arbitrary numbers of parameters and often ignore the symmetries of their respective systems. This work presents a simple model for the interaction of a periodic system of N coupled sites with one or more non-interacting boson modes using a minimal number of parameters [1]. A group theoretic approach allows one to partially diagonalize the Hamiltonian, providing numerical advantages, physical insight, and a gateway to accurate approximations. The single-mode two-site system reduces to the single-mode spin-boson model, also known as the Rabi Hamiltonian. Two higher dimensional generalizations are reviewed in the exciton-phonon/atom-field interpretations and related to a new integrability criterion [2]. The model predicts that $2N$ -level systems have parity symmetry and that the ground state of certain four-level atom-cavity systems will undergo parity change at large coupling.

[1] V. V. Albert, arXiv:1112.0849

[2] D. Braak, PRL **107**, 100401 (2011)

1:03PM Z1.00010 Thermal Effects on Quantum Sticking¹, YANTING ZHANG, DENNIS CLOUGHERTY, University of Vermont — Many-body effects on the threshold law of quantum sticking of a particle coupled to an ohmic bosonic bath are examined for finite temperature surfaces. Generalizing a variational mean-field method² previously applied to zero temperature surfaces, we obtain an explicit expression for the sticking probability of a particle with incident energy E . We find that there is a critical particle energy below which the probability of its sticking to the surface discontinuously drops to zero. We show that this singularity, whose origin is rooted by analogy to the localization transition in the spin-boson model, is experimentally accessible for ultracold particles. We provide detailed numerical results for this effect.

¹We gratefully acknowledge support by the National Science Foundation under DMR-0814377.

²Y. Zhang and D.P. Clougherty, arXiv:1012.4405

1:15PM Z1.00011 Theory of Non-Markovian dynamics in resonance fluorescence spectra, ABHISHEK KUMAR, SIGURDUR I. ERLINGSSON, School of Science and Engineering, Reykjavik University, Iceland, BILL COISH, Department of Physics, McGill University, Canada — Robust quantum coherence is an important prerequisite for any system that may be used to perform quantum information processing tasks. For systems that can be probed optically, the resonance fluorescence spectrum may provide indirect evidence of coherence times when supplemented with an appropriate model of the decay process. A common approach is to assume a Markovian system, resulting in exponential decay of correlation functions and Lorentzian features in the associated spectrum. For physical systems with strongly history-dependent (non-Markovian) dynamics, there is currently no satisfying systematic theoretical approach to establish the associated spectrum. We present a detailed theoretical method to obtain the resonance fluorescence spectrum for a general system undergoing non-Markovian dynamics. This procedure can be used to systematically account for features in resonance-fluorescence spectra due to genuine non-Markovian dynamics. Our approach is based on a Nakajima-Zwanzig generalised master equation for the dynamics of the reduced density matrix. We apply this theory to study the resonance fluorescence in the non-Markovian dynamics of a three level lambda system, relevant to recent experiments on heavy-hole spin dynamics in a quantum dot.

1:27PM Z1.00012 Quantum Revivals of the Morse Oscillator in Position Space and Momentum Space, ALVASON ZHENHUA LI, Microelectronics and Photonics Program, University of Arkansas at Fayetteville, AR 72701, WILLIAM HARTER, Department of Physics, University of Arkansas at Fayetteville, AR 72701 — Analytical solutions for the Morse oscillator are applied to investigate the quantum revivals both in position and momentum spaces. The properties of this anharmonic oscillator came across interesting space-time phenomena. These findings include simple Farey arithmetic revival structures. Such dynamic systems may have applications for quantum information technology and quantum computing.

1:39PM Z1.00013 Trapping of particles in the ray optics regime using DNG materials, JOSEPH SHAHBAZIAN, Tufts University — Optical tweezers use to confine and manipulate microscopic objects including living cells and bacteria, with high accuracy. The objective is calibrating the force on targets using DPS-DNG layered structure. Using this layered structure which acts as a tunable optical band-pass filter would assist calibration of the force on the target(s). Here shown that the proposed DNG-DPS structure would help to have highly focused calibrated tweezers without worrying about the polarization of optical wave. Calculation can describe well the experimental results.

Friday, March 2, 2012 11:15AM - 2:15PM –

Session Z2 DCMP DBIO: Invited Session: Active Responses of Biological Materials to Mechanical Stress 204AB

11:15AM Z2.00001 Cellular Mechanics and Mechanotransduction, DANIEL FLETCHER, University of California at Berkeley — No abstract available.

11:51AM Z2.00002 Force Transmission in the Actin Cytoskeleton, MARGARET GARDEL, U. Chicago — The ability of cells to sense and generate mechanical forces is essential to numerous aspects of their physiology, including adhesion, migration, division and differentiation. To a large degree, cellular tension is regulated by the transmission of myosin II-generated forces through the filamentous actin (F-actin) cytoskeleton. While transmission of myosin-generated stresses from the molecular to cellular length scale is well understood in the context of highly organized sarcomeres found in striated muscle, non-muscle and smooth muscle cells contain a wide variety of bundles and networks lacking sarcomeric organization. I will describe the *in vitro* and *in vivo* approaches we use to study force transmission in such disordered actomyosin assemblies. Our *in vivo* results are showing that highly organized stress fibers contribute surprisingly little to the overall extent of cellular tension as compared to disordered actomyosin meshworks. Our *in vitro* results are demonstrating the mechanisms of symmetry breaking in disordered actomyosin bundles that facilitate the formation of contractile bundles with well-defined “contractile elements.” These results provide insight into the self-organization of actomyosin cytoskeleton in non-muscle cells that regulate and maintain cellular tension.

12:27PM Z2.00003 Environmental properties set cell mechanics and morphology, PAUL JANMEY, University of Pennsylvania — Many cell types are sensitive to mechanical signals that are produced either by application of exogenous force to their surfaces, or by the resistance that their surroundings place on forces generated by the cells themselves. Cell morphology, motility, proliferation, and protein expression all change in response to substrate stiffness. Changing the elastic moduli of substrates alters the formation of focal adhesions, the assembly of actin filaments into bundles, and the stability of intermediate filaments. The range of stiffness over which different primary cell types respond can vary over a wide range and generally reflects the elastic modulus of the tissue from which these cells were isolated. Mechanosensing depends on the type of adhesion receptor by which the cell binds, and therefore on both the molecular composition of the extracellular matrix and the nature of its link to the cytoskeleton. Many cell types can alter their own stiffness to match that of the substrate to which they adhere. The maximal elastic modulus that cells such as fibroblasts can attain is similar to that of crosslinked actin networks at the concentrations in the cell cortex. The precise mechanisms of mechanosensing are not well defined, but they presumably require an elastic connection between cell and substrate, mediated by transmembrane proteins. The viscoelastic properties of different extracellular matrices and cytoskeletal elements strongly influence the response of cells to mechanical signals, and the unusual non-linear elasticity of many biopolymer gels, characterized by strain-stiffening, leads to novel mechanisms by which cells alter their stiffness by engagement of molecular motors that produce internal stresses. Cell cortical elasticity is dominated by cytoskeletal polymer networks and can be modulated by internal tension. Simultaneous control of substrate stiffness and adhesive patterns suggests that stiffness sensing occurs on a length scale much larger than single molecular linkages and that the time needed for mechanosensing is on the order of a few seconds.

1:03PM Z2.00004 Molecular Mechanotransduction: how forces trigger cytoskeletal dynamics¹, ALLEN EHRLICHER, Harvard University — Mechanical stresses elicit cellular reactions mediated by chemical signals. Defective responses to forces underlie human medical disorders, such as cardiac failure and pulmonary injury. Despite detailed knowledge of the cytoskeleton's structure, the specific molecular switches that convert mechanical stimuli into chemical signals have remained elusive. Here we identify the actin-binding protein, filamin A (FLNa) as a central mechanotransduction element of the cytoskeleton by using Fluorescence Loss After photoConversion (FLAC), a novel high-speed alternative to FRAP. We reconstituted a minimal system consisting of actin filaments, FLNa and two FLNa-binding partners: the cytoplasmic tail of β -integrin, and FilGAP. Integrins form an essential mechanical linkage between extracellular and intracellular environments, with β integrin tails connecting to the actin cytoskeleton by binding directly to filamin. FilGAP is a FLNa-binding GTPase-activating protein specific for Rac, which in vivo regulates cell spreading and bleb formation. We demonstrate that both externally-imposed bulk shear and myosin II driven forces differentially regulate the binding of integrin and FilGAP to FLNa. Consistent with structural predictions, strain increases β -integrin binding to FLNa, whereas it causes FilGAP to dissociate from FLNa, providing a direct and specific molecular basis for cellular mechanotransduction. These results identify the first molecular mechanotransduction element within the actin cytoskeleton, revealing that mechanical strain of key proteins regulates the binding of signaling molecules. Moreover, GAP activity has been shown to switch cell movement from mesenchymal to amoeboid motility, suggesting that mechanical forces directly impact the invasiveness of cancer.

¹This work was supported by grants NIH R01 HL19429 (T.P.S.) and NIH T32 HL07680 (A.J.E.) and by the Harvard University Science and Engineering Committee Seed Fund for Interdisciplinary Science (D.A.W., T.P.S., F.N.).

1:39PM Z2.00005 The physics of 3D cell migration, DENIS WIRTZ, Johns Hopkins — No abstract available.

Friday, March 2, 2012 11:15AM - 2:15PM –
Session Z3 DCMP DCOMP: Invited Session: Frontiers of Non-Equilibrium Transport Theories
205AB

11:15AM Z3.00001 DFT treatment of transport through Anderson junction: exact results and approximations¹, KIERON BURKE, Departments of physics and chemistry, University of California, Irvine — Since the pioneering break-junction experiments of Reed and Tour measuring the conductance of dithiolated benzene between gold leads, many researchers in physics and chemistry have been calculating conductance for such systems using density functional theory (DFT). Off resonance, the predicted current is often 10-100 times larger than that measured. This error is often ascribed to the application of ground-state DFT to a non-equilibrium problem. I will argue that, in fact, this is largely due to errors in the density functional approximations in popular use, rather than necessarily errors in the methodology. A stark illustration of this principle is the ability of DFT to reproduce the exact transmission through an Anderson junction at zero-temperature and weak bias, including the Kondo plateau, but only if the exact ground-state density functional is used. In fact, this case can be used to reverse-engineer the exact functional for this problem. Popular approximations can also be tested, including both smooth and discontinuous functionals of the density, as well as symmetry-broken approaches.

- [1] Kondo effect given exactly by density functional theory, J. P. Bergfield, Z. Liu, K. Burke, and C. A. Stafford, arXiv:1106.3104;
- [2] Broadening of the Derivative Discontinuity in Density Functional Theory, F. Evers, and P. Schmitteckert, arXiv:1106.3658;
- [3] DFT-based transport calculations, Friedel's sum rule and the Kondo effect, P. Tröster, P. Schmitteckert, and F. Evers, arXiv:1106.3669;
- [4] Towards a description of the Kondo effect using time-dependent density functional theory, G. Stefanucci, and S. Kurth, arXiv:1106.3728.

¹This work is funded by the U.S. Department of Energy (Grant No. DE-FG02-08ER46496).

11:51AM Z3.00002 Inelastic single-spin transport theory, STEFANO SANVITO, School of Physics, Trinity College Dublin — Spin-flip inelastic spectroscopy is a powerful tool for investigating the magnetic excitations of nano-scale magnets deposited on a metallic surface. In this talk I will present a perturbative approach to the calculation of the inelastic spin-flip spectra of magnetic adatoms, small magnetic clusters and magnetic molecules. The theory is based on the non-equilibrium Green's function formalism combined with a model spin Hamiltonian, where the conduction electrons are exchanged coupled to a system of quantum spins. By expanding the self-energy describing the electron-spin interaction to the third order we are able to capture both inelastic spin-flip events and the signature of Kondo resonances. Furthermore, when our approach is combined with a Master equation describing spin-relaxation, effects related to the spin-pumping at the single spin level can be described. In the talk I will demonstrate that the method offers an extremely good quantitative agreement with published experimental data. Importantly the formalism is amenable to be implemented together with highly accurate electronic structure methods.

12:27PM Z3.00003 Electron correlation effects on the diode properties and the local heating, YOSHIHIRO ASAI, Nanosystem Research Institute (NRI) "RICS," National Institute of Advanced Industrial Science and Technology (AIST) — Single molecular bridge junctions and atomic wires provide one of the best test fields for non-equilibrium transport theories whose progress gives benefits over wide range of physics. Experimental progresses in inelastic tunneling spectroscopy (IETS) and break junction techniques have played very important roles to make this possible. Inelastic scatterings between electrons and phonons give "local heating" of the junctions. The effective temperature due to the local heating was discussed successfully in terms of a fully self-consistent theory treating energy dissipation processes as well as inelastic heat generation on equal footing [1]. Recently, we found two cases where electron correlation gives distinct changes. The first case was found in the local heating problem in the resonant systems, where phonon damping due to its coupling with electron-hole excitation is suppressed by the correlation. The suppression enhances heat release to electrodes leading to the effective temperature suppression [2]. Another example is the single molecular rectifier. First principle NEGF-GGA calculation fails to explain the large rectification ratio (RR) at high bias voltage. Separate GW calculation based on Keldysh Green's function gives clear enhancement of RR over the mean field NEGF results suggesting that RR could be enhanced by the electron correlation effect [3]. Thus latest non-equilibrium transport theories enable us to treat the important physical processes accompanying electric conduction allowing us to make more direct comparisons with experimental phenomena at nano-scale.

[1] Y. Asai, Phys. Rev. B78, 045434 (2008).

[2] Y. Asai, Phys. Rev. B84, 085436 (2011).

[3] Y. Asai, H. Nakamura, J. Hihath, C. Bruot, and N.J. Tao, Phys. Rev. B 84, 115436 (2011).

1:03PM Z3.00004 Electron-ion correlations in electromigration: Coulomb's law and Landauer transport at the nanoscale, KIRK BEVAN, McGill University — Electromigration has gained increased prominence in recent years, as the rise of nanoelectronics has given way to higher current and power densities in computing interconnects and devices. In this context we address the fundamental materials question: what drives electromigration at the nanoscale? Our understanding of the forces that drive electromigration has remained at an uneasy juncture between the mesoscopic semi-classical and atomistic quantum mechanical regimes. At the nanoscale an atomistic understanding of materials is required. Through first-principles quantum transport calculations we show that a self-consistent Landauer transport framework provides much needed atomistic insight into the fundamental Coulombic forces which drive both current flow and electromigration at the nanoscale. These insights provide a general timely overview of the importance of electromigration in modern nanoelectronic devices and materials, not only from an operational perspective but also from a novel materials design perspective.

1:39PM Z3.00005 Probing DNA in nanopores via tunneling: from sequencing to "quantum" analogies, MASSIMILIANO DI VENTRA, University of California, San Diego — Fast and low-cost DNA sequencing methods would revolutionize medicine: a person could have his/her full genome sequenced so that drugs could be tailored to his/her specific illnesses; doctors could know in advance patients' likelihood to develop a given ailment; cures to major diseases could be found faster [1]. However, this goal of "personalized medicine" is hampered today by the high cost and slow speed of DNA sequencing methods. In this talk, I will discuss the sequencing protocol we suggest which requires the measurement of the distributions of transverse currents during the translocation of single-stranded DNA into nanopores [2-5]. I will support our conclusions with a combination of molecular dynamics simulations coupled to quantum mechanical calculations of electrical current in experimentally realizable systems [2-5]. I will also discuss recent experiments that support these theoretical predictions. In addition, I will show how this relatively unexplored area of research at the interface between solids, liquids, and biomolecules at the nanometer length scale is a fertile ground to study quantum phenomena that have a classical counterpart, such as ionic quasi-particles, ionic "quantized" conductance [6,7] and Coulomb blockade [8]. Work supported in part by NIH.

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Friday, March 2, 2012 11:15AM - 2:03PM – Session Z4 DAMOP: Disorder and Pairing in Ultracold Systems 205C

11:15AM Z4.00001 Many Body Localization in Incommensurate Potentials, SHANKAR IYER, California Institute of Technology, DAVID HUSE, Princeton University, GIL REFAEL, California Institute of Technology — A long-standing problem concerns the survival of Anderson localization in a many body system with interparticle interactions. In recent years, this problem has resurfaced due to work by Basko, Aleiner, and Altshuler, who have argued that highly excited states of an interacting, many body system can be localized in Fock space. Consequently, a dynamical quantum phase transition may separate such a many body localized phase from a delocalized, ergodic phase, and there is now numerical evidence for the existence of such a transition in disordered 1D systems. Meanwhile, 1D lattice models that lack genuine disorder, but which instead contain a periodic potential that is incommensurate with the lattice spacing, are known to have a localization transition even in the absence of interactions. Here, we numerically investigate whether this transition survives the introduction of interactions and, if so, how it is modified. These questions are increasingly experimentally relevant, because ultracold atom experiments sometimes use incommensurate potentials in place of true disorder to probe localization physics.

11:27AM Z4.00002 Mobile impurities in one-dimensional cold gases: subdiffusive, diffusive and ballistic regimes, ADRIAN KANTIAN, THIERRY GIAMARCHI, University of Geneva — Advances in cold gases physics are beginning to enable experiments involving the direct manipulation and observation of single- or few-atom mobile impurities [1] within a many-body quantum system, a topic of longstanding interest for condensed matter theory, where it is related to studies of e.g. conductivity and the X-ray edge problem. Further progress in this direction is expected from the latest generation of experiments offering single-site addressability in optical lattices [2,3]. In light of these developments we study the dynamics of mobile impurities in 1D quantum liquids using a DMRG technique. We address the recently proposed subdiffusive regime of impurity motion [4], a class of excitations beyond those described by the standard Tomonaga-Luttinger theory. We study the conditions for observing this regime and its' crossover to the ballistic regime. We furthermore examine the possibilities to observe the intermediate diffusive motion of impurities in these systems.

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11:39AM Z4.00003 Collective mode of an impurity and a Tonks-Girardeau gas¹, CHARLES MATHY, Institute for Theoretical Atomic, Molecular and Optical Physics, MIKHAIL ZVONAREV, EUGENE DEMLER, Physics Department, Harvard University — We investigate the quantum dynamics of an impurity immersed in a one-dimensional gas of strongly repulsive bosons, or equivalently fully-polarized fermions, interacting via a contact interaction. Using Bethe Ansatz we obtain essentially exact results at all timescales and for all couplings to the impurity. We find at strong coupling that if the impurity starts off with a momentum of the order of the Fermi momentum or higher a new type of collective mode is excited, corresponding to long lived oscillations of the impurity with respect to the background gas. We characterize this mode and discuss how it can be observed experimentally.

¹C.M. acknowledges support from the NSF through ITAMP at Harvard University and the Smithsonian Astrophysical Observatory.

11:51AM Z4.00004 Dynamics of mobile impurities in one-dimensional quantum liquids¹, MICHAEL SCHECTER, University of Minnesota, School of Physics and Astronomy, ALEX KAMENEV, University of Minnesota, School of Physics and Astronomy and Fine Institute for Theoretical Physics, DIMITRI GANGARDT, University of Birmingham, United Kingdom, AUSTEN LAMACRAFT, University of Virginia — We consider the dynamics of mobile impurities immersed in one-dimensional (1d) quantum liquids. Such systems have been realized experimentally in the context of ultracold atomic gases in optical lattices. We show that, on very general grounds, the dispersion relation of the impurity dressed by the liquid is a periodic function of momentum with period $2\pi\hbar n$, n being the 1d density. An impurity subject to a small external force thus exhibits the phenomenon of Bloch oscillations about a fixed point in real space, in the absence of a periodic potential. To compare with experiments, we set out to address the consequences of both finite temperature and finite force on the Bloch oscillation sequence. Our main results are as follows: (i) There exists a finite window of parameters where Bloch oscillations exist $F_{\min}(T) < F < F_{\max}$ (ii) The lower bound is fixed by thermal friction depending on temperature T , and interaction parameters. In particular, we show that $F_{\min} = 0$ for integrable impurity models. (iii) The upper bound $F_{\max}$ is set by friction associated with dipole radiation of phonons due to the accelerating impurity. The ensuing energy loss results in the uniform drift of the oscillation center.

¹This work was supported by DOE contract DE-FG02-08ER46482

12:03PM Z4.00005 Gapless superfluid phase with spin-dependent disorder, MI JIANG, RAVINDRA NANGUNERI, Physics Department, UC Davis, NANDINI TRIVEDI, Department of Physics, Ohio State University, GEORGE BATROUNI, INLN, Université de Nice-Sophia Antipolis, CNRS, RICHARD SCALETTAR, Physics Department, UC Davis — Motivated by the recent experimental development on spin-dependent optical lattices and disordered lattices, we show that the presence of a spin-dependent random potential on a superconductor or a superfluid atomic gas leads to distinct transitions at which the energy gap and average order parameter vanish, generating an intermediate gapless superfluid phase. This behavior is in marked contrast to the case of spin-symmetric randomness. The calculations are performed for a two dimensional attractive Hubbard model within Bogoliubov-de Gennes mean field theory. We characterize the different phases by correlating the local order parameter and the density of states.

12:15PM Z4.00006 Superdiffusive nonequilibrium transport of an impurity in a Fermi sea, HYUNGWON KIM, DAVID HUSE, Princeton University — We discuss a nonequilibrium transport of a single impurity atom immersed in a low-temperature Fermi sea with a short range interaction. We find that the impurity does a superdiffusive geometric random walk in which the characteristic momentum decay rate shows a quartic decrease in its momentum in three dimension. Then, we construct a master equation and its scaled form that governs the time evolution of the impurity. Next, we discuss two dimensional case in which the momentum decay rate decreases with the third power of its momentum.

12:27PM Z4.00007 Repulsive polarons in two-dimensional Fermi gases, VUDTIWAT NGAMPRIETIKORN, JESPER LEVINSSEN, University of Cambridge, MEERA PARISH, London Centre for Nanotechnology — We consider a single spin-down impurity atom interacting via an attractive, short-range potential with a spin-up Fermi sea in two dimensions (2D). Similarly to 3D, we show that the impurity can form a metastable state (the “repulsive polaron”) with energy greater than that of the non-interacting impurity. Moreover, we find that the repulsive polaron can acquire a finite momentum for sufficiently weak attractive interactions. Even though the energy of the repulsive polaron can become sizeable, we argue that saturated ferromagnetism is unfavorable in 2D because of the polaron’s finite lifetime and small quasiparticle weight.

12:39PM Z4.00008 Universal bound states of two atoms near a Feshbach resonance¹, SHINA TAN, Georgia Institute of Technology — The Efimov effect was traditionally thought to exist for three or more particles only. It will be shown how to make universal shallow bound states of TWO atoms only, which will exhibit a universal energy spectrum reminiscent of the Efimov effect, by using potentials to constrain the spatial motion of atoms. Several related types of such two-body states will be described. These diatomic “artificial molecules”, if isolated from each other, will be free from three-body recombination, and can have long lifetimes in principle.

¹ Alfred P. Sloan Foundation; National Science Foundation

12:51PM Z4.00009 Feshbach Correlations and Closed Channel Amplitudes, NICOLAS LOPEZ, SHAN-WEN TSAI, UC Riverside, EDDY TIMMERMAN, Los Alamos National Lab — The magnetically controlled Feshbach resonance is a prominent member of the cold atom toolkit. The ability to tune binary particle interactions in a quantum many body system has given access to collapsing BEC-physics in boson gases, to BEC-BCS crossover physics, to the unitarity regime, and to quantum phase transitions. The resonance is accessed by tuning the energy of a quasi-bound spin-rearranged molecular state near the vacuum of the interacting particles. Does the amplitude of the spin-rearranged or “closed channel” state play a significant role in the many body physics? We present a microscopic derivation of the Feshbach resonance interactions and obtain the parameters of the two-channel model in an optical lattice. We study two atoms interacting in a harmonic oscillator potential near a Feshbach resonance to derive the closed channel probability and to uncover the validity-range of the two channel lattice model.

1:03PM Z4.00010 Superfluid pairing in a mixture of a spin-polarized Fermi gas and a dipolar condensate¹, BEN KAIN, Department of Physics, College of the Holy Cross, Worcester, MA 01610, HONG LING, Department of Physics, Rowan University, Glassboro, NJ 08028 — We consider a mixture of a spin-polarized Fermi gas and a dipolar Bose-Einstein condensate in which s-wave scattering between fermions and the quasiparticles of the dipolar condensate can result in an effective attractive Fermi-Fermi interaction anisotropic in nature and tunable by the dipolar interaction. We show that such an interaction can significantly increase the prospect of realizing a superfluid with a gap parameter characterized by a coherent superposition of all odd partial waves. We formulate, in the spirit of the Hartree-Fock-Bogoliubov mean-field approach, a theory which allows us to estimate the critical temperature when the anisotropic Fock potential is taken into consideration and study how to prepare the mixture in order to optimize the critical temperature at which such a superfluid emerges before the system starts to phase separate.

¹This work is supported by the US National Science Foundation and the US Army Research Office

1:15PM Z4.00011 Superfluid transition temperature and its zero density limit extrapolation in a unitary atomic Fermi gas on a lattice¹, QIJIN CHEN, Zhejiang University — The superfluid transition temperature T_c of a unitary Fermi gas has been of great interest. One way to study T_c in a 3D continuum is to study fermions on a lattice at finite densities and then extrapolate to the zero density limit, as has been done in quantum Monte Carlo (QMC) simulation studies. For this extrapolation to work, it is essential to probe the densities in the asymptotic regime. In this talk, we study fermions on a three-dimensional isotropic lattice with an attractive on-site interaction as a function of density n , from half filling down to 5.0×10^{-7} per unit cell, using a pairing fluctuation theory. As n decreases towards $n = 0$, T_c/E_F increases to the leading order linearly in $n^{1/3}$, and reaches the zero density limit $T_c/E_F = 0.256$, consistent with that calculated directly in the continuum for a contact potential. Inclusion of the particle-hole channel reduces T_c/E_F to 0.217, in agreement with experiment. However, except for very low n , T_c/E_F exhibits significant higher order nonlinear dependence on $n^{1/3}$. The densities accessed by QMC studies are still not low enough to be in the asymptotic regime. References: Q.J. Chen, arXiv:1109.5327; arXiv:1109.2307; Q.J. Chen et al, PRL 81, 4708(1998); PRB 59, 7083(1999).

¹Supported by NSF, MOE and MOST of China

1:27PM Z4.00012 Pair Condensation in a Finite Trapped Fermi Gas¹, CHRISTOPHER GILBRETH, YORAM ALHASSID, Center for Theoretical Physics, Yale University — Cold atomic fermi gases are widely studied examples of strongly interacting quantum systems. Examples include ^4K , ^6Li and neutron matter. In the unitary regime, where the scattering length is very large compared to the mean inter-particle distance, they are nonperturbative and exhibit universal behavior. Moreover, they can be created in the lab, providing an excellent testing ground for theory. In this talk I will describe quantum Monte Carlo calculations we have been performing to study the signatures of pairing and the superfluid phase transition in finite-size systems. Using the Auxiliary Field Monte Carlo (AFMC) method, we study the pairing gap, condensate fraction, pair wavefunction and density profile as a function of temperature. Defining the onset of condensation T_{cond} as the temperature when the condensate fraction crosses its (finite) noninteracting limit, we consider the question of whether pairing occurs prior to condensation in the unitary regime.

¹Supported in part by the U.S. DOE grant No. DE-FG02-91ER40608, by facilities and staff of the Yale University Faculty of Arts and Sciences High Performance Computing Center, and by the NSF grant No. CNS 08-21132.

1:39PM Z4.00013 Cooling across the superfluid-normal interface of a unitary Fermi gas - an analogue of a dilution fridge?, ARIJEET PAL, DAVID HUSE, Princeton University — Phase separation between paired superfluid and partially polarized normal phases has been observed by various experimental groups around the world using resonantly-interacting spin-imbalanced, hyperfine states of fermionic atoms. In this work we phenomenologically study the effect of the evaporation of atoms and explore the possibility of realizing a non-equilibrium steady state with chemical potential and temperature gradients in some of these experiments.

1:51PM Z4.00014 Upper Branch Bosons at High Temperatures, WEIRAN LI, TIN-LUN HO, the Ohio State University — We use a generalized Nozieres-Schmitt-Rink (NSR) approach, which excludes the molecule poles in the T-matrix, to study the “upper branch” Bose gases at high temperatures. We show that when we tune the scattering length from positive side across the resonance, the Bose system can remain stable even with attractive interactions at relatively high temperatures. The energy of this upper branch Bose gas has a maximum at negative scattering length, which indicates pair formations are enhanced by Bose statistics in a many body system, in contrast to the Fermionic case where the maximum occurs at positive scattering length.¹

¹V.B.Shenoy and Tin-Lun Ho, arXiv:1106.0960, to appear in PRL.

Friday, March 2, 2012 11:15AM - 2:03PM –

Session Z5 DCMF: Synthesis, Transport, and Devices Based on Artificially Structured Materials
206A

11:15AM Z5.00001 Ultrasmall Silver Nanopores Fabricated by Femtosecond Laser Pulses¹, JIMIN ZHAO, F. BIAN, Y.C. TIAN, R. WANG, H.X. YANG, Institute of Physics, Chinese Academy of Sciences, HONGXING XU, Institute of Physics, CAS; Lund University, SHENG MENG, Institute of Physics, Chinese Academy of Sciences — Ultrasmall nanopores in silver thin films with a diameter of about 2 nm have been fabricated using femtosecond laser ablation in liquid [1]. Ultrafast laser pulse ablation generates highly nonequilibrium excited states, from which silver thin films emerge and progressively grow with the assistance of capping agent molecules. During this growth process, capping agent molecules are enclaves within the film, leaving individual ultrasmall pores in the thin film. Our first-principles calculations show that the pore size is critically determined by the dimension of the confined molecules. Furthermore, by using smaller capping agent molecules, we were able to fabricate smaller nanopores with 1.6nm diameter. Our approach advances the capability of optical methods in making nanoscale structures with potential applications in areas such as near-field aperture probes, imaging masks, magnetic plasmonic resonances, and biosensing with individual nanopores.

[1] F. Bian, Y. C. Tian, R. Wang, H. X. Yang, H. X. Xu, Sheng Meng, and Jimin Zhao, *Ultrasmall Silver Nanopores Fabricated by Femtosecond Laser Pulses*, Nano Lett. **11**, 3251–3257 (2011).

¹Financially supported by NSF of China, MOST of China, and CAS.

11:27AM Z5.00002 Effect of Li+3 Ion Irradiation on Properties of Ta and Dy Doped Bi_{1.5}Zn_{0.92}Nb_{1.5}O_{6.92} Pyrochlores, BILGEHAN YUMAK, Marmara University Department of Physics, MEHMET YUMAK, AY-HAN MERGEN, Marmara University Department of Metallurgical and Materials Eng, ANJUM QURESHI, Faculty of Engineering and Natural Sciences, Sabanci University — Pyrochlore compounds with a general formula of A₂B₂X₇ where A and B are B cations and X is anion exhibit a variety of interesting properties which allow for a broad range of applications, such as high-permittivity dielectrics, as cathode and electrolyte materials in solid electrolytes, host materials for the immobilization of fission products, catalysis, and thermal barrier coatings and fluorescence centers. Pyrochlore oxides can accommodate a wide range of solid solutions between BO₂ and A₂O₃ compounds. Radiation effects in a wide range of pyrochlore compositions have been extensively investigated due to the potential application of pyrochlores. In this study, Ta and Dy-doped Bi_{1.5}Zn_{0.92}Nb_{1.5}O_{6.92} (BZN) pyrochlore compounds were produced by mixed oxide technique. After determining the solubility limit of Ta and Dy in BZN by XRD, single phase Ta and Dy-doped BZN ceramics were irradiated with different fluences of Li³⁺ ion irradiation. The microstructures of sintered ceramics before and after irradiation were discovered by scanning electron microscopy. The effect of irradiation on dielectric properties at different frequencies and temperatures were also investigated.

11:39AM Z5.00003 Development of ZnO/Cu Nanolaminate Materials , SETH KING, LORALEE BILKE, JOSEPH KRUEGER, BENJAMIN OLESON, IAN SMITH, BENJAMIN STUROMSKI, University of Wisconsin - La Crosse — Promising materials to replace cost inhibitive indium-tin oxide as transparent conductive oxide layers are ZnO based alloys. Unlike In, Zn is cheap and abundant with a stable supply. Furthermore, ZnO is easily fabricated using standard industrial scale techniques. Therefore, the development of ZnO based materials may greatly advance modern electrical devices. The undoped bandgap of ZnO is 3.4 eV, and may be degenerately doped with donor species such as Al, B, or Ga. For pure ZnO, the electron mobility is ca. 200 cm²/V, but decreases significantly with doping due to impurity scattering. Recent studies have suggested that bilayers of doped ZnO and metal may offer low enough resistivity for industrial application. Therefore, it is a logical extension to investigate the properties of ZnO/metal nanolaminate films fabricated from multiple, thin, alternating layers of doped ZnO and a metal. We will present the preliminary results of the development of ZnO based nanolaminate materials consisting of alternating layers of ZnO and Cu fabricated by reactive DC sputter deposition. Our preliminary results suggest that these materials may have applications in photovoltaic devices as well as infrared mirrors.

11:51AM Z5.00004 Nano-structured Au surfaces by off-normal gas cluster ion beam technique , BUDDHI TILAKARATNE, DHARSHANA WIJESUNDERA, XUEMEI WANG, WEI-KÂN CHU, Department of Physics and Texas center for Superconductivity at University of Houston — Surface nano pattern formation has generated great interest in semiconductor, optoelectronics and bio-medical industries. For the past three decade cluster ion beam technology has developed significantly. A gas cluster ion consists thousands of atoms and usually energy per atom in the cluster is about 10eV and cluster ion surface penetration is minimum. Therefore, cluster ion impact form shallow depth modifications. When a cluster ion incident on to the surface off-normal beyond a certain angle from the normal surface target atoms gains forward momentum and creates clear surface nano-ripples between angles 40 to 60 degrees from surface normal. Even though many experiments have demonstrated cluster ion ripple formation, a mechanism of these formations has limited cluster ion beam industrial applications. We will discuss experimental results of surface evolution during the cluster ion off-normal incident irradiation and azimuthal sample rotation dependence of surface patterns, and compare results with a theoretical model.

12:03PM Z5.00005 Diamondoids enables 10nm resolution on X-ray PEEM , HITOSHI ISHIWATA, Stanford University, HENDRIK OHLDA, Stanford Synchrotron Radiation Laboratory, ANDREAS SCHOLL, Lawrence Berkeley National Laboratory, OLAV HELLWIG, Hitachi Global Storage Technologies, PETER SCHREINER, Justus-Liebig Universitaet, Institut fuer Organische Chemie, JEREMY DAHL, NICK MELOSH, Z.X. SHEN, Stanford University — Diamondoids are the smallest sp³ bonded carbon cage that can be found in different sizes and shapes, starting from single cage called adamantane that contain 10 carbons all hydrogen terminated on outside. While the electronic structure and material properties of diamondoids are based on bulk diamond, their nanostructure allows for tailoring their properties to a particular task. Diamondoids can be produced reliably and cost effective in different sizes and quantities. They exhibit a tremendous potential for real-world applications, e.g. as seed crystals in diamond growth, as robust mechanical coatings or as highly efficient electron cathodes. Here, we will focus on the latter, showing how diamondoid coating can be used to push the spatial resolution to the limit and significantly increasing the efficiency of an x-ray based cathode lens microscope (X-ray Photoemission Electron Microscope or XPEEM) by minimizing the effect of chromatic aberrations caused by the energy spread of the electrons emitted from the cathode. The unique feature of XPEEM microscopy is that it is capable of acquiring images with magnetic, chemical, structural as well as topographical contrast of surfaces and shallow interfaces. The capability to obtain such images with 10nm spatial resolution through simple, low-cost and readily available nanodiamond coating represents a major step forward towards real world application of these promising nano materials. (Presenting author: Z.X. Shen)

12:15PM Z5.00006 ABSTRACT HAS BEEN MOVED TO B17.00008 —

12:27PM Z5.00007 Quantum-Dot Cellular Automata On A Hydrogenated Silicon Surface: An Exact Diagonalization Study , BURKHARD RITTER, University of Alberta — Quantum-dot cellular automata (QCA) is an alternative computing paradigm for molecular-scale quantum devices. We present results from the first detailed exact diagonalization study of QCA systems using a richly extended Hubbard model. A controlled Hilbert space truncation alleviates the scaling problem and provides access to moderate system sizes. We characterize the static signal transmission for short wires and identify suitable material and system parameters for dangling bonds on a hydrogen-terminated silicon surface, a recent experimental realization. We discuss the challenges for a realistic, working implementation.

12:39PM Z5.00008 The chemical analysis about post annealing effect of HfO₂ on Si-passivated GaAs , SANG HAN PARK, HYO JIN KIM, DAE-KYONG KIM, MANN-HO CHO, Yonsei Univ., Sinchon-dong, Seodaemun-gu, Seoul, Korea, CHUNG YI KIM, LG Institute, Umyeong-dong, Seocho-gu, Seoul, Korea, HYOUNGSUB KIM, Sungkyunkwan Univ. Natural Sciences Campus, Cheoncheon-dong, Jangan-gu, Suwon-si, Gyeonggi-do, Korea — In order to develop a high performance MOS device, 3-5 based semiconductors as a high carrier transport semiconductors have been seriously considered. Especially, GaAs with HfO₂ as gate dielectric material attract as a candidate for future MOS FET device. Since, larger trap density at HfO₂/GaAs interface than for HfO₂/Si interface degrade device performance, Si interfacial layer was introduced to reduce interfacial trap. Moreover, Si reduces intrinsic defects at GaAs surface by reconstruct Ga or As homo bonds. In this study, we focused on changes in the chemical and structural characteristics of HfO₂/Si/GaAs film as a function of post annealing temperature. The interfacial reactions induced by post annealing were investigated by XPS, REELS, and XAS. The results show that Si layer decrease the diffusion and oxide formation of Ga and As. Also, the post nitridation significantly improve the diffusion barrier by forming the Ga-N layer. XAS result also consists with the fact that the post nitridation suppress Ga diffusion. The band offsets between GaAs and high-k gate dielectric were aligned using XPS and REELS.

12:51PM Z5.00009 Terahertz Generation Based on Gunn Oscillations in Unipolar Nanodiodes , MUBARAK ALI, AIMIN SONG, University of Manchester — A pressing concern in the terahertz (THz) deployment of technology is the lack of efficient, compact, solid-state THz emitters. Recently, self-switching devices (SSDs) have been demonstrated to offer a 2D planar technology with ultra-low parasitic capacitance, which enabled detection of microwave radiation up to 2.5 THz. Furthermore, it is possible to integrate a large array of SSDs in parallel in order to reduce overall impedance and hence reduce thermal noise. Monte Carlo simulations showed that the SSD can also emit radiation based on Gunn oscillations. In this work, we modeled using Silvaco Atlas to provide evidence of dipole domain formation in the channel and systematically study the dependence of emission frequency and intensity as a function of channel length and width as well as interface-charge density. The results showed that the fundamental oscillation frequency can reach as high as 400 GHz, whereas higher harmonics go well beyond 1.2 THz. By constructing an array that contains different geometries of SSDs placed in parallel, we expect to achieve frequency tuning in wide or narrow bands, which may have useful implications to practical applications.

1:03PM Z5.00010 Tuning electric and magnetic responses with structure evolution in a meta-material , XIANG XIONG, MU WANG, RUWEN PENG, Nanjing University — We demonstrated that in an assembly of double-layered metallic U-shaped resonators, magnetic and electric responses are realized respectively. The two different types of responses are realized at higher and lower frequency. When the U-shaped structure resonators evolve into H-shaped structure gradually, the electric and magnetic frequencies move forward to each other. In this case, when electric response and magnetic response are overlapped in frequency, negative refractive index can be realized.

1:15PM Z5.00011 Configuration interaction in a tunable wavelength shifter, ALEKSEJ MIALITSIN, National Renewable Energy Laboratory, ILIA SOLOV'YOV, Beckman Institute for Advanced Science and Technology, STEFAN SCHMULZ, Namlab, BRIAN FLUEGEL, ANGELO MASCARENHAS, National Renewable Energy Laboratory — It has recently been demonstrated how hybridized plasmon-phonon collective excitations in GaAs can be blue shifted by about 20 wavenumbers (0.6 THz) relative to the unperturbed longitudinal optical lattice vibration frequency as a function of excitation beam intensity [Fluegel et al., Nat. Phot. 1, 701 (2007)]. At beam intensities greater than 10 mW/cm^{-2} the wavelength shifted mode broadens and begins to exhibit a double-peak structure. We attribute this line-shape modification to configuration interaction of the named mode with the edge of the continuous background and discuss potential implications for coupled plasmon-phonon modes generated in semiconductor hetero-structures.

1:27PM Z5.00012 Secondary Electron Emission (SEE) Calculations, HAROLD P. HJALMARSON, RONALD P. KENSEK, Sandia National Laboratory, KENNETH E. KAMBOUR, Air Force Research Laboratory — Secondary electron emission (SEE) from solids is a consequence of energy loss by charged particles such as electrons. One important energy loss mechanism to be considered involves plasmon emission by the charged particle. Plasmons create electron-hole pairs when they decay. Under certain conditions, a sufficiently energetic electron, a secondary electron, may be emitted from the solid surface. In this presentation, results from two different approaches to this process will be presented. A particle-based Monte Carlo method and a continuum method will be used for these calculations. The results from the two different methods will be compared to each other to understand the effects of the various approximations in the two methods. The methods will be illustrated by an application to titanium dioxide (rutile). —Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

1:39PM Z5.00013 Dark Field Imaging of Plasmonic Resonator Arrays, ATILLA AYDINLI, SINAN BALCI, ERTUGRUL KARADEMIR, COSKUN KOCABAS, Bilkent University — We present critical coupling of electromagnetic waves to plasmonic cavity arrays fabricated on Moiré surfaces. The critical coupling condition depends on the superperiod of Moiré surface, which also defines the coupling between the cavities. Complete transfer of the incident power can be achieved for traveling wave plasmonic resonators, which have relatively short superperiod. When the superperiod of the resonators increases, the coupled resonators become isolated standing wave resonators in which complete transfer of the incident power is not possible. Dark field plasmon microscopy imaging and polarization dependent spectroscopic reflection measurements reveal the critical coupling conditions of the cavities. We image the light scattered from SPPs in the plasmonic cavities excited by a tunable light source. Tuning the excitation wavelength, we measure the localization and dispersion of the plasmonic cavity mode. Dark field imaging has been achieved in the Kretschmann configuration using a supercontinuum white light laser equipped with an acoustooptic tunable filter. Polarization dependent spectroscopic reflection and dark field imaging measurements are correlated and found to be in agreement with FDTD simulations.

1:51PM Z5.00014 Engineered Uniform Conduction Fronts in Memristive/Memcapacitive Systems, PATRICK MICKEL, CONRAD JAMES, Sandia National Laboratories — We introduce here a novel “memristor” design enabling the uniform propagation of the conduction front within the device, improving performance as well as device-to-device consistency. Typically, resistive switching in memristors occurs due to the localized formation of conductive filaments. Electric fields are magnified at filament tips (due to decreased separation, $E = V/d$), amplifying growth rates for select filaments and producing a localized and highly non-uniform conduction front. However, we show that by incorporating specifically spaced layers with alternating ionic mobilities the electric field magnification can be counterbalanced, resulting in a uniform conduction front. The uniform conduction front lowers device-to-device variability, improves analog tuning and significantly amplifies the memcapacitive properties of the device. These multilayered engineered nanostructures have potential applications in multi-bit memory storage and neuromorphic computing architectures.

Friday, March 2, 2012 11:15AM - 2:15PM –

Session Z6 DMP: Focus Session: Carbon Nanotube Electronics, Properties, and Devices 206B

11:15AM Z6.00001 ABSTRACT WITHDRAWN –

11:27AM Z6.00002 Exploring adiabatic/non-adiabatic phase transitions in suspended metallic carbon nanotubes, SHUN-WEN CHANG, Department of Physics and Astronomy, University of Southern California, ROHAN DHALL, Department of Electrical Engineering, University of Southern California, ZUWEI LIU, Department of Physics and Astronomy, University of Southern California, STEPHEN CRONIN, Department of Electrical Engineering, Physics and Astronomy, and Chemistry, University of Southern California, CRONIN'S GROUP TEAM — We investigate the non-adiabatic Kohn anomaly in suspended pristine metallic single-walled carbon nanotubes by studying the dependence of the Raman G band and $2D$ band frequency on Fermi energy. We find that by varying temperature, metallic nanotubes can switch between a regime in which the non-adiabatic Kohn anomaly is clearly observed, to a regime where the non-adiabatic Kohn anomaly is absent. Furthermore, we find that the non-adiabatic Kohn anomaly is always accompanied by a dramatic gate-induced modulation of the G band Raman intensity. By establishing a quantitative correlation between the strength of the non-adiabatic Kohn anomaly and the modulation of Raman intensity, we determine that the underlying mechanism that leads to both these effects is the same.

11:39AM Z6.00003 Current-Induced Cleaning of Adsorbates from Suspended Semiconducting Carbon Nanotube Diodes, ARGYRIOS MALAPANIS, EVERETT COMFORT, JI UNG LEE, College of Nanoscale Science and Engineering, SUNY, Albany, NY — Single-walled carbon nanotubes (SWNT) are prime candidates for future applications, including nanoelectronic and nanophotonic devices. Because of their large surface-to-volume ratio compared to that of a bulk semiconductor, however, SWNTs are very sensitive to their environment. Others have already established that their electronic properties can be dramatically changed by exposure to air, particularly oxygen or water. In this paper,¹ we show that the electronic and optical properties of $p-n$ diodes fabricated with suspended semiconducting SWNTs degrade over time with exposure to ambient conditions, mainly due to adsorption onto the tube's suspended part, which creates band-gap states. We provide the first correlation between adsorbate-generated electronic states and their impact on diode performance. Specifically, we show that the ideality factor, a fundamental parameter used to measure defect states in a $p-n$ diode, increases with the degree of adsorbate coverage. We also demonstrate a simple technique—current annealing—that can thermally reverse such degradation, returning device properties to their original characteristics.

¹A. Malapanis, E. Comfort, and J. U. Lee, Appl. Phys. Lett., 98, 263108 (2011).

11:51AM Z6.00004 Electronic performance of flexible single-wall carbon nanotube films: The role of electronic type, JOHN M. HARRIS, North Dakota State University, STEVEN D. HUDSON, JEFFREY A. FAGAN, NIST, ERIK K. HOBIE, North Dakota State University — Recent advances in the separation of single-wall carbon nanotubes (SWCNTs) by length and electronic type have made highly monodisperse SWCNT membranes a reality, opening up new realms of potential application in flexible electronics. By measuring the coupling between mechanical flexibility and electronic performance for thin transparent films of metallic and semiconducting SWCNTs assembled on elastic polymer substrates, we demonstrate a marked difference in the electronic manifestations of thin-film deformation for the two electronic SWCNT types. We relate these differences to mechanical and interfacial phenomena that stem from the distinct optical resonances characteristic of metallic or semiconducting nanotubes, and we evaluate the durability of each film type in response to repeated mechanical strain.

12:03PM Z6.00005 Origin of Capacitance Change in Semiconducting and Metallic Carbon Nanotubes, SEONG CHU LIM, DINH LOC DUONG, YOUNG WOO JO, TAE HYUNG KIM, SOO MIN KIM, Department of Energy Science, Sungkyunkwan University, JUNG HYUN YOON, HA RYONG HWANG, WISE CONTROL Inc., R&D Division, SLAVA ROTKIN, Department of Physics, Lehigh University, YOUNG HEE LEE, Department of Energy Science, Sungkyunkwan University, WISE CONTROL INC., R&D DIVISION COLLABORATION, DEPARTMENT OF PHYSICS, LEHIGH UNIVERSITY COLLABORATION — Different mechanisms are reported for the capacitance changes in metallic (m-) and semiconducting (s-) single-walled carbon nanotubes (SWCNTs) upon gas adsorption. The sensitivity, i.e., the change in capacitance, was high and reached approximately 2500% in the aligned s-SWCNT network, whereas the sensitivity was found to be low in the m-SWCNT network. The charge transfer/Fermi level shift and quantum capacitance related to the localized electronic density of states near the Fermi level were key contributors to sensitivity changes upon gas adsorption, although the polarization effect also played a role in the capacitance changes, particularly in the aligned CNTs, under a strong electric field.

12:15PM Z6.00006 Carbon based devices for molecular quantum spintronics¹, WOLFGANG WERNSDORFER, Institut Neel, CNRS, Grenoble — This presentation will address a new field called molecular quantum spintronics, which combines the concepts of spintronics, molecular electronics and quantum computing [1]. Various research groups are currently developing low-temperature scanning tunnelling microscopes to manipulate spins in single molecules, while others are working on molecular devices (such as molecular spin-transistors, spin valves and filters, and carbon-nanotube-based devices [1]) to read and manipulate the spin state and perform basic quantum operations. The talk will discuss the read-out of the spin states of single-molecule magnets using carbon based devices. In particular, carbon nanotube devices [2] and graphene nano-constrictions [3] will be discussed.

[1] L. Bogani & W. Wernsdorfer, Molecular spintronics using single-molecule magnets, *Nature Mat.* 7, 179 (2008).

[2] M. Urdampilleta, S. Klyatskaya, J.-P. Cleuziou, M. Ruben, W. Wernsdorfer. Supramolecular Spin Valves. *Nature Mat.* 10, 502 (2011).

[3] A. Candini, S. Klyatskaya, M. Ruben, W. Wernsdorfer, M. Affronte. Graphene Spintronic Devices with Molecular Nanomagnets. *Nano Lett.* 11, 2634, (2011).

¹This work is supported by the projects ANR-PNANO MolNanoSpin No. ANR-08-NANO-002, ERC Advanced Grant MolNanoSpin No. 226558, and STEP MolSpinQIP.

12:51PM Z6.00007 Poole-Frenkel emission by carbon nanotube defect sites, DENG PAN, BRAD CORSO, PHILIP COLLINS, Department of Physics and Astronomy, University of California Irvine — Single walled carbon nanotubes (SWCNTs) have a conductance that is particularly sensitive to the presence of defects and disorder. Here, we fabricate field effect devices out of individual SWCNTs in order to investigate this effect. The bias- and gate-dependent conductance of SWCNT devices is measured over a temperature range of 77 – 400 K. By performing these measurements on the same SWCNT before and after the incorporation of a point defect, we clearly discern the electronic consequences of the addition. Specifically, the initial recording of the pristine SWCNT determines the energy-dependent resistances of the SWCNT itself. After electrochemical point functionalization to introduce a defect site, the additional resistance and its energy-dependence is determined by properly accounting for the initial contributions. We find the defect scattering to be well fit by a Poole-Frenkel emission model, with the consequence that barrier widths and heights can be extracted for different defect types.

1:03PM Z6.00008 Scanning Probe Characterization of Electronic Scattering by Carbon Nanotube Defects, ELLIOT FULLER, STEVEN HUNT, BRAD CORSO, PHILIP COLLINS, Dept. of Physics and Astronomy, Univ. of California Irvine, Irvine, CA 92697 — Single-walled carbon nanotubes (SWCNTs) are quasi-ballistic, one-dimensional conductors with unique electronic properties. The controlled addition of a single covalent, sidewall defect interrupts this conduction pathway and produces a disproportionate change in the device properties. Here, we investigate the electronic effects in the immediate vicinity of a defect site using Kelvin force microscopy (KFM) and scanning gate spectroscopy (SGS). KFM images the local electrostatic surface potential along a SWCNT and thus can directly measure the potential drop at defects and other electronic surface features. Using KFM, we clearly observe the bias dependence of resistance at the site of defects and/or chemical attachments. The SGS technique provides complementary information by mapping their gate dependence. Combined, these two scanning probe techniques resolve the full energy dependence of scattering by a defect site and allow the determination of effective barrier widths and heights for different types.

1:15PM Z6.00009 Fundamental Limits of Current Flow in One-dimensional Carbon Nanomaterials, ALBERT LIAO, CHRISTOPHER NEUMANN, ERIC POP, Department of Electrical and Computer Engineering at the University of Illinois at Urbana-Champaign — Carbon nanotubes (CNTs) and graphene nanoribbons (GNRs) carry very high current densities given their strong sp² bonds and high carrier mobility. However, the fundamental limitations to their maximum current flow are still not well understood. We measured the maximum current flow of CNTs and GNRs in substrate-supported configurations in ambient air where devices break from Joule heating at ~600 C [1,2], revealing information about their power dissipation. Interestingly, thermal coupling with the substrate increases with CNT diameter but decreases with GNR width, due to competing roles of thermal boundary resistance and heat spreading into the substrate. To further study quasi-metallic single-wall CNTs at very high fields, we performed measurements in vacuum. We found some devices show current saturation as expected [3], but in many the current continues to increase with a constant slope of ~ 1 μ A/V at fields >10 V/ μ m. This is observed even in small-diameter (~1.2 nm) CNTs whose dimensions were verified by AFM and Raman spectroscopy. We suggest such behavior can be explained by a combination of better heat coupling with the substrate and higher subband conduction. [1] A. Liao *et al*, PRB **82**, 205406 (2010). [2] A. Liao *et al*, PRL **106**, 256801 (2011). [3] Z. Yao *et al*, PRL **84**, 2941 (2000).

1:27PM Z6.00010 Terahertz Detection in an Individual Single-Walled Carbon Nanotube¹, JOEL CHUDOW, DANIEL SANTAVICCA, Dept. of Applied Physics, Yale University, CHRIS MCKITTERICK, Dept. of Physics, Yale University, LUIGI FRUNZIO, Dept. of Applied Physics, Yale University, DANIEL PROBER, Dept. of Applied Physics and Physics, Yale University, PHILIP KIM, Dept. of Physics, Columbia University — Carbon nanotubes (CNTs) serve as a test experimental system for verification of physical models of one-dimensional (1-D) conduction. We aim to excite terahertz standing wave resonances on a CNT, which are predicted to display Luttinger-liquid behavior due to the lack of screening in 1-D. We describe measurements of terahertz (THz) absorption in individual single-walled carbon nanotubes and distinguish between two response mechanisms: bolometric detection due to heating a CNT with a temperature-dependent resistance and the response due to non-thermal electrical contact nonlinearities. This is the first frequency-domain demonstration of THz detection in an individual CNT. The effect of the contact nonlinearity is not decreased at THz frequencies and allows for analysis of the parallel contact capacitance to an individual CNT. Both detection mechanisms are expected to give evidence of the Luttinger-liquid resonant behavior. This experimental technique provides a method to study high-frequency charge excitations in the nanotube as a probe of the strength of the electron-electron interactions in this 1-D system.

¹This work supported by NSF-DMR.

1:39PM Z6.00011 Individual Single-Walled Carbon Nanotube Device Fabrication for Terahertz Detection¹, CHRIS MCKITTERICK, Physics Department, Yale University, JOEL CHUDOW, DANIEL SANTAVICCA, LUIGI FRUNZIO, Applied Physics Department, Yale University, DANIEL PROBER, Physics and Applied Physics Departments, Yale University, PHILIP KIM, Physics and Applied Physics Departments, Columbia University — We describe the fabrication process for the development of antenna-coupled single-walled carbon nanotube (CNT) terahertz (THz) detectors. This requires the development of a lithographically-defined gate electrode, as the device is fabricated on a THz-transparent insulating silicon substrate. Antenna development is geared towards accessing the largest possible bandwidth to facilitate the study of standing wave resonances in the CNT. These standing wave resonances are expected from the one-dimensional Tomonaga-Luttinger Liquid theory, which predicts collective charge oscillations, known as plasmons, which travel faster than the Fermi velocity. Using a Fourier transform interferometer, we excite the antenna-coupled CNT with a broadband blackbody source and probe the THz impedance of the CNT through Joule heating.

¹This work is supported by NSF-DMR and NSF-CHE.

1:51PM Z6.00012 In-situ TEM study of heat transfer between a carbon nanotube and contacting material, MERIJNTJE BRONGEEST, NORVIK VOSKANIAN, HANNA NILSSON, JOHN CUMINGS, University of Maryland — Due to their interesting intrinsic properties and 1D nature, carbon nanotubes may be (part of) the solution to the heat management challenge in nanoelectronics in multiple ways: e.g. as thermal interface material and/or interconnects in existing Si-based electronics, or as a building block in carbon-based electronics. Of crucial importance for any of these applications is the (in)ability to get heat in and out of the tube: the thermal contact resistance. Thermal contact resistance for carbon nanotubes is not fully understood yet, and theory is under construction. Measuring it is a challenge of its own as it is intimately connected to the thermal conductivity of the connected materials which are not necessarily known that well either. We study the thermal properties of carbon nanotubes with Electron Thermal Microscopy [T. Brintlinger et al., Nano Lett. 8, 582 (2008)], which allows for thermal imaging with a resolution of 150 nm, and combine that with finite-element modeling. With this approach we have already demonstrated that also on a substrate the CNT thermal conductivity is high, and that different heat transfer mechanisms (e.g. phonon-phonon, electron-surface polariton interaction) can be important. Our goal is to study and quantify thermal contact resistance between a carbon nanotube and its surroundings and we will present our latest results.

2:03PM Z6.00013 Remote Joule heating of crossed nanotube, NORVIK VOSKANIAN, KAMAL H. BALOCH, Materials Science and Engineering, University of Maryland, College Park, Maryland, MERIJNTJE S. BRONGEEST, Physics, University of Maryland, College Park, Maryland, JOHN CUMINGS, Materials Science and Engineering, University of Maryland, College Park, Maryland — The high thermal conductivity of carbon nanotubes makes them an excellent candidate for thermal management and thermal logic devices. We have studied the thermal characteristics of Joule-heated MWNTs in a crossed geometry, using an established thermal measurement technique that relies on the solid to liquid phase transition of indium islands [1]. Our experimental observations show the efficient transfer of heat from CNT to substrate but inefficient heat transfer past the crossing point. This supports the presence of a nonlocal joule heating phenomenon in which the hot electrons from the biased CNT directly transfer their energy to a nearby material. This talk will cover the developed thermal characterization technique, experimental results and simulations.

[1] T. Brintlinger, et al., Nano Lett. 8, 582 (2008).

Friday, March 2, 2012 11:15AM - 2:03PM —

Session Z7 DCMP: Transport and Optical Properties of Non-Carbon Nanotubes and Nanowires

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11:15AM Z7.00001 Exchange induced electron transport in heavily n-doped Si nanowires¹, JOONYEON CHANG, Korea Institute of Science & Technology, TAE-EON PARK, Yonsei University, Korea Institute of Science & Technology, BYOUNG-CHUL MIN, Korea Institute of Science & Technology, ILSOO KIM, Yonsei University, JAE-EUN YANG, MOON-HO JO, Postech, HEON-JIN CHOI, Yonsei University, KOREA INSTITUTE OF SCIENCE AND TECHNOLOGY TEAM, YONSEI UNIVERSITY TEAM, POSTECH TEAM — Silicon nanowires (Si NWs) have been used as building blocks in the “bottom-up” approach to nanoelectronics because of their excellent electrical properties. Despite the potential of Si NWs, unfortunately, there is little known about the electrical properties of heavily doped Si NWs. We have synthesized heavily doped *n*-type Si NWs and measured the electrical resistance using four-probe method. As we decrease the temperature, the resistivity of Si NWs decreases initially, shows a resistivity minimum around 60 K, and thereafter increases logarithmically. Below the resistivity minimum temperature (T_{min}), we have observed a dip around zero-bias in the differential conductance, and a negative magnetoresistance (MR) which depends on the angle between the applied magnetic field and current flow. These results are associated with the impurity band conduction and electron scattering by the localized spins at phosphorus donor states. The analysis on the MR reveals that the localized spins are coupled antiferromagnetically at low temperature via the exchange interaction.

¹Nano R&D and KIST Institutional program

11:27AM Z7.00002 Low-field mobility in ultrathin silicon nanowire junctionless transistors, BART SOREE, WIM MAGNUS, WILLIAM VANDENBERGHE, imec, UNIVERSITEIT ANTWERPEN COLLABORATION, KULEUVEN COLLABORATION — We theoretically investigate the phonon, surface roughness and ionized impurity limited low-field mobility of ultrathin silicon *n*-type nanowire junctionless transistors in the long channel approximation with wire radii ranging from 2 to 5 nm, as function of gate voltage. A few years ago, the junctionless nanowire transistor (JNT) or pinch-off nanowire was proposed by several research groups and was recently fabricated for the first time. The JNT is a uniformly doped nanowire with no junctions, i.e. source, channel and drain are doped with the same doping type. The main motivation for introducing this novel device concept are the absence of doping junctions which makes the fabrication easier, and the reduction of detrimental interactions occurring at the interface between the silicon body of the wire and the insulator (surface roughness). We investigate the case where due to quantum mechanical confinement the surface roughness scattering becomes again important and we report on the behavior of phonon, ionized impurity and surface roughness limited mobility as a function of radius and gate voltage.

11:39AM Z7.00003 Photovoltaic properties of axial in-situ doped SiGe heteronanowires, SON T. LE, Department of Physics, Brown University, A.D. MOHITE, D.E. PEREA, H. HTOON, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, P. JANNATY, A. ZASLAVSKY, School of Engineering, Brown University, S.T. PICRAUX, Center for Integrated Nanotechnologies, Los Alamos National Laboratory — We report on vapor-liquid-solid (VLS) growth and photovoltaic properties of axial in-situ doped Ge-Si heteronanowire (hetero-NW) solar cells. Modern VLS growth has recently demonstrated the growth of Si-Ge axial NWs with abrupt heterojunctions [1], and simultaneous control of both material composition and doping profiles. This advance allows for the integration of Ge with Si in a hetero-NW structure for broad-spectrum and high absorption efficiency solar cells. Our preliminary optical measurements on p -Ge/ i -Si/ n -Si wires provide important ingredients for a hetero-NW photovoltaic device. We achieved good rectification with $\sim 10^3$ ratio between forward and reverse bias currents at moderate voltage. Under laser illumination (532 nm), we measured a large open circuit voltage $V_{OC} \sim 0.54$ V and a high short-circuit current density $J_{SC} \sim 4 \times 10^3$ A/cm², comparable to state-of-the-art reported single NW results [2]. Additional optimization of separate Ge and Si pin NW structures and their integration in a combined Ge/Si tandem hetero-NW solar cell will be reported.

[1] D. E. Perea *et al.*, *Nano Lett.* **11**, 3117 (2011).

[2] B. Tian *et al.*, *Chem. Soc. Rev.* **38**, 16 (2009).

11:51AM Z7.00004 Strong Tuning of Spin Orbit Interaction in an InAs Nanowire by an Electrolyte Gate¹, DONG LIANG, XUAN P.A. GAO, Department of Physics, Case Western Reserve University — Manipulating electron spin in solid state devices has been the main target of spintronics. A key concept in many spintronic devices is to apply gate voltage or electric field (E) to tune spin precession via the Rashba spin orbit interaction (SOI). Quasi-one dimensional (1D) indium arsenide (InAs) nanowires are promising platforms in this regard due to InAs's strong intrinsic SOI and more effective control of Rashba SOI in 1D system with uni-directional momentum. Here, we demonstrate efficient control of Rashba SOI where E is created at the surface of InAs nanowire by solid electrolyte surrounding gate. Six-fold tuning of Rashba coefficient and 2.5 order of magnitude tuning of spin relaxation time are achieved within only 1 V of gate bias. Such a dramatic tuning of SOI paves a way towards quasi-1D nanowire spintronic devices with low power consumption.

¹The authors acknowledge ACS PRF (48800-DNI10) for partial funding support.

12:03PM Z7.00005 InAs/InSb axially heterostructured nanowires for small junction area semiconductor diodes, ALESSANDRO PITANTI, DANIELE ERCOLANI, LUCIA SORBA, STEFANO RODDARO, FABIO BELTRAM, NEST Scuola Normale Superiore & CNR NANO p.zza S. Silvestro 12 56127 Pisa Italy, LUCIA NASI, GIANCARLO SALVIATI, IMEM CNR parco Area delle Scienze 37/A 43010 Parma Italy, ALESSANDRO TREDICUCCI, NEST Scuola Normale Superiore & CNR NANO p.zza S. Silvestro 12 56127 Pisa Italy — Semiconductor nanowires are low-dimensional systems which appear as ideal candidates to enable ultra-fast electronic technology. Even if the realization of complex [1], nanowire-based electronic devices such as transistors and diodes has been demonstrated, the ultra-small axial electronic capacitance, related to the semiconductor tiny cross-section, is rarely exploited, due to the difficulty in creating homo/hetero-junctions within the nanowire itself. We propose a solution to produce axial, majority-carrier diodes, by employing growth interruption to create InAs/InSb heterojunction along the nanowire axis [2]. Despite being both InAs and InSb n -type materials, their broken gap band alignment produces strong asymmetry in the I-V characteristic, similarly to standard Schottky-barrier diodes. The band line-up determines a strong nonlinear current response at positive source-drain bias: when an additional InP barrier layer is inserted in-between the heterojunction, the maximum nonlinearity is drawn towards zero bias and the leakage current reduced, making these devices promising candidates for high cut-off frequency rectifying detectors/photomixers.

[1] N. Wang *et al.*, *Mat. Sci. Eng. R* **60**, 1 (2008).

[2] A. Pitanti *et al.* *Phys. Rev. X* **1**, 011006 (2011).

12:15PM Z7.00006 Growth and electrical properties of vertically oriented organic single-crystalline nanostructures¹, SAN THEINGI, Mount Holyoke College, TIM MIRABITO, ALEJANDRO BRISENO, University of Massachusetts (Amherst,MA), KATHERINE AIDALA, Mount Holyoke College — We present our growth of vertically oriented organic single crystalline nanowires of copper tetra-tertbutylphthalocyanine (t-butyl-CuPc) on highly ordered pyrolytic graphite (HOPG). The nanowires are grown by using physical vapor transport (PVT) method, with directed crystallization on ordered substrates. Single crystal nanostructures are free of grain boundaries and this promotes charge transport through the material. The pi-pi interactions between adjacent molecules of the single crystal provide a direct path for charge transfer, leading to high carrier mobility. Vertically oriented single-crystal nanostructures have applications as high surface area solar cells. We are studying the electrical conductivity of these nanostructures using conductive atomic force microscopy (CAFM). The AFM tip makes an electrical contact to an individual wire, and current is measured as a function of applied voltage.

¹We acknowledge support by NSF CAREER (DMR-0955348), Howard Hughes Medical Institute Summer Program, NSF Materials Research Science and Engineering Center on Polymers at UMass Amherst (DMR-0820506), and Center for Hierarchical Manufacturing (CMMI-0531171).

12:27PM Z7.00007 Rectification in an idealized model junction of strongly correlated electrons¹, FLORIAN SABOU, NATALIE BODINGTON-ROSEN, BRAD MARSTON, Brown University — Junctions of oppositely doped Mott insulators offer the possibility of rectification at extremely high frequencies. To simulate an idealized junction we use a model of spinless electrons moving in one dimension, the t-V chain, and control the chemical potential on the two halves of the chain to create a p-n junction. For short chains the many-body Schrodinger equation can be integrated forward in time numerically exactly, and we find that when subjected to an oscillating electric field the system rectifies by transferring charge in a preferred direction. Dissipation can be included in a phenomenological way by rotating time slightly off the real axis. The time dependent density-matrix renormalization-group may be used to extend the simulation to longer chains with spinning electrons.

¹Supported in part by NSF grant no. DMR-0605619.

12:39PM Z7.00008 Temperature effects on the Raman lineshape of cupric oxide thin films and nanowires, SHRIVIDYA RAVI, ALAN KAISER, Victoria University of Wellington, CHRISTOPHER BUMBY, Industrial Research Limited — The Raman spectrum can be used as a fingerprint for a given material but the details of the Raman spectrum (e.g. the peak lineshape) can also impart considerable information about various environmental effects. In this study, we will describe the effects of heating on the Raman lineshape using a temperature-dependent model. Homogeneous heating (i.e. spatially uniform temperature) leads to symmetrically broadened lineshapes while asymmetric lineshapes can be associated with electron-phonon coupling in or phonon confinement effects. Recently, several groups have found that asymmetric lineshapes from nanoparticles and nanowires require an additional term that describes the inhomogeneous heating - temperature gradients within the sample - due to a gaussian laser beam. In our samples, phonon confinement does not play a role at all as nanowire dimensions are well above 20 nm. Hence, we have invoked a purely temperature-dependent model. This model has considerable flexibility as it can explain both the symmetrical and asymmetrical broadening of the lineshape. We have used it to describe and compare a thin film of cupric oxide (which mostly exhibits homogeneous heating effects) and a vertical forest of cupric oxide nanowires (which exhibit effects of inhomogeneous heating).

12:51PM Z7.00009 Nonlocal Response of the Plasmonic Nanowire Metamaterials, BRIAN WELLS, Department of Physics and Applied Physics, University of Massachusetts Lowell, ANATOLY ZAYATS, Department of Physics, King's College London, VIKTOR PODOLSKIY, Department of Physics and Applied Physics, University of Massachusetts Lowell — Nanowire metamaterials are a class of composite photonic media formed by an array of aligned plasmonic nanowires embedded in a dielectric matrix. Depending on exact composition, geometry, and excitation wavelength, nanowire structures are known to exhibit elliptical, hyperbolic, or epsilon-near-zero (ENZ) responses. In the ENZ regime optical response of the composite becomes strongly nonlocal. Excitation of an additional wave, caused by nonlocality, has been experimentally demonstrated in nanowire-based metamaterials. Here we present numerical and analytical studies of the nonlocal optical response of plasmonic nanowire metamaterials. Dispersion of photonic modes of plasmonic metamaterials has been studied in finite-element-method (FEM) simulations as a function of wavelength, geometry, and material parameters. Analytical description of nonlocal effective permittivity tensor has been developed. These analytical results are in agreement with FEM simulations and experimental data.

1:03PM Z7.00010 ABSTRACT WITHDRAWN —

1:15PM Z7.00011 Equilibration of Luttinger liquid and conductance of quantum wires¹, K.A. MATVEEV, Argonne National Laboratory, A.V. ANDREEV, University of Washington — Luttinger liquid theory describes one-dimensional electron systems in terms of non-interacting bosonic excitations. In this approximation thermal excitations are decoupled from the current flowing through a quantum wire, and the conductance is quantized. We show that relaxation processes not captured by the Luttinger liquid theory lead to equilibration of the excitations with the current and give rise to a temperature-dependent correction to the conductance. In long wires, the magnitude of the correction is expressed in terms of the velocities of bosonic excitations. In shorter wires it is controlled by the relaxation rate.

¹Work supported by the U.S. Department of Energy under Contracts No. DE-AC02-06CH11357 and No. DE-FG02-07ER46452.

1:27PM Z7.00012 Rectification in Y-junctions of Luttinger liquid wires¹, CHENJIE WANG, D.E. FELDMAN, Brown University — We investigate rectification of a low-frequency ac bias in Y-junctions of one-channel Luttinger liquid wires with repulsive electron interaction. Rectification emerges due to three scatterers in the wires. We find that it is possible to achieve a higher rectification current in a Y-junction than in a single wire with an asymmetric scatterer at the same interaction strength and voltage bias. The rectification effect is the strongest in the absence of the time-reversal symmetry. In that case, the maximal rectification current can be comparable with the total current $\sim e^2V/h$ even for low voltages, weak scatterers and modest interaction strength. In a certain range of low voltages, the rectification current can grow as the voltage decreases. This leads to a bump in the I - V curve.

[1] Chenjie Wang and D. E. Feldman, Phys. Rev. B **83**, 045302 (2011).

¹We acknowledge funding for this project from NSF under grants number DMR-0544116 and PHY05-51164 and the U.S. Department of Energy, grant number DE-SC0001556.

1:39PM Z7.00013 Phonon scattering in a strongly-driven 1D electron system¹, KATHLEEN E. HAMILTON, LEONID P. PRYADKO, ALEXEY A. KOVALEV, UCR — We consider phonon relaxation kinetics of a non-equilibrium, one-dimensional electron system driven by a strong, high frequency electric field. For a single-band system, and assuming that the phonon scattering rate is small on the scale of the driving frequency ω , we derive and solve the coupled equations for the Keldysh Green's functions and self energies. In the presence of the periodic driving field, the electrons' energy is replaced by the Floquet quasienergy; in the single-band case it just equals the energy averaged over the period (modulo $\hbar\omega$). The energies of the phonons emitted or absorbed by the system correspond to transitions between the Floquet energy bands, and are strongly dependent on both the amplitude and the frequency of the driving field. Of note is a system in the regime of dynamical localization, where the average electron kinetic energy vanishes. Here, the phonon energies must be in resonance with harmonics of the driving frequency, and the stationary electron distribution function reduces to a constant, with infinite effective temperature.

¹Supported in part by the ARO grant W911NF-11-1-0027 and by the NSF grant 1018935

1:51PM Z7.00014 Nonequilibrium transport through a spinful quantum dot with superconducting leads, JENS PAASKE, BRIAN MOELLER ANDERSEN, KARSTEN FLENSBERG, Niels Bohr Institute, University of Copenhagen, VERENA KOERTING, NBIA, Niels Bohr Institute, University of Copenhagen — We study the nonlinear cotunneling current through a spinful quantum dot contacted by two superconducting leads. Applying a general nonequilibrium Green function formalism to an effective Kondo model, we study the rich variation in the IV-characteristics with varying asymmetry in the tunnel coupling to source and drain electrodes. The current is found to be carried respectively by multiple Andreev reflections in the symmetric limit, and by spin-induced Yu-Shiba-Rusinov bound states in the strongly asymmetric limit. The interplay between these two mechanisms leads to qualitatively different IV-characteristics in the cross-over regime of intermediate symmetry, consistent with recent experimental observations of negative differential conductance and re-positioned conductance peaks in sub-gap cotunneling spectroscopy.

Friday, March 2, 2012 11:15AM - 2:03PM —

Session Z8 DMP GMAG: Focus Session: Frustrated Magnetism - Magnetic insulators 208

11:15AM Z8.00001 Nature of the low energy excitations in the spin liquid state of Cs_2CuCl_4 ¹, ALTAN ALLAWALA, VESNA MITROVIC, BRAD MARSTON, GEORGIOS KOUTROULAKIS, Brown University, RADU COLDEA, Clarendon Laboratory, University of Oxford — We have performed detailed measurements as a function of temperature and applied magnetic field of the NMR rate in the spin liquid phase of the spin-1/2 frustrated antiferromagnet Cs_2CuCl_4 . Comparison of the magnetization and relaxation rate to the spin-1/2 antiferromagnetic chain α - CuNSal and to variational calculations using Gutzwiller-projected mean-field theory implies that the low energy excitations in Cs_2CuCl_4 are characterized by gapless fermionic excitations in the spin liquid phase at non-zero temperature and applied field. To investigate the ability of one dimensional versus two dimensional models to reproduce the low energy properties of Cs_2CuCl_4 ² we compare the measured T^{-1} NMR rate to a field theoretical description of a Luttinger liquid³.

¹Supported in part by NSF DMR-0547938 and DMR-0605619

²M.-A. Vachon *et al.*, New J. Phys. **13** 093029 (2011)

³H. Kühne *et al.*, Phys. Rev. B **83** 100407(R) (2011)

11:27AM Z8.00002 ESR studies of the quasi-2D frustrated Cs₂CuBr₄¹, S.A. ZVYAGIN, D. KAMENSKYI, J. WOSNITZA, HLD-HZDR, 01328 Dresden, Germany, M. IKEDA, T. FUJITA, M. HAGIWARA, KYOKUGEN, Osaka University, Toyonaka, Osaka 560-8531, Japan, O.A. STARYKH, Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112, USA, *R. HU, H. RYU, C. PETROVIC, Condensed Matter Physics and Materials Science Department, BNL, Upton, NY 11973, USA — We report low-temperature electron spin resonance (ESR) studies of single-crystalline samples of Cs₂CuBr₄, a spin-1/2 antiferromagnet with a triangular spin-lattice structure. A remarkable angular dependence of the resonance field, including the splitting of the ESR line for some orientations of the magnetic field, and the presence of a gap in the ESR excitation spectrum at temperatures above $T_N \sim 1.3$ K have been revealed. Our observations suggest that uniform Dzyaloshinskii-Moriya interaction affects the low-energy excitation spectrum in this frustrated compound. The results are compared with that obtained recently for the isostructural material Cs₂CuCl₄ [Povarov et al., Phys. Rev. Lett. 107, 037204 (2011)].

¹The work was supported in part by DFG and EuroMagNET II (EU Contract No. 228043). *Present address: University of Maryland, Center for Nanophysics and Advanced Materials, College Pk, MD 20742 USA

11:39AM Z8.00003 NMR Spectra in 2D Anisotropic Triangle Lattice¹, ADAM FREES, VESNA MITROVIC, Brown University — The spin 1/2 Heisenberg antiferromagnet on the 2D anisotropic triangle lattice represents an important example of the frustrated quantum magnets. The materials Cs₂CuCl₄ and Cs₂CuBr₄ are relevant model systems of such a frustrated magnet. In these compounds magnetic fields can induce numerous exotic quantum states. The states are characterized by their spin texture, which can be measured by NMR. In this talk, we discuss how to model different spin arrangements, and compute the resulting NMR spectra.

¹Supported in part by NSF DMR-0547938

11:51AM Z8.00004 Distinct magnetic regimes through site-selective atom substitution in the frustrated quantum antiferromagnet Cs₂CuCl_{4-x}Br_x, KATERYNA FOYEVTSOVA, HARALD O. JESCHKE, Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, 60438 Frankfurt, Germany, P.T. CONG, B. WOLF, M. DE SOUZA, N. KRUEGER, A.A. HAGHIGHIRAD, F. RITTER, W. ASSMUS, M. LANG, Physikalisches Institut, Goethe Universitaet Frankfurt, 60438 Frankfurt, Germany, ROSER VALENTI, Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, 60438 Frankfurt, Germany — A good realization of a spatially anisotropic spin 1/2 triangular lattice is provided by the isostructural layered compounds Cs₂CuCl₄ and Cs₂CuBr₄. In this talk, we shall present electronic structure calculations and magnetic susceptibility measurements[1] for the mixed systems Cs₂CuCl_{4-x}Br_x. We shall discuss the existence of three distinct concentration regimes which are separated by critical concentrations $x_{c1} = 1$ and $x_{c2} = 2$. The role of frustration effects at the critical concentrations will be highlighted.

[1] Cong et al. Phys. Rev. B 83, 064425 (2011)

12:03PM Z8.00005 Two-stage orbital order and dynamical spin frustration in KCuF₃¹, JAMES C.T. LEE, Frederick Seitz Materials Research Laboratory (FSMRL), UIUC, SHI YUAN, FSMRL, UIUC, SIDDHARTHA LAL², FSMRL and Institute for Condensed Matter Theory (ICMT), UIUC, YOUNG-IL JOE, YU GAN, SERBAN SMADICI, FSMRL, UIUC, PAUL M. GOLDBART, FSMRL and ICMT, UIUC, S. LANCE COOPER, PETER ABBAMONTE, FSMRL, UIUC, KEN FINKELSTEIN, Cornell High Energy Synchrotron Source, Cornell University, YEJUN FENG, Advanced Photon Source, Argonne National Laboratory, ANDRIVO RUSYDI, National University of Singapore — Results from our x-ray and Raman scattering studies on KCuF₃, a model orbital order system, strongly link a low-temperature orbital order transition to a previously unidentified structural phase transition at 50 K. Raman scattering shows softening of phonon modes linked to F—ions that ceases upon a splitting of a degenerate E_g mode at 50 K. This, along with the emergence of diffuse scattering around an orbital order Bragg peak at low temperature, suggests an onset of GdFeO₃-like octahedral tilting, which serves to stabilize the Neel spin order at 39 K. To explain these effects, we have added to the Kugel-Khomskii model a term for direct orbital exchange driven by electron-electron interactions and ligand distortions. This term creates a near degeneracy, which dynamically frustrates the spin order at high temperature, that is lifted by orbital—lattice interactions at low temperature.

¹Funding provided by grants from US DOE and NSF.

²Now at IISER-Kolkata

12:15PM Z8.00006 Evidence for pressure-tuned quantum structural fluctuations in KCuF₃, S. YUAN, M. KIM, J. SEELEY, S. LAL, P. ABBAMONTE, S.L. COOPER, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, IL 61801 — Frustrated magnetic systems are currently of great interest because of the possibility that these materials exhibit novel ground states such as orbital and spin liquids. We provide evidence in the orbital-ordering material KCuF₃ for pressure-tuned quantum melting of a static structural phase to a phase that dynamically fluctuates even near $T \sim 0$ K.[1] Pressure-dependent Raman scattering measurements show that applied pressure above $P^* \sim 7$ kbar reverses a low temperature structural distortion in KCuF₃, resulting in the development of a $\omega \sim 0$ fluctuational (quasielastic) response near $T \sim 0$ K. This pressure-induced fluctuational response is temperature independent and exhibits a characteristic fluctuation rate that is much larger than the temperature, $\Gamma \gg K_B T$, consistent with quantum fluctuations of the CuF₆ octahedra. We show that a previous developed model of pseudospin-phonon coupling qualitatively describes both the temperature- and pressure-dependent evolution of the Raman spectra of KCuF₃. Work supported by the U.S. Department of Energy under Award No. DE-FG02-07ER46453 and by the National Science Foundation under Grant NSF DMR 08-56321.

[1] S. Yuan et al., arXiv:1107.1433 (2011).

12:27PM Z8.00007 Bose metal phase in a simple honeycomb lattice model¹, CHRISTOPHER VARNEY, University of Massachusetts, Amherst / Georgetown University / University of Maryland, KAI SUN, VICTOR GALITSKI, University of Maryland, MARCOS RIGOL, Georgetown University — The existence of quantum spin liquids was first conjectured by Pomeranchuk some 70 years ago, who argued that frustration in simple antiferromagnetic theories could result in a Fermi-liquid-like state for spinon excitations. Here we present evidence that a simple quantum spin model on a honeycomb lattice hosts the long sought for Bose metal with a clearly identifiable Bose surface. The complete phase diagram of the model is determined via exact diagonalization and is shown to include four distinct phases separated by three quantum phase transitions. The stability of the Bose metal phase in the presence of other interactions is also discussed.

¹This research is supported by US-ARO, JQI-NSF-PFC, and the Office of Naval Research.

12:39PM Z8.00008 Spin liquid ground state on the honeycomb Heisenberg spin 1/2 model with nearest and next nearest neighbor interaction, ZHENYUE ZHU, STEVEN WHITE, University of California, Irvine, DAVID HUSE, Princeton University — We numerically investigate the $S=1/2$ Heisenberg model on the honeycomb lattice with nearest (J_1) and next-nearest neighbor (J_2) interactions with the density matrix renormalization group (DMRG). We are able to study open cylinders with widths up to 12 lattice spacings. For J_2/J_1 near 0.3, we find a spin liquid phase, bordered by an antiferromagnetic phase for smaller J_2 and a valence bond crystal for larger J_2 . For the spin liquid phase we find finite spin singlet and triplet gaps and short spin-spin and bond-bond correlation lengths. We also find that the energy splitting between the two different topological sectors decays exponentially with the system width, consistent with a gapped Z_2 spin liquid.

12:51PM Z8.00009 Exact Spin Liquid Ground States of the Quantum Dimer Model on the Square and Honeycomb Lattices, HONG YAO, Stanford University and Tsinghua University, STEVE KIVELSON, Stanford University — We study a generalized quantum hard-core dimer model on the square and honeycomb lattices, allowing for first and second neighbor dimers. At generalized Rohksar-Kivelson points, the exact ground states can be constructed, and ground-state correlation functions can be equated to those of interacting 1+1 dimensional Grassmann fields. When the concentration of second neighbor dimers is small, the ground state correlations are shown to be short-ranged corresponding to a (gaped) spin liquid phase. On a 2-torus, the ground states exhibit fourfold topological degeneracy. On a finite cylinder we have found a dramatic even-odd effect depending on the circumference, and propose that this can be used as a numerical diagnostic of the phase, more generally.

1:03PM Z8.00010 Physical solutions of the Kitaev honeycomb model¹, STEFANO CHESI, McGill University, FABIO L. PEDROCCHI, DANIEL LOSS, University of Basel — We have investigated the exact solution of the honeycomb model proposed by Kitaev and derived an explicit formula for the projector onto the physical subspace. The physical states are simply characterized by the parity of the total occupation of the fermionic eigenmodes. We consider a general lattice on a torus and show that the physical fermion parity depends in a nontrivial way on the vortex configuration and the choice of boundary conditions. In the vortex-free case with a constant gauge field we are able to obtain an analytical expression of the parity. For a general configuration of the gauge field the parity can be easily evaluated numerically, which allows the exact diagonalization of large spin models. We consider physically relevant quantities, as in particular the vortex energies, and show that their true value and associated states can be substantially different from the one calculated in the unprojected space, even in the thermodynamic limit.

¹F. L. Pedrocchi, S. Chesi, and D. Loss, Phys. Rev. B 84, 165414 (2011)

1:15PM Z8.00011 An FRG approach to the Heisenberg-Kitaev model, JOHANNES REUTHER, Karlsruhe Institute of Technology, RONNY THOMALE, Stanford University, SIMON TREBST, University of California, Santa Barbara — We apply the Functional Renormalization Group (FRG) method to frustrated spin-1/2 systems on two dimensional lattices such as the Heisenberg-Kitaev model. In order to be able to perform diagrammatic approximations, we use the pseudo fermion representation of spin operators. The FRG provides a systematic scheme for infinite order resummations in different interaction channels and hence allows to treat magnetic order and disorder effects on an equal footing. Calculating the magnetic susceptibility we identify different magnetically ordered and paramagnetic phases. In particular, the Heisenberg-Kitaev model exhibits magnetically ordered states well beyond the isotropic Heisenberg limit as well as an extended gapless spin-liquid phase around the highly anisotropic Kitaev limit. From the RG flow of the magnetic susceptibility we extract both, the Curie-Weiss scale and the critical ordering scale (for the magnetically ordered states). The Curie-Weiss scale changes sign, indicating a transition of the dominant exchange from antiferromagnetic to ferromagnetic, deep in the magnetically ordered regime. We discuss our results in light of recent experimental susceptibility measurements for Na_2IrO_3 and Li_2IrO_3 .

1:27PM Z8.00012 DMRG study of the spin-1/2 J1-J2 Honeycomb Antiferromagnetic Heisenberg Lattice¹, SHOU SHU GONG, DONGNING SHENG, Department of Physics and Astronomy, California State University Northridge, Northridge, California, 91325, USA, MATTHEW FISHER, Department of Physics, University of California, Santa Barbara, California 93106, USA — A possible quantum spin liquid state has been revealed in the Hubbard model on the honeycomb lattice by Quantum Monte Carlo study, which has stimulated a lot of recent interest in the quantum spin models on honeycomb lattice. In a recent paper (Phys. Rev. B 84, 024406 (2011)), the J1-J2-J3 Heisenberg model has been studied by exact diagonalization (ED), establishing a rich phase diagram with the Neel and plaquette valence-bond crystal (VBC) phases depending on couplings J2 and J3, while it remains unclear if there is a featureless spin liquid phase exists in such a model. Here, by implementing DMRG method with the full rotational $SU(2)$ symmetry, we study the J1-J2 Heisenberg model on honeycomb lattice at larger sizes. We analyze the spin-spin and dimer-dimer correlation functions for different sizes and extrapolate the structure factors to the thermodynamic limit to determine the nature of the quantum state. Our results suggest that the intermediate phase (with $J_2/J_1 \sim 0.2-0.35$) may be a spin liquid phase with vanishing spin/dimer correlations at the large distance limit. The nature of such a phase will be explored based on comparison with variational wavefunctions.

¹This work is supported by the NSF undergrants DMR-0906816, DMR-0611562 (S.S.G and D.N.S.) and DMR-1101912 (M.P.A.F.).

1:39PM Z8.00013 Searching for the Topological Degeneracy in the Hubbard Model on a Honeycomb Lattice, BRYAN CLARK, Princeton Center for Theoretical Science, Princeton University — Recent quantum Monte Carlo calculations by Meng, et. al [1] have produced strong numerical evidence for a topological Z_2 spin liquid on the Hubbard model on the honeycomb lattice. One feature of these spin liquids is the presence of a ground state degeneracy that depends on the manifold on which the system lives. Using finite temperature QMC calculations, we identify what states can live in the low-lying spectra, constraining the options for topologically degenerate ground states. In this talk we discuss these bounds and the implications for the Z_2 spin liquid. [1] Z. Y. Meng, T. C. Lang, S. Wessel, F. F. Assaad, and A. Muramatsu, Quantum spin-liquid emerging in two-dimensional correlated Dirac fermions, Nature 464, 847 (2010).

1:51PM Z8.00014 Emergent critical phase in a 2D frustrated Heisenberg model, PETER P. ORTH, Karlsruhe Institute of Technology (KIT), PREMALA CHANDRA, PIERS COLEMAN, Rutgers University, JOERG SCHMALIAN, Karlsruhe Institute of Technology (KIT) — It is well-known that a discrete Ising (Z_2) order parameter emerges in the frustrated square lattice J_1 - J_2 -Heisenberg model, which may be broken at finite temperature. We ask whether a different discrete symmetry Z_q with $q > 2$ may be found in other frustrated Heisenberg models, giving rise to a different finite temperature phase transition. Indeed, we identify an emergent Z_6 symmetry at low temperatures in a frustrated Heisenberg model on a 2D lattice that contains both the sites of the triangular and its dual honeycomb lattice. Our analysis combines a spin-wave expansion, susceptible to short-distance physics, with renormalization group arguments of the corresponding long-wavelength non-linear sigma model. Our results are even more appealing since the Z_6 clock model has a rich finite temperature phase diagram with two distinct Berezinskii-Kosterlitz-Thouless (BKT) phase transitions separated by a massless critical phase. We also discuss possible realizations of this phenomenon using cold-atoms in optical lattices.

Friday, March 2, 2012 11:15AM - 2:03PM —

Session Z9 DMP GMAG: Focus Session: Complex Bulk Oxide: General Properties 209

11:15AM Z9.00001 Local atomic structure of the layered compound SrFeO_2 , KAZUMASA HORIGANE, Department of Physics, University of Virginia, ANNA LLOBET, Los Alamos National Laboratory, KEESEONG PARK, DESPINA LOUCA, Department of Physics, University of Virginia — SrFeO_2 exhibits several unexpected structural and physical properties. Its antiferromagnetic transition temperature $T_N=473\text{K}$ is unusually high for a two-dimensional layered structure. First-principle calculations on SrFeO_2 showed that the Fe 3d down-spin electrons occupy the nondegenerate d_{z^2} level rather than the degenerate (d_{xz} , d_{yz}) levels. This is in good agreement with the absence of a Jahn-Teller instability and the existence of the three dimensional antiferromagnetic ordering because the out-of plane direct Fe-Fe exchange is comparable in strength to the in-plane Fe-O-Fe superexchange. Therefore, it is expected that there is no structure instability in SrFeO_2 . Using the pair distribution function (PDF) analysis to characterize the local structure of SrFeO_2 , we observed that the local symmetry is lower than the average P4/mmm crystal symmetry. In particular, the FeO_2 planes are buckled, with two unique buckling angles along the a-axis. The buckling angle of Fe-O-Fe is reduced from 180° with increasing temperature, accompanied by a reduction of the Fe magnetic moment. Thus the local structure instability correlates with the magnetism where the distortions suppress orbital overlap.

11:27AM Z9.00002 Phonon anomalies and critical fluctuations associated with charge stripes in $\text{La}_{1.67}\text{Sr}_{0.33}\text{NiO}_4$, SVETLANA ANISIMOVA, DAN PARSHALL, DMITRY REZNIK, University of Colorado at Boulder, DANIEL LAMAGO, LLB, CEA Saclay, DOUGLAS ABERNATHY, SNS, Oak Ridge National Laboratory, KAROL MARTY, MARK LUMSDEN, HFIR, Oak Ridge National Laboratory, G. GU, J.M. TRANQUADA, Brookhaven National Laboratory — We will report inelastic neutron scattering measurements of the spectrum of charge excitations in the stripe-ordered phase of $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$ ($x = \frac{1}{3}$). We identified clear signature of charge stripes at low energies in the nickelates. Our results imply that dynamic stripes are critical fluctuations associated with the stripe-ordering transition. We also observed a phonon anomaly correlated with dynamic stripes above the static-ordering transition, which occurs at 241 K. Our results elucidate the nature of dynamic charge stripes and their signature in the neutron spectra.

11:39AM Z9.00003 Rare orbital glass state in single crystalline $\text{Y}_2\text{Mo}_2\text{O}_7$, HARLYN SILVERSTEIN, University of Manitoba, HAIDONG ZHOU, National High Magnetic Field Laboratory, ALANNAH HALLAS, University of Manitoba, JASON GARDNER, YIMING QIU, National Institute of Standards and Technology, GEORG EHLERS, ANDREI SAVICI, Oak Ridge National Laboratory, ZAHRA YAMANI, Chalk River Laboratories, MICHEL GINGRAS, University of Waterloo, BRUCE GAULIN, KATHARINA FRITSCHKE, KATE ROSS, McMaster University, CHRISTOPHER WIEBE, University of Winnipeg — Perhaps one of the most curious cases of frustrated pyrochlores, $\text{Y}_2\text{Mo}_2\text{O}_7$ was first classified as a spin glass in 1986. Conventionally, spin glasses must exhibit some sort of chemical disorder although oxygen vacancies and Y-Mo site mixing is virtually absent in all studies to date. NMR and neutron PDF experiments show the presence of local disorder. While other studies have shown a lattice deformation occurring near $T_g=22\text{K}$, these distortions cannot be detected globally and may not be enough to explain the spin glass behavior. For 25 years, researchers have struggled to resolve spin glass theory with the data; the problem lies in that, until now, scientists have been unable to grow single crystal samples due to the oxidation of Mo^{4+} to Mo^{6+} at low temperatures. Here, we report the synthesis and characterization of the world's first single crystalline sample of $\text{Y}_2\text{Mo}_2\text{O}_7$. Unlike powder samples, single crystalline $\text{Y}_2\text{Mo}_2\text{O}_7$ heat capacity measurements show a T^2 dependence. Neutron scattering experiments show isotropic, broad, liquid-like collective modes and high-Q diffuse scattering characteristic of an orbital liquid to orbital glass transition at T_g .

11:51AM Z9.00004 Anisotropic magnetic properties of the KMo_4O_6 , M. ANDRADE, M. L. MAFFEI, C. A. M. DOS SANTOS, B. FERREIRA, A. F. SARTORI, Escola de Engenharia de Lorena - USP — Electrical resistivity measurements in the tetragonal KMo_4O_6 single crystals show a metal-insulator transition (MIT) near 100K. Magnetization measurements as a function of temperature show no evidence of magnetic ordering at this MIT [1]. Single crystals of KMo_4O_6 were obtained by electrolysis of a melt with a molar ratio of $\text{K}_2\text{MoO}_4:\text{MoO}_3 = 6:1$. The process were carried out at 930°C with a current of 20-25mA for 52h in argon atmosphere. After that, electrodes were removed from the melt alloying the crystals to cool down to room temperature rapidly. Scanning Electron Microscopy (SEM) showed that the black single crystals were grown on the platinum cathode. Typical dimensions of the single crystals are $1 \times 0.2 \times 0.2 \text{ mm}^3$. X-ray diffractometry confirmed that the single crystals have KMo_4O_6 tetragonal crystalline structure with space group $P\bar{4}$. Magnetization measurements were performed parallel and perpendicular to the c-axis from 2 to 300K. The results show anisotropic behavior between both directions. Furthermore, the temperature independence of the magnetization at high temperature and the upturn at low temperature are observed in agreement with previous results [1]. MxH curves measured at several temperatures show nonlinear behavior and a small magnetic ordering. The magnetic ordering seems to be related to the MIT near 100K. This material is based upon support by FAPESP (2009/14524-6 and 2009/54001-6) and CNPq/NSF (490182/2009-7). M. Andrade is CAPES fellow and C.A.M. dos Santos is CNPq fellow.

[1] K. V. Ramanujachary et al., J. Sol. State Chem.102 (1993) 69.

12:03PM Z9.00005 $\text{Cu}_3\text{Nb}_2\text{O}_8$: A Multiferroic with Chiral Coupling to the Crystal Structure, ROGER JOHNSON, Clarendon Laboratory, Department of Physics, University of Oxford, Oxford, OX1 3PU, United Kingdom, SUNIL NAIR, IISER Pune, Sai Trinity Building, Garware Circle, Sutarwadi, Pashan, Pune, Maharashtra 411021, India, LAURENT CHAPON, Institut Laue-Langevin, BP 156X, 38042 Grenoble, France., ALESSANDRO BOMBARDI, CARLO VECCHINI, Diamond Light Source, Harwell Science and Innovation Campus, Didcot, OX11 0DE, United Kingdom, D. PRABHAKARAN, ANDREW BOOTHROYD, PAOLO RADAELLI, Clarendon Laboratory, Department of Physics, University of Oxford, Oxford, OX1 3PU, United Kingdom — We will present recent bulk properties, neutron powder diffraction, and non-resonant x-ray diffraction measurements on a new multiferroic material, $\text{Cu}_3\text{Nb}_2\text{O}_8$. We demonstrate that an electric polarization evolves simultaneously with a generalised helicoidal magnetic ordering. Contrary to conventional models of multiferroicity, the electric polarization was found to lie perpendicular to the common rotation plane of the magnetic moments. We present a new model applicable to a specific class of crystals; those that support a macroscopic "ferroaxial" vector and adopt a helicoidal magnetic structure. Our new interpretation, which may explain the multiferroic properties of a number of systems reported in recent literature, is based upon the well-understood inverse Dzyaloshinskii-Moriya interaction, but requires an altogether different interpretation.

12:15PM Z9.00006 THz and infrared excitation spectrum below the Jahn-Teller transition in $\text{Sr}_3\text{Cr}_2\text{O}_8$, ZHE WANG, MICHAEL SCHMIDT, AXEL GÜNTHER, SEBASTIAN SCHAIKE, NIKOLA PASCHER, FRANZ MAYR, YURII GONCHAROV, HANS-ALBRECHT KRUG VON NIDDA, ALOIS LOIDL, Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany, DIANA QUINTERO-CASTRO, A.T.M.N. ISLAM, BELLA LAKE, Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany, JOACHIM DEISENHOFER, Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — We report on optical excitations observed recently in $\text{Sr}_3\text{Cr}_2\text{O}_8$ by THz and infrared spectroscopy. Low-energy excitations below 3 THz are detected by THz time domain spectroscopy. These excitations can be divided into two different classes according to the temperature-dependent properties. One is emergent right below the Jahn-Teller transition temperature, which is determined by specific heat measurement to occur at 285 K [1, 2]. The other appears only below 100 K, where the fluctuations are sufficiently suppressed, consistent with the temperature dependence of low-energy Raman modes [3]. Infrared transmission measurements reveal a broad crystal-field excitation, which can be associated with an electronic transition from E to T2 orbital states.

[1] Zhe Wang *et al.*, Phys. Rev. B **83**, 201102 (2011)

[2] D. L. Quintero-Castro *et al.*, Phys. Rev. B **81**, 014415 (2010)

[3] D. Wulferding *et al.*, Phys. Rev. B **84**, 064419 (2011)

12:27PM Z9.00007 Magnetic and Orbital Excitations in $\text{Sr}_3\text{CuIrO}_6$ ¹, J.P. HILL, X. LIU, M. DEAN, W. YIN, A. TSVELIK, Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, NY 11973, J. KIM, D. CASA, M.H. UPTON, APS, Argonne National Laboratory, Illinois 60439, USA, H. GRETARSSON, Y.-J. KIM, Dept. of Physics, University of Toronto, Canada M5S 1A7, T. QI, G. CAO, Dept. of Physics and Astronomy, U. Kentucky, Kentucky 40506, L. HOZOI, V. KATUKURI, J. V.D. BRINK, Institute for Theoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany — We report resonant inelastic x-ray scattering studies of the one-dimensional $\text{Sr}_3\text{CuIrO}_6$ at the Ir L_3 edge, with $\Delta E=40$ meV. At high energies, we find peaks at 0.6 eV, 0.9 eV, 3 eV, 4 eV and 6 eV. These peaks are non-dispersive, well-defined excitations. On the basis of quantum chemistry calculations, we are able to identify the first two as excitations within the t_{2g} manifold and the next two as between the t_{2g} and e_g manifolds, together with charge transfer excitations from the O $2p$ to the Ir $5d$. The 6 eV feature is another $t_{2g} - e_g$ excitation. From these we are able to determine both the spin-orbit and non-cubic crystal field splittings. We find that they are of comparable strength. In addition, magnetic excitations are observed, corresponding to excitations of the $j_{1/2}$ isospin. We find these are highly dispersive along the chain direction with a bandwidth of 20 meV and a gap of 30 meV. These results allow a complete modeling of the spin and orbital degrees of freedom in this model compound and we conclude an atomic, spin-orbit coupled description works well.

¹Work performed at BNL was supported by US DOE, Office of Science, DMSE under contract no. DE-AC02-98CH10886.

12:39PM Z9.00008 Probing Spin-Orbit Coupling in Iridium 5d Compounds with X-ray Absorption Spectroscopy, J.P. CLANCY, University of Toronto, N. CHEN, W.F. CHEN, C.Y. KIM, Canadian Light Source, K.W. PLUMB, Y.J. KIM, University of Toronto — Iridium-based transition metal oxides have begun to attract considerable interest following recent proposals of exotic electronic and magnetic ground states (topological insulators, topological semi-metals, spin liquids, and spin-orbital Mott insulators) driven by large spin-orbit coupling effects. We have performed x-ray absorption spectroscopy (XAS) measurements on a series of iridium-based compounds (such as Ir, IrCl₃, IrO₂, Na₂IrO₃, Sr₂IrO₄, and Y₂Ir₂O₇) in order to investigate the magnitude of the spin-orbit interactions in these systems. By determining the branching ratio of the XAS white-line intensities at the Ir L₂ and L₃ absorption edges, we obtain a direct measure of the expectation value for the spin-orbit operator ($L \cdot S$). These measurements reveal remarkably strong spin-orbit interactions in almost all Ir-based compounds, with branching ratios up to several times larger than the statistical value. The branching ratio is found to be largely independent of electronic properties (metal or insulator), ionization state (Ir³⁺ [5d⁶] or Ir⁴⁺ [5d⁵]), and chemical composition (oxide or halide), although it does appear to be correlated with local Ir site symmetry and Ir-Ir bond distances.

12:51PM Z9.00009 Investigation of magnetic phase transitions in B-site disordered $\text{PbBxB}'\text{-xO}_3$ ($B = \text{Fe, Co}$ and $B' = \text{Nb, Ta}$), SHRAVANI CHILLAL, ETH Hoenggerberg, Switzerland, ELENA POPOVA, Saint Petersburg State University and Ioffe Physico-Technical Institute RAS, Russia, ERIK EULF, SEVERIAN GVASALIYA, ETH Hoenggerberg, Switzerland, TATIANA SHAPLYGINA, SERGEY LUSHNIKOV, Ioffe Physico-Technical Institute RAS, Russia, ANDREY ZHELUDEV, ETH Hoenggerberg, Switzerland, LABORATORY FOR NEUTRON SCATTERING AND MAGNETISM, ETH HOENGGERBERG, 8093 ZURICH, SWITZERLAND TEAM, IOFFE PHYSICO-TECHNICAL INSTITUTE RAS, 194021 ST. PETERSBURG, RUSSIA COLLABORATION, SAINT PETERSBURG STATE UNIVERSITY, DEPARTMENT OF CRYSTALLOGRAPHY, 199034, ST. PETERSBURG, RUSSIA COLLABORATION — Materials such as $\text{PbFe}_{0.5}\text{Nb}_{0.5}\text{O}_3$ (PFN-0.5)/ $\text{PbFe}_{0.5}\text{Ta}_{0.5}\text{O}_3$ (PFT-0.5) and $\text{PbCo}_{0.33}\text{Nb}_{0.67}\text{O}_3$ (PCN-0.33) are relaxor ferroelectrics. $\text{PbFe}_{0.5}\text{Nb}_{0.5}\text{O}_3$ (PFN-0.5) also shows anti-ferromagnetic order below ~ 143 K. Though multiferroicity is an important property of PFN-0.5, its uniqueness stems from coexisting anti-ferromagnetic and spinglass phases below ~ 12 K. Presently, it is the only known such case in a Heisenberg 3D spin system. We report a first systematic study of the H-T phase diagram of PFN-0.5 and discuss the results in the context of existing theories. In addition, we study the magnetic properties of PFT-0.5 and PCN-0.33. While PFN-0.5 and PFT-0.5 demonstrate similar behavior, PCN-0.33 does not show any anomalies that could signify magnetic ordering. We propose that the observed dramatic differences may result from partial B-site ordering.

1:03PM Z9.00010 Direct neutron scattering-based observation of spin excitons in LaCoO_3 ¹, S. EL-KHATIB, American University of Sharjah, D. PHELAN, University of Minnesota, J.A. BORCHERS, J. BARKER, P. BUTLER, NIST Center for Neutron Research, H. ZHENG, J.F. MITCHELL, Argonne National Laboratory, C. LEIGHTON, University of Minnesota — We report temperature-dependent small angle neutron scattering (SANS) results on undoped LaCoO_3 single crystals. The data reveal two main scattering components; a high q signal increasing with T above 50 K, and a low q component that turns on sharply below 60 K. The former is shown to be due to inelastic scattering quantitatively consistent with the excitations associated with the spin-state transition. Of greater interest, the low q scattering is shown to be of Guinier form, revealing scattering from a dilute assembly of magnetic objects of size approximately 15-20 nm. The abrupt onset of this scattering at 60 K, i.e. very close to the point at which prior work provided evidence of formation of interacting magnetic excitons, suggests that this represents the first direct scattering-based observation of magnetic excitons forming around O defects in LaCoO_3 .

¹Work supported by DOE (neutron scattering) and NSF

1:15PM Z9.00011 High-pressure studies on Ba-doped cobalt perovskites by neutron diffraction¹, HUIBO CAO, VASILE GARLEA, Oak Ridge National Laboratory, FANGWEI WANG, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, ANTONIO DOS SANTOS, Oak Ridge National Laboratory, ZHAOHUA CHENG, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences — Cobalt perovskite possess rich structural, magnetic and electrical properties depending on the subtle balance of the interactions among the spin, charge, and orbital degrees of freedom. Divalent hole-doped cobalt perovskites $\text{LaA}^{2+}\text{CoO}_3$ exhibit structural phase transitions, metal-insulator transitions, and multi-magnetic phase transitions. High-pressure measurement is believed to mimic the size effects of the doped ions. We performed neutron diffraction experiments on selected Ba-doped LaCoO_3 under pressures up to 6.3 GPa at SNAP at Spallation Neutron Source of ORNL. This work focuses on the high-pressure effects of the selected Ba-doped samples and the change of the phase diagram with pressure.

¹This research is supported by UT Battelle, LLC, Contract DE-AC05-00OR22725 for U.S. D.O.E., and the National Basic Research Program of China (973 Program, 2010CB833102).

1:27PM Z9.00012 Electric field tuning of the metal-magnetic transition in ionic liquid gated $\text{Ca}_3\text{Ru}_2\text{O}_7$ flakes, CONOR PULS, XINXIN CAI, Physics Department, The Pennsylvania State University, JIN PENG, ZHIQIANG MAO, Physics Department, Tulane University, YING LIU, Physics Department, The Pennsylvania State University — The recent application of ionic liquids in electric field-effect devices has provided for unprecedentedly high surface charge accumulations ($\approx 10^{14} \text{ cm}^{-2}$) due to the formation of an electronic double layer at their interface with various materials. This technique provides a tool to explore metal-insulator transitions and superconductivity in various materials including transition metal oxides. We extend this technique to the study of the physics of strongly correlated electrons in complex oxides such as the Ruddlesden-Popper (R-P) series $\text{Ca}_{n+1}\text{Ru}_n\text{O}_{3n+1}$, where $n = 1, 2, \dots \infty$. $\text{Ca}_3\text{Ru}_2\text{O}_7$, the $n = 2$ member of the R-P series, features antiferromagnetic ordering below 56 K and a first-order metal-insulator transition along with a structural transition at 48 K. We developed a technique for fabricating Hall bar devices on $\text{Ca}_3\text{Ru}_2\text{O}_7$ flakes prepared by mechanical exfoliation from bulk crystals, and performed low-temperature measurements using the ionic liquid DEME-TFSI in a top-gate configuration. We will discuss electrical transport results and the metal-magnetic transition with gate voltage tuning in these devices.

1:39PM Z9.00013 p-Electron Magnetism in anion doped BaTiO_{3-x}X_x (X=C,N,B), CHRISTOPH GRUBER, PEDRO OSVALDO BEDOLLA VELAZQUEZ, JOSEF REDINGER, PETER MOHN, Vienna University of Technology, MARTIJN MARSMAN, University of Vienna — We present VASP calculations using the HSE functional for carbon, nitrogen, and boron doped BaTiO_{3-x}X_x (X=C,N,B). We calculate a 40-atom supercell and replace one oxygen atom by C,N, or B. For all three substituents we find a magnetically ordered groundstate which is insulating for C and N and halfmetallic for B. The changes in the electronic structure between the undoped and the doped case are dominated by the strong crystal field effects together with the large band splitting for the impurity p-bands. Using an MO picture we give an explanation for the pronounced changes in the electronic structure between the insulating non-magnetic state and the as well insulating magnetic state for doped BaTiO₃. p-element doped perovskites could provide a new class of materials for various applications ranging from spin-electronics to magneto-optics.

1:51PM Z9.00014 Spin-dependent Optical Properties of Multiferroic EuO and GdN, CHUN-GANG DUAN, Key Laboratory of Polar Materials and Devices, Ministry of Education, East China Normal University — We present a first-principles study on the linear and non-linear optical properties of multiferroic EuO and GdN. In particular, we have decomposed the linear and non-linear optical spectra into spin-dependent terms, i.e., we could obtain optical spectra from individual spin channel. With the help of such method, a regular optical spectrum could present information of spin-dependent band structures, which is of great importance to the study of ferromagnetic insulators.

Friday, March 2, 2012 11:15AM - 2:15PM – Session Z11 DMP: Focus Session: Graphene Devices - Hybrid Structures 210B

11:15AM Z11.00001 Nano-patterning of fluorinated graphene by electron beam, SAVERIO RUSSO, FREDDIE WITHERS, THOMAS BOINTON, Centre for Graphene Science, University of Exeter, Exeter, United Kingdom, MARC DUBOIS, Clermont Université, UBP, Laboratoire des Matériaux Inorganiques, Aubière, France, MONICA CRACIUN, Centre for Graphene Science, University of Exeter, Exeter, United Kingdom — The development of transparent electronics is reliant on achieving high conductivity materials with a gate tuneable carrier mobility and low contact resistance at the interface with metals. Graphene — a layer of carbon atoms in a honeycomb lattice — offers just such a possibility. Functionalizing graphene with fluorine induces the opening of a band gap in the otherwise semimetallic graphene. Here we demonstrate that fluorinated graphene — a wide gap semiconductor with sp³ electron orbital hybridization — can be selectively reduced to graphene by electron-beam irradiation. We employ this functionality to pattern conductive nanostructures in a sheet of fluorinated graphene, realizing transparent graphene-based electronic devices such as nanoribbons without the need for etching of graphene. Electrical transport experiments over a wide range of temperatures (from 300K to 4K) of the ribbons show a transport gap whose size is inversely proportional to the width of the patterned ribbons. In this gap, electrons are localized, and charge transport is dominated by variable range hopping. Charging effects constitute a significant portion of the activation energy, and we find that the activation energy scales well with the width of the ribbons [Nano Lett. 11, 3912 (2011)].

11:27AM Z11.00002 Room-temperature gating of molecular junctions using few-layer graphene nanogap electrodes¹, AMELIA BARREIRO, FERRY PRINS, JUSTUS RUITENBERG, JOHANNES SELDENTHUIS, Kavli Institute of Nanoscience, TU Delft, NURIA ALIAGA-ALCALDE, ICREA, Universitat de Barcelona, LIEVEN VANDERSYPEN, HERRE VAN DER ZANT, Kavli Institute of Nanoscience, TU Delft, KAVLI INSTITUTE OF NANOSCIENCE, TU DELFT COLLABORATION — We report on a new method based on feedback controlled electroburning to controllably form nanogaps in few-layer graphene [1]. The gaps have separations on the order of 1-2 nm as estimated from a Simmons model for tunneling. Furthermore, molecules are deposited in the nanogaps. These molecular junctions display gateable IV-characteristics at room temperature. Gateable transport through molecules contacted between the electrodes demonstrates the potential of room-temperature operation of our molecular devices. Combined with the observed stability in time, our study shows that few-layer graphene nanogaps are an interesting alternative to metal electrodes. [1] Ferry Prins, Amelia Barreiro, Justus Ruitenber, Johannes Seldenthuis, Núria Aliaga-Alcalde, Lieven Vandersypen, Herre van der Zant, Nanoletters 11 (2011) 4607 - 4611

¹Fundamental Research on Matter (FOM)

11:39AM Z11.00003 Graphene Nanogap for Gate Tunable Quantum Coherent Single Molecule Electronics, TOMAS LOFWANDER, ANDERS BERGVALL, KRISTIAN BERLAND, PER HYLDGAARD, SERGEY KUBATKIN, Dep. of Microtechnology and Nanoscience - MC2, Chalmers University of Technology, SE-412 96 Goteborg, Sweden — We present atomistic calculations¹ of quantum coherent electron transport through fulleropyrrolidine terminated molecules bridging a graphene nanogap. We predict that three difficult problems in molecular electronics with single molecules may be solved by utilizing graphene contacts: (1) a back gate modulating the Fermi level in the graphene leads facilitate control of the device conductance in a transistor effect with high on/off current ratio; (2) the size mismatch between leads and molecule is avoided, in contrast to the traditional metal contacts; (3) as a consequence, distinct features in charge flow patterns throughout the device are directly detectable by scanning techniques. We show that moderate graphene edge disorder is unimportant for the transistor function.

¹ A. Bergvall, K. Berland, P. Hyldgaard, S. Kubatkin, and T. Lofwander, Phys. Rev. B. **84**, 155451 (2011).

11:51AM Z11.00004 The Role of Surfactant Adsorbates on Hysteresis and Carrier Mobility in Graphene Transistors, CHIH-JEN SHIH, GERALDINE PAULUS, QING HUA WANG, ZHONG JIN, MOON-HO HAM, DANIEL BLANKSCHTEIN, MICHAEL STRANO, Massachusetts Institute of Technology, MIT TEAM — Understanding the role of polar and ionic adsorbates on the transport characteristics of graphene transistors is important for the development of graphene-based sensor devices and printable electronics using graphene solutions. We have investigated the effects of commonly used surfactants for graphene dispersion in aqueous solution on transport characteristics of graphene transistors. The adsorbates are found to transfer electrons to graphene, scatter carrier transport, and induce more electron-hole puddles when the graphene is on an SiO₂ substrate. We relate the change in transport characteristics to specific properties of a series of anionic, cationic, and neutral surfactants using a modification of a self-consistent transport theory. To understand the effects of surfactant adsorbates trapped on either side of the graphene, suspended devices were fabricated. Strong hysteresis is observed when both surfaces were exposed to the surfactants, attributable to their function as charge traps. This work is the first to demonstrate the control of hysteresis, allowing us to eliminate it for sensor and device applications or enhance it for non-volatile memory applications.

12:03PM Z11.00005 Model results for graphene electrodes in molecular junctions, CARLO MOTTA, Dept. Materials Science, Università di Milano-Bicocca (Italy), MARIO ITALO TRIONI, CNR – National Research Council of Italy, ISTM (Italy), GIAN PAOLO BRIVIO, ETSF, Dept. Materials Science, Università di Milano-Bicocca (Italy), KIZHAKEYIL LUKOSE SEBASTIAN, IPC Department Indian Institute of Science, Bangalore (India), DANIEL SÁNCHEZ PORTAL, Centro Mixto CSIC-UPV/EHU and Donostia International Physics Center (DIPC) — Graphene is a material with a high potential for nanoelectronic applications as transparent conductive electrode. In view of a graphene-based electronics, a possible way to bridge graphene electrodes is by molecular linkers either organic molecules or graphene-derived systems such as graphene nanoribbons (GNR). In the present work, we investigated the electronic and conductive properties of such junctions for two different devices. First we modeled a photochromic switch based on diarylethene molecules, which can be activated/deactivated by light. We found a large on/off current ratio, which can be improved by modifying the functional groups of the molecule. We then investigated the properties of graphene/GNR/graphene junctions, showing that their conductive properties can be tailored by changing the length and width of the GNR. The calculations have been carried out by using the non-equilibrium Green's function method combined with density functional theory.

12:15PM Z11.00006 ABSTRACT WITHDRAWN —

12:27PM Z11.00007 Graphene Chemical sensors on Flexible Substrates, BENJAMIN MAILLY, ALLEN HSU, Massachusetts Institute of Technology, FRANCESCO PAPPALARDO, STMicroelectronics, DAWN NIDA, NSRDEC, ELIO GUIDETTI, LUIGI OCCHIPINTI, SALVATORE COFFA, STMicroelectronics, JING KONG, TOMAS PALACIOS, Massachusetts Institute of Technology, TOMAS PALACIOS TEAM — Thanks to its all-surface 2D structure combined with a very high carrier mobility, Graphene is a very promising candidate for high sensitivity and low noise chemical sensing. Indeed, graphene devices can perform electrical detection for chemical sensing in a wide variety of applications, including pH monitoring in electrolytes and glucose measurements in blood. Furthermore, the fabrication of low cost and flexible sensors can be made possible by enabling the integration of graphene on plastic substrates. Our group has developed the first solution-gated graphene field effect transistor (SGFET) on a flexible substrate, PolyEthylene Naphthalate (PEN). For this purpose, graphene grown by chemical vapor deposition is transferred on the PEN substrate, where the metal contacts had already been evaporated. The characterization of our devices in a phosphate buffer solution displays good transconductance around $0.9 \text{ mS} \cdot \text{mm}^{-1}$. pH measurements have been performed using these devices and a sensitivity as high as 22 mV/pH have been demonstrated. In addition, long term pH monitoring was demonstrated in these devices. Our on-going work focuses on studying the influence of the substrate as well as the presence of residues on the graphene surface in the pH sensing mechanism.

12:39PM Z11.00008 Graphene field-effect biosensor arrays, B. WANG, Department of Physics, Penn State University, K.L. LIDDELL, C.D. KEATING, Department of Chemistry, Penn State University, J. ZHU, Department of Physics, Penn State University — We report on the study of chemical and biological sensing using graphene field-effect transistor (GFET) arrays. Large-scale single layer graphene sheets are synthesized by low-pressure chemical vapor deposition on copper. We fabricate GFET arrays capable of operating in solutions by passivating the graphene channel with a thin oxide layer. This oxide layer also serves as the electrolyte gate dielectrics and the sensing surface. The GFET arrays exhibit an average field-effect mobility of $\sim 5000 \text{ cm}^2/\text{Vs}$ and small hysteresis in gate sweeps. We demonstrate the sensing operation of the GFET via measuring the pH value of phosphate buffer solutions. Gate sweeps indicate an approximately linear shift of the Dirac point with increasing pH, with an average slope of $+46 \text{ mV/pH}$. The viability of using GFETs to detect the specific binding of biomolecules will also be discussed.

12:51PM Z11.00009 A model of large volumetric capacitance in graphene supercapacitors based on ion clustering, BRIAN SKINNER, University of Minnesota, MICHAEL FOGLER, University of California, San Diego, BORIS SHKLOVSKII, University of Minnesota — Electric double layer supercapacitors are promising devices for high-power energy storage based on the reversible absorption of ions into porous, conducting electrodes. Graphene is a particularly good candidate for the electrode material in supercapacitors due to its high conductivity and large surface area. In this paper we consider supercapacitor electrodes made from a stack of graphene sheets with randomly-inserted “spacer” molecules. We show that the large volumetric capacitances $C > 100 \text{ F/cm}^3$ observed experimentally can be understood as a result of collective intercalation of ions into the graphene stack and the accompanying nonlinear screening by graphene electrons that renormalizes the charge of the ion clusters.

1:03PM Z11.00010 Morphology-controlled graphene aerogel for energy storage, SON TRUONG NGUYEN, Department of Mechanical Engineering - National University of Singapore, HOA TIEN NGUYEN, School of Chemical and Biomedical Engineering - Nanyang Technological University, HAI MINH DUONG, Department of Mechanical Engineering - National University of Singapore — The development of new anode/cathode materials with highly conductive, non-corrosive, high specific surface area and high porosity for energy storage devices is highly desirable. Graphene aerogels have been focused emergently recently due to novel properties of the graphene. However, the aerogel-based application performance strongly depends on the morphology and structure of the graphene aerogels. The graphene aerogels with low-density have thinner struts, a different distribution of particle sizes, and less internal connectivity. This, in turn, changes the way the material can transport electric charge. As a result, the highest surface area graphene aerogels end up having the worst electrical conductivity, and the most conductive graphene aerogels have lowest surface areas. So the best designs of the developed graphene aerogel nanostructures in terms of pore size, porosity, density and mechanical properties for energy storage devices are essential. In this work, we develop a new fabrication method of graphene aerogels with well-controlled morphology and high electrical conductivity from graphene oxide through the supercritical drying process. The morphology and electrical conductivity of the graphene aerogels are controlled by the precursor contents and the synthesis conditions. The experimental results are very useful for experimentalists deciding the best graphene aerogel nanostructures for their needs.

1:15PM Z11.00011 Electrostatic control of many-body interactions in graphene: Observation of the effects of doping on the saddle-point exciton, KIN FAI MAK, Columbia University, KELIANG HE, Case Western Reserve University, NICK PETRONE, JIM HONE, Columbia University, JIE SHAN, Case Western Reserve University, TONY HEINZ, Columbia University — Significant excitonic effects were recently identified in the optical response of graphene through the asymmetric resonance feature at 4.62 eV in the optical conductivity. The peak, which is red-shifted by nearly 600 meV from the predicted band-to-band transition energy,¹ can be considered as a saddle-point exciton. Here we report a systematic study of this excitonic feature as a function of the doping density, for densities extending up to the metallic regime² ($\sim 10^{14} \text{ cm}^{-2}$). With increasing density of either electrons or holes, the excitonic resonance is found to shift to the red and to become more symmetric in form. These experimental features agree very well with a recent ab-initio GW-Bethe-Salpeter calculation³ and can be understood as a consequence of enhanced “metallic” screening of the graphene dielectric function.⁴ In addition, analysis of the width of the excitonic peak provides information on the quasiparticle lifetime. Mechanisms for the inferred rapid quasiparticle decoherence will be discussed.

¹Mak et al. Phys. Rev. Lett. 106, 046401, (2011).

²Efetov & Kim, Phys. Rev. Lett. 105, 256805, (2010).

³Felipe H. da Jornada, J. D., Steven G. Louie. Private communications. (2011).

⁴Hwang, E. H. & Das Sarma, S. Phys. Rev. B 75, 205418

1:27PM Z11.00012 Chemically Tunable Transport Phenomena of Functionalized Graphene, NICOLAS LECONTE, AURÉLIE LHERBIER, FRANCOIS VARCHON, JEAN-CHRISTOPHE CHARLIER, Université Catholique de Louvain, Institut de la Matière Condensée et des Nanosciences (IMCN), NAPS-ETSF, Belgium, JUAN JOSE PALACIOS, ICREA, Institutio Catalana de Recerca i Estudis Avançats, Spain, DAVID SORIANO, PABLO ORDEJON, STEPHAN ROCHE, CIN2 (ICN-CSIC) and Universitat Autònoma de Barcelona, Catalan Institute of Nanotechnology, Spain — We present an ab initio multiscale study and quantum transport simulations using the Kubo formalism [1] of chemically modified graphene based materials, whose properties are tuned by changing the density and nature of grafted molecular units. Depending on the nature of the introduced molecular bonding different conduction mechanism are obtained, including transition from weak to strong Anderson localization [2,3], as well as spin-dependent phenomena [4] and magnetoresistive fingerprints [5].

References: [1] H. Ishii, F. Triozon, N. Kobayashi, K. Hirose, and S. Roche, C. R. Physique 10, 283 (2009) [2] N. Leconte, J. Moser, P. Ordejon, H. Tao, A. Lherbier, A. Bachtold, F. Alsina, C.M. Sotomayor Torres, J.-C. Charlier, and S. Roche, ACS Nano 4, 7, 4033-4038 (2010) [3] N. Leconte, A. Lherbier, F. Varchon, P. Ordejon, S. Roche, and J.-C. Charlier (accepted in PRB) [4] N. Leconte, D. Soriano, S. Roche, P. Ordejon, J.-C. Charlier, and J.J. Palacios, ACS Nano 5, 5, 3987-3992 (2011) [5] D. Soriano, N. Leconte, P. Ordejon, J.-C. Charlier, J.J. Palacios, and S. Roche, Phys. Rev. Lett. 107, 016602 (2011)

1:39PM Z11.00013 First-principles study of hybrid Graphene/MnO₂ bilayers, MIGUEL PRUNEDA, Centro de Investigación en Nanociencia y Nanotecnología (CIN2-CSIC) — Oxide nanosheets are an important and promising component for creating new materials. Their capacitance properties are particularly appealing for electric batteries. Manganese oxide nanosheets are abundant, environmental friendly, have low cost, and high electrochemical activity. However MnO₂ poor electrical conductivity and chemical stability limits its applicability as electrode material. Hybrid graphene/oxide nanostructures have been proposed to overcome these difficulties. Here, density functional theory calculations are performed to better understand the electronic properties of heterobilayers made from graphene and MnO_x monolayers. The charge transfer between graphene and MnO₂ monolayers are analyzed and related to the presence of oxygen vacancies in different concentrations, which are known to induce atomic reconstructions and phase transformations of the oxide. Magnetic properties of the heterobilayers will also be discussed.

1:51PM Z11.00014 Boron Nitride Nanoribbons: Synthesis and Future Directions¹, ASHLEY GIBB, KRIS ERIKSON, UC Berkeley, ALEX SINITSKII, University of Nebraska Lincoln, MICHAEL ROUSSEAS, NASIM ALEM, UC Berkeley, JAMES TOUR, Rice University, ALEX ZETTL, UC Berkeley, Lawrence Berkeley National Lab — Boron Nitride Nanoribbons (BNNR) have been theorized to have many interesting electrical and magnetic properties and edge states, but these characteristics have not been experimentally verified due to challenges in synthesis and purification. We have produced BNNRs by longitudinally splitting boron nitride nanotubes (BNNT) using potassium vapor as an intercalant. Due to the strong interactions between boron nitride sheets, separation of nanoribbons from their parent tubes is challenging. We have used various solvent systems to assist with separation of the ribbons with the goal of probing their properties.

¹Research supported in part by the National Science Foundation.

2:03PM Z11.00015 Electron-Hole Polarization Dynamics in Graphene Oxide¹, ANNEMARIE L. EXARHOS, MICHAEL E. TURK, ZHENG TANG LUO, A.T.C. JOHNSON, JAMES M. KIKKAWA, Department of Physics and Astronomy, University of Pennsylvania — Graphene oxide (GO) has been shown to emit broadband visible and near infrared photoluminescence (PL). Here we use polarization sensitive optical spectroscopy to study spectral diffusion and temporal dynamics of electron-hole polarization in this material. Steady state polarization memory measurements show strong polarization memory close to the excitation energy, which weakens gradually in moving toward lower emission energies. To understand the dynamics underlying this behavior, we also perform time-resolved PL studies using an optical Kerr gate with sub-picosecond temporal resolution. Polarization memories show ultrafast dynamics within the PL lifetime in solid GO preparations where the incident light lies fully in the plane of the GO flakes. Using additional knowledge gained from optical anisotropy measurements, we discuss the relevance of our polarization memory data to the origins of PL in these systems.

¹We gratefully acknowledge the primary support of NSF DMR-0907226. Construction of the Kerr gate system was supported by the Department of Energy Office of Basic Energy Sciences Award DE-SC0002158. Sample fabrication supported under NSF NSEC DMR08-32802

Friday, March 2, 2012 11:15AM - 2:15PM – Session Z12 DCMP: Graphene: Electronic Structure and Interactions - Spectroscopy 210C

11:15AM Z12.00001 Phonon self-energy corrections to non-zero wavevector phonon modes in single-layer graphene, PAULO ARAUJO, Massachusetts Institute of Technology, DANIELA MAFRA, Universidade Federal de Minas Gerais, KENTARO SATO, RICHIRO SAITO, Tohoku University, JING KONG, MILDRED DRESSELHAUS, Massachusetts Institute of Technology — Phonon self-energy corrections have mostly been studied theoretically and experimentally for phonon modes with zone-center ($q=0$) wave-vectors. Here, gate-modulated Raman scattering is used to study phonons of a single layer of graphene (1LG) in the frequency range from 2350 to 2750 cm⁻¹, which shows the G* and the G'-band features originating from a double-resonant Raman process with $q \neq 0$. The observed phonon renormalization effects are different from what is observed for the zone-center $q=0$ case. To explain our experimental findings, we explored the phonon self-energy for the phonons with non-zero wave-vectors ($q \neq 0$) in 1LG in which the frequencies and decay widths are expected to behave oppositely to the behavior observed in the corresponding zone-center $q=0$ processes. Within this framework, we resolve the identification of the phonon modes contributing to the G* Raman feature at 2450 cm⁻¹ to include the iTO+LA combination modes with $q \neq 0$ and the 2iTO overtone modes with $q=0$, showing both to be associated with wave-vectors near the high symmetry point K in the Brillouin zone.

11:27AM Z12.00002 Impact of Graphene-Metal Interfaces on the Raman and Transport Properties of Graphene Devices¹, ALLEN HSU, MARIO HOFMANN, WENJING FANG, KI KANG KIMG, JING KONG, TOMAS PALACIOS, MIT — Graphene is an amazing nano-material with many exciting properties and applications. However, due to its low dimensionality, the performance of this material is mainly limited by interfaces and surface properties. One of these interfaces, important for graphene field effect transistors and catalysts supported on graphene membranes, is that between the graphene and a metal layer. In this study, we experimentally examine the impact of various metals on graphene through Raman and Transmission Electron Microscopy. We find that strong graphene-metal interactions have significant impacts on the phonon structure in graphene. Furthermore, we observe changes in our Raman spectra relating to the crystallographic orientation between a metal and graphene.

¹Army Research Labs, MSD Focus Center, ONR Gate Muri, ISN

11:39AM Z12.00003 Raman spectroscopy of sputtered metal-graphene and metal-oxide-graphene interfaces, CHING-TZU CHEN, MARCIN GAJEK, MARCUS FREITAG, MARCELO KURODA, VASILI PEREBEINOS, SIMONE RAOUX, IBM TJ Watson Research Center — In this talk, we report our recent development in sputtering deposition of magnetic and non-magnetic metal and metal-oxide thin films on graphene for applications in spintronics and nanoelectronics. TEM and SEM images demonstrate homogeneous coverage, uniform thickness, and good crystallinity of the sputtered films. Raman spectroscopy shows that the structure of the underlying graphene is well preserved, and the spectral weight of the defect D mode is comparable to that of the e-beam evaporated samples. Most significantly, we report the first observation of graphene-enhanced surface excitations of crystalline materials. Specifically, we discover two pronounced dispersive Raman modes at the interface of graphene and the nickel-oxide and cobalt-oxide films which we attribute to the strong light absorption and high-order resonant scattering process in the graphene layer. We will present the frequency-dependent, polarization-dependent Raman data of these two modes and discuss their microscopic origin.

11:51AM Z12.00004 Effects of sliding on Raman spectrum of bilayer graphene¹, SEON-MYEONG CHOI, Korea Institute for Advanced Study, Seoul 130-722, Korea, SEUNG-HOON JHI, Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea, YOUNG-WOO SON, Korea Institute for Advanced Study, Seoul 130-722, Korea — Electronic properties of graphene are changed by various external effects such as strain, doping, and defects, etc. Such effects can be measured by Raman spectroscopy. For example, doping and defects increase the intensities of D-peak of single layer graphene, while the external strains generate splitting of G- and 2D-peaks respectively. In bilayer graphene, sliding motions between two layers also can change its electric and optical properties. Based on the first principles calculation methods, the sliding between two layers of bilayer graphene is shown to change the electronic and phonon dispersions, thereby altering its Raman spectrum significantly.

¹Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2011-C1-21).

12:03PM Z12.00005 Electronic Structure of Suspended Bilayer Graphene¹, PO-CHUN YEH, KEVIN KNOX, WENCAN JIN, JERRY DADAP, PHILIP KIM, RICHARD M. OSGOOD, Columbia University, ALEXEI BARINOV, ELETTRA TRIESTE — Bilayer graphene is an important medium for achieving band-gap tuning for graphene applications in digital electronics, such as in graphene nanoribbon FETs. ARPES is an important tool for measuring the electronic structure of crystals in the vicinity of the Dirac point. While accurate measurements have been made on the bilayer graphene band-structure on SiC, similar effort on free-standing graphene has not yet been reported. In this paper, we describe measurements of the band-structure of a $\sim 650 \mu\text{m}^2$ sample of exfoliated bilayer graphene suspended over $5\text{-}\mu\text{m}$ -diameter wells formed in SiO_2 on a Si substrate. The measurements, performed at the Spectromicroscopy Beamline at ELETTRA with photon energy of 27eV, show that this material is essentially undoped and we compare its band structure with that expected from tight-binding calculations.

¹Work is supported by DOE grant DE-FG 02-04-ER-46157. Sample preparation is supported by AFOSR MURI Grant FA9550-09-1-0705

12:15PM Z12.00006 Electrical transport between single-crystal domains in graphene: bigger is not always better, ADAM TSEN, LOLA BROWN, MARK LEVENDORF, Cornell University, FERESHTE GHAAHARI, Columbia University, PINSHANE HUANG, CARLOS RUIZ-VARGAS, DAVID MULLER, Cornell University, PHILIP KIM, Columbia University, JIWOONG PARK, Cornell University — Single-layer graphene can now be produced on the centimeter or even meter scale using chemical vapor deposition. These large-scale graphene films are polycrystalline, consisting of many separate single-crystal domains, as was recently identified using transmission electron microscopy. Understanding the electrical transport across these domains is relevant not only for device applications, but has also been the focus of many fundamental studies. Here, we first examine the structure of graphenes produced under different growth conditions using dark-field transmission electron microscopy (DF-TEM). We find three classes of grain boundaries—continuous, amorphous, and overlapped. Next, we study the electrical properties of graphene devices consisting of individual grain boundaries that have been first imaged by DF-TEM. We find that the grain boundaries exhibit an additional gate-dependent resistance that is keenly sensitive to growth conditions. Surprisingly, this resistance is an order of magnitude greater for growths with larger grain size due to more poorly-connected domains. Our results show that domain size is not the single most important parameter determining electrical performance of large-scale graphene films—the quality of inter-domain connections is just as crucial.

12:27PM Z12.00007 Trapping Image State Electrons on Graphene Layers and Islands¹, JERRY DADAP, Columbia University, DANIEL NIESNER, THOMAS FAUSTER, Universitat Erlangen-Nurnberg, NADER ZAKI, KEVIN KNOX, PO-CHI YEH, ROHAN BHANDARI, RICHARD M. OSGOOD, Columbia University, MARIN PETROVIC, MARKO KRALJ, Institut za Fiziku, Croatia — The understanding of graphene-metal interfaces is of utmost importance in graphene transport phenomena. To probe this interface we use time- and angle-resolved two-photon photoemission to map the bound, unoccupied electronic structure of the weakly coupled graphene/Ir(111) system. The energy, dispersion, and lifetime of the lowest three image-potential states are measured. In addition, the weak interaction between Ir and the smooth, epitaxial graphene permits observation of resonant transitions from an unquenched Shockley-type surface state of the Ir substrate to graphene/Ir image-potential states. The image-potential-state lifetimes are comparable to those of mid-gap clean metal surfaces. Evidence of localization of the excited image-state electrons on single-atom-layer graphene islands is provided by coverage-dependent measurements.

¹Columbia work supported by DOE grant DE-FG 02-04-ER-46157

12:39PM Z12.00008 Image potential states of Graphene/Ru(0001) interface, SHENGMIN ZHANG, XUEFENG CUI, LEIMING WANG, HRVOJE PETEK, Department of Physics and Astronomy, University of Pittsburgh, LABORATORY OF ULTRAFAST DYNAMICS TEAM — Graphene, the parent of all graphitic forms, has become one of the most exciting topics in condensed matter physics. It is now well understood that the low-energy electronic properties of graphene are described by two-dimensional Dirac equation for massless particles, but the unoccupied bands are hardly unexplored in experimental research. In this talk we will present new results on the unoccupied electronic structure, namely the image potential states (IPS), measured by two-photon photoemission spectroscopy (2PPS). The single layer graphene is prepared by thermal decomposition of ethylene on a Ru(0001) surface. Through low energy electron diffraction (LEED) and 2PPS, we verify formation of high-quality, single layer thick graphene samples. Based on the graphene/Ru(0001) system, we first measured the surface structure and IPS on Ru(0001) by angle-resolved 2PP. From the angle-resolved spectra, we obtain the effective mass $m_{eff} = 1.1m_e$, which is close to the expected value for a free electron state of $m_{eff} = 1m_e$. With the same method, we measured the IPS on the graphene/Ru(0001) surface. However, we observe complex structure consisting of two nearly degenerate states that reflect the mutual interactions between graphene and Ru(0001) substrate.

12:51PM Z12.00009 Energy loss spectroscopy of epitaxial and free-standing multilayer graphene, OLEKSIY ROSLYAK, GODFREY GUMBS, Department of Physics and Astronomy, Hunter College at the City University of New York, 695 Park Avenue New York, NY 10065, USA, DANHONG HUANG, Air Force Research Laboratory, Space Vehicles Directorate, Kirtland Air Force Base, NM 87117, USA — We present a formalism and numerical results for the energy loss of a charged particle scattered at an arbitrary angle from epitaxially grown multilayer graphene (MLG). It is compared with that of free-standing graphene layers. Specifically, we investigated the effect of the substrate induced energy gap on one of the layers. The gap yields collective plasma oscillations whose characteristics are qualitatively and quantitatively different from those produced by Dirac fermions in gapless graphene. The range of wave numbers for undamped self-sustaining plasmons is increased as the gap is increased, thereby substantially increasing and red-shifting the MLG stopping power for some range of charged particle velocity. We also applied our formalism to interpret several distinct features of experimentally obtained electron energy loss spectroscopy (EELS) data.

1:03PM Z12.00010 Interface Science in Graphene Materials: An Electronic Structure View of Soft X-Ray Spectroscopy , LIANG ZHANG, JUNFA ZHU, University of Science and Technology of China, WEI-CHENG WANG, CHINGLIN CHANG, Tamkang University, PER-ANDERS GLANS, JINGHUA GUO, Lawrence Berkeley National Laboratory — The ability to control the morphology of nanostructured carbon-based materials is of crucial importance for the applications of photovoltaic, energy storage such as Li-ion batteries, etc. The properties of matter at nanoscale dimensions are dramatically different from the bulk. The differences arise through quantum confinement, altered thermodynamics or changed chemical reactivity. In general, electronic structure ultimately determines the properties of matter, thus understanding of electronic structure is crucial for tailoring the properties of nanoscale systems. The graphene/Cu and SiO₂ composites have been studied using XAS, XES and RIXS. New electronic states in the conduction band are observed, which are ascribed to the monovacancy defect state and interfacial interaction. The polarized XAS spectra demonstrate that the graphene/Cu exhibits high alignment and weak corrugation. Significant intensity modulation of resonant XES spectral shape upon different excitation energies near the C K-edge, indicates that graphene preserves an intrinsic symmetry and the interaction between graphene and Cu has unique influence on the electronic structure of graphene. The broad RIXS features and subtle shifts are observed in the RIXS spectra of graphene/Cu, which can be attributed to the strong electron-phonon scattering, charge transfer from the Cu sites

1:15PM Z12.00011 Electron-Phonon Coupling and Large Intrinsic Bandgap in Highly-Screened Graphene , DAVID SIEGEL, University of California, Berkeley / Lawrence Berkeley National Lab, CHOONGYU HWANG, Lawrence Berkeley National Laboratory, ALEXEI FEDOROV, Advanced Light Source, Lawrence Berkeley National Laboratory, ALESSANDRA LANZARA, University of California, Berkeley / Lawrence Berkeley National Lab — The electron-electron and electron-phonon interactions are two of the most fundamental interactions in many-body physics, leading to Mott insulating behavior and superconductivity. In graphene, the pointlike Fermi surface and linear band dispersions give these interactions distinctive characteristics with respect to normal metals. Here we present data on the electron-phonon interaction in highly-screened graphene, which we have analyzed by angle-resolved photoemission spectroscopy (ARPES). In contrast with every previous ARPES study, the magnitude of our extracted electron-phonon coupling constants generally agree with theoretical predictions. We also demonstrate the presence of a 400 meV bandgap at the Dirac point in epitaxial graphene on a copper substrate. These results shed light on the nature of the electron-phonon interaction and the tunability of the Dirac quasiparticles in graphene.

1:27PM Z12.00012 Photoemission on highly-ordered arrays of structured epitaxial graphene , JEREMY HICKS, J. PALMER, H. TINKEY, K. SHEPPERD, Georgia Institute of Technology, A. TEJEDA, A. TALEB-IBRAHIMI, P. LE FÈVRE, Synchrotron SOLEIL, C. BERGER, Georgia Institute of Technology & CNRS-Institut Néel, W.A. DE HEER, E.H. CONRAD, Georgia Institute of Technology — We use the recently-demonstrated method of growing pre-patterned epitaxial graphene directly from structured silicon carbide (SiC) to produce dense, highly-ordered arrays of graphene nanoribbons suitable for macroscopic characterization methods. Specifically, we use angle-resolved photoemission spectroscopy (ARPES) to observe the ensemble-averaged band structure of nanoribbons with nominal widths of 10nm and 30nm. A Dirac-like cone is visible down to 10nm and, although the graphene is a single layer, it is undoped, in contrast to single layer graphene nanoribbons on either the Si- or C-terminated faces of SiC.

1:39PM Z12.00013 Spectroscopic Ellipsometry, Auger and STM Characterization of Epitaxial Graphene grown on 6H-SiC (0001) , FLORENCE NELSON, ALAIN C. DIEBOLD, College of Nanoscale Science and Engineering, University at Albany, ANDREAS SANDIN, DAN DOUGHERTY, DAVE ASPNES, JACK ROWE, Department of Physics, North Carolina State University — Graphene grown by the thermal decomposition of SiC has become of interest to the semiconductor industry due to its unique, high-mobility electronic structure. The growth is of a more scalable nature when compared to exfoliated flakes produced from the “scotch tape” method. The resulting film rests on a “buffer layer” separating the graphene from the underlying substrate, which is thought to consist of a mixture of sp² and non-sp² bonding due to the sp³ bonding of the SiC substrate. The mobilities of the graphene layer have previously been shown to differ from that of the interface layer. We investigate the difference in the optical response of the two layers using Spectroscopic Ellipsometry and find a red-shift of the ~4.5 eV absorbance found in graphene due to the exciton-dominated transition at the M point of the Brillouin Zone. The structural characterization of the films are performed through Auger and STM on substrates which were cleaned by CMP and chemical etching methods prior to the epitaxial growth in UHV.

1:51PM Z12.00014 Vibrational spectroscopy of molecules adsorbed on graphene , YAQING BIE, JASON HORNG, FENG WANG, UC Berkeley — Graphene, being a monolayer membrane, is extremely sensitive to the environment. Understanding how it interacts with adsorbed molecules and polymers is fundamental for improving graphene electronic devices. Previous studies show that electrons in graphene can couple efficiently to phonon vibrations of the substrate, which can become a limiting factor for graphene mobility. Here we investigate the interactions between vibrations of adsorbed molecules with graphene using vibrational spectroscopy. We performed the vibrational spectroscopy using a broadband tunable infrared laser source and a high precision spectrometer. We will discuss how the vibration frequencies of the adsorbed molecules get modified through their interactions with graphene.

2:03PM Z12.00015 Magneto-phonon resonance of shear modes of bilayer graphene , KOSTYANTYN KECHEDZHI, Department of Physics and Astronomy, Rutgers The State University of New Jersey, 136 frelinghuysen rd, Piscataway, 08854 NJ, USA, MARK OLIVIER GOERBIG, JEAN-NOEL FUCHS, Laboratoire de Physique des Solides, Université Paris-Sud, CNRS UMR 8502, F-91405 Orsay, France, VLADIMIR FAL'KO, Department of Physics, Lancaster University, Lancaster, LA1 4YB, UK — We describe the frequency renormalization of the recently observed shear phonon mode of bilayer graphene due to electron-phonon coupling. In presence of a relatively strong magnetic field resonances with electronic inter-Landau level transitions are possible. When the resonance condition is satisfied a fine structure of the Raman line corresponding to the shear mode arises which is linear in electron-phonon coupling constant. This effect can be used to measure the strength of the electron-phonon coupling for the shear mode.

Friday, March 2, 2012 11:15AM - 2:03PM –

Session Z13 DMP GMAG: Focus Session: Magnetic Nanostructures-Nanoparticles and Granular Systems 211

11:15AM Z13.00001 Unexpected magnetization in highly pure metal oxide nanoparticles , C.B. HANNA, GORDON ALANKO, BOONE BEAUSOLEIL, JORDAN CHESS, AARON THURBER, ALEX PUNNOOSE, Boise State University — We report the synthesis and characterization of a large set of highly pure metal oxide (CeO₂, SnO₂ and ZnO) nanoparticles of ultra-small size (2-10 nm). While the metal oxide systems in this study are non-magnetic as bulk materials, our prepared nanoparticles possess an unexpected small room-temperature ferromagnetic magnetization on the order of 0.001 emu/g. This magnetization is shown to not be a result of magnetic impurities, and is discussed in terms of modification of the electronic structure and crystal lattice. These nanoparticles were thoroughly characterized in their size and phase by x-ray diffraction, morphology by transmission electron microscopy, chemical state and elemental purity by x-ray photoelectron spectroscopy, electronic bandgap by UV-vis absorption spectroscopy, and magnetic properties by vibrating sample magnetometry and electron paramagnetic resonance.

11:27AM Z13.00002 Magnetic Transitions in Granular FeRh¹, B. KAESWURM, F. JIMÉNEZ-VILLACORTA, R. BARUA, D. HEIMAN, L.H. LEWIS, Northeastern University — The relationship between the crystallographic lattice and magnetism in materials undergoing first order thermodynamic phase transitions, where structural and magnetic phase transitions occur simultaneously, are not fully understood. Nanostructuring of such materials offers a route to tailor these transitions through alteration of free energy terms dependent upon the surface area and volume of finite systems. Previous studies in melt spun ribbons of FeRh nanoprecipitates in a Cu matrix have shown a reduced phase transition compared to bulk [1]. In this study nanostructured FeRh films were obtained by RF sputter deposition in nonmagnetic matrices of Cu, Si and alumina. After vacuum annealing, the structure and magnetism of the samples were studied. Preliminary results highlight the relationships between chemistry, nanostructuring and magnetic response in the FeRh system.

[1] Evidence for Highly Suppressed Magnetostructural Transition Temperature in Nanostructured FeRh, R. Barua; F. Jimenez-Villacorta; H. Jiang; J.E. Shield; D. Heiman; L.H. Lewis, IEEE MMM Conference 2011, Scottsdale, Arizona, US, Abstract No CE-05

¹Research funded by U.S. DOE [DE-SC0005250]

11:39AM Z13.00003 Investigation of Local Structures and Magnetism in Mn-doped Y₂O₃ Nanocrystals¹, T.S. WU, S.L. CHANG, Y.L. SOO, National Tsing Hua University — Nanocrystals of Mn-doped Y₂O₃ were prepared by thermal decomposition method and alternately annealed in oxygen and forming gas to vary the oxygen deficiency. X-ray diffraction (XRD), high-resolution transmission electron microscopy (HR-TEM), x-ray absorption fine structures (XAFS), and superconducting quantum interference device (SQUID) techniques were applied before and after each annealing to monitor structural and magnetic variations of the sample. The XRD data show that these annealing treatments do not appreciably change the average particle size of the sample. An amorphous-to-crystalline long-range-order structural change was observed for the first annealing applied to the as-made samples. The short-range-order structure exhibited by XAFS reveals that O vacancies surrounding magnetic impurity atoms were appreciably increased by forming-gas-annealing and decreased by oxygen-annealing in the samples. The increase and decrease of O vacancies are accompanied by enhanced and reduced saturation magnetization as demonstrated by SQUID, respectively. Our experimental results demonstrate clear correlation between magnetism and O vacancies around magnetic ions and therefore strongly support the bound magnetic polaron model in these nanocrystal DMO samples.

¹This work has been supported by NSC in Taiwan.

11:51AM Z13.00004 Preparation and Characterization of Mg Substituted NiCuZn Nano Ferrites for Multilayer Chip Inductors, R.C. REDDY A, SUJATHA CH, VENUGOPAL REDDY K, SOWRI BABU K, National Inst. of Technology Warangal - 506004 (A.P) India, H.RAO K, Andhra University Visakhapatnam - 530003 (A.P) India — The present paper examines the effect of magnesium substitution on structural and magnetic properties of NiCuZn nano ferrites synthesized by sol - gel method. Formation of single phase spinel structure was confirmed both from XRD and FTIR. The initial permeability shows decreasing trend with increasing Mg concentration due to reduced magnetization, grain size and increased magneto - crystalline anisotropy constant. At the same time, the cut off frequency increases with increasing Mg content. This is attributed to domain wall pinning arising due to the presence of non magnetic magnesium ions. Also the permeability is observed to be constant up to 10MHz frequency range showing compositional stability and quality of the material. The magnetic loss factor shows very low values at higher frequencies. It is concluded that even though both zinc and magnesium are non magnetic ions, substitution of one cation by another prone to influence the magnetic properties due to their change in dimension and cation distribution among the two available sites of a spinel system. These samples have advantages of low sintering temperature find applications in multilayer chip inductors due to their high and constant permeability even at higher frequencies.

12:03PM Z13.00005 Ferromagnetic Resonance on Micro- and Nanoferrites in Millimeter Waves, KONSTANTIN KOROLEV, Tufts University, JOHN MCCLOY, Glass and Materials Science Team, Pacific Northwest National Laboratory, Richland, WA, USA, MOHAMMED AFSAR, Tufts University, TUFTS UNIVERSITY TEAM, GLASS AND MATERIALS SCIENCE TEAM TEAM, EXTREMELY HIGH FREQUENCY MEDICAL AND TECHNICAL ASSOCIATION TEAM — Complex magnetic permeability and dielectric permittivity of micro- and nano-sized powdered barium ferrite (BaFe₁₂O₁₉) and strontium ferrite (SrFe₁₂O₁₉) have been studied in a broadband millimeter wave frequency range for the first time. Transmittance measurements have been performed using a free space quasi-optical millimeter wave spectrometer, equipped with a set of high power backward wave oscillators. Backward wave oscillators have been used as sources of tunable coherent radiation at each individual *Q*-, *V*- and *W*- frequency bands. Real and imaginary parts of dielectric permittivity for both types of micro- and nanoferrites have been calculated using analysis of recorded high precision transmittance spectra. Frequency dependences of the magnetic permeability have been obtained from Schlömann's equation for partially magnetized ferrites. Tunable millimeter wave absorber, based on micro- and nano-sized powdered ferrite materials is presented.

12:15PM Z13.00006 Polarized Magnetic Induced Broadening of Plasmon-photonics in Fe₃O₄-Silicone Elastomer Composite Films¹, DANHAO MA, DEREK CAPLINGER, DUSTIN HESS, KOFI ADU, Department of Physics, The Pennsylvania State University, Altoona College, Altoona, PA 16601, RICHARD BELL, Department of Chemistry, The Pennsylvania State University, Altoona College, Altoona, PA 16601 — We report systematic studies of polarization dependence of magneto-optical response of Fe₃O₄-silicone elastomer composite. The Fe₃O₄ particles were aligned in the elastomer matrix with static magnetic field. The optical response of two composites containing 5wt% and 15wt% of 20nm-30nm diameter Fe₃O₄ particle aligned in- and out-of-plane were measured with an absorption spectrometer. We observed a systematic redshift in the optical response of the out-of-plane samples with increasing static magnetic field. Furthermore, the observed redshift increases with increasing weight percent of Fe₃O₄ in the composite; obtaining a maximum shift of ~ 174 nm at 600 Gauss in the 15wt% Fe₃O₄-elastomer composite films. The observed redshift in the optical response of the out-of-plane composite is attributed to the effect of magnetic field strength and the metal particle/cluster size in the elastomer. However, there were no observable shifts in the in-plane samples, suggesting that the orientation (polarization) of the magnetic dipole and the induced electric dipole play a crucial role in the optical response.

¹This Work is Funded by Penn State Altoona Undergraduate Research Grant.

12:27PM Z13.00007 Precipitation of coherent FeRh nanoparticles with highly suppressed magnetostructural transition temperatures in rapidly solidified (FeRh)₅Cu₉₅ alloys¹, RADHIKA BARUA, Department of Chemical Engineering, Northeastern University, XIUJUAN JIANG, JEFF SHIELD, Department of Mechanical Engineering, University of Nebraska, DON HEIMAN, Department of Physics, Northeastern University, LAURA LEWIS, Department of Chemical Engineering, Northeastern University — Magnetostructural phase transitions have the capability of delivering large functional effects in response to small excursions in magnetic field, temperature and strain; this potential might be amplified in nanostructured systems by virtue of large surface:volume ratios. Nanoprecipitates (~10nm) of FeRh, a well-known magnetostructural material, were studied with structural and magnetic probes in a rapidly solidified phase-separated system of (FeRh)₅Cu₉₅. Magnetization studies indicate a dramatic reduction in the magnetostructural phase transition temperature (T_t) of the nanoscaled FeRh phase relative to the bulk value ($\Delta T = T_{t,Bulk} - T_{t,Nano} = 220$ K). Transmission electron microscopy (TEM) and selected area electron diffraction (SAED) reveals a coherent orientational relationship between the FeRh ($a_{FeRh} = 3.09$ Å) and Cu ($a_{Cu} = 3.78$ Å) phases. At the matrix/precipitate interface a constrained misfit strain of $\epsilon = 0.18$ is observed. The reduction of the magnetostructural phase transition temperature and evolution of the magnetic properties with system annealing is analyzed in the context of the strain between the FeRh nanoparticles and the Cu matrix.

¹Research conducted under the auspices of U.S. Department of Energy (DOE Grant DE-SC0005250)

12:39PM Z13.00008 Biomimetic Control of Magnetite Shape and Morphology using Polyaminoacids, CEM LEVENT ALTAN, SEYDA BUCAK, T.C. Yeditepe University, NICO SOMMERDIJK, Eindhoven University of Technology — Inspired by nature, this work explores the use of randomly sequenced poly(amino acids) to control the size, morphology and magnetic properties of magnetite via synthetic methods in a controlled manner as in the case of magnetotactic bacteria. Aqueous partial oxidation and chemical precipitation methods are employed for the synthesis of 7 - 50 nm iron oxide nanoparticles at room temperature. X-ray diffraction (XRD) and Transmission Electron Microscopy (TEM) revealed formation of iron oxide nanoparticles both in the presence and absence of poly(amino acids). In the presence of random poly(amino acid)s with different compositions consisting of E, K and A amino acids the mean particle size for the chemical precipitation method is decreased regardless of amino acid composition. For partial oxidation method, mean particle size is also decreased and nanoparticle strings are observed while synthesized in the presence of poly(aspartic acid). Magnetic properties of particles obtained via different routes are also investigated. This provides a bio-inspired route for control over size, morphology and magnetic properties of magnetite nanoparticles.

12:51PM Z13.00009 High Resolution Far Infrared Study of Antiferromagnetic Resonance Transitions in α -Fe₂O₃ (hematite), SHIN GRACE CHOU, DAVID F. PLUSQUELLIC, PAUL E. STUTZMAN, SHUANGZHEN WANG, EDWARD J. GARBOCZI, WILLIAM F. EGELHOFF¹, National Institute of Standards and Technology — In this study, we report high resolution optical measurements of the temperature dependence of the antiferromagnetic (AFM) transition in α -Fe₂O₃ (hematite) between (0.5 and 10) cm⁻¹. The absorption peak position, over a large temperature range, is found to be in agreement with a modified spin-wave model at both the high and low temperature phases, where the temperature is above and below the Morin transition temperature, respectively. The high spectral resolution optical measurements as demonstrated in this study allow unprecedented zero-field spectral analysis of the zone center AFM magnon in a previously challenging spectral region, giving insights into the role of temperature and strain on the exchange and anisotropy interactions in the system. The results also suggest that the frequency-resolved measurement platform could be extended for room-temperature non-destructive examination and imaging applications for antiferromagnetic materials and devices.

¹deceased

1:03PM Z13.00010 Mapping Nanomagnetic Fields Using a Radical Pair Reaction¹, HOHJAI LEE, Department of Chemistry and Chemical Biology, Harvard University, NAN YANG, School of Engineering and Applied Sciences, Harvard University, ADAM COHEN, Department of Chemistry and Chemical Biology and Department of Physics, Harvard University — We visualized the magnetic field around ferromagnetic nanostructures using a combination of a standard epifluorescence microscope and a fluorescence chemical indicator of magnetic field (H. Lee et al., Nano Lett. DOI: 10.1021/nl202950h). The indicator was a chain-linked electron donor-acceptor molecule, phenanthrene-(CH₂)₁₂-O-(CH₂)₂-dimethylaniline, that forms spin-correlated radical pairs upon photoexcitation. The magnetic field altered the coherence spin dynamics, yielding an 80% increase in exciplex fluorescence in a 0.1 T magnetic field. The magnetic field distributions were quantified to precision of 1.8×10^{-4} T by image analysis and agreed with finite-element nonmagnetic simulations.

¹This work was supported by the Defense Advanced Research Projects Agency (DARPA) YFA Grant N66001-091-2104 and the Office of Naval Research (ONR) YIP Grant N000140910868.

1:15PM Z13.00011 Electrostatic Force Microscopy of Fe₃O₄ nanoparticles, A. MOTTAGHIZADEH, LPEM, ESPCI-ParisTech-UPMC-CNRS, Paris, France, P.L. LANG, LPEM, ESPCI-ParisTech-UPMC-CNRS, Paris, France; School of Science, BUPT, Beijing, China, L. CUI, LPEM, ESPCI-ParisTech-UPMC-CNRS, Paris, France; IOP and Beijing Nat. Lab. for Cond. Matt. Phys., CAS, Beijing, China, J. LESUEUR, A. ZIMMERS, H. AUBIN, LPEM, ESPCI-ParisTech-UPMC-CNRS, Paris, France, J. LI, D.N. ZHENG, IOP and Beijing Nat. Lab. for Cond. Matt. Phys., CAS, Beijing, China, V. REBUTTINI, Dept. of Chemistry, CICECO, University of Aveiro, Aveiro, Portugal, N. PINNA, Dept. of Chem., CICECO, Univ. of Aveiro, Portugal; WCU, C2E2, School of Chem. and Biological Engineering, College of Engineering, SNU, Seoul, Korea — The electronic compressibility is a fundamental property that characterizes the electronic properties of materials submitted to an external electric field. In metals (insulators), the electronic compressibility is large (small) and leads to a small (large) screening length. Variations of the screening length can be observed through measurements of the “quantum” capacitance between one material and a metallic counter-electrode. Using an Electrostatic Force Microscope (EFM), we measured maps of the local capacitance of 8 nm magnetite nanoparticles synthesized following the “benzyl alcohol route” deposited on a metallic substrate. Magnetite, an inverse spinel structure of composition Fe₃O₄, is a material with strongly correlated electronic properties and presents a metal-insulator transition at 120 K, the so-called Verwey transition. We present EFM measurements of these nanoparticles as a function of tip-sample distance and temperature.

1:27PM Z13.00012 Nano-scaled magnetic domains in CMR-manganites, YOSHIHIKO TOGAWA, Nanoscience and Nanotechnology Research Center, Osaka Prefecture University, TSUKASA KOYAMA, KEN HARADA, SHIGEO MORI, Department of Materials Science, Osaka Prefecture University — La_{1-x}Sr_xMnO₃ (LSMO) is one of interesting materials with strongly-correlated electrons, wherein a complex variety of ground states are generated depending on the Sr doping concentration x . In this work, we have microscopically investigated changes of the magnetic states by applying magnetic fields in single crystals of LSMO by using Lorentz transmission electron microscopy. In the specimen with $x = 0.175$, the magnetic stripe domains appear at regular intervals of about 200 nm as a magnetic ground state in zero magnetic field at 110 K. Importantly, we have clarified that magnetic domains as large as 100 nm are generated in the magnetic stripe domains in vertical magnetic fields and take a form of the magnetic vortex with tilted magnetic components. To the best of our knowledge, these magnetic domains are new kinds of magnetic ground states (spin textures) in manganites. In the presentation, we will explain detailed responses of magnetic vortices to various experimental parameters of external magnetic fields and discuss the nucleation and growth mechanism of magnetic vortices in the magnetic stripe domains and the expected functionality of magnetic vortices in manganites.

1:39PM Z13.00013 Anomalous thermal hysteresis in the high-field magnetic moments of magnetic nanoparticles embedded in multi-walled carbon nanotubes, GUO-MENG ZHAO, California State University, Los Angeles, JUN WANG, Ningbo University, YANG REN, Argonne National Lab, PIEDER BEELI, California State University, Los Angeles — We report high-temperature (300-1120 K) magnetic properties of Fe and Fe₃O₄ nanoparticles embedded in multi-walled carbon nanotubes. We unambiguously show that the magnetic moments of Fe and Fe₃O₄ nanoparticles are seemingly enhanced by a factor of about 3 compared with what they would be expected to have for free (unembedded) magnetic nanoparticles. What is more intriguing is that the enhanced moments were completely lost when the sample was heated up to 1120 K and the lost moments at 1120 K were completely recovered through several thermal cycles below 1020 K. The anomalous thermal hysteresis of the high-field magnetic moments is unlikely to be explained by existing physical models except for the high-field paramagnetic Meissner effect due to the existence of ultrahigh temperature superconductivity in the multi-walled carbon nanotubes.

1:51PM Z13.00014 Carbon Nanostraws with Novel Magnetic Properties for Microwave Devices and Biomedical Applications¹, K. STOJAK, S. CHANDRA, S. PAL, H. KHURSHID, M.H. PHAN, H. SRIKANTH, University of South Florida-Physics — Carbon nanotubes (CNTs) have stirred interest in many areas of current research because of their unique electrical properties and potential use in the biomedical field. Here, we report on the synthesis, structural, and magnetic characterization of “nanostraws,” which consist of nanoparticle-filled CNTs made by a template-assisted chemical vapor deposition method. In this study, the nanoparticle fillers are magnetite, cobalt ferrite, and nickel ferrite. These high-aspect ratio magnetic nanostructures have a tunable anisotropy in addition to enhanced magnetic interactions amongst the CNT-encapsulated magnetic nanoparticles. Enhanced magnetic interactions include higher saturation magnetization and higher blocking temperature. These properties are desirable for microwave devices and biosensing applications.

¹Work Funded by CIFM and FCASST

Friday, March 2, 2012 11:15AM - 2:03PM – Session Z16 DCMP: Disordered and other Strongly Correlated Systems 251

11:15AM Z16.00001 Composition-tuned smeared phase transitions, DAVID NOZADZE, FAWAZ HRAHSEH, CHRISTOPHER SVOBODA, THOMAS VOJTA, Missouri University of Science and Technology — Phase transitions in random systems are smeared if individual spatial regions can order independently of the bulk system. We study such smeared phase transitions (both classical and quantum) in substitutional alloys A_{1-x}B_x that can be tuned from an ordered phase at composition $x = 0$ to a disordered phase at $x = 1$. We show that the ordered phase develops a pronounced tail that extends over all compositions $x < 1$. Using optimal fluctuation theory, we derive the composition dependence of the order parameter and other quantities in the tail of the smeared phase transition. We also investigate the influence of spatial disorder correlations on smeared phase transitions. We compare our results to computer simulations of a toy model, and we discuss experiments.

11:27AM Z16.00002 Understanding zero-bias anomalies in disordered strongly-correlated electron systems: An atomic-limit perspective¹, RACHEL WORTIS, LISTER MULINDWA, Trent University — Many interesting phenomena arise in strongly-correlated electron systems which are disordered, either intrinsically or due to doping. In trying to understand these phenomena, the single-particle density of states provides a useful bridge between theory and experiment. Progress has recently been made in understanding the origins of the zero-bias anomaly that appears in these systems, and how this zero-bias anomaly differs from that studied by Altshuler and Aronov in weakly-correlated systems. Because both interactions and disorder reduce the importance of kinetic energy, the atomic limit provides a useful perspective. The case of long-range 1/r interactions in the atomic limit was addressed by Efros and Shklovskii, who showed the density of states is suppressed to zero at the Fermi level. However, the argument they used does not address screened interactions or the effect of double occupancy. This talk presents classical Monte Carlo results for the density of states in the atomic limit of the extended Anderson-Hubbard model. The origin of the zero-bias anomaly in this system is explained, and the results are compared both with those obtained when hopping is allowed and with those of Efros and Shklovskii.

¹Research supported by the National Science and Engineering Research Council (NSERC) of Canada.

11:39AM Z16.00003 Novel critical point in the random quantum Ashkin-Teller model, FAWAZ HRAHSEH, THOMAS VOJTA, Missouri University of Science and Technology — The first order phase transition of the quantum Ashkin-Teller model has been intensely studied over many decades. In this work, we study the effect of disorder on this quantum phase transition using a strong-disorder renormalization group approach. Specifically, we develop an implementation of the strong-disorder renormalization group that works for both weak and strong four-spin couplings. For large four-spin coupling, we find a novel type of infinite-randomness fixed point. We investigate the critical properties of this fixed point, and we discuss broader implications for the fate of the first-order quantum phase transitions in disordered systems.

11:51AM Z16.00004 Spectral function of two-dimensional disordered Hubbard model¹, OINAM NGANBA MEETEI, NANDINI TRIVEDI, The Ohio State University — We show that moderate disorder introduces extended states in the Mott gap which upon further increase of disorder strength become localized states [1]. We propose that the inverse of the Lorentzian broadening of the spectral function $A(\mathbf{k}, \omega=0)$ as a function of $\mathbf{k}$ can be used as an order parameter for describing the both the transition from a Mott insulator to an unusual metallic state and the transition from the metal to a localized insulator of spin singlets. We further track the evolution of $A(\mathbf{k}, \omega)$ as a function of disorder and interaction strength. We also obtain the screening length of an external Coulomb potential from the density-density correlation function and find that the screening length is shortest at intermediate disorder in the metallic region. Our calculations are performed within an exact eigenstate formalism that treats the disorder exactly. The single particle Green's function is calculated within self-consistent mean field theory. In real space the bubble diagrams for this on-site interaction are an exact representation of density-density correlation function.

[1] D. Heidarian and N. Trivedi, Phys. Rev. Lett. **93**, 126401 (2004)

¹This work was supported by NSF-MRSEC grant DMR-0820414 (ONM) and by DOE grant number DE-FG02-07ER46423 (NT).

12:03PM Z16.00005 Variational Monte Carlo Study of Anderson Localization in the Hubbard Model¹, WILLIAM ATKINSON, AVID FARHOODFAR, Trent University, ROBERT J. GOODING, Queen's University — We have studied the effects of interactions on persistent currents in half-filled and quarter-filled Hubbard models with weak and intermediate strength disorder. Calculations are performed using a variational Gutzwiller ansatz that describes short range correlations near the Mott transition. A persistent current is induced with an Aharonov-Bohm flux, and the Anderson localization length is extracted from the scaling of the current with system size. We find that, at half filling, the localization length grows monotonically with interaction strength, even though the current itself is suppressed by strong correlations. This supports earlier dynamical mean field theory predictions that the elastic scattering rate is reduced near the Mott transition.

¹work supported by NSERC of Canada and the SHARCNET computing network.

12:15PM Z16.00006 Spin fluctuations near a spin-density-wave instability in periodic Anderson model studied by two-particle approach in dynamical mean field theory, WENHU XU, Department of Physics and Astronomy, Rutgers University, CEDRIC WEBER, Cavendish Laboratories, Cambridge University, United Kingdom, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University — We study the magnetic properties of periodic Anderson model when the system approaches to the vicinity of a spin-density-wave(SDW) instability from paramagnetic phase. Static and dynamical Q -dependent susceptibility are calculated using a two-particle approach in dynamical mean field theory. The SDW instability at a critical value of hybridization V_c is identified by the divergence of static susceptibility at low temperature and at a wavevector Q_c which connects the “hot zones” of the conduction band. Away from V_c , spin fluctuations at Q_c is suppressed at low energy and at low temperature in the heavy Fermi liquid regime, while near V_c , spin fluctuations at Q_c are significantly enhanced as temperature decreases. This indicates that the SDW instability is due to the competition between RKKY interaction and Kondo coupling in the crossover regime.

12:27PM Z16.00007 Large Disorder Renormalization Group Study of Singularities in the Insulating Phase of the Anderson Model of Localization¹, SONIKA JOHRI, Department of Electrical Engineering, Princeton University, Princeton NJ 08544-5263, R.N. BHATT, Department of Electrical Engineering and Princeton Center for Theoretical Science, Princeton University, Princeton NJ 08544-5263 — A recent study² of Anderson's 1958 model of localization³ reveals singular behavior of electronic eigenstates, as displayed by the density of states and inverse participation ratio, as a function of energy. This behavior occurs inside the insulating phase and separates typical Anderson localized from rare configuration, resonant Lifshitz states. Here, we use the large disorder renormalization group (LDRG) approach to study this problem. In particular, we study, using the LDRG approach, how the singular behavior evolves as a function of system size, starting from a toy model with two-sites which can be solved analytically. We assess the accuracy of the LDRG approach in obtaining the singular behavior in the thermodynamic limit for different disorder strengths, by comparing with results obtained by exact numerical diagonalization.

¹This work was supported by Department of Energy Grant No. DE-SC0002140.

²S. Johri, R.N. Bhatt, arXiv:1106.1131v2

³P. W. Anderson, Physical Review **109**, 1492 (1958).

12:39PM Z16.00008 Long-range spatial correlations in one-dimensional Anderson models¹, GREG PETERSEN, NANCY SANDLER, Ohio University, NQPI TEAM — The study of metal-insulator transitions (MIT) in one-dimensional (1d) Anderson disordered systems remains an active topic of research. Analytic and numerical results have confirmed the scaling prediction on the absence of MIT for short-range correlated disorder potentials. Solutions for long-range correlated potential models (i.e. the dimer model and those with power-law spectral densities) have shown MITs in 1d. However, long-range correlations remain poorly understood. In order to gain some insight, we study a 1d Anderson model with disorder potential correlations described by a power-law model with $\langle \epsilon_i \epsilon_0 \rangle = 1/(1 + r/a)^\alpha$. Here ϵ_i , r , a , and α are the on-site energy, position, lattice constant, and strength of the correlation respectively. We obtained results with various methods (wave packet diffusion, participation ratio, transfer matrix and Green's function) that support the absence of a MIT in these models in. We further show that an analysis of the beta function provides evidence for the validity of the same one-parameter scaling law valid for short-range correlated potentials.

¹This work has been supported by the NSF-PIRE mwn/ciam and NSF Grant DMR-0710581.

12:51PM Z16.00009 Dispersive Impurities in one-dimensional Fermi Gases: From one to two Channel Kondo Polarons, KAREN HALLBERG, Centro Atomico Bariloche and Instituto Balseiro, CNEA, CONICET, Bariloche, Argentina, JULIAN RINCON, Oak Ridge National Laboratory, USA, DANIEL GARCIA, Centro Atomico Bariloche and Instituto Balseiro, CNEA, CONICET, Bariloche, Argentina, MATTHIAS VOJTA, Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — We consider the problem of a dispersive magnetic impurity interacting antiferromagnetically with a one dimensional fermionic gas. By combining general considerations and extensive numerical simulations we show that the problem displays a quantum phase transition between two-channel and one-channel Kondo behaviour upon increasing the Kondo coupling and construct a phase diagramme. We also discuss possible experimental realisations.

1:03PM Z16.00010 ABSTRACT WITHDRAWN —

1:15PM Z16.00011 Charge fractionalization on quantum Hall edges, MARIANNE RYPESTOEL, University of Oslo, MATS HORS DAL, University of Leipzig, HANS HANSSON, Stockholm University, JON MAGNE LEINAAS, University of Oslo — Interactions between edges of quantum Hall bars give rise to Luttinger Liquid behavior with a nontrivial interaction parameter g . This leads to fractionalization of localized charges that propagate along the edges. We focus on fractionalization in systems with variable g and the separation of a charge into a sharply defined front pulse and a broader tail. The possibility of detecting the front pulse through noise measurement is discussed and illustrated by numerical simulations of a simplified Hall bar model.

1:27PM Z16.00012 Study of spontaneous anomalous Hall effect in 2-D electron fluid by bosonization, WATHID ASSAWASUNTHONNET, EDUARDO FRADKIN, Department of Physics, University of Illinois at Urbana-Champaign — We explore spontaneous time-reversal symmetry breaking in two-dimensional electron fluids using the method of higher dimensional bosonization. We focus on a fluid phase in which time-reversal symmetry and chiral symmetry are broken, but the space inversion and the combination of chiral and time-reversal symmetries are intact. This phase exhibits non-quantized anomalous Hall effect in the absence of external magnetic fields which corresponds to the Berry curvature on the Fermi surface. Furthermore we investigate the Berry phase connection and its representation in terms of bosonized fields.

1:39PM Z16.00013 Non-chiral Bosonization of Fermions in One Dimension¹, GIRISH SETLUR², Associate Professor, Department of Physics, Indian Institute of Technology Guwahati 781039, India — An alternative to the conventional approach to bosonization in one dimension that invokes the Dirac equation in 1+1 dimension with chiral “right-movers” and “left-movers” is proposed that works directly with the bounded parabolic energy bands relevant to Condensed Matter problems. This technique allows us to use a basis different from the plane wave basis that makes this non-chiral approach ideally suited to study Luttinger liquids that have boundary or impurities that break translational symmetry. We provide a simple solution to the electron Green function for the problem of Luttinger liquid (LL) with a boundary and also for a LL with a single impurity. The present method is significantly easier than the g-ology based standard bosonization and other methods that require a combination of RG along with bosonization/refermionization techniques. Our results are broadly consistent with these more established approaches.

¹Partially supported by Department of Science and Technology and SERC, Govt. of India

²In collaboration with Dr. V. Meera, DST NanoScience Initiative Research Fellow, JNCASR, Bangalore.

1:51PM Z16.00014 A Partially-ordered-set Based Approach to the Dirac Equation in 3+1 space-time¹, KEITH EARLE, KEVIN KNUTH, University at Albany (SUNY) — Recent work by Knuth and co-workers has shown how insights into Einstein's Theory of Special Relativity may be obtained by careful reasoning about consistent quantification of a poset. The Feynman Chessboard problem in 1+1 spacetime can be treated from this perspective, for example. Alternative methods of solution based on techniques borrowed from statistical mechanics have also been developed over the years to solve the Feynman Chessboard model in 1+1 spacetime. One particularly intriguing solution is based on a master-equation approach developed by McKeon and Ord for 1+1 spacetime. We will show how this model may be extended to 3+1 spacetime using techniques developed by Bialynicki-Birula, thus providing an alternative derivation of the Dirac equation. An external electromagnetic field can be accommodated very naturally in the formalism from which a pleasing pictorial representation of electromagnetic interactions in the lattice picture emerges.

¹Partially supported by FRAP, University at Albany.

Friday, March 2, 2012 11:15AM - 2:15PM – Session Z17 DCMP: 2D Crystals: Beyond Graphene 252A

11:15AM Z17.00001 Electronic and Transport Properties of Few-Layer MoS₂ Crystals, DORON NAVEH, Electrical & Computer Engineering, Carnegie Mellon University, Pittsburgh, PA, United States, ASHWIN RAMASUBRAMANIAM, Mechanical & Industrial Engineering, University of Massachusetts Amherst, Amherst, MA, United States, ELIAS TOWE, Electrical & Computer Engineering, Carnegie Mellon University, Pittsburgh, PA, United States — We investigate the electronic properties of few-layer MoS₂ flakes prepared by mechanical exfoliation. Field-effect transistors from MoS₂ flakes were fabricated and their properties were systematically characterized as a function of sample thickness. Scanning probe measurements are employed to characterize the interface between MoS₂ flakes and metal contacts. Transport properties of these devices and their correlation to electronic structure calculations are discussed.

11:27AM Z17.00002 Optical pump-probe studies of carrier dynamics in few-layer MoS₂, RUI WANG, BRIAN RUZICKA, NARDEEP KUMAR, MATTHEW BELLUS, HSIN-YING CHIU, HUI ZHAO, University of Kansas — Molybdenum disulfide is a transition metal dichalcogenide with an indirect band gap of 1.29 eV. Its layered structure allows fabrication of atomically-thin films where the quantum confinement can significantly modify the electronic and optical properties. We demonstrate that a femtosecond pump-probe technique can be used to study charge carrier dynamics in few-layer MoS₂ samples fabricated on Si/SiO₂ substrates by mechanical exfoliation. Carriers are injected by a 780-nm pump pulse via phonon assisted indirect absorption in bilayers or through edge states. Their dynamics are probed by measuring differential reflection of a probe pulse tuned to the excitonic transition near 670 nm. We found that the magnitude, the sign, and the decay time of the signal change dramatically as the probe wavelength is tuned within the excitonic resonance. With a fixed probe wavelength, the differential reflection signal is proportional to the carrier density. The decay time is independent of the carrier density. Besides providing quantitative information on the carrier dynamics in this promising two-dimensional material, our experiment may stimulate further optical studies of carrier dynamics in this material system.

11:39AM Z17.00003 Integrated circuits and logic operations with high room temperature voltage gain based on single-layer MoS₂, ANDRAS KIS, BRANIMIR RADISAVLJEVIC, MICHAEL WHITWICK, EPFL — Two-dimensional materials such as single-layer MoS₂ represent the ultimate limit of miniaturization in the vertical dimension, are interesting as building blocks of low-power nanoelectronic devices and are suitable for integration due to their planar geometry. Because they are less than 1 nm thin, 2D materials in transistors could also lead to reduced short channel effects and result in fabrication of smaller and more power efficient transistors. Here, we report on the first integrated circuit based on a two-dimensional semiconductor MoS₂. Our integrated circuits are capable of operating as inverters, converting logical “1” into logical “0”, with room-temperature voltage gain higher than 4.5, making them suitable for incorporation into digital circuits. We also show that electrical circuits composed of single-layer MoS₂ transistors are capable of performing the NOR logic operation, the basis from which all logical operations and full digital functionality can be deduced. We have also fabricated suspended single-layer MoS₂ membranes and have performed mechanical measurements using an atomic force microscope. Our results show that single-layer MoS₂ has a Young's modulus higher than steel and can withstand deformation up to 11%, making it suitable for integration with flexible electronic devices.

11:51AM Z17.00004 ABSTRACT WITHDRAWN —

12:03PM Z17.00005 ABSTRACT WITHDRAWN —

12:15PM Z17.00006 Transient Photoluminescence in MoS₂ layered crystals, TUNG-WU HSIEH, CHIH-WEI LAI, Michigan State University — We report sub-10-ps transient exciton photoluminescence (PL) in mechanically exfoliated few- and mono-layered crystals of MoS₂. We characterize layered crystals with thickness of $\sim 1\mu\text{m}$, 100 nm, 10nm, and down to few-layers on SiO₂/Si and mica substrates using luminescence and Raman spectroscopy. A frequency shift of $\sim 2\text{ cm}^{-1}$ is observed on sub-10-nm-thick samples for the in-plane E_{2g}^1 and the out-of-plane A_{1g} Raman modes. The relative intensities of Stokes and Anti-Stokes Raman components are used to determine the lattice temperature under a laser excitation with a spot diameter of $1\mu\text{m}$ and an average power 0.5 to 20mW. PL spectra are measured for lattice temperatures from $\sim 70\text{K}$ to 500K. We observe two groups of luminescence emissions with comparable peak intensities centered at 1.85eV (VIS) and 1.35eV for samples of a thickness $1\mu\text{m}$ down to 10 nm under a cw laser excitation at a wavelength of 532nm (2.33eV). The VIS luminescence emissions are enhanced under a 2-ps pulsed laser excitation at a wavelength of 633nm (1.96eV). The rise and decay times of the luminescence are found to be less than 5 ps. Our results suggest that excitonic effects play a role in enhancing the luminescence quantum efficiency.

12:27PM Z17.00007 Quasiparticle self-consistent GW calculations of monolayer, bilayer and bulk MoS₂, TAWINAN CHEIWCHANHAMNANGIJ, WALTER LAMBRECHT, JIE SHAN, Department of Physics, Case Western Reserve University, 10900 Euclid Avenue, Cleveland, Ohio 44106 — Photoluminescence and absorption spectra of monolayer MoS₂ indicate a direct gap behavior while bulk MoS₂ is known to have an indirect gap. The details of these spectra and the band structure are not yet fully understood. Here, the quasiparticle self-consistent GW method is used to study the electronic structure of monolayer, bilayer, and bulk MoS₂. Band structures, effective masses, and dielectric functions are extracted from our calculations. In contrast to another recent GW calculation, we find the monolayer to have a direct gap of 2.84 eV at K, which is large compared to the photoluminescence energies. The exciton binding energy for this transition is estimated within an effective mass approximation using our calculated effective masses and dielectric constants and amounts to about 0.90 eV, leading to good agreement with the experimental data for the lowest direct transition. We find a second conduction band local minimum along Γ -K about 0.44 eV higher but do not find it to give rise to a bound state exciton. When spin-orbit coupling is included, we find a spin-splitting of the levels along Γ -K in the monolayer related to the absence of an inversion center. In the bilayer, we find an indirect gap from Γ -K and a splitting of the valence band at K, mainly due to the interlayer interaction but also increased by spin-orbit coupling. The splitting between the lowest two absorption features A and B is consistent with the slightly larger splitting calculated in the bilayer than the monolayer.

12:39PM Z17.00008 High Performance Two Dimensional MoS₂ MOSFET with ALD Al₂O₃ Gate Stacks, HAN LIU, KUN XU, PEIDE YE, Purdue University — We study the growth mechanism of atomic layer deposition (ALD) of Al₂O₃ on layered MoS₂. We demonstrate the feasibility of direct growth of Al₂O₃ on this 2D material by trimethylaluminum (TMA) and water as precursors. Atomic force microscopy study shows that the quality of the Al₂O₃ film is degraded at elevated temperatures, originated from impeded surface absorption of precursors. We also apply density functional theory (DFT) study of the reaction which is in good agreement with our experimental observations. In addition, we fabricate dual gate MoS₂ metal-oxide-semiconductor field effect transistors (MOSFET). From the transport study we find out the lowering the growth temperature will result in a huge negative threshold voltage shift, which can be improved by either forming gas anneal after Al₂O₃ deposition or insertion of an Al seeding layer which would facilitate higher growth temperature with better film quality. Further details will be provided in the presentation.

12:51PM Z17.00009 Novel valley and spin physics in monolayer MoS₂¹, DI XIAO, Oak Ridge National Laboratory, G.B. LIU, The University of Hong Kong, WENGUANG ZHU, University of Tennessee & Oak Ridge National Laboratory, XIAODONG XU, University of Washington, WANG YAO, The University of Hong Kong — We show that the valley Hall effect and valley-dependent optical selection rule can be realized in monolayer MoS₂, which is a direct bandgap semiconductor with non-central valleys. In addition, spin-orbit coupling in this materials is large, which gives rise to novel spin physics tied to the valley degree of freedom.

¹Research sponsored by the DOE, Office of BES, Materials Sciences and Engineering Division, and by Research Grant Council of Hong Kong

1:03PM Z17.00010 Enhanced thermal conductivity and isotope effect in single-layer hexagonal boron nitride¹, DAVID BROIDO, Boston College, LUCAS LINDSAY, Naval Research Laboratory — We have calculated the lattice thermal conductivity, k , of both naturally occurring and isotopically enriched single layers of hexagonal boron nitride (h-BN) as well as bulk h-BN using an exact numerical solution of the Boltzmann transport equation for phonons [1]. Good agreement is obtained with measured bulk h-BN data [2], and the stronger phonon-phonon scattering identified in these systems explains why their k values are significantly lower than those in graphene and graphite. A reduction in such scattering in the single layer arising mainly from a symmetry-based selection rule leads to a substantial increase in k , with calculated room temperature values of more than 600 W/m-K. Additional enhancement is obtained from isotopic enrichment, which exhibits a strong peak as a function of temperature, with magnitude growing rapidly with crystallite size. [1] L. Lindsay and D. A. Broido, Phys. Rev. B 84, 155421 (2011). [2] E. K. Sichel, R. E. Miller, M. S. Abrahams, and C. J. Buicocchi, Phys. Rev. B 13, 4607 (1976).

¹Supported by NSF, NRC/NRL and DARPA.

1:15PM Z17.00011 Two-dimensional Dirac fermions and quantum transport in (Sr/Ca)MnBi₂, KEFENG WANG, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory Upton, New York 11973 USA, D. GRAF, National High Magnetic Field Laboratory, Florida State University, LIMIN WANG, HECHANG LEI, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory Upton, New York 11973 USA, S.W. TOZER, National High Magnetic Field Laboratory, Florida State University, CEDOMIR PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory Upton, New York 11973 USA — We report two dimensional Dirac fermions and quantum transport behavior in single crystals of SrMnBi₂ and CaMnBi₂. The non-zero Berry's phase, small cyclotron resonant mass and first-principle band structure suggest the existence of the Dirac fermions in the Bi square nets. Angular dependent magnetoresistance and quantum oscillations suggest dominant two-dimensional (2D) Fermi surfaces. The in-plane transverse magnetoresistance exhibits a crossover at a critical field B^* from semiclassical weak-field B^2 dependence to the high-field unsaturated linear magnetoresistance ($\sim 120\%$ in 9 T at 2 K) due to the quantum limit of the Dirac fermions. The temperature dependence of B^* satisfies quadratic behavior, which is attributed to the splitting of linear energy dispersion in high field. Our results demonstrate the universal existence of two dimensional Dirac fermions in different materials with Bi square nets.

1:27PM Z17.00012 Field-induced polarization of Dirac valleys in bismuth, KAMRAN BEHNIA, ZENGWEI ZHU, AURELIE CALLAUDIN, BENOIT FAUQUE, ESPCI, WOUN KANG, Ewha Womans University — The principal challenge in the field of "valleytronics" is to lift the valley degeneracy of electrons in a controlled way. In graphene, a number of methods to generate a valley-polarized flow of electrons have been proposed, which are yet to be experimentally realized. In bulk semi-metallic bismuth, the Fermi surface includes three cigar-shaped electron valleys lying almost perpendicular to the high-symmetry axis known as the trigonal axis. The in-plane mass anisotropy of each valley exceeds 200 as a consequence of Dirac dispersion, which drastically reduces the effective mass along two out of the three orientations. We present a study of angle-dependent magnetoresistance in bismuth which shows that a flow of Dirac electrons along the trigonal axis is extremely sensitive to the orientation of in-plane magnetic field. The effect is visible even at room temperature. Thus, a rotatable magnetic field can be used as a valley valve to tune the contribution of each valley to the total conductivity. At high temperature and low magnetic field, the three valleys are interchangeable and the three-fold symmetry of the underlying lattice is respected. As the temperature is decreased or the magnetic field increased, this symmetry is spontaneously lost. This loss may be an experimental manifestation of the recently proposed valley-nematic Fermi liquid state.

1:39PM Z17.00013 STM measurements of Charge Density Waves in S-doped NbSe₂, ULRICH WURSTBAUER, ETHAN ROSENTHAL, ERICK F. ANDRADE, CARLOS ARGUELLO, SUBBAIAH P. CHOCKALINGAM, Dept. of Physics, Columbia University, SHUANG JIA, ROBERT J. CAVA, Dept. of Chemistry, Princeton University, ABHAY N. PASUPATHY, Dept. of Physics, Columbia University — Recent scanning tunneling microscopy (STM) measurements have shown that crystal defects have a profound influence on the nature of the charge density wave (CDW) transition in the transition-metal dichalcogenides (TMD). In order to examine this effect systematically, we employ low temperature STM to visualize the CDW transition in intentionally doped TMD crystals. We use a newly designed homebuilt ultra-low-loss, variable temperature STM to perform measurements on crystal samples of NbS_xSe_{2-x}. We describe the effect of the sulphur atoms on both the local and global charge order in this material.

1:51PM Z17.00014 Imaging Charge Density Wave Nucleation in NbSe₂, ETHAN ROSENTHAL, CARLOS ARGUELLO, SUBBAIAH CHOCKALINGAM, WOO CHANG CHUNG, LIUYAN ZHAO, CHRISTOPHER GUTIERREZ, JOON HO KANG, ABHAY PASUPATHY, Columbia University, SHUANG JIA, ROBERT CAVA, Princeton University — Understanding the effects of spatial inhomogeneity in complex materials is necessary to achieve a fundamental understanding of their quantum states. NbSe₂ serves as a clean and relatively simple system for understanding the emergence of one such state – the charge density wave (CDW) phase. Using variable temperature scanning tunneling microscopy (STM), we visualize the nucleation of CDWs about crystal defects at temperatures well above T_{CDW} . The CDW correlation length increases with decreasing temperature, until global order is reached below T_{CDW} . We also employ scanning tunneling spectroscopy in order to visualize the energy-dependent, spatial phase of the CDW state. With both topographic and spectroscopic data, we will provide a clear picture of the CDW transition and insight into the microscopic mechanisms at work.

2:03PM Z17.00015 Nature of Electronic States in Ultrathin MoS₂ Field Effect Transistor, SUBHAMOY GHATAK, ATINDRA NATH PAL, ARINDAM GHOSH, Indian Institute of Science, Bangalore, LOW TEMPERATURE NANO-ELECTRONICS GROUP TEAM — Molybdenum disulphide (MoS₂) is a layered transition metal dichalcogenide with a Mo layer sandwiched between two S layers (S-Mo-S), which forms its basic unit. Each basic unit is attached to other units only with weak Van der Waals force. This enables to make an atomically thin single layer of MoS₂ with a bandgap 1.9 eV. The presence of bandgap has made it an interesting material in thin film transistors. It has been reported [1] recently that very high on/off ratio ($\sim 10^8$) can be obtained in single layer MoS₂ transistor due to the presence of this bandgap. Though the on/off ratio is very high, mobility in these transistors are considerably low. Here we have investigated the origin of such low mobility. From our temperature dependent study we find that atomically thin MoS₂ layer becomes highly disordered in the presence of the substrate and electron got localised in the traps created by the charge impurities at substrate-MoS₂ interface. We propose that high mobility can be obtained in these transistors by removing the charge impurity background.

[1] Radisavljevic, B. *et al.* Nature Nanotechnology **2011**, 6, 147–150.

[2] Ghatak, S. *et al.* ACS Nano **2011**, 5, 7707.

Friday, March 2, 2012 11:15AM - 2:15PM –
Session Z18 DCMP: Enhanced Optical Properties Using Plasmonics, Metamaterials, and Nanoparticles 252B

11:15AM Z18.00001 Nonresonant Broadband Funneling of Light via Ultrasubwavelength Channels¹, GANAPATHI SUBRAMANIA, Sandia National Laboratories, Albuquerque, NM, USA, STAVROULA FOTEINOPOULOU, School of Physics, University of Exeter, Exeter, UK, IGAL BRENER, Sandia National Laboratories, Albuquerque, NM, USA — Efficient control of light-matter interaction, which is key to many photonics applications such as detectors, sensors and novel light sources, can be achieved by enhancing and funneling light efficiently through deep subwavelength channels. Thus far, this has been accomplished by exciting the structural surface plasmon resonances of perforated nanostructured metal films, a phenomenon known as extraordinary optical transmission. The resonant nature of the phenomenon makes it inherently narrowband. Here, we introduce a new paradigm structure consisting of double-grooved metallic structure that possesses all the capabilities of extraordinary optical transmission platforms, yet operates nonresonantly and across broadband (Phys. Rev. Lett. 107, 163902(2011)). As a result, our proposed platform demonstrates efficient ultrabroadband funneling of optical power confined to an area as small as $\sim (\lambda/500)^2$, where optical fields are enhanced, thus exhibiting functional possibilities beyond resonant platforms. We explain the nonresonant mechanism underlying this phenomenon with a simple quasistatic picture that shows excellent agreement with our numerical simulations.

¹Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE's National Nuclear Security Administration under contract DE-AC04-94AL85000.

11:27AM Z18.00002 Measurement of Near-Field Thermal Radiation through a Nanometer-Sized Gap, ANASTASSIOS MAVROKEFALOS, POETRO SAMBEGORO, GANG CHEN, Massachusetts Institute of Technology — Radiation heat transfer in nanostructures can differ significantly from that in macrostructures due to wave effects. Theory has predicted that thermal radiation heat transfer between two surfaces separated by tens of nanometers can exceed that of Planck's blackbody radiation law by several orders of magnitude. Our AFM-inspired heat flux sensor, comprising of a sphere attached to the tip of a bimetallic cantilever, can measure the radiation exchange across nanometer-scale gaps between a sphere and a flat surface. The objective of this work is to experimentally study thermal radiative transfer at very small separation gaps. In previous experiment, our group has successfully measured near-field radiative heat transfer through gap as small as 30 nm. In this work, we extend this technique to decrease the gap down to a few nanometers and show that existing fluctuating electrodynamics theory cannot predict experimental results in the extreme limit of small separation between two surfaces. Our experiments raise interesting question on the convergence of radiation heat transfer mechanism and interfacial heat conduction mechanism. Theoretical approaches bridging these two regimes will be discussed.

11:39AM Z18.00003 Making metals transparency for white light by surface plasmons¹, RU-WEN PENG, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China, XIAN-RONG HUANG, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA, REN-HAO FAN, JIA LI, QING HU, MU WANG, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China, NATIONAL LABORATORY OF SOLID STATE MICROSTRUCTURES COLLABORATION, ARGONNE NATIONAL LABORATORY COLLABORATION — We demonstrate both experimentally and theoretically that metallic gratings consisting of narrow slits become transparent for extremely broad bandwidths under oblique incidence. This phenomenon can be explained by a concrete picture in which the incident wave drives free electrons on the conducting surfaces and part of the slit walls to form surface plasmons (SPs). The SPs then propagate on the slit walls but are abruptly discontinued by the bottom edges to form oscillating charges that emit the transmitted wave. This picture explicitly demonstrates the conversion between light and SPs and indicates clear guidelines for enhancing SP excitation and propagation. Making structured metals transparent may lead to a variety of applications. References: Xian-Rong Huang, Ru-Wen Peng, and Ren-Hao Fan, Phys. Rev. Lett. (2010)105, 243901; and Ren-Hao Fan, Ru-Wen Peng, Xian-Rong Huang, Jia Li, Qing Hu, and Mu Wang, manuscript prepared(2011).

¹Supported by NSF and MOST in China, and DOE in USA.

11:51AM Z18.00004 Fabrication of Broad Band Mid-Infrared Absorber based on Periodic Dielectric-Thin Metal Film Multilayer Structures, SHY-HAUH GUO¹, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742, ANDREI B. SUSHKOV, Department of Physics, University of Maryland, College Park, MD 20742, TIMOTHY CORRIGAN, Department of Physical Sciences, Concord University, Athens, WV 24712, DONG PARK², Department of Electrical Computer Engineering, University of Maryland, College Park, MD 20742, H. DENNIS DREW³, Department of Physics, University of Maryland, College Park, MD 20742, PAUL KOLB, WARREN HERMAN, Laboratory for Physical Sciences, College Park, MD 20740, RAYMOND PHANEUF⁴, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742 — We present results from measurements on periodic multilayer structure of alternating dielectric and thin metal layers to achieve a broadband absorber of mid-infrared radiation. We examine the effect on performance of a back-reflective metallic bottom layer, surface roughness at interfaces, the metal conductance, the thickness of dielectric layers, and a patterned anti-reflective layer. We determine optimum structure parameters for absorption of a 500 K-black body spectrum, and find that the numerical results agree well with the measured absorption spectra. We also investigate the possibility of fabricating a patterned anti-reflective layer to further increase the absorption.

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12:03PM Z18.00005 Simultaneous Bulk and Surface Plasmon Resonance and Radiative Polaritons excited in RuO₂ films grown on glass and on TiO₂ (001)¹, L. WANG, C. CLAVERO, K. YANG, E. RADUE, College of William and Mary, G. SCAREL, James Madison University, I. NOVIKOVA, R. LUKASZEW, College of William and Mary — Conducting oxides, such as RuO₂, have a much lower carrier concentration as compared to metals, leading to a lower plasma frequency of 3.3eV which lies in the infrared (IR) region. This unique feature of conducting oxides allows for simultaneous observation of surface and bulk polariton modes in the IR range. Here we have investigated bulk and surface plasmons as well as radiative polaritons in RuO₂ thin films. The RuO₂ thin films investigated were grown using DC magnetron sputtering on glass and on TiO₂ (001). We have used X-ray Diffraction and Reflection High-Energy Electron Diffraction to characterize the microstructure of these samples. Four-point probe and ellipsometry were used to investigate the electrical conductivity and the optical properties. The optical measurements were carried out using HeNe red laser (632nm) and IR laser (1520nm) radiations to illuminate RuO₂ thin films. We will show that bulk plasmons can be excited in RuO₂ thin films in the visible red region, while simultaneous bulk plasmons as well as surface plasmons excitation are observed in the IR region. We also studied the substrate influence on the radiative polaritons in the middle IR region ($20\text{-}2.2\mu\text{m}$) by measuring films grown on glass and on TiO₂ (001).

¹This work was financially supported by NSF (DMR-1006013).

12:15PM Z18.00006 Simulations of enhanced absorption in composite embedded, insulated metal nanopatterns for ultrathin film photovoltaics, XINYU LIU, FAN YE, MICHAEL J. BURNS, MICHAEL J. NAUGHTON, Department of Physics, Boston College, Chestnut Hill, 02467 — In recent work [1], a concept of employing embedded metallic nanopatterns (EMN) in ultrathin film solar cells was discussed. Elsewhere in this conference, Fan *et al.* advance this with a scheme for embedded insulated metallic nanopatterns (EIMN) that is designed to avoid deleterious carrier recombination as would result from bare metal inclusions in a PV film. However, a practical route to fabricating EIMNs of desired shapes for eventual scale production is nontrivial. Here, we introduce two notions toward that goal, nano-stamping and spin-coating, of compact arrays of metallic core/insulating shell nanoparticles (MNP). We show by simulations that optical absorption of an EIMN composed of arrays of core-shell MNPs having SiO₂ coatings is essentially the same as that of an EMN composed of solid metals without insulation, with absorption concentrated in the surrounding PV medium. These concepts may provide practical routes for scalability of EIMN-based ultrathin film plasmonic solar cells.

[1] F. Ye, M. J. Burns, M. J. Naughton, Proc. SPIE 8111, 811103 (2011), and this conference.

12:27PM Z18.00007 Embedded insulated metallic nanopatterns for enhanced optical absorption and photovoltaics, FAN YE, MICHAEL J. BURNS, MICHAEL J. NAUGHTON, Department of Physics, Boston College, Chestnut Hill, 02467 — Recently, we have shown embedded metallic nanopatterns (EMN) in ultrathin PV films to be candidates for high efficiency thin-film solar cells, owing to prominent metamaterial/plasmonic-enhanced light trapping, as compared to unpatterned, surface- or bottom-patterned [1]. We also showed that hot electron effects emerge in ultrathin a-Si-based solar cells [2]. The EMN in the semiconductor layer, however, can also serve as a source of recombination for photogenerated electrons and holes, leading to decreased current. Here, we propose the idea of an embedded insulated metallic nanopattern (EIMN) to efficiently avoid the recombination effect while maintaining high light absorption in an ultrathin film format in which hot electron physics can contribute. Simulations show that an EIMN with a 10 nm layer of dielectric insulation provides essentially the same absorption as its EMN counterpart. Measurements on several EMN structures will be presented. This EIMN architecture may provide a practical route to high efficiency, hot electron solar cell technology using ultrathin films.

[1]F. Ye, M.J. Burns, M.J. Naughton, Proc. SPIE 8111, 811103 (2011).

[2]K. Kempa, M.J. Naughton, Z.F. Ren, A. Herczynski, T. Kirkpatrick, J. Rybczynski, Y. Gao, Appl. Phys. Lett. 95, 233121(2009)

12:39PM Z18.00008 An effective medium formulation to estimate the plasmonic dispersion of a randomly distributed gallium nanoparticle ensemble, YANG YANG, Physics Dept, Duke University, JOHN M. CALLAHAN, Nanogenesis Div, AEGIS Technology, TONG-HO KIM, APRIL S. BROWN, ECE Dept, Duke University, MARIA LOSURDO, GIANNI BRUNO, IMIP-CNR, HENRY O. EVERITT, Physics and ECE, Duke University; Army Aviation and Missile RD&E Center — Quantum confinement causes the dielectric function of nanometer-sized metal particles to depart from metallic bulk dispersion in a manner correlating with the size, shape, and spacing of the nanostructures. An improved effective medium approximation is formulated to reconcile angle-dependent ultraviolet/visible spectroscopy and spectroscopic ellipsometry measurements of the collective optical dispersion of randomly distributed hemispherical gallium nanoparticles deposited on a sapphire surface using ultra high vacuum molecular beam epitaxy. Atomic force microscopy and scanning electron microscopy analyze the size distribution of the nanoparticle ensembles to estimate their volume fraction. The optical constants are then estimated using a modified Maxwell-Garnett effective medium approximation that treats the ambient vacuum as a host and the bare sapphire substrate as a semi-infinite layer. The refined dielectric function improves estimates of the collective plasmonic response of the nanoparticle ensemble.

12:51PM Z18.00009 Plasmon responses and optical chirality of helical nanoparticle assemblies¹, ZHIYUAN FAN, ALEXANDER GOVOROV, Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701, United States, OHIO UNIVERSITY TEAM — Helical gold nanoparticle assemblies exhibit strong circular dichroism (CD) in the plasmonic band. This CD effect comes from dipolar Coulomb and electromagnetic interactions between spherical gold nanoparticles. A typical CD spectrum of chiral plasmonic assembly includes positive and negative bands. The shape of CD spectra is sensitive to geometrical parameters of the assembly. In this study, we show that the CD signal is stable against structural defects, which makes experimental realizations of strong CD effect feasible. To date, several recent experimental papers reported CD effects in helical plasmonic systems. In addition, we found that the sign of CD signal can flip as a function of the inter-particle distance and, for very long helices, the long-range electrodynamic interactions become essential. These results are important for designing nanocomposite materials with strong optical chirality in the visible wavelength range.

¹This work was supported by Volkswagen Foundation and NSF (project number CBET-0933415)

1:03PM Z18.00010 Determining 3D Relative Orientation between Plasmonic Nanoparticles¹, FARBOD SHAFIEI, CHIHUI WU, PATRICK PUTZKE, YANWEN WU, AKSHAY SINGH, GENNADY SHVETS, XIAOQIN LI, University of Texas at Austin — Polarization resolved far-field scattering measurements were used to determine 3D relative orientation between plasmonic nanoparticles placed few nanometers apart. The metallic nanostructure was assembled using the atomic force microscope (AFM) nanomanipulation method. When a gold nanosphere (150 nm in diameter) was placed within a few nanometers to the end of a gold nanorod (20 nm in diameter and 180 nm in length), near field coupling between them introduced new features in the scattering spectra. Specifically, a Fano resonance emerged, due to the interference between a dark mode, corresponding to the quadrupole charge distribution on the rod, and the bright, dipole mode of the sphere. As linear polarizer in the path of the incident and emission light was rotated, the scattering spectra evolve systematically, enabling us to determine the 3D relative orientation between these two plasmonic nanoparticles. This orientation information cannot be accurately and dynamically obtained using other scanning probe techniques, especially when one nanoparticle is partially hidden under the other nanoparticles.

¹Financial supports from NSF, ONR, AFOSR, ARO, and the Welch Foundation are acknowledged

1:15PM Z18.00011 Plasmonic Circular Dichroism Effect in Nanomaterials¹, HUI ZHANG, ZHIYUAN FAN, ALEX GOVOROV, Ohio University — By employing a numerical solution of Maxwell's equations beyond the dipole limit, we studied the circular dichroism (CD) signal of a chiral molecule in the presence of a gold nanoparticle (NP) dimer. The CD signals come from two parts: The first one is Coulomb interaction within the molecule-dimer complex giving rise to the plasmon peak in the CD spectrum, while the other one is the plasmonic enhancement of the absorption process in a chiral molecule. Typically, the CD signals of chiral molecules are very weak in the visible range, but are strong in the UV range. In the presence of gold dimer, however, we found a strong CD signal emerges in the visible range of photon energies, where the plasmon effect makes the main contribution to CD signal at the plasmon frequency. Furthermore, we propose that, by using the plasmon-induced CD signals, one can design optical sensors to study chirality of biomolecules.

¹This work was supported by Volkswagen Foundation and NSF (project number CBET-0933415).

1:27PM Z18.00012 Metamaterial Enhanced Terahertz Spectroscopy of Biomolecules, LOGAN CHIEFFO, GEORGE KEISER, ANDREW STRIKWERDA, Boston University, Department of Physics, KEBIN FAN, Boston University, Department of Mechanical Engineering, SHYAMSUNDER ERRAMILLI, Boston University, Department of Physics, XIN ZHANG, Boston University, Department of Mechanical Engineering, RICHARD AVERITT, Boston University, Department of Physics — As the field of metamaterials experiences exponential growth, an increasing number of studies have focused on understanding near-field coupling between arrays of metamaterials and their local environment. Examples include a second array of metamaterials, phonon bands in semiconductors, and even small molecules. In this work, we demonstrate metamaterial coupling to a thin film of biomolecules. Protein films are deposited onto arrays of gold split ring resonators (SRRs) on thin silicon nitride substrates. As the LC resonance of the SRR is tuned across the low frequency terahertz (THz) modes of the biomolecule, hybridization results in mode splitting. The thin substrates (400nm) and the large electric field enhancement intrinsic to the SRRs provide ultrasensitive detection of the THz modes in the protein, allowing for the THz response to be measured from thin films which would otherwise not be observable.

1:39PM Z18.00013 Poynting vector in magnetic materials: from thermomagnetic effects to metamaterials, ANDREI SERGEEV, MICHAEL REIZER, VLADIMIR MITIN, SUNY at Buffalo — In a finite sample, besides the bulk currents given by the Kubo formula, additional charge and energy are transferred by surface magnetization currents. We show that for the energy current, the corresponding surface correction to the Kubo's current is expressed in terms of the magnetization component of the Poynting vector, $\mathbf{M} \times \mathbf{E}$. Magnetization currents, like persistent currents, are dissipationless and do not transfer entropy. Only in this way, one can obtain the Nernst and Ettingshausen coefficients that satisfy to the Onsager relation. In the microscopic transport theory, for maintaining gauge invariance in a magnetic field, the heat current operator should include the magnetic term. Both magnetization-related effects - the dissipationless nature and strong surface contribution to the energy transfer - have been also overlooked in the recent works on the Poynting vector in metamaterials. The paradoxes in this area are resolved, if one accurately considers a balance of electromagnetic energy transferred by bulk and surface magnetization currents.

1:51PM Z18.00014 Polarization Conversion Using the Cavity Resonances of Plasmonic Patch Nanoantennas, FENG WANG, AYAN CHAKRABARTY, Liquid Crystal Institute, Kent State University, FRED MINKOWSKI, Department of Physics, Kent State University, QI-HUO WEI, Liquid Crystal Institute, Kent State University — The control of light polarization is essential to all optical experiments and photonic devices. Here we propose and demonstrate a novel method to realize the polarization conversion by using an array of non-chiral plasmonic patch nano-antennas. The patch nano-antennas are composed of a 2D array of elliptical Ag nano-disks and a base Ag substrate spaced by an ultra-thin dielectric layer. The Ag nano-disks and the base metal substrate would form an array of plasmonic nanocavities with ultrasmall mode volumes. We will show the excitation of the fundamental mode of the plasmonic cavity resonance could introduce a 90° phase delay to the reflected light from the patch antenna. This phase delay can be utilized to realize the polarization conversion between linearly polarized light and elliptically or circularly polarized light.

2:03PM Z18.00015 Plasmonic nanowire transmission lines, YUN PENG, KRIS KEMPA, Physics Department, Boston College — Metallic nanowires could be used as nano-optical transmission lines. The important factors characterizing such lines are the subwavelength operation, long propagation length, and low penetration of the propagating modes into the environment outside wires. In this work we study these factors in silver nanowires operating as surface plasmon polariton (SPP) waveguides, by employing the finite difference time domain (FDTD) and the finite difference frequency domain (FDFD) simulations. In addition to the dispersion relation of the SPP mode, we investigate the inter-wire crosstalk, an important feature of the nano-optical circuits. We compare our results with the available experimental results.

Friday, March 2, 2012 11:15AM - 2:15PM –

Session Z19 DCMP: Invited Session: Non-Abelian States in the 1st Excited Landau Level: Experimental Status and Theoretical Outlook 253AB

11:15AM Z19.00001 Interferometric evidence for non-Abelian quasiparticles at filling factor $5/2$, ROBERT WILLETT, Bell Laboratories, Alcatel-Lucent — The $5/2$ fractional quantum Hall state charge $e/4$ excitations are proposed to follow non-Abelian statistics [1]. In edge state interference these purported non-Abelian quasiparticles should display period $e/4$ Aharonov-Bohm oscillations if the interfering quasiparticle encircles an even number of localized $e/4$ charges, but suppression of oscillations if an odd number is encircled [2-3]. To test this, we have performed swept area interference measurements at $5/2$ [4-5]. We observe an alternating pattern of $e/4$ and $e/2$ period oscillations in resistance for a large change in the interferometer area, with the area sweep changing the enclosed localized $e/4$ quasiparticle number. This observed aperiodic alternation is consistent with proposed non-Abelian $e/4$ properties: the $e/4$ oscillations occur for encircling an even number of localized quasiparticles over their aperiodic spatial distribution, and the lower amplitude $e/2$ oscillations are observed when encircling an odd number as the $e/4$ oscillations are suppressed, allowing observation of the persistent smaller Abelian $e/2$ oscillations. Importantly, adding localized quasiparticles to the encircled area by changing magnetic field can change the parity of the enclosed quasiparticle number and should induce interchange of the expressed $e/4$ and $e/2$ periods: such interchange is observed in these measurements. In further experiments with the goal of understanding specific $e/4$ edge propagation properties, a series of interferometers of different sizes have been tested. The range of device dimensions has allowed measurement of the $e/4$ quasiparticle propagation attenuation length, demonstrating that small interferometric pathlengths are necessary to observe the interference oscillations. The stability in phase and amplitude of the $e/4$ oscillations has been tested with respect to sample dimensions, time, and temperature using this set of interferometers, and these results will be discussed.

- [1] Moore, G. and Read, N., Nucl. Phys. B360, 362 (1991).
- [2] Stern, A. and Halperin, B. I., Phys. Rev. Lett. 96, 016802-016805 (2006).
- [3] Bonderson, P., Kitaev, A. and Shtengel, K., Phys. Rev. Lett. 96, 016803-016806 (2006).
- [4] Willett, R.L., Pfeiffer, L.N., West, K.W., PNAS 106: 8853-8858 (2009).
- [5] Willett, R.L., Pfeiffer, L.N., West, K.W., PRB 82: 205301 (2010).

11:51AM Z19.00002 Observation of Braiding Statistics in the Fractional Quantum Hall Effect¹, WOOWON KANG, University of Chicago — It has been postulated that the quasiparticles excitations of fractional quantum Hall (FQH) states are Abelian anyons with fractional statistical angles. More interestingly, non-Abelian anyons have been predicted for certain FQH states such as that found at filling factors $\nu = 5/2$ and $12/5$. To date experimental detection of anyons and their braiding statistics in quantum interference experiments has remained controversial. In this talk I will present results from the study of Abelian and non-Abelian braiding statistics of anyons in the fractional quantum Hall (FQH) systems through Fabry-Perot interferometry. In the $\nu = 7/3$ FQHE state we confirm the anyonic braiding statistics by detecting the postulated statistical phase angle of $2\pi/3$. This result is consistent with a change of the anyon number by one. In the interference study of the $\nu = 5/2$ FQH state we observe phase slips $5\pi/4, \pi$, and $\pi/4$. These observed statistical phase slips agree with a theoretical model of braiding of Majorana modes of the $\nu = 5/2$ non-Abelian state that is strongly coupled to each other and to the edge modes of interferometer in presence of Coulomb interaction. Our results provide compelling support for the existence of non-Abelian anyons.

¹Work performed in collaboration with Sanghun An, P. Jiang, H. Choi, S.H. Simon, L.N. Pfeiffer, K.W. West, and K.W. Baldwin; supported by Microsoft and NSF MRSEC.

12:27PM Z19.00003 Quantum Hall interferometry in abelian and non-abelian states, ADY STERN¹, Weizmann Institute of Science — This talk deals with the theory of quantum Hall interferometers. I will first consider an idealized model of such interferometers and review how they may potentially identify anyonic quasi-particles, both abelian and non-abelian. I will then describe lessons learned from experiments regarding this idealized model, and how it should be amended to take into account effects of coupling between the bulk and the edge. In particular, I will describe how electron-electron interaction affects the outcome of interferometry experiments and distinguishes between “Aharonov-Bohm” and “Coulomb-dominated” regimes. These two regimes are characterized by different magnetic field periodicities and different directions of the equi-phase lines in the plane of magnetic field and voltage applied to a side gate. I will discuss how the contributions of the Aharonov-Bohm effect, the Coulomb interaction and the fractional statistics (abelian and non-abelian) may be distinguished from one another in the two regimes. Finally, I will address issues unique to non-abelian states, particularly the effect of bulk-edge tunnel coupling on the interference, and comment on experimental observations of interference in the $\nu = 5/2$ state.

¹The works I will describe have been carried out with B.I. Halperin (Harvard), I. Neder (Harvard & Tel-Aviv), Bernd Rosenow (Leipzig) and S.H. Simon (Oxford)

1:03PM Z19.00004 Plasma Analogy and non-Abelian Braiding Statistics in Ising-type Quantum Hall States, PARSA BONDERSOON, Microsoft Station Q — Quantum Hall systems are effectively two-dimensional and thus allow for quasiparticle excitations with exotic exchange statistics based on the braid group. These may be “anyons” with fractional statistics that lie somewhere between that of bosons and fermions, or, even more exotically, “non-Abelian anyons” with quasiparticle exchange represented by matrices. The quasiparticle statistics of candidate quantum Hall states (universality classes) is usually conjectured, but in some instances can be deduced from their representative trial wavefunctions. I will explain how this can be done for wavefunctions with a “plasma analogy” similar to Laughlin’s. Then I will construct a plasma analogy for the non-Abelian Ising-type states, e.g. the Moore-Read Pfaffian state. This provides the first complete proof of the non-Abelian braiding statistics of quasiparticles in these states, which are likely candidates to explain the observed Hall conductivity plateaus in the second Landau level, most notably the one at filling fraction $\nu = 5/2$.

1:39PM Z19.00005 Insights into the Nature of the Exotic Fractional Quantum Hall States from Ultra-low Temperature Transport, GABOR CSATHY, Purdue University — It is believed that the $\nu = 5/2$ and $12/5$ fractional quantum Hall states (FQHS) in the second Landau level of a two-dimensional electron gas support excitations with non-Abelian braiding statistics. Two outstanding questions concerning the nature of the both the odd and even denominator FQHS of the second Landau level as probed by transport measurements at temperatures as low as 5mK will be addressed. We report the discovery of a new odd denominator FQHS state at $\nu = 2 + 6/13$. The energy gaps of this and other states at $\nu = 2 + 1/3, 2 + 2/3$, and $2 + 2/5$ reveal a markedly different dependence on the effective magnetic field as compared to that of the corresponding lowest Landau level states at $6/13, 1/3, 2/3$, and $2/5$. If, in addition, we assume a Landau level-independent effective mass, we find that the $7/3$ and $8/3$ states are consistent, whereas the $2 + 2/5$ and the $2 + 6/13$ states show a strong deviation from the predictions of the model of free composite fermions. For the even denominator states at $\nu = 5/2$ and $7/2$ we extended measurements to the new regime of very low densities and to samples grown in two MBE chambers: one at Princeton and one at Purdue. Comparisons found in the literature of the experimentally measured intrinsic gaps at $\nu = 5/2$ with numerical results are confusing: three methods find a large difference whereas a fourth method finds a good agreement. Our data suggests that the former three methods have deficiencies and therefore cannot be used. Using the fourth and a new method we introduce we find an excellent agreement of the experimental and numerical intrinsic gaps at $\nu = 5/2$. These findings lend a strong support to the Pfaffian description of the $\nu = 5/2$ fractional state. Work done in collaboration with A. Kumar, N. Samkharadze, N. Deng, J. Watson, G. Gardner, M. Manfra, L. Pfeiffer, and K. West. G.A.C. has been supported by the NSF DMR-0907172 and DOE DE-SC0006671 grants.

Friday, March 2, 2012 11:15AM - 2:15PM –

Session Z20 DCMP: Invited Session: Optical Processes in Nitrides and Other Wide-Band-Gap Semiconductors 253C

11:15AM Z20.00001 Electronic Properties of ZnO: Reconciling Multiple Techniques¹, STEVEN M. DURBIN, University at Buffalo, The State University of New York — Significant progress has been made recently in our understanding of the electronic properties of ZnO and their physical origins, and yet we are far from being in possession of a complete picture despite decades of effort. Given the ultraviolet bandgap of this semiconductor (essentially the same as GaN), its easy synthesis using a wide variety of crystal growth techniques, the ready availability of high-quality single crystals, and intrinsic highly efficient luminescence, it is a material of great interest for a wide variety of device applications. Still, reliable p-type doping remains a considerable obstacle to realizing junction devices, and luminescence features often attributed to acceptor related transitions in fact have alternative physical origins. The role of impurities is reasonably well-understood, but a detailed understanding of dominant defects is somewhat elusive, although several techniques based directly and indirectly on Schottky contacts have provided some illumination on the topic. In this talk, I will summarize recent results in the field, and outline some of the key issues to which definitive answers are desirable if ZnO is going to be commercially competitive with GaN.

¹This work was supported in part by the MacDiarmid Institute for Advanced Materials and Nanotechnology; the Marsden Fund; and the State University of New York, and represents a collaboration with Canterbury Univ., Warwick Univ. and the Univ. of Michigan.

11:51AM Z20.00002 Loss mechanisms in nitrides¹, CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara — Indium gallium nitride alloys are successfully being used for light emitting diodes (LEDs) and laser diodes (LDs) in the green to ultraviolet part of the optical spectrum. These devices are the key enablers to Solid-State Lighting, which promises to significantly cut electricity consumption. Applications are still limited, however, by the declining efficiency of LEDs at high currents ("droop") and by absorption losses of undetermined origin in LDs. Several mechanisms have been suggested as the cause of this efficiency loss, such as Auger recombination and free carrier absorption. Experimentally it is very difficult to discriminate between different nonradiative processes. We have therefore addressed the loss mechanisms based on state-of-the-art first-principles computational theory. We use ab initio wave functions and bands that are accurate throughout the entire Brillouin zone (as opposed to k.p band structures). For Auger recombination we find that both electron-electron-hole and hole-hole-electron processes contribute, and that indirect processes assisted by alloy scattering and by electron-phonon coupling dominate. The magnitude of the resulting Auger coefficient indicates that Auger recombination is indeed responsible for the efficiency reduction at high carrier densities. Strategies for overcoming this limitation will be discussed. For free-carrier absorption, the relevant optical processes are again indirect. We determine the optical absorption coefficient and the corresponding photon mean free path as a function of carrier concentration. The computed values indicate that the effect is weak in LEDs but constitutes an important loss mechanism in LDs.

¹Work performed in collaboration with E. Kioupakis, P. Rinke, K. Delaney, and D. Steiauf, and supported by DOE and by the UCSB SSLEC.

12:27PM Z20.00003 Carrier localisation mechanisms and efficiency droop in nitride quantum wells, COLIN HUMPHREYS, University of Cambridge — A variety of experimental evidence indicates that the carriers in InGaN quantum wells (QWs) in InGaN/GaN QW structures are localised at room temperature, for example the S-shape temperature dependence of the peak photoluminescence (PL) energy with increasing excitation power density, a key fingerprint of carrier localisation. This localisation is believed to be responsible for the high efficiency of light emission from InGaN QWs since it prevents the carriers from moving to non-radiative recombination centers such as dislocations. In-rich clusters in the InGaN QWs were widely believed to be responsible for the localisation of the carriers. However, careful electron microscopy (EM) and atom probe tomography (APT) have shown that such clusters do not exist in InGaN QWs, at least for In contents less than 25%, and hence such clusters cannot be responsible for the localisation of the carriers. So what mechanisms are localising the carriers? APT and EM have shown that the InGaN in the QWs is a random alloy, with the In atoms distributed at random on the Ga sites. They have also shown that the InGaN QWs have monolayer and bilayer thickness fluctuations. Quantum mechanical calculations show that the holes in the InGaN QWs are localised on a scale of 1-2nm by the random indium fluctuations, and the electrons are localised on a scale of about 5nm by the QW thickness fluctuations. This localisation prevents the carrier from diffusing to dislocations and hence results in a high efficiency of light emission at room temperature. At high carrier densities the localised states saturate with carriers and the additional non-localised carriers can then diffuse to defects and recombine non-radiatively. It is suggested that this is a significant contributory factor to the efficiency droop observed in InGaN/GaN QW structures at higher current densities.

1:03PM Z20.00004 Photoluminescence as a tool for characterizing point defects in semiconductors, MICHAEL RESHCHIKOV, Physics Department, Virginia Commonwealth University — Photoluminescence is one of the most powerful tools used to study optically-active point defects in semiconductors, especially in wide-bandgap materials. Gallium nitride (GaN) and zinc oxide (ZnO) have attracted considerable attention in the last two decades due to their prospects in optoelectronics applications, including blue and ultraviolet light-emitting devices. However, in spite of many years of extensive studies and a great number of publications on photoluminescence from GaN and ZnO, only a few defect-related luminescence bands are reliably identified. Among them are the Zn-related blue band in GaN, Cu-related green band and Li-related orange band in ZnO. Numerous suggestions for the identification of other luminescence bands, such as the yellow band in GaN, or green and yellow bands in ZnO, do not stand up under scrutiny. In these conditions, it is important to classify the defect-related luminescence bands and find their unique characteristics. In this presentation, we will review the origin of the major luminescence bands in GaN and ZnO. Through simulations of the temperature and excitation intensity dependences of photoluminescence and by employing phenomenological models we are able to obtain important characteristics of point defects such as carrier capture cross-sections for defects, concentrations of defects, and their charge states. These models are also used to find the absolute internal quantum efficiency of photoluminescence and obtain information about nonradiative defects. Results from photoluminescence measurements will be compared with results of the first-principle calculations, as well as with the experimental data obtained by other techniques such as positron annihilation spectroscopy, deep-level transient spectroscopy, and secondary ion mass spectrometry.

1:39PM Z20.00005 Numerical Simulation of III-Nitrides Materials and Light Emitting Devices¹, ENRICO BELLOTTI, Boston University — The versatility of III-Nitrides semiconductors has led to their use in an increasing number of technologically important applications. Their ability to operate over a wide spectral range from the infrared to the deep ultraviolet has propelled this material system into the field light emitters and detectors. Furthermore, their desirable high field transport properties make III-Nitrides an ideal platform for power semiconductor devices. Along with the experimental activity to fabricate and characterize optoelectronic and electronics devices, a number of significant theoretical efforts are underway to understand the novel properties of this material system. This presentation will discuss the unique characteristics that the III-Nitrides material presents from the point of view of the carrier transport and optical properties. The quantum mechanical processes that are responsible for breakdown at high fields will also be discussed. In particular it will be shown that these quantum mechanical effects have to be taken into account to reproduce a number of experimental results. Furthermore, an analysis of the non-radiative recombination processes that are relevant in analyzing the quantum efficiency data of III-Nitride based light emitters will be presented. Finally the model used and the results obtained for the direct and assisted (phonons and electrons) Auger recombination rates and their impact on the calculated quantum efficiency of III-Nitrides based LEDs will be presented.

¹This work was supported by NSF, ARL and BU Photonics Center.

Friday, March 2, 2012 11:15AM - 2:15PM –

Session Z22 DMP DCOMP: Focus Session: Fe-based Superconductors - Orbital Order and Chalcogenides 254B

11:15AM Z22.00001 Orbital Order and Orthorhombic Anisotropy in Iron Pnictides¹, CHENG-CHIEN CHEN, Stanford Institute for Materials and Energy Science, SLAC National Accelerator Laboratory — Orthorhombic anisotropy has been reported in iron-pnictide superconductors by a broad range of experiments, including neutron scattering, transport measurements, and a variety of spectroscopies. We explore the idea that these observed anisotropies of broken tetragonal symmetry stem from an ordering of the partially-filled iron d-orbitals. In particular, we will consider a model Hamiltonian that couples the spin and orbital variables, and show that this spin-orbital model captures several observed behaviors in the iron-pnictide materials. We will conclude the talk by discussing x-ray absorption linear dichroism and other recent experiments supportive of theories highlighting the orbital degrees of freedom.

¹Research supported by the U.S. Department of Energy under contract No. DE-AC02-76SF00515. Work in collaboration with the research groups of Thomas Devereaux and Rajiv Singh.

11:51AM Z22.00002 Orbital ordering in Ba(Fe_{1-x}Co_x)₂As₂ revealed by X-ray absorption Spectroscopy, Y.K. KIM, W.S. JUNG, G.R. HAN, C. KIM, Yonsei Univ., K.-Y. CHOI, Seoul National Univ., A.P. SINGH, J.Y. KIM, Pohang accelerator lab., J. MIYAWAKI, Y. TAKATA, A. CHAINANI, Excitation order research team, RIKEN SPing-8 Center — Recently, anomalous in-plane anisotropy was observed by various experiment in iron pnictide systems. To explain the anomalous in-plane anisotropic behavior observed in iron pnictide system, orbital ordering was suggested as an origin of it. Among the various possible ordering, Ferroorbital ordering was proposed which occurs unequal occupation number of d_{yz} and d_{zx} orbital. It was theoretically predicted that such orbital ordering could be observed by performing X-ray Linear Dichroism experiment. To figure out, we performed the experiment on the most studied iron pnictide system, Ba(Fe_{1-x}Co_x)₂As₂. We obtained linear dichroism signal which indicates different occupation number for different orbital. And we observed temperature and doping dependence of the dichroism signal. Our results support the existence of ferro-orbital ordering.

12:03PM Z22.00003 Non-Fermi Liquid due to Orbital Fluctuations in Iron Pnictide Superconductors, WEI-CHENG LEE, PHILIP PHILLIPS, University of Illinois at Urbana-Champaign — We propose that the quantum fluctuations associated with quasi-1D d_{xz} and d_{yz} bands could result in a non-Fermi liquid behaviour in iron-pnictide superconductors. Using a five orbital tight binding model with generalized Hubbard on-site interactions, we find that within a one-loop treatment, a branch of overdamped collective modes develops at low frequency in channels associated with quasi-1D d_{xz} and d_{yz} bands. When the critical point for the C₄ symmetry broken phase (structural phase transition) is approached, the overdamped collective modes soften, and acquire increased spectral weight, leading to a non-Fermi liquid behavior at the Fermi surface. We argue that this non-Fermi liquid behavior is responsible for the recently observed zero-bias enhancement in the tunneling signal in quantum point contact spectroscopy. A key experimental test of this proposal is the absence of the non-Fermi liquid behaviour in the hole-doped materials. Our result suggests that quantum criticality plays an important role in understanding the normal state properties of iron-pnictide superconductors.

12:15PM Z22.00004 Spin and orbital characters of excitations in iron arsenide superconductors revealed by simulated resonant inelastic x-ray scattering, TAKAMI TOHYAMA, Yukawa Institute for Theoretical Physics, Kyoto University, EIJI KANESHITA, Sendai National College of Technology, KENJI TSUTSUI, Synchrotron Radiation Research Center, Japan Atomic Energy Agency — We theoretically examine the orbital excitations coupled to the spin degree of freedom in the parent state of the iron-arsenide superconductor, based on the calculation in a five-band itinerant model [1]. The calculated Fe L₃-edge resonant inelastic x-ray scattering (RIXS) spectra disclose the presence of spin-flip excitations involving several specific orbitals. Magnon excitations predominantly composed of a single orbital component can be seen in experiments, although its spectral weight is smaller than spin-flipped interorbital high-energy excitations. The detailed polarization and momentum dependence is also discussed with predictions for the experiments. [1] E. Kaneshita, K. Tsutsui, and T. Tohyama, Phys. Rev. B **84**, 020511(R) (2011)

12:27PM Z22.00005 Orbital fluctuation mediated superconductivity and structure transition in iron-based superconductors, HIROSHI KONTANI, Nagoya University — The main features in Fe-based superconductors are summarized as (i) orthorhombic transition accompanied by remarkable softening of the shear modulus C₆₆, (ii) high-T_c superconductivity close to the orthorhombic phase, and (iii) stripe-type magnetic order induced by orthorhombicity. To understand them, we analyze the multiorbital Hubbard-Holstein model with Fe-ion optical phonons. In the random-phase-approximation (RPA), a small electron-phonon coupling constant ($\lambda \sim 0.2$) is enough to produce large orbital (=charge quadrupole) fluctuations. The most divergent susceptibility is the O_{xz}-antiferro-quadrupole (AFQ) susceptibility, which causes the s-wave superconductivity without sign reversal (s₊₊-wave state). ¹ The s₊₊-wave state is robust against impurities, ² consistently with experimental observations. At the same time, divergent development of O_{x²-y²}-ferro-quadrupole (FQ) susceptibility is brought by the “two-orbital process” with respect to the AFQ fluctuations.

¹H. Kontani and S. Onari, Phys. Rev. Lett. **104**, 157001 (2010).

²S. Onari and H. Kontani, Phys. Rev. Lett. **103**, 177001 (2009).

12:39PM Z22.00006 A Monte Carlo simulation study of phase transitions in spin-orbital models for iron pnictides¹, RYAN APPLGATE, RAJIV SINGH, Department of Physics, University of California, Davis, CHENG-CHIEN CHEN, THOMAS DEVEREAUX, Department of Physics, Stanford University, Stanford — The common phase diagrams of superconducting iron pnictides show interesting material specificities in the structural and magnetic phase transitions. In some cases the two transitions are separate and second order, while in others they appear to happen concomitantly as a single first order transition. We explore these differences using Monte Carlo simulations of a two-dimensional Hamiltonian with coupled Heisenberg-spin and Ising-orbital degrees of freedom. In this spin-orbital model, the finite-temperature orbital-ordering transition results in a tetragonal-to-orthorhombic symmetry reduction and is associated with the structural transition in the iron-pnictide materials. With a zero or very small spin space anisotropy, the magnetic transition separates from the orbital one in temperature, and the orbital transition is found to be in the Ising universality class. With increasing anisotropy, the two transitions rapidly merge together and tend to become weakly first order. We also study the case of a single-ion anisotropy and propose that the preferred spin-orientation along the antiferromagnetic direction in these materials is driven by orbital order.

¹Supported in part by NSF-DMR1004231 and US DOE DE-AC02-76SF00515

12:51PM Z22.00007 Local Quantum Criticality of an Iron-Pnictide Tetrahedron¹, TZE TZEN ONG, PIERS COLEMAN, Center for Materials Theory, Department of Physics & Astronomy, Rutgers University — Motivated by the close correlation between transition temperature (T_c) and the tetrahedral bond angle of the As-Fe-As layer observed in the iron-based superconductors, we study the interplay between spin and orbital physics of an isolated iron-arsenide tetrahedron embedded in a metallic environment. Whereas the spin Kondo effect is suppressed to low temperatures by Hund's coupling, the orbital degrees of freedom are expected to quantum mechanically quench at high temperatures, giving rise to an overscreened, non-Fermi liquid ground-state. Translated into a dense environment, this critical state may play an important role in the superconductivity of these materials.

¹This work is supported by DOE grant DE-FG02-99ER45790.

1:03PM Z22.00008 Hint of a condensate in $K_{0.8}Fe_{2-y}Se_2$ ¹, C.C. HOMES, J.S. WEN, Z.J. XU, G.D. GU, Condensed Matter Physics and Materials Science Dept., Brookhaven National Laboratory, Upton, New York — The optical properties of the iron-chalcogenide superconductor $K_{0.8}Fe_{2-y}Se_2$ with a critical temperature $T_c = 31$ K have been measured over a wide frequency range in the a - b planes above and below T_c . The conductivity is incoherent at room temperature, but becomes coherent (Drude-like) with $\omega_{p,D} \simeq 430 \pm 20$ cm⁻¹ and $1/\tau_D \simeq 70 \pm 5$ cm⁻¹ at $T \simeq T_c$; however, $\omega_{p,D}$ is an order of magnitude smaller than what is observed in other iron-based superconductors. The highly anisotropic nature of these materials suggests that the transport is best described by a sheet resistance $R_{\square} = \rho_{dc}/d \simeq 64$ k Ω (per sheet), well above the threshold for the superconductor-insulator transition at $R_{\square} = h/4e^2 \simeq 6.9$ k Ω . Below T_c , $\omega_{p,S} \simeq 220 \pm 20$ cm⁻¹ resulting in a superfluid density $\rho_{s0} \equiv \omega_{p,S}^2 \simeq 48 \times 10^3$ cm⁻², placing this material on the scaling line $\rho_{s0}/8 \simeq 4.4 \sigma_{dc} T_c$ observed for the cuprates, but in a region associated with Josephson coupling, suggesting this material is inhomogeneous and constitutes a Josephson phase.²

¹Supported by the DOE under Contract No. DE-AC02-98CH10886.

²C. C. Homes *et al.*, arXiv:1110.5529

1:15PM Z22.00009 Optical spectroscopy of $K_xFe_{2-y}Se_{2-z}S_z$ superconductors¹, CATALIN MARTIN, K. MILLER, University of Florida, Gainesville, FL 32611, HECHANG LEI, C. PETROVIC, Brookhaven National Laboratory, Upton, NY 11973, D. B. TANNER, University of Florida, Gainesville, FL 32611 — We measured the temperature dependent optical reflectivity $R(\omega)$ and extracted the complex optical conductivity $\sigma(\omega)$ of the $K_xFe_{2-y}Se_{2-z}S_z$ superconductors. At room temperature, both $R(\omega)$ and $\sigma_1(\omega)$ have semiconducting behavior. Upon cooling, at temperatures depending on the S-concentration, the low frequency reflectivity increases in absolute value and shows a sharp upturn, consistent with metallic behavior. The phonon spectrum of $\sigma_1(\omega)$, which is very different from similar Fe-based superconductors and also doping dependent will be explained in terms of the changes in occupancy of the Fe-sites with doping. An anomalous feature in optical reflectivity is observed in the superconducting state and its possible origin and association with the condensation of free carriers will be discussed.

¹Supported by US DOE under contract DE-FG02-02ER45984 and under contract DE-AC02-98CH10886

1:27PM Z22.00010 Electronic Structure of $K_{0.8}Fe_2Se_2$ High Temperature Superconductor, SHIZHONG YANG, RUI GUO, EBRAHIM KHOSRAVI, GUANG-LIN ZHAO, DIOLA BAGAYOKO, Southern University and A&M College, ELECTRONIC STRUCTURE TEAM, HPC TEAM — Since the synthesis of the first ones in 2008, iron-based high temperature superconductors have been the subject of many studies. This great interest is partly due to their higher, upper magnetic field, smaller Fermi surface around the Γ point, and a larger coherence length. This work is focused on $A_xFe_2Se_2$ structural superconductor (FeSe, 11 hierarchy; A=K, Cs) as recently observed. ARPES data show novel, electronic structure and a hole-free Fermi surface which is different from previously observed Fermi surface images. *Ab initio* density functional theory GW method was used to simulate the electronic structure of the novel superconductor $A_xFe_2Se_2$. We compare this electronic structure with those of other Fe-based superconductors. Possible explanations for the hole-free Fermi surface were discussed.

1:39PM Z22.00011 ARPES studies of the AFe_2Se_2 (A=K, Rb, Cs) iron-based superconductors, MING YI, Stanford University, D.H. LU, SLAC National Accelerator Laboratory, Z.K. LIU, S. RIGGS, J.-H. CHU, Stanford University, B. LV, University of Houston, S.-K. MO, Lawrence Berkeley National Laboratory, M. HASHIMOTO, SLAC National Accelerator Laboratory, R.G. MOORE, Stanford Institute for Materials and Energy Sciences, Z. HUSSAIN, Lawrence Berkeley National Laboratory, I.R. FISHER, Stanford University, C.W. CHU, University of Houston, Z.-X. SHEN, Stanford University — The AFe_2Se_2 (A=K, Rb, Cs) family is one of the newest iron-based superconductors that has attracted considerable attention in the pnictide community due to its many differences with the other iron pnictide compounds, including a very large magnetic moment indicative of strong electron correlation, insulating behavior in non-superconducting compounds, and even in superconducting compounds resistivity shows a bad metallic behavior that crosses over into insulating behavior at higher temperatures. Despite such marked differences with the other pnictides, T_c in AFe_2Se_2 can be as high as 30K. Such interesting properties suggest that the AFe_2Se_2 superconductors may be close to a Mott insulating state, and many theoretical efforts have followed in this regard. Here we present detailed angle-resolved photoemission studies of AFe_2Se_2 to address the issue of whether these materials are indeed close to a Mott insulating state.

1:51PM Z22.00012 One-Fe versus Two-Fe Brillouin Zone of Fe-Based Superconductors: Creation of the Electron Pockets via Translational Symmetry Breaking¹, CHIA-HUI LIN, Brookhaven National Laboratory/ Stony Brook University, TOM BERLIJN, LIMIN WANG, CHI-CHENG LEE, WEI-GUO YIN, Brookhaven National Laboratory, WEI KU, Brookhaven National Laboratory/ Stony Brook University — We investigate the physical effects of translational symmetry breaking in Fe-based high-temperature superconductors due to alternating anion positions [1]. In the representative parent compounds, including the newly discovered Fe-vacancy-ordered $K_{0.8}Fe_{1.6}Se_2$, an unusual change of orbital character is found across the one-Fe Brillouin zone upon unfolding the first-principles band structure and Fermi surfaces [2], suggesting that covering a larger one-Fe Brillouin zone is necessary in experiments. Most significantly, the electron pockets (critical to the magnetism and superconductivity) are found only created with the broken symmetry, advocating strongly its full inclusion in future studies, particularly on the debated nodal structures of the superconducting order parameter. [1] C.-H. Lin et al, arXiv:1107.1485 (2011). [2] Wei Ku et al, Phys. Rev. Lett. 104, 216401 (2010).

¹Work supported by DOE DE-AC02-98CH10886.

2:03PM Z22.00013 Metal-to-Insulator Transition in Multi-Orbital Models for $A_xFe_ySe_2$, RONG YU, QIMIAO SI, Department of Physics and Astronomy, Rice University, Houston, TX 77005 — The degree of electron correlations remains a central issue in the iron-based superconductors. Compared to other compounds, the newly discovered $A_xFe_ySe_2$ family is unique in some aspects: the Fermi surface consists of only electron pockets, while T_c is as high as 30 K; the superconducting compound is close to an antiferromagnetically insulating phase with a large magnetic moment. These features suggest that the $A_xFe_ySe_2$ system contains stronger electron correlations than pnictides. To investigate the correlation effects in $A_xFe_ySe_2$, we study the metal-to-insulator transition in multi-orbital models for this system using slave-spin mean-field method. We show that when electron correlations are tuned, the system undergoes a metal-to-Mott-insulator transition at commensurate electron filling. We also find that the Mott insulator is close to an orbital-selective Mott phase in the phase diagram.

Friday, March 2, 2012 11:15AM - 2:15PM –

Session Z23 DCMP: Superconductivity: Magnetic Field & Vortex Related (Experimental) 255

11:15AM Z23.00001 Flux avalanches triggered by microwave depinning of superconducting vortices, AHMAD AWAD, FARKHAD ALIEV, Universidad Autonoma de Madrid Spain, WELDESCLASSIE ATAKLTI, ALEJANDRO SILHANEK, VICTOR MOSHCHALKOV, Katholieke Universiteit Leuven Belgium, YURI GALPERIN, University of Oslo Norway, VALERI VINOKUR, Argonne National Laboratory USA — We observe abrupt changes in broadband microwave permeability of thin Pb superconducting films as functions of the microwave frequency and intensity, as well as of external magnetic field. These changes are attributed to vortex avalanches generated by microwave induced depinning of vortices close to the sample edges. We map the experimental results on the widely used theoretical model assuming reversible response of the vortex motion to a. c. drive. It is shown that our measurements provide an efficient method of extracting the main parameter of the model- depinning frequencies for different pinning centers. The observed dependences of the extracted depinning frequencies on the microwave power, magnetic field and temperature support the idea that the flux avalanches are generated by microwave induced thermomagnetic instabilities.

11:27AM Z23.00002 Free flux flow: a probe into the field dependence of vortex core size in clean single crystals¹, A.A. GAPUD, O. GAFAROV, S. MORAES, University of South Alabama, J.R. THOMPSON, University of Tennessee and Oak Ridge National Laboratory, D.K. CHRISTEN, Oak Ridge National Laboratory, A.P. REYES, National High Magnetic Field Laboratory — The free-flux-flow (FFF) phase has been attained successfully in a number of clean, weak-pinning, low-anisotropy, low- T_c , single-crystal samples as a unique probe into type II superconductivity that is independent of composition. The “clean” quality of the samples have been confirmed by reversible magnetization, high residual resistivity ratio, and low critical current densities J_c with a re-entrant “peak” effect in $J_c(H)$ just below the critical field H_{c2} . The necessity of high current densities presented technical challenges that had been successfully addressed, and FFF is confirmed by a field-dependent ohmic state that is also well below the normal state. In these studies, the FFF resistivity $\rho_f(H)$ has been measured in order to observe the field-dependent core size of the quantized magnetic flux vortices as modeled recently by Kogan and Zelezhina (KZ) who predicted a specific deviation from Bardeen-Stephen flux flow, dependent on normalized temperature and scattering parameter λ . The compounds studied are: V_3Si , $LuNi_2B_2C$, and $NbSe_2$, and results have shown consistency with the KZ model. Other applications of this method could also be used to probe normal-state properties, especially for the new iron arsenides, as will be discussed.

¹Funded by the Research Corporation and by an NSF-RUI grant.

11:39AM Z23.00003 Vortex exclusion transition¹, MILIND KUNCHUR, MANLAI LIANG, University of South Carolina, ALEXANDER GUREVICH, Old Dominion University — Ordinarily, Abrikosov vortices penetrate a type-II superconductor in a magnetic field larger than the lower critical field. However if the sample dimensions/s transverse to the applied magnetic field become smaller than some limit (found by Likharev to be $d < 4.4\xi$ for a film of thickness d where ξ is the coherence length), the formation of a parallel vortex in a film is excluded. We measured the transport response of a Molybdenum-Germanium superconducting film in parallel magnetic field and observed a sharp change in the V-I characteristics at a temperature which corresponds to the condition that $d \approx 4.4\xi(T)$. We present the evolution of the observed transport behavior as a function of temperature and magnetic field.

¹This work was supported by the U. S. Department of Energy under Grant No. DE-FG02-99ER45763

11:51AM Z23.00004 Vortex motion in superconducting single-crystal microstructures of $NbSe_2$ ¹, SHAUN MILLS, NEAL STALEY, CONOR PULS, The Pennsylvania State University, CHENYI SHEN, LINJUN LI, ZHUAN XU, Zhejiang University, YING LIU, The Pennsylvania State University — Superconducting microstructures prepared by advanced nanofabrication methods can be used to address long-standing, fundamental questions concerning vortex motion, including vortex tunneling and the Aharonov-Casher effect of vortices. The observation of these phenomena requires devices with minimal disorder and the fewest dissipative normal electrons. We have developed a process to fabricate superconducting microstructures from single-crystal ultrathin flakes of the layered Type II superconductor $NbSe_2$. Our process utilizes a multi-step electron beam lithography technique, whereby a $NbSe_2$ flake is cut into a desired microstructure with appropriate electrical leads. Despite the small device dimensions, which feature line widths less than 40 nanometers, our devices are superconducting. We are currently working on superconducting microstructures of $NbSe_2$ that involve integration of aluminum leads, aiming at the control and measurement of vortices in these novel structures.

¹Work supported by NSF under grant CMMI 09-00692

12:03PM Z23.00005 Evidence of Vortex Jamming in Abrikosov Vortex Flux Flow Regime¹, GORAN KARAPETROV, Physics Department, Drexel University, V. YEFREMENKO, G. MIHAJLOVIC, J.E. PEARSON, Argonne National Laboratory, M. IAVARONE, Temple University, V. NOVOSAD, S.D. BADER, Argonne National Laboratory — We report on dynamics of non-local Abrikosov vortex flow in mesoscopic superconducting Nb channels. Magnetic field dependence of the non-local voltage induced by the flux flow shows that vortices form ordered vortex chains. Voltage asymmetry (rectification) with respect to the direction of vortex flow is evidence that vortex jamming strongly moderates vortex dynamics in mesoscopic geometries. The findings can be applied to superconducting devices exploiting vortex dynamics and vortex manipulation, including superconducting wires with engineered pinning centers.

¹This work was supported by UChicago Argonne, LLC, Operator of Argonne National Laboratory. Argonne, a U.S. Department of Energy Office of Science Laboratory, is operated under Contract No. DE-AC02-06CH11357 and US DOE Grant No. DE-FG02-10ER46710

12:15PM Z23.00006 Vortex Pinning Enhancement in Patterned MoGe Thin Films Coated with Permalloy, MICHAEL LATIMER, ZHILI XIAO, Northern Illinois University, Argonne National Laboratory, RALU DIVAN, IL WOONG JUNG, WAI-KWONG KWOK, Argonne National Laboratory — Resistivity measurements on permalloy (Py) coated MoGe thin films containing periodic hole arrays were carried out to study the effects of magnetic material filling the hole array. Thin films of MoGe were patterned via focused-ion-beam (FIB) milling to create pinning sites for the vortex lattice. A Py layer was deposited onto the hole array using magnetron sputtering. We investigate periodic hole arrays coated with magnetic material to determine the change in transport properties with varying magnetic fields. Samples with and without a Py coating were tested to determine the effect of magnetic material filling the hole array on the vortex lattice. Significant pinning enhancement was found in the Py coated samples.

12:27PM Z23.00007 Vortex Confinement in Planar S/F Hybrid Structures¹, S. MOORE, Physics Department, Temple University, Philadelphia, PA 19122 USA, V. NOVOSAD, V.G. YEFREMENKO, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439 USA, G. KARAPETROV, Physics Department, Drexel University, Philadelphia, PA 19104 USA, M. IAVARONE, Physics Department, Temple University, Philadelphia, PA 19122 USA — We have investigated the effect of periodic stray fields of the ferromagnet on the vortex dynamics in superconductor/ferromagnet (S/F) systems. Magnetization measurements were performed using SQUID magnetometry for Permalloy/Niobium (Py/Nb) samples of varying Py domain widths and Nb thicknesses. The hysteresis loops show an increase of the critical current for some values of magnetic domain width and superconductor thickness in some portion of the H-T phase diagram. However, below a threshold temperature sudden jumps in magnetization are observed during a slow sweep of the external magnetic field, which indicate the occurrence of vortex avalanches. These avalanches have been confirmed by scanning probe microscopy and they can cause a collapse of the critical state below a threshold temperature. Static and dynamics of these systems will be discussed.

¹This work was supported by US DOE Grant No. DE-FG02-10ER46710 and UChicago Argonne, LLC, Operator of Argonne National Laboratory. Argonne, a U.S. Department of Energy Office of Science Laboratory, is operated under Contract No. DE-AC02-06CH11357.

12:39PM Z23.00008 Spatial resolution of MFM measurements of penetration depth, ERIC SPANTON, Stanford Institute for Materials and Energy Science, SLAC, LAN LUAN, Harvard, JOHN KIRTLEY, KATHRYN MOLTER, Stanford Institute for Materials and Energy Science, SLAC — The penetration depth and its temperature dependence are key ways to characterize superconductors. Measurements of the local Meissner response of a superconductor can determine the local penetration depth. To quantify the spatial resolution of such measurements, we seek to characterize the point spread function of magnetic force microscope (MFM) measurements of the penetration depth both numerically and experimentally. Modeling various geometries of MFM tips (pyramid, dipole, and long thin cylinder) in the presence of various geometries of spatial variation in the penetration depth (point variation, columnar defects, and planar defects or twin boundaries) shows the importance of the MFM tip geometry to achieving both excellent spatial resolution and quantitatively interpretable results. We compare these models to experimental data on pnictides and cuprates to set upper limits on the sub-micron-scale variation of the penetration depth. These results demonstrate both the feasibility and the technical challenges of submicron penetration depth mapping.

12:51PM Z23.00009 Direct observation of jamming of superconducting vortices in a funnel structure, VITALII VLASKO-VLASOV, TIM BENSEMAN, ULRICH WELP, WAI KWOK, Argonne National Laboratory — Arrest of the vortex dynamics at elevated temperatures is an imperative for using benefits of high T_c in cuprate superconductors. Here we explore experimentally a possibility of using funnel geometries for attenuation of the vortex motion. A single funnel structure is sculptured into a twin free single crystal of YBCO using laser lithography and ion milling. The magnetic field penetration patterns are studied using magneto-optical imaging technique at different temperatures below T_c . In ramping up fields we observe an increase of the vortex density in the throat of the funnel structure showing the jamming of vortices at the entry into narrow vortex channel. The effect is discussed using results of recent numerical simulations. This work was supported by UChicago Argonne, LLC, under contract No. DE-AC02-06CH11357.

1:03PM Z23.00010 Interplay between Superconducting Vortices in the Dynamic Regime and Magnetism in Borocarbides, MARCUS WEIGAND, CHRISTIAN BATISTA, LEV BULAEVSKII, SHIZENG LIN, FRANCISCO BACA, LEONARDO CIVALE, Los Alamos National Laboratory, SERGEY BUD'KO, PAUL CANFIELD, Ames Laboratory, BORIS MAIOROV, Los Alamos National Laboratory — In superconductors with coexisting magnetic order an interaction is expected between vortices moving above a certain speed and the intrinsic magnetic moments. It has been predicted that in this dynamic regime vortices emit energy through the radiation of spin waves, thus slowing down and reducing the dissipation associated with their movement.¹ While of potential interest for applications, this effect has not yet been proven experimentally. In order to elucidate the phenomenon, we have carried out electrical transport measurements on $\text{ErNi}_2\text{B}_2\text{C}$ single crystals, covering a broad range of temperatures, applied magnetic fields and field orientations. We observe a distinct change in the shape of current-voltage curves measured above and below the Néel temperature (T_N), which implies that the features seen below T_N are related to the material's antiferromagnetism. We complement these results with measurements of the irreversible magnetization, which also show significant anomalies around T_N . Angular critical current measurements have also been performed to investigate the influence of the material's intrinsic magnetic moments on its current-carrying capabilities.

¹A. Shekhter, L. N. Bulaevskii, and C. D. Batista, Phys. Rev. Lett. 106, 037001 (2011).

1:15PM Z23.00011 Vortex pinning effects in the Corbino geometry¹, YANIV ROSEN, STEFAN GUÉNON, IVAN SCHULLER, Center for Advanced Nanoscience, University of California San Diego — We probed a dynamic system of superconducting vortices with an artificial pinning landscape in the Corbino geometry. Current was applied from the center of the disc and propagated radially outward to produce a circular force with strength proportional to $1/r$ on the vortices. For small injection currents the vortex lattice is rigid, however large currents can cause shearing of the lattice. In order to investigate the temperature, current, and pinning lattice dependencies in different samples, we have defined Nb discs with a diameter of $60\text{ }\mu\text{m}$ on a circularly symmetric lattice of magnetic dots. In particular we present data that show steps instead of minima in the magnetoresistance curves at the position of the matching field indicating an unexpected influence of the pinning array on the motion of the vortex lattice.

¹This work was supported by the US-NSF

1:27PM Z23.00012 Zero average and net flows of vortices in hybrid nanostructures with asymmetric pinning potentials¹, JOSE L. VICENT, Universidad Complutense and IMDEA-Nanociencia (Madrid), DAVID PEREZ DE LARA, IMDEA-Nanociencia and Universidad Complutense (Madrid), ALICIA GOMEZ, FERNANDO GALVEZ, Universidad Complutense (Madrid), MIGUEL A. GARCIA, CSIC and IMDEA-Nanociencia (Madrid), ELVIRA M. GONZALEZ, Universidad Complutense (Madrid) — We have fabricated hybrid nanostructures with superconducting film on top of an array of magnetic nanotriangles. In these structures, non-zero DC and AC voltages (V_{DC} , V_{AC}) are generated by alternating currents injected in the hybrid device. The V_{DC} and V_{AC} behaviors give us an overall picture of the vortex dynamics and the rectification effects in these superconducting devices.

¹Spanish MICINN, CM and Santander-Complutense

1:39PM Z23.00013 Vortex configurations and geometrical shapes of superconducting MoGe networks revealed by scanning SQUID microscope¹, TAKEKAZU ISHIDA, HO THANH HUY, TSUTOMU YOTSUYA, Osaka Prefecture University, MASAHIKO HAYASHI, Akita University — We prepared square networks of MoGe films by a standard photolithographic technique to observe vortex penetration into the network by means of a scanning SQUID microscope under different conditions of applied magnetic fields and temperatures. We found that vortex distribution in network evolves with applied magnetic field. At half matching field, vortices showed a checkerboard pattern, being in good agreement with theoretical predictions. We also investigated how vortices occupy network holes at different temperatures. Vortices tend to align in a “diagonal” direction at high temperatures while vortices repel each other to become isolated vortices at lower temperatures. Our results are consistent with theoretical calculation for nanoscopic superconducting network using the nonlinear Ginzburg-Landau equation. We also demonstrate that our data processing method appreciably improved a spatial resolution of the SQUID microscope.

¹This work was partly supported by a Grant-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology of Japan (Grant Nos. 19206104, 23246173, 23226019).

1:51PM Z23.00014 Threshold Critical Current Density to Trigger Flux Avalanches in Superconducting Thin Films, W.A. ORTIZ, DF/UFSCar, Brazil and Centre for Advanced Study, Norwegian Academy of Science and Letters, M. MOTTA, F. COLAUTO, DF/UFSCar, Brazil, R. ZADOROSNY, DFQ/UNESP, Brazil, T.H. JOHANSEN, Physics, Univ of Oslo and Centre for Advanced Study, Norwegian Academy of Science and Letters, R. DINNEN, M. BLAMIRE, Materials Science, Cambridge Univ, UK, G.W. ATAKLTI, V.V. MOSHCHALKOV, A.V. SILHANEK, K.U.Leuven, Belgium — Under certain conditions of temperature and magnetic field, sudden flux bursts (avalanches) develop into superconducting films, as a consequence of thermomagnetic instabilities, which occur when heat dispersion is slower than magnetic diffusion. Based on a systematic study of the magnetic response (including magneto-optical imaging) of two Nb films - one plain and the other decorated with a square array of square antidots - we have found the existence of a threshold critical current density above which vortex avalanches are triggered. The experimental results reveal that this threshold value is nearly constant within the whole range of temperatures and magnetic fields investigated. The fact that an avalanche is triggered once the critical current reaches the threshold is in close correspondence with the behavior of granular material in sandpiles, which slides down whenever the slope exceeds the threshold repose angle. Our results are in perfect agreement with the predictions of a model for thermomagnetic instabilities in superconducting films, published previously by Yurchenko and coworkers [PRB 76, 092504 (2007)].

2:03PM Z23.00015 Vortex-state electrodynamics in superconducting thin films studied by infrared spectroscopy¹, XIAOXIANG XI, D.B. TANNER, Department of Physics, University of Florida, G.L. CARR, Photon Sciences, Brookhaven National Laboratory, J.-H. PARK, D. GRAF, National High Magnetic Field Laboratory, Florida State University — In a type-II superconductor, a magnetic field above the lower critical field creates vortices and dramatically changes the superconductor's electrodynamic response. Such changes have been observed in thin film samples by our infrared magneto-spectroscopy experiments with field normal to the film surface. The complex optical conductivity was extracted, and was compared to existing models for the effective electrodynamic response of the vortex state. We found a good agreement between our optical data and a calculation using Maxwell Garnett theory, which treats the mixed state as having normal-metal disks (representing the vortex cores) surrounded by superconductor. Our data also show the effect of magnetic-field-induced pair breaking on the superconducting fraction outside of the vortices.

¹Supported by the US DOE through contracts DE-FG02-02ER45984 at UF, DE-AC02-98CH10886 at the NSLS, and DE-FG52-10NA29659 at the NHMFL.

Friday, March 2, 2012 11:15AM - 12:39PM – Session Z26 DCOMP: General Theory / Computational Physics II 257B

11:15AM Z26.00001 Corrections to the geometrical interpretation of bosonization¹, MANFRED STEINER, BRAD MARSTON, Brown University — Bosonization is a powerful approach for understanding certain strongly-correlated fermion systems, especially in one spatial dimension but also in higher dimensions². The method may be interpreted geometrically in terms of deformations of the Fermi surface, and the quantum operator that effects the deformations may be expressed in terms of a bilinear combination of fermion creation and annihilation operators. Alternatively the deformation operator has an approximate representation in terms of coherent states of bosonic fields³. Calculation of the inner product of deformed Fermi surfaces within the two representations reveals corrections to the bosonic picture both in one and higher spatial dimensions. We discuss the implications of the corrections for efforts to improve the usefulness of multidimensional bosonization.

¹Supported in part by NSF DMR-0605619.

²A.Houghton, H.-J. Kwon and J. B. Marston, Adv. in Phys. **49**, 141 (2000).

³A. H. Castro Neto and E. Fradkin, Phys. Rev. B **49**, 10877 (1994).

11:27AM Z26.00002 Emergent Anyons in Exactly Solvable Discrete Models for Topological Phases in Two Dimensions¹, YUTING HU, SPENCER STIRLING², YONG-SHI WU³, Department of Physics and Astronomy, University of Utah — Anyons can emerge as collective excitations in models of topological phases. Exactly solvable discrete models that describe two-dimensional topological phases were proposed by Kitaev, and Levin and Wen respectively. I will present the explicit form of the operators that create and move fluxons (anyonic quasiparticles living at the plaquettes) in the Levin-Wen models. The exchange and exclusion statistics of these fluxons are studied. In particular, I will discuss the topological properties of Fibonacci anyons emerging in a particular Levin-Wen model.

¹YSW is supported in part by US NSF grant PHY-1068558.

²Department of Mathematics, University of Utah

³Key State Laboratory of Surface Physics, and Department of Physics, Fudan University

11:39AM Z26.00003 Uniform Approximation from Symbol Calculus on a Spherical Phase Space, LIANG YU, U.C. Berkeley — We use symbol correspondence and quantum normal form theory to develop a more general method for finding uniform asymptotic approximations. We then apply this method to derive a uniform approximation of the $6j$ -symbol in terms of the rotation matrices. The derivation is based on the Stratonovich-Weyl symbol correspondence between matrix operators and functions on a spherical phase space. The resulting approximation depends on a canonical, or area preserving, map between two pairs of intersecting level sets on the spherical phase space.

11:51AM Z26.00004 Searching for B-modes with QUIET: Latest results from the maximum-likelihood pipeline, INGUNN KATHRINE WEHUS, University of Oslo, QUIET COLLABORATION — The polarisation of the cosmic microwave background (CMB) gives us unique information about the existence of primordial gravitational waves and the energy scale of inflation. QUIET is a ground-based CMB polarisation experiment, taking advantage of the world's most sensitive microwave radiometers, to search for B-modes in the CMB polarisation. The pilot phase data taking was finished in December 2010, consisting of around 250 000 diode hours of Q-band data at 43 GHz and about ten times more W-band data at 94 GHz. The data are analyzed by two independent pipelines, the maximum-likelihood (ML) pipeline and the pseudo- C_ℓ (PCI) pipeline. I will present the ML pipeline and our latest results.

12:03PM Z26.00005 The Fourth Dimension and Transaction Line, PETER SCHICK, Columbia University — The fourth dimension is basically the depth between two objects or the depth between an object. It is the z compared to the length, width, height. When one looks at a few objects the depth in between them is the fourth dimension. The transaction line is a relationship between two objects that are falling. This line allows the relationship to form so that they fall at the same time, regardless how much they weigh.

12:15PM Z26.00006 Reconsidering Dark Matter, SOL AISENBERG, International Technology Group — There is a difference between (a) distances of remote standard candles, SN Type Ia, and (b) distances based upon their red shifts. It was believed that these galaxies had accelerated and used Dark Energy. There are 2 assumptions not supported by observations. The first is that the red shifts for remote galaxies are due to the Doppler Effect associated with receding velocity. Hubble only observed red shifts as a function of distances of known stars, and never measured receding velocities. He suggested the Doppler Effect as a cause, but expressed doubt about the suggestion. There are other causes for a red shift - gravity red shift of light from the sun, and loss of photon energy by gravity interaction of photons with dust and gas in interstellar space. The second assumption is that Hubble's linear relationship between the observed red shift and the distance will be valid at very large distances. Increasing red shift corresponds to a decrease of photon energy towards zero, and cannot be used for very remote stars - where the photon energy approaches zero and the red shift dependence becomes nonlinear and asymptotic to a constant value. This predicts the difference between the galaxy distances and the distances determined from their observed red shifts. The recent Nobel Prize (to Schmidt, Reis, and Perlmutter) needs reexamination. Two basic assumptions that are the foundation of their work may not be accurate. Details are in my earlier essays in "The Misunderstood Universe", © 2009. .

12:27PM Z26.00007 The Exact Solution of The Pioneer Anomaly According to The General Theory of Relativity and The Hubble's Law, AZZAM ALMOSALLAMI, University of Malaya — Radio metric data from Pioneer 10/11 indicate an apparent anomalous, constant, acceleration acting on the spacecraft with a magnitude $\sim 8 \times 10^{-10}$ m/s², directed towards the Sun[1,2]. Turyshev [7] examined the constancy and direction of the Pioneer anomaly, and concluded that the data a temporally decaying anomalous acceleration $-2 \times 10^{-11} \frac{m}{s^2 yr}$ with an over 10% improvement in the residuals compared to a constant acceleration model. Anderson, who is retired from NASA's Jet Propulsion Laboratory (JPL), is that study's first author. He finds, so "it's either new physics or old physics we haven't discovered yet." New physics could be a variation on Newton's laws, whereas an example of as-yet-to-be- discovered old physics would be a cloud of dark matter trapped around the sun[12]. In this paper I introduce the exact solution for the Pioneer anomaly depending on the general theory of relativity and the Hubble's law. According to my solution, there are two terms of decelerations that controls the Pioneer anomaly. The first is produced by moving the Pioneer spacecraft through the gravitational field of the Sun, which causes the velocity of the spacecraft to be decreased according to the Schwarzschild Geometry of freely infalling particle. This deceleration is responsible for varying behaviour of the Pioneer anomaly in Turyshev [7], depending on $1/r^{2.5}$ the distance from the sun. The second term is produced by the attractive force of the dark matter which is constant and equals to the Hubble's constant multiplied by the speed of light in vacuum.

Friday, March 2, 2012 11:15AM - 2:15PM –
Session Z27 DCMP: Invited Session: Interaction Driven Broken Symmetry States in Bilayer Graphene 258AB

11:15AM Z27.00001 Theoretical Approach to Many-body Instabilities in Bilayer Graphene¹, OSKAR VAFEK, National High Magnetic Field Laboratory and Florida State University — I will review current theoretical approach to electron-electron interaction driven many-body instabilities in bilayer graphene at the neutrality point. The role of competing interactions and the dependence of different ordering tendencies on the range of the interaction will be examined. In particular, I will argue that within the renormalization group approach, for longer range interaction giving predominantly forward scattering, the leading ordering tendency is towards a gapless electronic nematic state. For shorter range interactions giving additional back scattering comparable to the forward scattering, the leading ordering tendency is towards a gapped Neel antiferromagnet. These results will be discussed in the context of recent experiments reporting signatures of broken symmetry states in suspended bilayer graphene.

¹NSF CAREER Award under Grant no. DMR-0955561

11:51AM Z27.00002 Interaction-Driven Spectrum Reconstruction in Bilayer Graphene, KOSTYA NOVOSELOV, University of Manchester — The nematic phase transition in various two-dimensional electronic systems is a fascinating subject of an ongoing investigation. Driven by electron-electron interactions it represents a new class of strongly correlated electronic ground states. Thus it is extremely important and interesting to expand the list of materials where such transitions are observed to those with particularly unusual electronic dispersion. Here we show indications that bilayer graphene – a truly two-dimensional material with complex chiral electronic spectrum – undergoes such transition. This is especially surprising as no interaction effects have been observed so far in either mono- or bilayer graphene without a help of magnetic field. Gaining access to low-energy physics in bilayer graphene devices (by suspending our samples and achieving quasiparticle mobilities larger than 10^6 cm²/V.s) allowed us to observe strong spectrum reconstructions and electron topological transitions which we attribute being due to such nematic transition.

12:27PM Z27.00003 Spontaneous Quantum Hall Liquids, FAN ZHANG, (1) UT-Austin (2) UPenn — Driven by electron-electron interactions, bilayer graphene and its thicker cousins, chirally (ABC) stacked multilayers, exhibit a variety of distinct broken symmetry states in which each spin-valley flavor spontaneously transfers charge between layers, because of their flat touching bands and large pseudospin chiralities. These gapped states are accompanied by large momentum space Berry curvatures and different types of topological orders. These competing ground states are distinguished by their flavor Hall conductivities, orbital magnetizations, edge state properties, and response to external fields. These spontaneous quantum Hall (SQH) states at zero field smoothly evolve into quantum Hall ferromagnet states at finite field. Various phase transitions occur by tuning carrier densities, temperature, and external fields. Recently, SQH states have started to be observed and explored in transport and Hall experiments on suspended devices with dual gates.

1:03PM Z27.00004 Interaction-Driven Insulating States in Bilayer Graphene, CHUN NING LAU, University of California, Riverside — Bilayer graphene (BLG) at the charge neutrality point (CNP) is unstable to electronic interactions, and expected to host a ground state with spontaneously broken symmetries. Here I will present our transport spectroscopy measurements on singly- and dual-gated suspended BLG devices, which have field effect mobility values up to 250,000 and 100,000 cm²/Vs, respectively. We observe an insulating state at CNP with a gap ~2 meV, which can be closed by elevated temperature, finite doping or a perpendicular electric field of either polarity. For magnetic field B>1T, the gap increases linearly with B. Our work contributes towards understanding the rich interaction-driven physics in BLG.

1:39PM Z27.00005 Electronic structure of multilayer graphene¹, EDWARD MCCANN, Lancaster University — The single-particle low-energy Hamiltonian of bilayer graphene describes chiral quasiparticles with a dominantly parabolic dispersion exhibiting Berry phase 2π . This chiral Hamiltonian produces a doubly-degenerate zero-energy Landau level incorporating two different orbital states with the same energy. Taking into account spin and valley degeneracies, the zero-energy Landau level in a bilayer is eightfold degenerate, as compared to the fourfold degeneracy of other bilayer states and the fourfold degeneracy of all levels in a monolayer. Such levels can be split by interlayer asymmetry, due to the presence of an external gate or doping, or by interaction effects. This talk will describe the electronic behavior of multilayer graphene, focusing on three, four and five layers. The goal will be to identify features that are distinct from those observed in monolayers and bilayers, and to highlight effects - such as level splitting and crossing - that can be explained either within the single-particle picture or that require an understanding of electronic interactions. For example, the low-energy Hamiltonian of ABA-stacked multilayer graphene may be partially diagonalized into an approximate block-diagonal form, with each diagonal block contributing parabolic bands except for an additional block describing Dirac-like bands with a linear dispersion in a multilayer with an odd number of layers. By taking into account the symmetry of the crystal structure, it is possible to fully include the band parameters and to analyze their effect on the block-diagonal Hamiltonian. Next-nearest-layer couplings are shown to be particularly important in determining the low-energy spectrum and the phase diagram of the quantum Hall conductivity by causing energy shifts, level anti-crossings, and valley splitting of the low-lying Landau levels.

This work was done in collaboration with Mikito Koshino of the Department of Physics, Tohoku University, Sendai 980-8578, Japan.

¹This work was funded by the JST-EPSRC Japan-UK Cooperative Programme Grant No. EP/H025804/1.

Friday, March 2, 2012 11:15AM - 1:27PM –
Session Z29 GQI: Focus Session: Superconducting Qubits: Noise and Anomalous Temperature
259A

11:15AM Z29.00001 Measurement-induced qubit state mixing from upconverted low frequency noise¹, D.H. SLICHTER, R. VIJAY, S.M. WEBER, I. SIDDIQI, UC Berkeley, QNL — We observe readout-induced qubit state mixing in a flux-tunable transmon qubit coupled to a planar resonator. Our results indicate that dephasing noise at the qubit-cavity detuning frequency Δ is upconverted by photons in the readout cavity, causing spurious qubit state transitions in agreement with theory [1]. Using a superconducting parametric amplifier to perform continuous high-fidelity qubit measurement, we characterize the transition rate dependence on cavity photon population and the intensity of added low frequency noise injected from a broadband fast flux excitation line. From the remnant excitation rate in the absence of added noise, we extract a noise spectral density at frequencies ~ 1 GHz. We also measure the noise spectral density from 0.02-0.5 Hz and 1-20 MHz using Ramsey fringes and Rabi oscillations, respectively. Postulating that flux noise is the dominant source of dephasing in our qubit, we fit the measured noise to a $1/f^\alpha$ power law, finding a slope $\alpha = 0.6$ and amplitude $(1.4\mu\Phi_0)^2/\text{Hz}$ at 1 Hz. These values are in agreement with other measurements of low-frequency flux noise. Our results suggest that $1/f$ flux noise persists to GHz frequencies.

[1] Boissonneault et al., PRA 79, 013819 (2009).

¹This research was supported by the ARO QCT program.

11:27AM Z29.00002 $1/f$ Noise of Josephson Tunnel Junction Embedded Microwave Resonators at Single Photon Energies and Millikelvin Temperatures¹, I. SIDDIQI, KATER MURCH, STEVEN WEBER, ELI LEVENSON-FALK, R. VIJAY, UC Berkeley, QNL — We present measurements of the $1/f$ frequency noise of superconducting aluminum lumped and distributed element resonators in the low power, low temperature operating regime characteristic of superconducting qubits. A comparison was made between these devices and similar co-fabricated linear resonators to infer the level of critical current noise associated with the tunnel junctions. At 25 mK and in the single photon regime, the observed frequency fluctuations of junction embedded and linear resonators were comparable. Attributing all the observed noise to critical current fluctuations, we report an upper bound for $1/f$ critical current fluctuations in 0.5-2 μA junctions of $3 \times 10^{-8} (1/\sqrt{Hz})$ at 1 Hz. We note that for some samples we observed the activation of a single fluctuator above 50 mK which increased the level of noise significantly.

¹This research is supported by the IARPA CSQ program.

11:39AM Z29.00003 Flux Noise in SQUIDS Due to Hyperfine Interactions¹, JIANSHEG WU, CLARE YU, Department of Physics and Astronomy, University of California, Irvine, — Although there have been significant advances in superconducting qubits, they continue to be plagued by noise and decoherence. Low frequency $1/f$ flux noise in superconducting quantum interference devices (SQUIDS) is one of the dominant sources of noise in superconducting flux and phase qubits. Recent experiments implicate spins on the surface of metals as the source of flux noise in SQUIDS, and indicate that these spins are able to relax without conserving total magnetization. We present a model of $1/f$ flux noise in which electron spins on the surface of metals can relax via hyperfine interactions. Our results indicate that flux noise would be significantly reduced in superconducting materials where the most abundant isotopes do not have nuclear moments such as zinc and lead.

¹This work was supported by Army Research Office grant W911NF-10-1-0494.

11:51AM Z29.00004 Pure dephasing in flux qubits due to flux noise with spectral density scaling as $1/f^{\alpha_1}$, STEVEN ANTON, UC Berkeley, C. MULLER, Univ de Sherbrooke, J.S. BIRENBAUM, S.R. O'KELLEY, A.D. FEFFERMAN, UC Berkeley, D.S. GOLUBEV, Karlsruhe Institute of Technology, G.C. HILTON, H.-M. CHO, K.D. IRWIN, NIST, Boulder, F.C. WELLSTOOD, Univ of Maryland, GERD SCHON, A. SHNIRMAN, Karlsruhe Institute of Technology, JOHN CLARKE, UC Berkeley — Magnetic flux noise is a major source of pure dephasing in superconducting flux qubits. This noise, common to SQUIDs, is believed to arise from localized electrons whose spins reverse randomly. We present representative measurements on dc SQUIDs over a range of temperatures showing, in general, $S_{\Phi}(f) = A^2/(f/(1 \text{ Hz}))^{\alpha}$. In our measurements, A is of the order of $1 \mu\Phi_0\text{Hz}^{-1/2}$ and $0.6 < \alpha < 1$. Motivated by these results, for arbitrary values of α we calculate pure dephasing times for both Ramsey and echo pulse sequences assuming linear coupling between the energy level splitting and the flux through the qubit. We find that the dephasing time τ_{ϕ} decreases dramatically as α is reduced. In addition, the frequency bandwidth to which the qubit is sensitive—defined by the infrared and ultra-violet cutoff frequencies—can significantly affect τ_{ϕ} in a manner depending on the type of sequence and value of α . For each sequence, τ_{ϕ} becomes independent of the ultra-violet cutoff frequency when its value exceeds $1/\tau_{\phi}$. Finally, we present calculated dephasing times corresponding to our measured spectra.

¹This work was supported by ARO and IARPA.

12:03PM Z29.00005 Very-low-frequency spectroscopy of both flux and tunnel-coupling noise in a flux qubit, JONAS BYLANDER, FEI YAN, SIMON GUSTAVSSON, Massachusetts Institute of Technology, FUMIKI YOSHIHARA, Institute of Physical and Chemical Research (RIKEN), Japan, DAVID G. CORY, IQC, University of Waterloo, and Perimeter Institute, Canada, YASUNOBU NAKAMURA, NEC Corp. and RIKEN, Japan, WILLIAM D. OLIVER, MIT and MIT Lincoln Laboratory — We inferred the very-low-frequency noise (0.01 to 100 Hz) of a superconducting flux qubit by repeatedly subjecting it to free induction during a fixed length of time and sampling the binary read-out signal. The excited-state probability varies as the qubit-transition frequency fluctuates due to noise, and we control the sensitivities to noise in the energy and tunnel coupling terms of the Hamiltonian by tuning the static flux (energy) bias. At low temperature, interestingly, both types of low-frequency noise follow the same $1/f$ -type power laws observed at much higher frequencies. We will further present the temperature dependence of both noises from 10 to 200 mK.

12:15PM Z29.00006 $T_{1\rho}$ experiment as a noise spectrum analyzer, FEI YAN, SIMON GUSTAVSSON, JONAS BYLANDER, Massachusetts Institute of Technology, FUMIKI YOSHIHARA, The Institute of Physical and Chemical Research, YASUNOBU NAKAMURA, The Institute of Physical and Chemical Research, NEC, DAVID CORY, University of Waterloo, WILLIAM OLIVER, MIT Lincoln Laboratory — We performed a $T_{1\rho}$ (spin-locking) experiment on a superconducting flux qubit, enabling us to resolve the environmental noise in the intermediate-frequency range. By driving the qubit along its state polarization, in the rotating frame, it is effectively spin-locked: the decohering effect of low-frequency noise is thereby dramatically reduced compared to Rabi oscillations. We measured the $T_{1\rho}$ relaxation rate in the rotating frame, under different driving amplitudes and flux biases. Relating this driven relaxation rate to the noise at the corresponding Rabi frequency, we extracted the noise power spectral densities of the energy-bias (flux) and tunnel-coupling terms of the qubit's Hamiltonian at frequencies ranging from 0.5 to 100 MHz. In the flux-noise spectrum, we observed features due to non-Gaussian noise, which can be modeled by a strong random-telegraph fluctuator, supporting observations in the decoherence of a spin-echo.

12:27PM Z29.00007 Characterization of critical-current noise in Josephson junctions and its implications for qubit dephasing¹, CHRISTOPHER D. NUGROHO, VLADIMIR ORLYANCHIK, DALE J. VAN HARLINGEN, University of Illinois at Urbana-Champaign — Critical-current noise in Josephson junctions may ultimately limit the coherence of superconducting qubits. Presently qubit coherence times are limited by energy relaxation or other dephasing mechanisms, but recent qubit advances may put the coherence times in the regime where critical-current noise play an important role. We report on the measurement of I_c -noise in Josephson junctions and compare them to fluctuations in the normal state resistance when superconductivity is suppressed in a magnetic field. We measure the noise scaling with the junction area, normal state resistance, and temperature. We will then discuss the implication of this noise to qubit decoherence.

¹Work supported by IARPA grant Army UCB-00006692.

12:39PM Z29.00008 Pure dephasing from quasiparticle tunneling in superconducting qubits, GIANLUIGI CATELANI, Yale University — Quasiparticles tunneling across Josephson junctions provide an intrinsic decoherence mechanism in superconducting qubits. The quasiparticle current spectral density $S_{qp}(\omega)$ determines both the relaxation rate and the pure dephasing rate. The latter is in general proportional to the spectral density evaluated at zero frequency. In the case of quasiparticle, however, $S_{qp}(\omega)$ diverges logarithmically as frequency goes to zero, potentially leading to very fast dephasing. Here we show how to regularize this divergence in a self-consistent way. This enable us to estimate the dephasing rate due to quasiparticle tunneling and to study its magnetic flux dependence for various qubit designs.

12:51PM Z29.00009 Anomalous Temperatures of Superconducting Qubits¹, K. GEERLINGS, S. SHANKAR, Z. LEGHTAS, M. MIRRAHIMI, L. FRUNZIO, R.J. SCHOEKOPF, M.H. DEVORET, Applied Physics Dept., Yale University — We present qubit temperature measurements on several superconducting transmon qubits coupled to compact resonators. By addressing multiple transitions of the artificial atom and cavity system, we measured the temperature as a function of qubit and cavity frequency and cavity Q. For high cavity Q and large detuning, qubit temperatures were found to be greater than 120mK, well in excess of the dilution refrigerator base temperature of 15mK. This unanticipated effect can be explained by the decoupling of the qubit to the cold load damping the cavity. We will present our attempts to produce lower qubit temperatures with additional filtering and dynamical cooling experiments.

¹Work supported by IARPA, ARO and the NSF.

1:03PM Z29.00010 Minimizing environmental decoherence for a superconducting phase qubit - transmon architecture, RAMI BARENDTS, J. WENNER, M. LENANDER, Y. CHEN, J. KELLY, J. BOCHMANN, B. CHIARO, E. LUCERO, P. O'MALLEY, M. MARIANTONI, A. MEGRANT, C. NEILL, D. SANK, P. ROUSHAN, A. VAINSENER, H. WANG, T. C. WHITE, Y. YIN, A. N. CLELAND, JOHN M. MARTINIS, UC Santa Barbara, J. J. A. BASELMANS, SRON Netherlands Institute for Space Research — The coherence of superconducting quantum systems is currently a major obstacle towards high gate fidelity and long-lived memory. We found that quasiparticle generation from stray infrared light is a significant source of energy relaxation. We show that resonator quality factors and phase qubit energy relaxation times are limited by a quasiparticle density of approximately $200 \mu\text{m}^{-3}$, induced by 4 K blackbody radiation from the environment. We demonstrate how this influence can be fully removed by isolating the devices from the radiative environment using multistage shielding. In addition, we analyze the decoherence due to circuitry in our new phase qubit-transmon architecture. This architecture - consisting of transmon qubits, resonators, and phase qubits using a frequency domain multiplexed readout - is less affected by Purcell decay. At present, fabrication of samples is ongoing.

1:15PM Z29.00011 Designs towards improved coherence times in superconducting qubits, ANTONIO CORCOLES, JERRY CHOW, JAY GAMBETTA, CHAD RIGETTI, JIM ROZEN, GEORGE KEEFE, MARY BETH ROTHWELL, STEFANO POLETTI, MARK KETCHEN, MATTHIAS STEFFEN, IBM TJ Watson Research Center — Coherence times for superconducting qubits in a planar geometry have increased drastically over the past 10 years with improvements exceeding a factor of 1000. However, recently these appeared to have reached a plateau around 1-2 microseconds, the limits of which were not well understood. Here, we present experimental data showing that one limit is due to infra-red radiation, confirming observations from other groups. We observe increased coherence times after appropriate IR shielding. Further improvements are shown to be possible by increasing the feature size of the interdigitated shunting capacitor, strongly indicating that surface losses at the metal/substrate interface are limiting qubit coherence times. In our experiments we kept the ratio of line width to gap size constant, but increased the overall feature size. We will discuss this and other similar design approaches towards better coherence in superconducting qubits.

Friday, March 2, 2012 11:15AM - 2:15PM –
Session Z30 GQI: Focus Session: Quantum Information for Quantum Foundations - Quantumness versus Classicality 259B

11:15AM Z30.00001 Nonequilibrium quantum correlations and Leggett-Garg inequalities¹, J.C. CASTILLO, F.J. RODRIGUEZ, L. QUIROGA, Universidad de los Andes — Theoretical guides to test 'macroscopic realism' in condensed matter systems under quantum control are highly desirable. We report the evaluation of Leggett-Garg inequalities (LGI) in an out-of-equilibrium set up consisting in two interacting qubits coupled to independent baths at different temperatures as can occur for two dipolar coupled spins or superconducting qubits in diverse solid-state environments. We find that LGI violations persist for a longer time in a thermal nonequilibrium scenario as compared with similar results at thermodynamic equilibrium. We contrast these findings with the behavior of non-locality-dominated quantum correlation measurements, such as concurrence, between the two qubits under similar temperature gradients.

¹Facultad de Ciencias Research Funds, Universidad de los Andes.

11:27AM Z30.00002 Quantum Correlations in Large-Dimensional States of High Symmetry, ERIC CHITAMBAR, University of Toronto — Multiparty quantum systems can possess non-classical correlations more general than those characterized by entanglement. In this talk, I will discuss various proposed measures of quantum correlations and investigate how these measures behave for the so-called Werner and isotropic families of states. In particular, I will provide closed expressions for the quantum discord (QD) and the relative entropy of quantumness (REQ) in these states for arbitrary dimensions. The QD and REQ will be shown to equal one another, as well as other well-known measures of quantum correlations. For all Werner states, the classical correlations are seen to vanish in high dimensions while the amount of quantum correlations becomes independent of whether or not the state is entangled. For isotropic states, nearly the opposite effect is observed with both the quantum and classical correlations growing without bound as the dimension increases and only as the system becomes more entangled.

11:39AM Z30.00003 Nonnegative subtheories of qubits: stabilizer states and more, STEPHEN BARTLETT, JOEL WALLMAN, The University of Sydney — Negativity in a quasi-probability representation is typically interpreted as an indication of nonclassical behavior. However, this does not preclude bases that are nonnegative from having interesting applications—the single-qubit stabilizer states have nonnegative Wigner functions and yet play a fundamental role in many quantum information tasks. We determine what other sets of quantum states and measurements of a qubit can be nonnegative in a quasi-probability distribution, and identify nontrivial groups of unitary transformations that permute such states. These sets of states and measurements are analogous to the single-qubit stabilizer states. We show that no quasi-probability representation of a qubit can be nonnegative for more than 2 bases in any plane of the Bloch sphere. Furthermore, there is a unique set of 4 bases that can be nonnegative in an arbitrary quasi-probability representation of a qubit. We provide an exhaustive list of the sets of single-qubit bases that are nonnegative in some quasi-probability distribution and are also closed under a group of unitary transformations, revealing two families of such sets of 3 bases with quasi-probability distributions defined on a space of 8 ontic states. We extend several of these results to higher dimensions.

11:51AM Z30.00004 Symmetric States on the Octonionic Bloch Ball¹, MATTHEW GRAYDON, University of Waterloo, Perimeter Institute for Theoretical Physics, Institute for Quantum Computing — Finite-dimensional homogeneous self-dual cones arise as natural candidates for convex sets of states and effects in a variety of approaches towards understanding the foundations of quantum theory in terms of information-theoretic concepts. The positive cone of the ten-dimensional Jordan-algebraic spin factor is one particular instantiation of such a convex set in generalized frameworks for quantum theory. We consider a projection of the regular 9-simplex onto the octonionic projective line to form a highly symmetric structure of ten octonionic quantum states on the surface of the octonionic Bloch ball. A uniform subnormalization of these ten symmetric states yields a symmetric informationally complete octonionic quantum measurement. We discuss a Quantum Bayesian reformulation of octonionic quantum formalism for the description of two-dimensional physical systems. We also describe a canonical embedding of the octonionic Bloch ball into an ambient space for states in usual complex quantum theory.

¹This work was supported in part by the U. S. Office of Naval Research (Grant No. N00014-09-1-0247).

12:03PM Z30.00005 Magically, the negativity of the discrete Wigner function is useful, VICTOR VEITCH, CHRISTOPHER FERRIE, JOSEPH EMERSON, Institute for Quantum Computing and Department of Applied Mathematics, University of Waterloo — It is possible to represent d -dimensional quantum states as probability distributions over a phase space of d^2 points. However, to encompass the full quantum formalism we must allow negative representations. The well known magic state model of quantum computation gives a recipe for universal quantum computation using perfect Clifford operations and repeat preparations of a noisy ancilla state. It is an open problem to determine which ancilla states enable universal quantum computation in this model. In this talk we will show that for systems of odd dimension a necessary condition for a state to enable universal quantum computation is that it have negative representation in a particular quasi-probability representation. This representation is a natural discrete analogue to the Wigner function. This condition implies the existence of a large class of bound states for magic state distillation: states which cannot be prepared using Clifford operations but which are not useful for quantum computation. This settles in the negative the conjecture that all states not representable as a convex combination of stabilizer states enable universal quantum computation.

12:15PM Z30.00006 Anderson localization modeled by means of numerical solutions of the Schrödinger equation¹, NAGENDRA DHAKAL, SERGIO TAFUR, MICHAEL LEUNBERGER, UCF — We developed codes for simulating the Schrödinger equation based on the finite-difference time-domain (FDTD) method. We model the 2 dimensional free electron gas system using perfectly matched layers for the open surrounding space. We study the effect of localized impurities on the time evolution of the electron wave function, thereby observing dephasing introduced by the impurities. Our numerical simulations show the decoherence due to the impurities at moderate impurity densities and Anderson localization at high impurity densities. Our results are important for the implementation of quantum computing, quantum communication, and spintronics.

¹NSF Grant No. ECCS-0901784, AFOSR Grant No. FA9550-09-1-0450, and NSF Grant No. ECCS-1128597.X Prefer Oral Session Prefer Poster

12:27PM Z30.00007 Quench dynamics in the Anderson impurity model, DEEPAK IYER, NATAN ANDREI, Department of Physics and Astronomy, Rutgers, The State University of New Jersey — We study the non-equilibrium behavior of an interacting quantum dot following a quench, where it is suddenly attached to a lead. The system is modeled by a single level Anderson impurity model with infinite on-site repulsion attached via tunneling to non-interacting leads. We use the open system Bethe Ansatz solution of the Anderson model and develop a formal framework to implement Yudson's contour integral formalism in the presence of a Fermi sea. This framework allows the calculation of the full time evolution of the multi-particle wave function and various observables of the system.

12:39PM Z30.00008 Consistent quantum prediction and decoherence in quantum cosmology, DAVID CRAIG¹, Le Moyne College and Perimeter Institute for Theoretical Physics — A complete "consistent histories" framework for certain symmetry-reduced models of quantum gravity is given, within which probabilities may be consistently extracted from quantum amplitudes. The decoherence functional for both a standard "Wheeler-DeWitt" quantization and a loop quantization of a flat Friedmann-Robertson-Walker cosmological model is constructed, from which consistent quantum predictions may be made in mathematically precise models of quantum cosmologies. Consistent (decoherent) families of histories are exhibited, with an emphasis on the crucial role played by the decoherence of histories in arriving at self-consistent quantum predictions for these closed quantum systems. By way of example, the problem of resolution of the classical "big bang" singularity is compared and contrasted in these two models. Special attention is given to consistent quantum predictions in these theories which are *certain i.e.* predictions for which the problem of interpretation of probabilities for a closed quantum system is not present.

¹Based in part on joint work with Parampreet Singh, LSU.

12:51PM Z30.00009 Wavefunction Collapse via a Nonlocal Relativistic Variational Principle, ALAN HARRISON, Los Alamos National Laboratory — We propose a relativistically covariant variational principle (VP) capable of describing wavefunction collapse. This produces a nonlinear, nonlocal, time-reversal-invariant theory; the hidden variable is the phase of the wavefunction. The VP is $\delta(A_1 + A_2) = 0$, in which A_1 and A_2 are positive definite integrals over all spacetime of functions of $\psi(t, \vec{x})$. A_1 is quadratic in deviations of the wavefunction from compliance with the standard quantum mechanical (SQM) wave equation. A_2 takes a minimum value when the wavefunction is a state of minimal uncertainty, penalizing certain kinds of superpositions and thus driving collapse. A multiplier sets the relative size of the terms so that (1) A_1 dominates in isolated microscopic systems, so they evolve according to the SQM wave equation; and (2) macroscopic superpositions cause A_2 to dominate, driving the system to collapse. Since any macroscopic measurement apparatus is entangled with the system being measured, process (2) explains the empirical observation that measurement collapses the wavefunction. We show that A_2 enforces the Born rule, under suitable assumptions and approximations. As an example, the theory predicts the results of the two-slit experiment, including the delayed-choice variant.

1:03PM Z30.00010 New proofs of the Kochen-Specker theorem for a system of three qubits, MORDECAI WAECELL, P.K. ARAVIND, Worcester Polytechnic Institute — In 1995 Kernaghan and Peres gave a transparent state-independent "parity proof" of the Kochen-Specker theorem by using a system of three qubits. They did this by using the observables of the 3-qubit system to construct a set of 40 rays in a real 8-dimensional space that formed 25 bases, and then picked out a subset of the bases that gave a parity proof. They showed that there are 320 different (but unitarily equivalent) versions of their proof in this 40-ray set. We extend their result in a number of ways. Firstly, we show that this 40-ray set contains five new types of parity proofs in addition to the one found by Kernaghan and Peres, and that the total number of versions of all six types of proofs under the symmetries of the system is $2^{11} = 2048$. Secondly, we point out the existence of a large number of state-independent KS proofs in the 3-qubit system that are structurally different from the Kernaghan-Peres proof, and we explore their features. The geometry of mutually unbiased bases (MUBs) in the 3-qubit system, which played a crucial role in the discovery of these new proofs, will be discussed.

1:15PM Z30.00011 New Algorithms for Generating Arbitrary Kochen-Specker Sets, NORMAN D. MEGILL, Boston Information Group, Lexington, MA 02420, USA, MLADEN PAVIČIĆ, University of Zagreb, Croatia — The Kochen-Specker (KS) sets (constructive proofs of quantum contextuality) have recently obtained a special significance as building blocks of quantum information protocols since quantum contextuality was revealed as property complementary to nonlocality and entanglement. [A. Cabello, *Phys. Rev. Lett.* **104**, 220401 (2010).] Thus, generating arbitrary KS sets becomes as needed as generating Bell states and this has been enabled by recent findings of a vast amount ($> 10^{20}$) of new KS sets—we call them a "KS sea." [N.D. Megill, K. Fresl, M. Waegell, P.K. Aravind, and M. Pavičić, *Phys. Lett. A*, **375** 3419 (2011); M. Waegell and P.K. Aravind, *Int. J. Phys. A* [to appear] (2011).] Here we present our newest algorithms and computer programs which enable us to obtain any desired KS set from the KS sea in a very short time without ever making a complete data base of KS sets—which would be an impossible task anyhow. This was made possible with the help of our representation of the KS sea as well as individual KS sets by means of MMP hypergraphs.

1:27PM Z30.00012 How Different Can Quantum States with the Given Fidelity Be?, VIKTOR DODONOV, MATHEUS HOROVITS, Institute of Physics, University of Brasilia, Brazil — We address the following question: how big can the relative energy difference between two states of a harmonic oscillator (field mode) with the fixed value of fidelity F be? Exact analytical bounds are found for several popular families of quantum states: coherent, squeezed, arbitrary (mixed) Gaussian, binomial and negative binomial. Numerical bounds are calculated for various superpositions of coherent states ("Schrödinger cat states") and their generalizations. The restrictions on the minimal admissible fidelity levels for quite arbitrary (unknown) states belonging to selected families appear rather strong. For example, one can find two squeezed states with $F = 0.9$ but with the relative mean energy difference exceeding 100%. To guarantee the relative energy difference less than 10% for arbitrary coherent states, the fidelity must exceed the level 0.995. For many other sets of states (e.g., squeezed and negative binomial) the restrictions can be much stronger.

1:39PM Z30.00013 Physical meaning of the de Broglie waves, JINGZHENG QIN, SIMON BERKOVICH, The George Washington University — Commonly regarded as an abstract entity, de Broglie waves represent a real thing making the wave-particle duality an operative factor with a wealth of consequences. Waves as probabilities in Schrödinger's quantum mechanics are due to interactive holography that builds up on top of the suggested cellular automaton model of the physical Universe [1]. This model implementing a rule of mutual synchronization produces a set of helicoidal solitons that corresponds exactly to the whole spectrum of elementary particles of matter, no more and no less. The particle-like behavior of the solitons exhibits periodic synchro activities that constitute a wave. The wavelength is inversely proportional to the momentum of these elementary particles, and they distinctly show characteristic qualities of the micro world. The condition of translation-rotation congruity foresees a very small decrease of photons speed with their frequency and polarization, while smoothness of this condition for neutrinos accounts for their already observed faster-than-light propagation. Helicoidal solitons create identical impacts from rotation resulting in the same value of spin for different particles irrespective of variations in mass and speed that are related to translational motion. For any given orientation, spin is either "up" or "down" since helicoidal solitons are flipping this way with every half-turn. Deep inelastic scattering performs sampling of the wave structure of the helicoidal solitons deceptively portraying the outcomes as isolated quarks. [1] S. Berkovich, "A comprehensive explanation of quantum mechanics," <http://www.cs.gwu.edu/research/technical-report/170>

1:51PM Z30.00014 No Drama Quantum Theory? , ANDREY AKHMETELI, LTASolid Inc. — Is it possible to offer a “no drama” quantum theory? Something as simple (in principle) as classical electrodynamics – a theory described by a system of partial differential equations (PDE) in 3+1 dimensions, but reproducing unitary evolution of a quantum field theory in the configuration space? The following results suggest an affirmative answer: 1. The scalar field can be algebraically eliminated from scalar electrodynamics; the resulting equations describe independent evolution of the electromagnetic field (EMF). 2. After introduction of a complex 4-potential (producing the same EMF as the standard real 4-potential), the spinor field can be algebraically eliminated from spinor electrodynamics; the resulting equations describe independent evolution of EMF. 3. The resulting theories for EMF can be embedded into quantum field theories. Another fundamental result: in a general case, the Dirac equation is equivalent to a 4th order PDE for just one component, which can be made real by a gauge transform. Issues related to the Bell theorem are discussed. A. Akhmeteli, Int'l Journal of Quantum Information, Vol. 9, Suppl., 17-26 (2011) A. Akhmeteli, Journal of Mathematical Physics, Vol. 52, 082303 (2011) A. Akhmeteli, quant-ph/1108.1588

2:03PM Z30.00015 Type 2 local realism is alive and well in the quantum world , JEFFREY BOYD, retired — It is often, but incorrectly said, that there is no local realism in the quantum world. This is wrong because there is a second type of local realism. Type two local realism is drastically different than how most people think of their world, including Einstein. It starts with the idea that we are immersed in a sea of invisible elementary waves, traveling in all directions, at all wavelengths. Whenever a photon or other particle moves, it follows one of these waves in the reverse direction. Although this may sound preposterous, this theory can explain several quantum experiments: Jacques (2007) Wheeler thought experiment with delayed choice, Kim (1999), Quantum eraser experiment with delayed choice, all the Bell test experiments with delayed choice, and the double slit experiment. Using the Theory of Elementary Waves (TEW), all these experiments can, surprisingly, be explained using this unconventional type of local realism, with time going forward.

Friday, March 2, 2012 11:15AM - 2:15PM – Session Z31 DCMP: Topological Insulators: Junctions and Interfaces 260

11:15AM Z31.00001 Topological p-n Junction , JING WANG, SHOU-CHENG ZHANG, Department of Physics, Stanford University — $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ is an ideal topological insulator with truly insulating bulk and tunable surface state across the Dirac point. We consider a junction between surface p-type and surface n-type on these ideal topological insulators in which carrier type and density in two adjacent regions are locally controlled by electrostatic gating or planar grade doping. Such junction setting on topological insulators are fundamental to device development. We find a gapless chiral edge state localized at the p-n interface arises when applying a magnetic field, which can be detected by scanning tunneling microscopy. The two-terminal conductance of such p-n junction in the quantum Hall regime will be $1/4$ times the quantum of conductance e^2/h , which signifies the half-quantum Hall effect of a topological insulator surface.

11:27AM Z31.00002 Andreev Reflection in two-dimensional Topological Insulators , AWADHESH NARAYAN, STEFANO SANVITO, Trinity College Dublin — A metal-superconductor interface may reflect an incident electron from the metal as a positively charged hole with opposite spin, while a Cooper pair is formed in the superconductor. This electron-hole conversion is Andreev reflection (AR) and has served as a useful probe for spin-polarized currents. In this work we study AR at topological insulator-superconductor interface, for both time-reversal symmetric (Z_2) and time-reversal broken (*Chern*) cases. We model Z_2 insulators using the proposal of Kane and Mele, while for *Chern* insulator we use a spinful version of the Haldane model. By employing Landauer-Büttiker scheme we find for both cases perfect AR, which is highly robust to disorder and persists as long as the edge states are present. Further, we propose an experiment to distinguish between the two types of topological insulators. The proposal involves a local doping with magnetic impurities at one of the edges of the two-dimensional material. This suppresses one of the channels for reflection and the AR coefficient drops by a factor of two. No such suppression is seen for the *Chern* insulator.

11:39AM Z31.00003 Theory of Odd-Parity Superconductivity: from Gap Function to Topological Invariants and Surface Andreev Bound States , YANG QI, Institute for Advanced Study, Tsinghua University, LIANG FU, Department of Physics, Massachusetts Institute of Technology — Three-dimensional superconductors with a nodeless pairing gap can be classified by an integer topological invariant, and gapless Andreev bound states exist on the surface when the topological invariant is nontrivial. In this letter we give a general criterion for determining the topological invariant for centrosymmetric superconductors with *odd-parity* pairing. We show that in a general system with spin-orbit coupling, the superconducting gap function can be expressed by a pseudospin d-vector, and the topological invariant can be determined from the total winding number of the pseudospin d-vector on the Fermi surfaces. We also discuss Andreev surface states, and we found gapless surface states when the topological invariant in the bulk is topologically nontrivial.

11:51AM Z31.00004 Current-phase relation for Josephson effect through helical metal , ERHAI ZHAO, George Mason University, CHRIS OLUND, University of Virginia — We compute the current-phase relation of Josephson junctions fabricated on the surface of three-dimensional topological insulators. The Josephson coupling between two superconductors is mediated by the two-dimensional helical metal. It gives rise to the so-called fractional Josephson effect. A short junction is previously known to be a quantum wire of Majorana fermions. We discuss the dependence of the current-phase relation on the length of the junction, the chemical potential of the helical metal, and temperature.

12:03PM Z31.00005 Interface engineering of quantum Hall effects in digital transition-metal oxide heterostructures¹ , SATOSHI OKAMOTO, DI XIAO, Materials Science and Technology Division, Oak Ridge National Laboratory, WEN-GUANG ZHU, Department of Physics and Astronomy, University of Tennessee & Materials Science and Technology Division, Oak Ridge National Laboratory, YING RAN, Department of Physics, Boston College, NAOTO NAGAO, Department of Applied Physics, The University of Tokyo & CMGR and CERG, RIKEN-ASI — Based on tight-binding modeling and first-principles calculations, we investigate possible quantum Hall effects in transition-metal oxide heterostructures. Bilayers of perovskite-type transition-metal oxides grown along the [111] crystallographic axis are found to be potential candidates for two-dimensional topological insulators. The topological band structure of these materials can be tune-tuned by changing dopant ions, substrates, and external gate voltages. We predict that LaAuO_3 bilayers have a topologically-nontrivial energy gap of about 0.15 eV, which is sufficiently large to realize the quantum spin-Hall effect at room temperature. We also discuss intriguing phenomena associated with the nearly flat topologically-nontrivial bands found in eg systems, such as fractional quantum Hall effect.

¹S.O. and W.Z. were supported by US DOE, BES, MSE Division. D.X. was supported by LDRD, ORNL. N.N. was supported by MEXT (19048008, 19048015, 21244053). Computational support was provided by NERSC of US DOE.

12:15PM Z31.00006 Proximity effects at semiconductor/topological insulator interfaces¹, GUFENG ZHANG, JIE WANG, Univ. of Sci. & Tech. of China, XIAOGUANG LI, Fudan Univ., Shanghai, China, U of Tennessee, Univ. of Sci. & Tech. of China, DIMITRIE CULCER, Univ. of Sci. & Tech. of China, ZHENYU ZHANG, Univ. of Sci. & Tech. of China, Harvard Univ. — Using phenomenological model Hamiltonians, we study the spatial distribution of topological surface states (TSS) in semiconductor/topological insulator (TI) heterostructures. Due to proximity effects induced by the TI substrate, the location of the TSS can be shifted perpendicularly to the interface. We show that both the direction and magnitude of the shift can be tuned by the cooperative effects of the spin-orbit coupling within the hybrid system, the bandgap of the overlayer, and the thickness of the overlayer. Potential technological applications of these salient properties of the TSS will also be discussed.

¹Supported by DMSE of USDOE, USNSF, and NNSF of China.

12:27PM Z31.00007 Abrikosov Vortex Lattice in 3D Topological Insulator – Superconductor Heterostructures¹, HSIANG-HSIUAN HUNG, Department of Electrical and Computer Engineering, the University of Illinois at Urbana-Champaign, TAYLOR HUGHES, Department of Physics, the University of Illinois at Urbana-Champaign, MATTHEW GILBERT, Department of Electrical and Computer Engineering, the University of Illinois at Urbana-Champaign — Majorana fermions have been predicted to exist on the surface of the three-dimensional (3D) topological insulator/s-wave superconductor heterostructures by proximity effects [Phys. Rev. Lett. **100**, 096407 (2008)]. In the diffuse vortex limit, the physics of these non-abelian anyons is theoretically well-understood c.f. Phys. Rev. B **84**, 144507 (2011). However, the dilute vortex limit is unlikely to be available in experimental systems. In this work, we study the dense vortex limit in 3D topological insulator/s-wave superconductor heterostructures using the self-consistent Bogoliubov-de Gennes (BdG) equations under the application of a uniform magnetic flux. We find that as we approach the dense limit of vortices on the surface, that the hybridization between the vortices leads to the formation of a “Majorana bandstructure” which exists within the superconducting gap. We describe the physics of the system as we move from the dilute limit to the dense limit as we vary the surface chemical potentials and the magnetic field magnitudes.

¹This work is supported by the AFOSR under grant FA9550-10-1-0459.

12:39PM Z31.00008 Quantum Hall Superfluids in Topological Insulator Thin Films, DAGIM TILAHUN, BYOUNGHAK LEE, Texas State Univ/ Univ of Texas at Austin, EWELINA HANKIEWICZ, Universitaet Wuerzburg, ALLAN MACDONALD, University of Texas at Austin — Three-dimensional topological insulators have protected Dirac-cone surface states. In this work we argue that gapped excitonic superfluids with spontaneous coherence between top and bottom surfaces can occur in the TI-thin-film quantum-Hall regime. We find that the large dielectric constants of TI materials increase the layer separation range over which coherence survives and decrease the superfluid sound velocity, but have little influence on the superfluid density or on the charge gap. The coherent state at total Landau-level filling factor $\nu_T = 0$ is predicted to be free of edge modes, qualitatively altering its transport phenomenology compared to the widely studied case of $\nu_T = 1$ in GaAs double quantum wells.

12:51PM Z31.00009 Junction between surfaces of two topological insulators¹, DIPTIMAN SEN, QINDRILA DEB, Indian Institute of Science, Bangalore, India — We study scattering from a line junction which separates the surfaces of two three-dimensional topological insulators; some aspects of this problem were recently studied in Takahashi and Murakami, Phys. Rev. Lett. **107**, 166805 (2011). The velocities of the Dirac electrons on the two surfaces may be unequal and may even have opposite signs; in the latter case, we find that the electrons must, in general, go into the two-dimensional interface separating the two topological insulators. We also study what happens if the two surfaces are at an angle ϕ with respect to each other. We find in this case that there are bound states which propagate along the line junction with a velocity and direction of spin which depend on the bending angle ϕ .

¹D. S. thanks DST, India for financial support under SR/S2/JCB-44/2010.

1:03PM Z31.00010 Dirac cones in the gapless interface states between two topological insulators, RYUJI TAKAHASHI, SHUICHI MURAKAMI, Department of Physics, Tokyo Institute of Technology — When two topological insulators are attached together, the states on the interface become gapped due to the hybridization between the surface states. We have shown that if the two topological insulators have the opposite signs for the Dirac velocities, there exist gapless interface states [1]. In the last March meeting we showed a general proof for the existence of the gapless states using the mirror Chern number, which fixes the chirality of the surface states. In this presentation, we report the dispersions of these gapless interface states. They are in general a collection of Dirac cones. For example, if the system has threefold rotational symmetry, the interface states have six Dirac cones. By using the Fu-Kane-Mele model, which is the tight-binding model on the diamond lattice with the spin-orbit interaction, we calculate the dispersion of this gapless interface states, and discuss the relationship with the mirror Chern number.

[1] R. Takahashi, S. Murakami, Phys. Rev. Lett. **107**, 166805 (2011).

1:15PM Z31.00011 Conductance through step junctions in 3D topological insulators¹, MIREIA ALOS-PALOP, RAKESH P. TIWARI, MIRIAM BLAAUBOER, Delft University of Technology, Kavli Institute of Nanoscience — An effective continuous model for low-energy surface states of a 3D topological insulator was presented by Zhang *et al.*, Nat. Phys. **5**, 438 (2009). We present a general solution for this 3D model in a surface different from the standard (111)-surface. In our solution, surface states consist of a single Dirac cone with a Fermi velocity different from the one in (111)-surfaces, and the energy has an elliptical dispersion in k -space. We then study transport through a step junction composed of a (111)-surface – side-surface – (111)-surface and predict that the conductance saturates at $2/3 G_0$, independent of eccentricity and velocity mismatch at the interfaces. We compare our model with a junction in a plane with only (111)-states where conductance saturation does depend on velocity mismatch. We also analyze the Fano factor and highlight experimentally relevant situations where our predictions could be tested.

¹This research was supported by the Dutch Science Foundation NWO/FOM.

1:27PM Z31.00012 Inter-band Tunneling between Doped Topological Insulator Surface States, GEN YIN, DARSHANA WICKRAMARATNE, ROGER LAKE, University of California Riverside — Thin films of 3D topological insulators (TIs) have been experimentally synthesized recently. Impurity doping of the TI surface has been reported to modify the position of the Fermi level and generate Rashba-like splitting of the surface band structure. Our research uses a Non-Equilibrium Green's Function (NEGF) method to simulate inter-surface transport properties for TI thin films. A tight-binding model is established by discretizing a 4×4 k.p Hamiltonian for 3D TIs. Because of confinement, thin TI slabs of several nanometers allows inter-surface tunneling at quantum number matching states. The tunneling intensity can be tuned by surface Coulomb impurity doping or applying an external bias. Unlike regular topologically trivial surface states, inter-band tunneling between TI surfaces presents a conduction minimum when the dispersions of the two surfaces align perfectly over each other. The suppression of transport originates from the momentum coupling with time reversal symmetry, leading to significant non-linear I-V properties for the P-N tunneling at forward bias. This leads to a NDR current minimum when an external bias completely compensates the built-in potential. The study on inter-surface tunneling in TI thin films benefits the understanding of the transport behavior of TI surface states, which calls for further experimental investigations in the future.

1:39PM Z31.00013 Spin Texture on the Fermi Surface of Strained HgTe, SAAD ZAHEER, STEVE YOUNG, University of Pennsylvania, DANIEL CELLUCCI, University of Georgia, JEFFREY TEO, CHARLES KANE, EUGENE MELE, ANDREW RAPPE, University of Pennsylvania — We present *ab initio* and $\mathbf{k} \cdot \mathbf{p}$ calculations of the Fermi surface of strained HgTe obtained by stretching the Zinc-Blende lattice along the (111) axis. Near the Fermi level, strained HgTe exhibits point-like accidental degeneracies between a two-fold degenerate and two non-degenerate bands along the (111) axis. The three bands disperse linearly in all directions about the degenerate points and their low energy physics is described by an effective four band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian. The Fermi surface consists of two ellipsoids which contact only at the point where the Fermi level crosses the two-fold degenerate band along the (111) axis. The spin expectation value on both ellipsoids is constrained to vanish along the (111) axis due to mirror symmetry about a plane that contains that axis. Furthermore the winding number of spins around the two ellipsoids changes from one end to the other indicating the existence of singular points in the spin texture. Indeed, the *ab initio* and $\mathbf{k} \cdot \mathbf{p}$ calculations confirm the existence of such spin singularities on the Fermi ellipsoids. We show that doping HgTe with Zinc atoms chemically strains the HgTe Zinc-Blende lattice and present *ab initio* calculations on HgZnTe that confirm the above results.

1:51PM Z31.00014 Spin-transfer torque and spin-polarization in topological-insulator-based magnetic tunnel junctions¹, FARZAD MAHFOUZI, Department of Physics and Astronomy, University of Delaware, Newark, DE 19716-2570, USA, NAOTO NAGAOSA, Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan, BRANISLAV NIKOLIĆ, Department of Physics and Astronomy, University of Delaware, Newark, DE 19716-2570, USA, QUANTUM TRANSPORT THEORY GROUP COLLABORATION — We derive a nonequilibrium Green function-based formula for spin-transfer torque (STT) exerted by the conduction electrons on the magnetization of a free ferromagnetic (F) layer where *strong* spin-orbit coupling (SOC) is present either in the bulk or at the interface of the F layer. This nonequilibrium Born-Oppenheimer approximation-type formula is employed to predict unconventional STT in N|TI|F semi-magnetic tunnel junction (MTJ) containing a three-dimensional topological insulator (TI). The STT is driven by the SOC on the surface of TI, as well as by the charge current becoming spin-polarized in the direction of transport as it flows from the normal metal (N) through the bulk of the TI layer. The in-plane and perpendicular STT components in N|TI|F semi-MTJ are an order of magnitude larger than in conventional F|I|F MTJ, or N|I|F semi-MTJ with the strong Rashba SOC at the I|F interface, assuming comparable resistance of all three junctions.

¹F. M. and B. K. N. were supported by DOE Grant No. DE-FG02-07ER46374 and N. N. was supported by Grant-in-Aids for Scientific Research (21244053) from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

2:03PM Z31.00015 Time reversal symmetric Kitaev model and topological superconductor, RYOTA NAKAI, Department of Physics, University of Tokyo, SHINSEI RYU, Department of Physics, University of Illinois, AKIRA FURUSAKI, Condensed Matter Theory Laboratory, RIKEN — We study a time reversal symmetric quantum spin model in two dimensions that is introduced as a higher spin extension of the Kitaev model and is exactly solvable [1]. The ground state of the topological phase of this model can be viewed as a time reversal symmetric topological superconductor in two dimensions. The helical Majorana edge modes which appear in time reversal pair in the topological phase are explained by topological argument. The correlation functions along the edge are derived from the gapless edge theory.

[1] R. Nakai, S. Ryu, and A. Furusaki, arXiv:1111.1230.

Friday, March 2, 2012 11:15AM - 1:39PM – Session Z32 DCMP: Topological Insulators: General Theory II 261

11:15AM Z32.00001 Room temperature quantum spin Hall thin film for buckled honeycomb structures of silicon, germanium, and tin, TAY-RONG CHANG, National Tsing Hua U., Hsinchu, Taiwan, HSIN LIN, Northeastern U., HORNG-TAY JENG, National Tsing Hua U., Hsinchu, Taiwan and Institute of Physics, Academia Sinica, Taipei, Taiwan, M.Z. HASAN, Princeton U., ARUN BANSIL, Northeastern U. — We have carried out first-principles calculations on buckled honeycomb structures of silicon, germanium and tin. When the spin-orbit coupling is included in the computations, these two dimensional (2D) systems are found to be in a quantum spin Hall phase with nontrivial topological invariant $Z_2 = -1$, and a band gap that increases with increasing atomic number. In particular, we predict that buckled honeycomb Sn thin film is a room temperature quantum spin Hall insulator with 0.25 eV band gap.

11:27AM Z32.00002 Topological order and semions in a strongly correlated quantum spin Hall insulator, ANDREAS RUEGG, GREGORY A. FIETE, University of Texas at Austin — We provide a self-consistent mean-field framework to study the effect of strong interactions in a quantum spin Hall insulator on the honeycomb lattice. We identify an exotic phase for large spin-orbit coupling and intermediate Hubbard interaction. This phase is gapped and does not break any symmetry. Instead, we find a four-fold topological degeneracy of the ground state on the torus and fractionalized excitations with semionic mutual braiding statistics. Moreover, we argue that it has gapless edge modes protected by time-reversal symmetry but a trivial Z_2 topological invariant. Finally, we discuss the experimental signatures of this exotic phase. Our work highlights the important theme that interesting phases arise in the regime of strong spin-orbit coupling and interactions.

11:39AM Z32.00003 Spontaneous breakdown of time reversal symmetry in the doped honeycomb lattice with enlarged unit cell, ADOLFO G. GRUSHIN, EDUARDO V. CASTRO, ALBERTO CORTIJO, MARIA A. H. VOZMEDIANO, BELÉN VALENZUELA, Instituto de Ciencia de Materiales de Madrid, CSIC, Spain, FERNANDO DE JUAN, Department of Physics, Indiana University, Bloomington, IN — Enlarging the unit cell of simple lattice models is proposed as a simple means to get spontaneous breakdown of time reversal symmetry (T) and to stabilize non trivial topological phases. As a case study we explore the nearest neighbor tight binding model for spinless fermions interacting through short range Coulomb interactions in the honeycomb lattice. Using a variational mean field approach and an enlarged six atom unit cell we obtain a very rich phase diagram as doping and interaction strength are varied. Two broken T phases, with orbital currents (fluxes) arranged in a Kekulé pattern, show up above the Van Hove filling. One of them realizes a topological Fermi liquid with a finite anomalous Hall conductivity. Instabilities towards charge modulated and superconducting phases are also discussed.

11:51AM Z32.00004 Synchronous and Asynchronous Mott Transitions in Topological Insulator Ribbons¹, AMAL MEDHI, VIJAY B. SHENOY, H.R. KRISHNAMURTHY, Center for Condensed Matter Theory, Indian Institute of Science, Bangalore 560012, India — We address how the nature of linearly dispersing edge states of two dimensional (2D) topological insulators evolves with increasing electron-electron correlation engendered by a Hubbard like on-site repulsion U . We consider finite ribbons of two systems of topological band insulators with local electronic interactions incorporated. Using an inhomogeneous cluster slave rotor mean-field method developed here, we show that electronic correlations drive the topologically nontrivial phase into a Mott insulating phase via two different routes. In a synchronous transition, the entire ribbon attains a Mott insulating state at one critical U . In the second, asynchronous route, Mott localization first occurs on the edge layers at a smaller critical value of electronic interaction which then propagates into the bulk as U is further increased until all layers of the ribbon become Mott localized.

¹Work supported by DAE, SRC and DST, India

12:03PM Z32.00005 Interaction-driven topological and nematic phases on the Lieb lattice, WEI-FENG TSAI, National Sun Yat-sen University, CHEN FANG, Purdue University, HONG YAO, Stanford University, JIANGPING HU, Purdue University — We investigate the interaction-driven instabilities of the band crossing point (BCP), which occurs in the band structure resulting from spinless/spinful fermions moving on the (extended) Lieb lattice. In the non-interacting limit, we show the topological stability of the BCP both from momentum and real space arguments, provided time reversal and C_4 point group symmetries are preserved. With short-range repulsive interactions, we find that at zero temperature this BCP is marginally unstable against infinitesimal repulsions and results in topological quantum anomalous/spin Hall, charge nematic, and nematic-spin-nematic phases, separately, depending on the interaction strengths. Possible physical realizations and the existence of a topological nearly flat band are also discussed.

12:15PM Z32.00006 Geometric effects on surface states in topological insulator Bi_2Te_3 nanowire, PARIJAT SENGUPTA, TILLMAN KUBIS, MICHAEL POVOLOTSKYI, GERHARD KLIMECK, Purdue University — Bismuth Telluride (BT) is a 3D topological insulator (TI) with surface states that have energy dispersion linear in momentum and forms a Dirac cone at low energy. In this work we investigate the surface properties of a BT nanowire and demonstrate the existence of TI states. We also show how such states vanish under certain geometric conditions. An atomistic model (sp3d5s* TB) is used to compute the energy dispersion in a BT nanowire. Penetration depth of the surface states is estimated by ratio of Fermi velocity and band-gap. BT possesses a tiny band-gap, which creates small localization of surface states and greater penetration in to the bulk. To offset this large spatial penetration, which is undesirable to avoid a direct coupling between surfaces, we expect that bigger cross-sections of BT nanowires would be needed to obtain stable TI states. Our numerical work validates this prediction. Furthermore, geometry of the nanowire is shown to influence the TI states. Using a combined analytical and numerical approach our results reveal that surface roughness impact electronic structure leading to Rashba type splits along z-direction. Cylindrical and square cross-sections are given as illustrative examples.

12:27PM Z32.00007 Spinless massless and massive Dirac fermions in a checkerboard lattice magnet¹, JORN VENDERBOS, MARIA DAGHOFER, JEROEN VAN DEN BRINK, IFW Dresden, SANJEEV KUMAR, Indian Institute of Science Education and Research (IISER) — We investigated the theory of the interplay of itinerant electrons and localized magnetic moments on the frustrated checkerboard lattice as function of the super-exchange interaction between the localized moments and the band filling of fermions. We find that at half filling a very robust magnetic “flux” phase is lowest in energy. The ordering of the localized spins induces an effective gauge field flux of π for the electrons. Consequently, this phase preserves time-reversal symmetry and the low-energy effective theory of the electrons is that of massless Dirac fermions, resembling the situation in graphene except that the spin degree of freedom is absent here. The robustness of this state originates from the geometrical frustration of the checkerboard lattice. In the crossover regime from this flux state and the saturated FM state at vanishing super-exchange coupling, these Dirac fermions become massive with opposite sign of the mass at the two degeneracy points. This chiral spin state is then equivalent to a time-reversal breaking anomalous Quantum Hall phase, precisely in the way once envisioned by Haldane in graphene.

¹Supported by DPG (Emmy Noether program) and the Dutch Science Foundation NWO/FOM (Interphase program)

12:39PM Z32.00008 Kondo lattice on the edge of a 2D topological insulator, JOSEPH MACIEJKO, Princeton Center for Theoretical Science — Much attention has been devoted recently to the experimental and theoretical study of the effect of magnetic impurities on the stability of the gapless boundary modes of topological insulators. When the quantum dynamics of the impurities is considered, those boundary modes constitute novel types of fermionic baths which may affect the nature of possible impurity phases and phase transitions. We study a regular one-dimensional array of quantum magnetic impurities interacting with the helical edge liquid of a two-dimensional time-reversal invariant topological insulator. Exact solutions at the special Toulouse and Luther-Emery points as well as a renormalization group analysis à la Anderson-Yuval allow us to construct a phase diagram in the space of Kondo coupling, electron-electron interaction strength, and electron density. We point out similarities and differences with the Kondo lattice in an ordinary one-dimensional electron gas.

12:51PM Z32.00009 Non-Abelian Berry transport, spin coherent states, and Majorana points, YUN LIU, ABHISHEK ROY, MICHAEL STONE, University of Illinois at Urbana-Champaign — We consider the adiabatic evolution of Kramers degenerate pairs of spin states in a half-integer spin molecular magnet as the molecule is slowly rotated, for which it is possible to encounter non-Abelian Berry's phase. To understand the full details of the adiabatic quantum evolution, we invoke Majorana's parametrization of a general spin- j state in terms of the $2j$ Majorana points. As an illustration we consider molecular magnets of the $j = 9/2$ Mn4 family and compute the frequency with which the magnetization varies. This frequency is generally different from the frequency of the rotation.

1:03PM Z32.00010 Exploring Diabolical points and Berry Phases in the Majorana Representation, ABHISHEK ROY, University of Illinois, Urbana-Champaign — Diabolical points or level crossings are often observed in spin hamiltonians, where they give rise to a Berry phase. We study their geometric structure using the Majorana representation which associates a spin state to a set of points on the Bloch sphere. Each crossing carries a Chern number which is found to be directly related to the wrapping of Majorana points around it. We apply our method to study model hamiltonians for molecular magnets in an external magnetic field, in which a rich pattern of diabolical points are seen. Our result enables a simple visualization of the Berry phases without the use of perturbation theory.

1:15PM Z32.00011 Quasiparticle effects in the bulk and surface-state bands of Bi_2Se_3 and Bi_2Te_3 topological insulators¹, OLEG V. YAZYEV, UC Berkeley/LBNL/EPFL, EMMANOUIL KIOUPAKIS, U of Michigan, JOEL E. MOORE, STEVEN G. LOUIE, UC Berkeley/LBNL — We investigate the bulk band structures and the surface states of Bi_2Se_3 and Bi_2Te_3 topological insulators using first-principles many-body perturbation theory based on the GW approximation. The quasiparticle self-energy corrections introduce significant changes to the bulk band structures, surprisingly leading to a decrease in the direct band gaps in the band-inversion regime as opposed to the usual situation without band inversion. Parametrized “scissors operators” derived from the bulk studies are then used to investigate the electronic structure of slab models which exhibit topologically protected surface states. The introduction of self-energy corrections results in significant shifts of the surface-state Dirac point energies relative to the bulk bands and in enlarged gap openings from the interactions between the surface states across the thin slab, both in agreement with experimental data.

¹Reference: arXiv:1108.2088. Support by NSF Grant No. DMR10-1006184, US DOE Cont. No. DE-AC02-05CH11231 and Swiss NSF Grant No. PP002-133552. Computer resources from NICS.

1:27PM Z32.00012 Search for new topological insulators: ternary Li_2AgSb -class semiconductors and related compounds, HSIN LIN, Northeastern U., TANMOY DAS, LANL and Northeastern U., Y.J. WANG, Northeastern U., L.A. WRAY, LBNL and Princeton U., S.-Y. XU, M.Z. HASAN, Princeton U., ARUN BANSIL, Northeastern U. — Topological insulators host a rare quantum phase of electrons which is characterized by a topological invariant number of bulk states of combined spin-orbit and time-reversal symmetry origin. Despite recent progress the available classes of topological insulators are still quite limited for use in device applications and experimental exploration of exotic topological phenomena. For this reason, the search for new materials with greater structural flexibility and tunability in various local order broken symmetry phases is continuing worldwide with great intensity. Here we discuss our effort based on first-principles calculations to show that the adiabatic continuation method can provide a very powerful tool for predicting non-trivial topological phases with the example of ternary intermetallic series, $\text{Li}_2M'X$ ($M'=\text{Cu, Ag, Au, and Cd}$, $X=\text{Sb, Bi, and Sn}$) as well as other compounds with zinc-blende type sublattice. [1-3] Work supported by the Office of Basic Energy Sciences, US DOE.

[1] H. Lin, *et al.* Nature Materials **9**, 546 (2010).
 [2] Y. J. Wang, *et al.* New J. Phys. **13**, 085017 (2011).
 [3] H. Lin, *et al.*, arXiv:1007.5111.

Friday, March 2, 2012 11:15AM - 1:51PM – Session Z40 DBIO: Biomechanics - Organismic Motion 156A

11:15AM Z40.00001 The mechanics of anisotropic cytoskeletal networks, TAO ZHANG, MOUMITA DAS, Syracuse University, D.A. QUINT, UC-Merced, J.M. SCHWARZ, Syracuse University — At the leading edge of a crawling cell, the actin cytoskeleton extends itself via a branched, crosslinked network of filaments, otherwise known as the lamellipodium. The filaments in this network have an average preferred orientation of around ± 30 degrees with respect to the normal of the leading edge. This preferred orientation of filaments leads to a material that is structurally anisotropic. To better understand the forces generated by the lamellipodium, we analytically and numerically study the mechanical properties of a model branched and crosslinked filamentous network where the filaments are preferentially oriented along one direction. We investigate the interplay between geometry, elasticity and anisotropy in the network. In particular, we show how anisotropy modulates the onset of rigidity and non-linear mechanical response of the network.

11:27AM Z40.00002 Self-Organized Cell Motility from Motor-Filament Interactions, XINXIN DU, KONSTANTIN DOUBROVINSKI, MIRIAM OSTERFIELD, Princeton University — Cell motility is driven primarily by the dynamics of the cell cytoskeleton, a system of filamentous proteins and molecular motors. It has been proposed that cell motility is a self-organized process; that is, local short-range interactions determine much of the necessary dynamics required for the whole-cell organization that leads to polarization and directional motion. Here we present a mesoscopic meanfield description of filaments, motors, and cell boundaries; this description gives rise to a dynamical system exhibiting multiple self-organized states. We discuss several qualitative aspects of the asymptotic states and compare them to those of living cells.

11:39AM Z40.00003 Modeling of a crawling *C. elegans* in a micro-structured environment¹, AMAR PATEL, VENKAT PADMANABHAN, DEEPAK SOLOMON, ZEINA KHAN, Texas Tech University, FRANK VAN BUSSEL, Max Planck Institute for Dynamics and Self-Organization, SIVA VANAPALLI, Texas Tech University, KENDRA RUMBAUGH, Texas Tech University Health Sciences Center, JERZY BLAWZDZIEWICZ, Texas Tech University — A simple curvature-based model is used to study crawling *C. elegans* in a micro-structured environment of periodic pillars. In our model system, the shape of the worm is described by a simple sinusoidal expression in curvature representation. The gait of the worm is determined by a set of parameters including the amplitude, frequency, and phase of the curvature. The moving worm is subject to the friction with the underlying substrate, and the forces due to interaction of the worm body with pillars. If the friction is isotropic the worm has to interact with the pillars to move forward. We find that only a narrow range of worm gaits leads to efficient propulsion in this case. To investigate how the worm adjusts its gait to the environment microstructure, we implement a simple control system that chooses the right set of parameters based on the past interactions of the worm with its surroundings. Results of our simulations of the worm motion are compared with our experimental observations of *C. elegans* crawling in an agar environment containing an array of fabricated pillars.

¹We acknowledge financial support by NSF grant CBET 1059745.

11:51AM Z40.00004 Fluctuations, Dynamics, and the Stretch-Coil Transition of Single Actin Filaments in Extensional Flows, VASILY KANTSER, RAYMOND E. GOLDSTEIN, DAMTP, University of Cambridge, DEPARTMENT OF APPLIED MATHEMATICS AND THEORETICAL PHYSICS TEAM — Semi-flexible polymers (actin filaments) subject to hydrodynamic forcing play an important role in cytoskeletal dynamics in the cell. The non-equilibrium problem of semi-flexible polymer dynamics is highly challenging due to the coupling between the objects deformations and the flow. This leads to a free-boundary hydrodynamic problem, where the object's shape is not given *a priori*, but determined by an interplay between the fluid stresses, bending energy and the length constrain of the actin filaments. We have investigated experimentally and analytically dynamics of actin filaments in elongational flow. Near hyperbolic stagnation points of the flow filaments experience a competition between bending elasticity and tension induced by the flow, and are predicted to display suppressed thermal fluctuations in the steady regime and a buckling instability under sudden change of the velocity gradient. Using a microfluidic cross-flow geometry we verify these predictions in detail, including a fluctuation-rounded stretch-coil transition of actin filaments.

12:03PM Z40.00005 Cell Shape Dynamics: From Waves to Migration, MEGHAN DRISCOLL, University of Maryland, College Park, COLIN MCCANN, University of Maryland, College Park and National Cancer Institute, National Institutes of Health, XIAOYU SUN, JOHN FOURKAS, University of Maryland, College Park, CAROLE PARENT, National Cancer Institute, National Institutes of Health, WOLFGANG LOSERT, University of Maryland, College Park — We observe and quantify wave-like characteristics of amoeboid migration. Using the amoeba *Dictyostelium discoideum*, a model system for the study of chemotaxis, we demonstrate that cell shape changes in a wave-like manner. Cells have regions of high boundary curvature that propagate from the leading edge toward the back, usually along alternating sides of the cell. Curvature waves are easily seen in cells that do not adhere to a surface, such as cells that are electrostatically repelled from surfaces or cells that extend over the edge of micro-fabricated cliffs. Without surface contact, curvature waves travel from the leading edge to the back of a cell at $\sim 35 \mu\text{m}/\text{min}$. Non-adherent myosin II null cells do not exhibit these curvature waves. At the leading edge of adherent cells, curvature waves are associated with protrusive activity. Like regions of high curvature, protrusive activity travels along the boundary in a wave-like manner. Upon contact with a surface, the waves stop moving relative to the surface, and the boundary shape thus reflects the history of protrusive motion. The wave-like character of protrusions provides a plausible mechanism for the ability of cells to both swim in viscous fluids and to navigate complex 3-D topography.

12:15PM Z40.00006 A curvature-based description for the kinematics of *C. Elegans*¹, VENKAT PADMANABHAN, ZEINA KHAN, DEEPAK SOLOMON, SIVA VANAPALLI, Texas Tech University, KENDRA RUMBAUGH, Texas Tech University Health Sciences Center, JERZY BLAWDZIEWICZ, Texas Tech University — *Caenorhabditis Elegans* is a free-living soil nematode that propels itself in various complex environments by producing undulatory body motion. Such nematodes display a rich variety of body shapes and trajectories during their locomotion. Here we show that the complex shapes and trajectories of *C. Elegans* have a simple analytical description in curvature representation. Our model is based on the assumption that the curvature wave is generated in the head segment of the worm body and propagates backwards. We have found that a simple sinusoidal function for the curvature can capture multiple worm shapes during the undulatory movement. The worm body trajectories can be well represented by piece-wise sinusoidal curvature with abrupt changes in amplitude, frequency, and phase.

¹We acknowledge financial support by NSF grant CBET 1059745.

12:27PM Z40.00007 Paramecia Swim with a constant propulsion in Solutions of Varying Viscosity¹, JAMES M. VALLES, JR., ILYONG JUNG, HARRY MICKALIDE, HOJIN PARK, THOMAS POWERS, Brown University — Paramecia swim through the coordinated beating of the 1000's of cilia covering their body. We have measured the swimming speed of populations of Paramecium Caudatum in solutions of different viscosity, η , to see how their propulsion changes with increased drag. We have found the average instantaneous speed, V to decrease monotonically with increasing η . The product ηv is roughly constant over a factor of 7 change in viscosity suggesting that paramecia swim at constant propulsion force. The distribution of swimming speeds is Gaussian. The width appears proportional to the average speed implying that both fast and slow swimmers exert a constant propulsion. We discuss the possibility that this behavior implies that the body cilia beat at constant force with varying viscosity.

¹This work was supported by NSF PHY0750360 and at the NHMFL by NSF DMR-0084173

12:39PM Z40.00008 Response of Swimming Paramecia to *in situ* changes in their apparent weight¹, ILYONG JUNG, HARRY MICKALIDE, JAMES M. VALLES, JR., Brown University — There is a class of marine micro-organisms that are small enough that low Reynold's number hydrodynamics dictates their swimming mechanics and large enough that the force of gravity exerts a noticeable influence on their motion. Experiments on populations of paramecia suggest that they exert a greater propulsion when swimming against gravity. This negative gravi-kinesis is surprising because it suggests that they sense their tiny apparent weight of about 80 pN. To understand this response in more detail, we are investigating how individual paramecia caudatum change their swimming speed and helical trajectories in response to changes in their apparent weight. We vary the apparent weight with the technique of Magnetic Force Buoyancy Variation employing a high field resistive magnet at the National High Magnetic Field Laboratory. We will present analysis of the swimming for apparent weight changes as large as a factor of 8.

¹This work was supported by NSF PHY0750360 and at the NHMFL by NSF DMR-0084173

12:51PM Z40.00009 Capillary Action may act as a cooling method in Plants and Animals, RICHARD KRISKE, University of Minnesota — A capillary tube in a plant may lead from its roots to the leaves. It takes no work for the column of water to rise from the roots to the leaves, and if there is capillarity in the soil, it takes no work for the water to flow through the ground to the roots. It does take work for a molecule of water to evaporate from the tube into the atmosphere. When a molecule of water evaporates another molecule travels through the soil and up the plant to replace it. The lost molecule creates a "hole" in the water column which like a signal is sent to the root and the sea of water in the soil replaces it. Since the water molecules are not unique this is the same situation as if the water vapor were condensed back to a liquid in a refrigeration cycle. Another interesting aspect of this sort of refrigeration is that the "hole" itself may be used to do work along the wall of the capillary tube, which may have Fermi Levels in it. An Hydraulic Semi Conductor, and in it is a method of cooling the Semi Conductor. This may be applicable to other similar systems using other liquids, or substances such as nanotube systems, where the hole signals,cools and performs chemical reactions involving not only orbitals but Fermi Levels, a transition between Quantum and Classical Mechanics, with surprises.

1:03PM Z40.00010 Data-Driven Classification of Animal Behavior, GORDON BERMAN, WILLIAM BIALEK, JOSHUA SHAEVITZ, Princeton University — The last decades have seen an explosion in our ability to characterize the molecular, cellular and genetic building blocks of life; the ingredients out of which we try to explain the rich and compelling behavior of living organisms. Our characterization of behavior itself, however, has advanced more slowly. Since modern ethology was founded over a century ago, behavioral experiments have focused largely on a restricted set of behaviors within the scope of a limited environment. Moreover, the set of behaviors to be examined is often user-defined, creating the potential for human bias and anthropomorphism. The research presented here describes a data-driven methodology for analyzing animal behavior, focusing on the fruit fly, *Drosophila melanogaster*, as a model system. Towards this end, we have built an imaging system that can track single flies as they move about a relatively unencumbered environment. Utilizing this capacity to generate large data sets of animal behavior, we have developed a method for automatically identifying behavioral states using techniques from image analysis, machine learning, and nonlinear dynamics. Identifying these states provides the starting point for many analyses and creates the possibility for automatic phenotyping of subtle behavioral traits.

1:15PM Z40.00011 Multiscale Analysis of Head Impacts in Contact Sports¹, MARK GUTTAG, Brown University, SUBHAM SETT, SIMULIA, JENNIFER FRANCK, KYLE MCNAMARA, EYAL BAR-KOCHBA, Brown University, JOSEPH CRISCO, Rhode Island Hospital, JANET BLUME, CHRISTIAN FRANCK, Brown University — Traumatic brain injury (TBI) is one of the world's major causes of death and disability. To aid companies in designing safer and improved protective gear and to aid the medical community in producing improved quantitative TBI diagnosis and assessment tools, a multiscale finite element model of the human brain, head and neck is being developed. Recorded impact data from football and hockey helmets instrumented with accelerometers are compared to simulated impact data in the laboratory. Using data from these carefully constructed laboratory experiments, we can quantify impact location, magnitude, and linear and angular accelerations of the head. The resultant forces and accelerations are applied to a fully meshed head-form created from MRI data by Simpleware. With appropriate material properties for each region of the head-form, the Abaqus finite element model can determine the stresses, strains, and deformations in the brain. Simultaneously, an in-vitro cellular TBI criterion is being developed to be incorporated into Abaqus models for the brain. The cell-based injury criterion functions the same way that damage criteria for metals and other materials are used to predict failure in structural materials.

¹Support from Rhode Island Science and Technology Advisory Council, and NIH BRP.

1:27PM Z40.00012 The fern sporangium: an ultrafast natural catapult, XAVIER NOBLIN, LPMC, UMR 6622 CNRS-UNS, Parc Valrose, 06108 Nice cedex 2, France, MEDERIC ARGENTINA, LJAD, UMR 6621 CNRS-UNS, Parc Valrose, 06108 Nice cedex 2, France, JARED WESTBROOK, Department of Botany, University of Florida, Gainesville, FL, 32611 USA, CORALINE LLORENS, NICOLAS ROJAS, LJAD, UMR 6621 CNRS-UNS, Parc Valrose, 06108 Nice cedex 2, France, JACQUES DUMAIS, OEB, Harvard University, 16 Divinity Avenue, 02138 Cambridge, MA, USA — Plants have developed fascinating mechanisms to create ultra fast movements that often reach the upper limit allowed by physical laws. Inspiration for new technologies is one of the reasons for the strong interest for these mechanisms, along with the deep interest of understanding complex, natural systems. The fern sporangium is a capsule that contains the spores, it is surrounded by a row of cells called the annulus which acts as a beam. Due to the water evaporation from its cells, the annulus bends strongly and induces elastic energy storage during an opening phase. The tension in the cells breaks when cavitation bubbles appear in the cells, leading to a fast release of the elastic energy. The fern sporangium then acts as a catapult which ejects rapidly its spores by closing back to the initial closed shape. We have analyzed the slow opening motion and the fast catapulting mechanism. We found that the catapult motion involves two time scales, showing a very original behavior. In man-made catapults, the recoil motion needs to be arrested by a cross bar so that the projectile is released from the arm. We show here that the fern sporangium replaces the essential cross bar by an elegant poroelastic damping, leading to a completely autonomous, efficient device.

1:39PM Z40.00013 Hydrodynamics of Active Permeating Gels, ANDREW CALLAN-JONES, University of Montpellier II, FRANK JÜLICHER, Max Planck Institute for the Physics of Complex Systems — We present a hydrodynamic theory of active viscoelastic gels in which a polymer network is embedded in a background fluid. This work is motivated by active processes in the cell cytoskeleton in which motor molecules generate elastic stresses in the network which can drive permeation flows of the cytosol. Our approach differs from earlier ones by considering the elastic strain in the polymer network as a slowly relaxing dynamical variable. We discuss a specific case that illustrates the role of permeation in active gels: the self-propulsion of a thin slab of gel relative to a substrate driven by filament polymerization and depolymerization.

Friday, March 2, 2012 11:15AM - 1:51PM –

Session Z41 DBIO GSNP: Focus Session: Non-Covalent Protein Interactions 156B

11:15AM Z41.00001 Novel Aspects of Hydrogen Bonding in Protein Function: Active Site Ionic Hydrogen Bonds, WOUTER D. HOFF, Oklahoma State University — We use photoactive yellow protein (PYP), a bacterial photoreceptor, to explore novel aspects of the role of hydrogen bonding in protein function. PYP exhibits photochemical activity based on its ionized p-coumaric acid (pCA) chromophore, which is hydrogen bonded to Tyr42 and Glu46. We report that these active site ionic hydrogen bonding interactions cause unexpected molecular and functional properties of PYP. First, we describe a novel spectroscopic isotope effect (SIE) in which dissolving PYP in D₂O causes a red-shift in its electronic absorbance spectrum. We assign this SIE to the ionic hydrogen bond between pCA and Glu46, which—in contrast to standard hydrogen bonds—is weakened upon H/D exchange. These findings extend the effects of H/D exchange from kinetic isotope effects to include shifts in absorbance spectrum, and illustrate the biological relevance of ionic hydrogen bonding to protein active sites. Secondly, we examine how the protein environment achieves the unusual strong preference of the pCA to remain ionized in the protein interior. We use the rescue of the Y42F mutant of PYP by incorporation of a trans-locked analog of pCA to dissect the contributions of active site hydrogen bonding to the large down-shift in the pK_a of the pCA. Together, the Tyr42 and Glu46 hydrogen bonds to the pCA account for ~80% of this shift, which can be quantitatively explained by the loss of ionic hydrogen bonding upon pCA protonation from the solvent. Since ionic hydrogen bonds occur in many proteins, this mechanism of pK_a tuning is likely to be of general relevance.

11:51AM Z41.00002 Computational design of protein interactions: designing proteins that neutralize influenza by inhibiting its hemagglutinin surface protein, SAREL FLEISHMAN, Weizmann Institute of Science — Molecular recognition underlies all life processes. Design of interactions not seen in nature is a test of our understanding of molecular recognition and could unlock the vast potential of subtle control over molecular interaction networks, allowing the design of novel diagnostics and therapeutics for basic and applied research. We developed the first general method for designing protein interactions. The method starts by computing a region of high affinity interactions between dismembered amino acid residues and the target surface and then identifying proteins that can harbor these residues. Designs are tested experimentally for binding the target surface and successful ones are affinity matured using yeast cell surface display. Applied to the conserved stem region of influenza hemagglutinin we designed two unrelated proteins that, following affinity maturation, bound hemagglutinin at subnanomolar dissociation constants. Co-crystal structures of hemagglutinin bound to the two designed binders were within 1Å RMSD of their models, validating the accuracy of the design strategy. One of the designed proteins inhibits the conformational changes that underlie hemagglutinin's cell-invasion functions and blocks virus infectivity in cell culture, suggesting that such proteins may in future serve as diagnostics and antivirals against a wide range of pathogenic influenza strains. We have used this method to obtain experimentally validated binders of several other target proteins, demonstrating the generality of the approach. We discuss the combination of modeling and high-throughput characterization of design variants which has been key to the success of this approach, as well as how we have used the data obtained in this project to enhance our understanding of molecular recognition. References: Science 332:816 JMB, in press Protein Sci 20:753

12:27PM Z41.00003 The power of simple hard-sphere models in protein structure prediction¹, LYNNE REGAN, Yale University — There are several force-fields that are currently used to describe the potential energy of biological macromolecules such as proteins. These typically include many parameters, derived from a combination of statistical, experimental sources. These work on average to describe a protein, but the large number of parameters moves this description further away from a true physical understanding than is desirable. Our approach is to investigate to what extent simple hard sphere models can be used to model and predict the behavior of different aspects of protein structure. We present the results of specific calculations. The distributions of the side-chain dihedral angle χ_1 of Val and Thr in proteins of known structure show distinctive features: Val side chains predominantly adopt dihedral angle, χ_1 , of 180, whereas Thr side chains typically adopt a dihedral angle, χ_1 , of 60 or 300. Several hypotheses have been proposed to explain these differences, including inter-residue steric clashes and hydrogen-bonding interactions. In contrast, we show that the observed side-chain dihedral angle distributions for both Val and Thr can be explained using only local steric interactions in a dipeptide mimetic. Our results emphasize the power of a simple physics-based approaches and their importance for future advances in protein engineering and design.

¹In collaboration with Alice Zhou and Corey O'Hern, Yale University.

1:03PM Z41.00004 Acetylation of LYS-16 of H4 Histone Tail May Sequester the Tail and Inhibit its Interactions with Neighboring Nucleosomes, DAVIT POTOYAN, GAREGIN PAPOIAN, University of Maryland — Histone tails are highly flexible N terminal protrusions of histone proteins, which help to fold DNA into dense superstructures known as chromatin. On a molecular scale histone tails are poly-electrolytes with high degree of conformational disorder, allowing them to function as bio-molecular “switches,” regulating various genetic regulatory processes via diverse types of covalent modifications. Because of being intrinsically disordered, the structural and dynamical aspects of histone tails are still poorly understood. Using multiple explicit solvent and coarse-grained MD simulations we have investigated the impact of the acetylation of LYS-16 residue on the conformational and DNA-binding propensities of H4 histone tail. The potential of mean force computed as a function of distance between a model DNA and histone tail center of mass showed a dramatic enhancement of binding affinity upon mono-acetylation of the H4 tail. The estimated binding free energy gain for the wild type is 2kT, while for the acetylated it reaches 4-5 kT. Additionally our structural analysis shows that acetylation is driving the chain into collapsed states, which get enriched in secondary structural elements upon binding to the DNA. We suggest a non-electrostatic mechanism that explains the enhanced binding affinity of the acetylated H4 tail. At last our findings lead us to propose a hypothesis that can potentially account for the celebrated chromatin “fiber loosening effects” observed in many experiments.

1:15PM Z41.00005 Exploring copper chelation in Alzheimer's disease protein, FRISCO ROSE, MIROSLAV HODAK, JERRY BERNHOLC, CHiPS/NCsu — Alzheimer's disease (AD) is a neurodegenerative disorder affecting millions of aging people in the U.S. alone. Clinical studies have indicated that metal chelation is a promising new approach in alleviating the symptoms of AD. Our study explores the as yet undetermined mechanism of copper chelation in amyloid- β , a protein implicated in AD. The structure of amyloid- β is derived from experimental results and incorporates a planar copper-ion-binding structure in a semi-solvated state. We investigate the chelation process using the nudged elastic band method implemented in our *ab initio* real-space multigrid code. We find that an optimal sequence of unbonding and rebonding events as well as proton transfers are required for a viable chelation process. These findings provide fundamental insight into the process of chelation that may lead to more effective AD therapies.

1:27PM Z41.00006 Transition-metal prion protein attachment: Competition with copper, MIROSLAV HODAK, JERRY BERNHOLC, North Carolina State University — Prion protein, PrP, is a protein capable of binding copper ions in multiple modes depending on their concentration. Misfolded PrP is implicated in a group of neurodegenerative diseases, which include "mad cow disease" and its human form, variant Creutzfeld-Jacob disease. An increasing amount of evidence suggests that attachment of non-copper metal ions to PrP triggers transformations to abnormal forms similar to those observed in prion diseases. In this work, we use hybrid Kohn-Sham/orbital-free density functional theory simulations to investigate copper replacement by other transition metals that bind to PrP, including zinc, iron and manganese. We consider all known copper binding modes in the N-terminal domain of PrP. Our calculations identify modes most susceptible to copper replacement and reveal metals that can successfully compete with copper for attachment to PrP.

1:39PM Z41.00007 Steric clashes determine differences in side chain dihedral angle distributions: A study of Thr versus Val¹, ALICE ZHOU, COREY O'HERN, LYNNE REGAN, Yale University — With the long-term goal to improve the design of protein-protein interactions, we develop a simple hard sphere model for dipeptides that can predict the side-chain dihedral angle distributions of Val and Thr in both the α -helix and β -sheet backbone conformations. We find that it is essential to include the non-polar hydrogens in the model; indeed interatomic clashes involving the non-polar hydrogens largely determine the form of side-chain dihedral angle distributions. Further, we are able to explain key differences in the side-chain dihedral angle distributions for Val and Thr from intra-residue steric clashes rather than inter-residue steric clashes or hydrogen bonding. These results are the crucial first step in developing computational models that can predict the side chain conformations of residues at protein-peptide interfaces.

¹NSF-DMR-1006537

Friday, March 2, 2012 11:15AM - 1:03PM –

Session Z42 DBIO: Focus Session: Physics of Biomaterials: Mechanics, Dynamics, and Transport 156C

11:15AM Z42.00001 Highly parallel computational study of amphiphilic molecules using the Wang-Landau method¹, THOMAS VOGEL, DAVID LANDAU, The Center for Simulation Physics, University of Georgia, Athens, GA, 30602, U.S.A. — The self-assembly process in amphiphilic solutions is a phenomenon of broad interest. Molecular dynamics simulations generally used to study micelle formation or lipid layer assembly in an explicit solvent are limited in time scale. Vast studies of structure formation processes via standard Markov-chain based Monte Carlo simulations are challenging, but the Wang-Landau method [1] provides a way to efficiently study such systems in a generalized thermodynamic ensemble. This makes it possible, for example, to get results over a broad temperature range from a single simulation. In an attempt to develop highly parallel applications using this method, we study the thermodynamic behavior of a generic coarse-grained model for amphiphilic molecules [2] as well as of a new coarse-grained lipid model specifically designed for dimyristoyl phosphatidylcholine (DMPC) [3]. Here, we focus on the design and the performance of our parallel Wang-Landau simulation on multi-CPU and GPU systems.

[1] F. Wang and D.P. Landau, Phys. Rev. Lett. **86**, 2050 (2001)

[2] S. Fujiwara et al., J. Chem. Phys. **130**, 144901 (2009)

[3] W. Shinoda et al., J. Phys. Chem. B **114**, 6836 (2010)

¹Research supported by NSF.

11:27AM Z42.00002 Spatial response variations within biosensor flow cells, NICOLA CANT, SARAH HARRISON, Dstl — Biosensors are currently being developed for the detection of a wide range of analytes in a variety of scenarios. One such area is that of environmental monitoring for the presence of biological threats, from toxins through to viruses and bacteria. The varying nature, and in particular disparate size, of such a variety of analytes poses a significant challenge in the development of effective high confidence instruments. Many existing biosensors employ functionalised flow cells in which spatially defined arrays of surface immobilised recognition elements are present to specifically capture their analyte of interest. Experimental data obtained using a grating coupled SPR instrument, the BIAcoreTM Flexchip, has revealed spatial dependency differences in response behaviours between proteinaceous and particulate analytes. In particular, the magnitude of responses seen with *Bacillus anthracis* spores across the instruments flow cell appear to be influenced by shear and gravitational effects whilst those from soluble proteins are more uniform. We have explored this dependence to understand its fundamental impact on the successful implementation of multi-analyte environmental biological detection systems.

11:39AM Z42.00003 Size-dependent mechanical properties of low-dimensional materials: coupling between deformation modes, YITING DING, ZHIPING XU, Computational Energetics Laboratory, Department of Engineering Mechanics & Center for Nano and Micro Mechanics — Coupling between deformation modes, such as tension, bending, shear, and twisting, are widely observed in low-dimensional materials, especially biological materials. In this talk we will present our study on microtubules (MT) mechanics, where significance of mode coupling leads remarkable size-dependence in structural and mechanical properties. Using molecular dynamics (MD) simulations, we find a distinct dependence of bending rigidity on the contour length of a MT that agrees well with experimental data. We develop a simple model by including basic parameters to explain and predict this interesting phenomenon. An extended discussion will be made to general low-dimensional materials, with focuses not only on the mechanism, but also applications in optimal materials design.

11:51AM Z42.00004 A QM/MM method for simulating the sequencing of DNA using graphene nanopores: solvent effects on nucleobase selectivity, ALEXANDRE ROCHA, GUSTAVO FELICIANO, Universidade Federal do ABC - Brazil, YUHUI HE, Osaka University - Japan, RALPH SCHEICHER, Department of Physics and Astronomy, Uppsala University - Sweden, MAURICIO COUTINHO, Universidade Federal do ABC - Brazil — The possibility of using graphene nanopores for DNA sequencing is driving a significant research effort with the aim of obtaining cheaper, more efficient, sequencing techniques. In this work we will present electronic transport calculations of graphene nanopores used for sequencing DNA strands. We consider both single layer and double layer graphene with different types of functionalization of the pore edges. The simulations were performed using a QM/MM method which allows us to treat the graphene sheet containing the nanopore and a segment of DNA within the pore via ab initio DFT methods (QM) whereas the effects of the water molecules, the counter-ions and the remainder of the DNA strand is taken into consideration using a classical potential (MM). The electronic transport properties along graphene are subsequently calculated using non-equilibrium Green's functions including the classical potential. Different time steps of classical molecular dynamics simulations of the DNA strand passing through the nanopore are considered in order to simulate the translocation process. This way we are able to address the effects of the solvent on the selectivity of the device to different nucleobases using atomistic methods.

12:03PM Z42.00005 First-Principles Study of Muon Trapping in Singlet and Triplet States of Oxyhemoglobin, ROGER PINK, S.R. BADU, T.P. DAS, Department of Physics, University at Albany, SUNY, N. SAHOO, UTMD Anderson, LEE CHOW, Department of Physics, University of Central Florida, R.H. SCHEICHER, Uppsala University, K. NAGAMINE, Department of Physics, UCR — There is great current interest in the possibility of magnetic character in oxyhemoglobin (OxyHb) due to the detection [1] of muon spin-lattice relaxation in OxyHb. First-Principles variational Hartree-Fock Many Body Perturbation Theory (VHFMBPT) technique investigations on the singlet and triplet states of pure OxyHb have shown² that the triplet state is considerably higher than the singlet state ruling out magnetic character. However the charge distribution obtained by the VHFMBPT procedure in both states show a number of sites that have negative charges where the trapping of muon is being investigated to examine if the energy gap in the ordering of singlet and triplet states can be reduced or reversed leading to magnetic effects. Other possible sources of magnetism in Oxyhemoglobin will also be discussed. 1. K. Nagamine et al. Proc. Japan. Acad. B-Physics 83, 120 (2007); 2. S.R. Badu et al. Reported at Third Joint HFI-NQI International Conference, CERN, Geneva, September 2010.

12:15PM Z42.00006 Branched Polymer Models and the Mechanism of Multilayer Film Buildup, PRADEEP WADUGE, DHAN KHADKA, DONALD HAYNIE, University of South Florida — The “in and out diffusion” hypothesis does not provide a sufficient explanation of the exponential buildup displayed by some polyelectrolyte multilayer film systems. Here, we report initial tests of an alternative view, on which the completion of each adsorption cycle results in an increase in the number of polymer binding sites on the film surface. Polycationic dendrimeric peptides, which can potentially bind several oppositely-charged peptides each, have been designed, synthesized and utilized in comparative film buildup experiments. Material deposited, internal film structure and film surface morphology have been studied by ultraviolet spectroscopy (UVS), circular dichroism spectroscopy (CD), quartz crystal microbalance (QCM) and atomic force microscopy (AFM). Polycations tended to contribute more to film buildup than did polyanions on quartz but not on gold. Increasing the number of branches in the dendrimeric peptides from 4 to 8 reproducibly resulted in an increase in the film growth rate on quartz but not on gold. Peptide backbones tended to adopt a β -strand conformation on incorporation into a film. Thicker films had a greater surface roughness than thin films. The data are consistent with film buildup models in which the average number of polymer binding sites will increase with each successive adsorption cycle in the range where exponential growth is displayed.

12:27PM Z42.00007 Reduction of Scattered Light by Müller Cells in the Human Retina, OLIVER BENDIX, RAGNAR FLEISCHMANN, THEO GEISEL, MPI for Dynamics and Self-Organization — It is a long standing question why in the mammalian eye photoreceptors are positioned at the back of the retina, forcing photons to travel through various neuronal layers of the retina before the light-sensitive rods and cones can detect them. Recent studies suggest that certain retinal glial cells—called Müller cells (MCs)—play an important role in answering that question. It has been experimentally shown that MCs extracted from the retina can act as optical fibers [1]. To understand the light guiding properties of the MC in the natural fluctuating optical environment, we developed a model to analyze the light reflection and transmission of MCs embedded in a random medium neuronal tissue. With these quantities and a simplified geometrical eye model we study how light is scattered in the eye. We found that MCs can lead to a substantial increase of the signal-to-noise ratio (SNR), the ratio of the intensity of direct incident light at a photoreceptor to the intensity of back-scattered light from other areas of the retina. The SNR is most pronounced in the vicinity of the fovea and can be more than an order of magnitude.

[1] Franze et. al., Proc Natl Acad Sci USA, 2007, 104, 8287-8292.

12:39PM Z42.00008 Quantifying the deformation of the red blood cell skeleton in shear flow¹, ZHANGLI PENG, Massachusetts Institute of Technology, QIANG ZHU, University of California San Diego — To quantitatively predict the response of red blood cell (RBC) membrane in shear flow, we carried out multiphysics simulations by coupling a three-level multiscale approach of RBC membranes with a Boundary Element Method (BEM) for surrounding flows. Our multiscale approach includes a model of spectrins with the domain unfolding feature, a molecular-based model of the junctional complex with detailed protein connectivity and a whole cell Finite Element Method (FEM) model with the bilayer-skeleton friction derived from measured transmembrane protein diffusivity based on the Einstein-Stokes relation. Applying this approach, we investigated the bilayer-skeleton slip and skeleton deformation of healthy RBCs and RBCs with hereditary spherocytosis anemia during tank-treading motion. Compared with healthy cells, cells with hereditary spherocytosis anemia sustain much larger skeleton-bilayer slip and area deformation of the skeleton due to deficiency of transmembrane proteins. This leads to extremely low skeleton density and large bilayer-skeleton interaction force, both of which may cause bilayer loss. This finding suggests a possible mechanism of the development of hereditary spherocytosis anemia.

¹This work was supported by the National Heart, Lung and Blood Institute under award number R01HL092793.

12:51PM Z42.00009 Theoretical study of electron transport in DNA, BIKAN TAN, MIROSLAV HODAK, WENCHANG LU, JERRY BERNHOLC, CHIPS/NCSS — Multiple experiments have indicated high conductivity of DNA, but its origin has not yet been satisfactorily explained. In this work, we explore the conductivity of double stranded B-DNA using a nonequilibrium Green's function method based on density-functional theory. The DNA is sandwiched between metallic nanotube leads and we investigate the effect of various linkers connecting the DNA to the leads. Our results show that the alkane linker, $(CH_2)_n$, which is often used in experiments, dramatically decreases the conductivity due to its large band gap around the Fermi level. We also find that conductivity can be greatly enhanced by aligning the highest occupied molecule orbital energy of DNA with the Fermi level of the leads by applying a gate bias to the DNA. Finally, we examine the effects of misalignment and mismatches on conductivity of DNA.

Friday, March 2, 2012 11:15AM - 2:15PM –

Session Z43 GSNP DFD: Invited Session: Applications of Jamming 157AB

11:15AM Z43.00001 Robotics using sand, HEINRICH JAEGER, Univ of Chicago — No abstract available.

11:51AM Z43.00002 Shocks in fragile matter, VINCENZO VITELLI, Instituut Lorentz for Theoretical Physics — Non-linear sound is an extreme phenomenon typically observed in solids after violent explosions. But granular media are different. Right when they unjam, these fragile and disordered solids exhibit vanishing elastic moduli and sound speed, so that even tiny mechanical perturbations form supersonic shocks. Here, we perform simulations in which two-dimensional jammed granular packings are continuously compressed, and demonstrate that the resulting excitations are strongly nonlinear shocks, rather than linear waves. We capture the full dependence of the shock speed on pressure and compression speed by a surprisingly simple analytical model. We also treat shear shocks within a simplified viscoelastic model of nearly-isostatic random networks comprised of harmonic springs. In this case, anharmonicity does not originate locally from nonlinear interactions between particles, as in granular media; instead, it emerges from the global architecture of the network. As a result, the diverging width of the shear shocks bears a nonlinear signature of the diverging isostatic length associated with the loss of rigidity in these floppy networks.

12:27PM Z43.00003 Controlling the jamming transition of sheared hard spheres, THOMAS HAXTON, Lawrence Berkeley National Laboratory — Many applications require understanding how disordered materials flow under an external load such as a shear stress. Since external loads drive systems out of equilibrium, their behavior cannot be described solely in terms of equilibrium parameters like temperature and pressure. However, simulations and experiments show that sheared spherical particles possess an *effective* temperature that relates low-frequency fluctuations of various observable quantities to their associated response functions. Here, we show that the mobility of a mixture of sheared hard spheres is largely controlled by the dimensionless ratio of effective temperature to pressure, $T_{\text{eff}}/p\sigma^3$, where σ is the sphere diameter. We define the effective temperature as the consistent value that relates the amplitudes of low-frequency shear stress and density fluctuations to their associated response functions. We find that the relaxation time τ characterizing the mobility depends on $T_{\text{eff}}/p\sigma^3$ according to two distinct mechanisms in two distinct regimes. In the *solid response* regime, the behavior at fixed packing fraction ϕ satisfies $\tau\dot{\gamma} \propto \exp(-c\rho\sigma^3/T_{\text{eff}})$, where $\dot{\gamma}$ is the strain rate and c depends weakly on ϕ , suggesting that the effective temperature controls the average local yield strain. In the *fluid response* regime, τ depends on $T_{\text{eff}}/p\sigma^3$ as it depends on $T/p\sigma^3$ in equilibrium. This regime comprises a large part of the hard-sphere jamming phase diagram including both near-equilibrium conditions where T_{eff} is similar to the kinetic temperature T_{kin} and far-from-equilibrium conditions where $T_{\text{eff}} \neq T_{\text{kin}}$. In particular, the dynamic jamming transition is largely controlled by the fluid-response mechanism; like equilibrium hard spheres, sheared hard spheres can flow only if low-frequency fluctuations are large enough compared to the pressure. By presenting our results in terms of the dimensionless jamming phase diagram, we show how these mechanisms likely apply to systems with soft repulsive interactions.

1:03PM Z43.00004 Density-Temperature-Softness Scaling of the Dynamics of Glass-forming Soft-sphere Liquids¹, MAGDALENO MEDINA-NOYOLA, Instituto de Física, Universidad Autónoma de San Luis Potosí — We employ the principle of dynamic equivalence between soft-sphere and hard-sphere fluids [Phys. Rev. E **68**, 011405 (2003); Phys. Rev. Lett. **107**, 155701 (2011)] to describe the interplay of the effects of varying the density n , the temperature T , and the softness (characterized by a softness parameter ν^{-1}) on the dynamics of glass-forming soft-sphere liquids in terms of simple scaling rules. The main prediction is the existence of a dynamic universality class associated with the hard sphere fluid, constituted by the soft-sphere systems whose dynamic parameters, such as the α -relaxation time and the long-time self-diffusion coefficient, depend on n , T , and ν only through the reduced density $n^* \equiv n\sigma_{HS}^3(n, T, \nu)$, where the effective hard-sphere diameter $\sigma_{HS}(n, T, \nu)$ is determined by the Andersen-Weeks-Chandler condition for soft-sphere-hard-sphere structural equivalence. A number of scaling properties observed in recent experiments and simulations involving glass-forming fluids with repulsive short range interactions are found to be a direct manifestation of this general dynamic equivalence principle. The self-consistent generalized Langevin equation (SCGLE) theory of colloid dynamics [Phys. Rev. E **76**, 041504, 062502 (2007)] is shown to accurately capture these scaling rules. The non-equilibrium extension of this theory [Phys. Rev. E **82**, 061503, 061504 (2010)] is employed to describe the manifestation of this scaling on the aging of instantaneously-quenched soft-sphere liquids.

¹Work supported by the Consejo Nacional de Ciencia y Tecnología (CONACYT, México), through Grants No. 84076 and 132540, and through the Red Temática de Materia Condensada Blanda.

1:39PM Z43.00005 Active Jamming: Self-propelled particles at high density¹, SILKE HENKES, Syracuse University — What determines the mechanical properties of dense collections of active particles? The answer to this question is highly relevant to a wide range of physical and biological phenomena from tissue formation to the dynamics of vibrated granular layers. We present a numerical study of the phases and dynamics of a dense collection of self-propelled particles with soft repulsive interactions and polar alignment in a two-dimensional confined geometry. The phase diagram consists of a polar liquid phase at low packing fraction and high self-propulsion speed, and an active jammed phase at high density and low self-propulsion speed. The liquid phase exhibits local alignment and giant number fluctuations typical of the Vicsek class of models. The dynamics of the jammed phase is dominated by oscillations along the low frequency modes of the underlying packing. We show analytically that at long times the energy is carried entirely by the lowest available excitations of the system. Recent experiments on epithelial cell monolayers using force traction microscopy have revealed stress distributions that resemble those observed in granular materials. We measure and compare the local stresses in our active system, with added attraction, to both granular materials and the tissue experiments.

¹This work was done in collaboration with Yaouen Fily and M. Cristina Marchetti and supported by the NSF through grants DMR-0806511 and DMR-1004789. The computations were carried out on SUGAR, a cluster supported by NSF-PHY-1040231.

Friday, March 2, 2012 11:15AM - 2:15PM –
Session Z46 DPOLY DBIO: Invited Session: Self-Assembly of Proteins: From Capsids to Crystals 160AB

11:15AM Z46.00001 Experimental and theoretical studies of capsid self-assembly, ADAM ZLOTNICK, Indiana University — No abstract available.

11:51AM Z46.00002 Theoretical approach to crystallization: foundations and application to proteins¹, JAMES LUTSKO, Center for Nonlinear Phenomena and Complex Systems, Universite Libre de Bruxelles — A fundamental issue in the modern study of phase transitions is the description of the process of nucleation, i.e. the choices of nucleation pathways. Proteins, in particular, are well-known to sometimes crystallize by passing through a meta-stable amorphous state and simulation and theory have shown that this is also true of many other systems. The issue also arises in the important case of polymorphic materials. In all cases, the goal is to understand which pathway is favored and how this is affected by the external control parameters. In this talk, I discuss a theoretical description of nucleation that allows for the direct determination of nucleation pathways and of their relative probability of realization that takes into account both thermodynamics and kinetic effects. It is based on a formulation of nucleation as a fundamentally non-equilibrium process and fully incorporates the effect of free-energy landscapes, determined e.g. via Density Functional Theory, in a consistent manner.

¹This work was supported in part by the European Space Agency under contract number ESA AO-2004-070.

12:27PM Z46.00003 Elasticity Theory of Viral Capsids, ROBIJN BRUINSMA¹, Department of Physics and Astronomy, University of California, Los Angeles — The continuum elasticity theory of icosahedral thin shells has been applied with success to shape transitions of the protein shell surrounding the viral genome, the capsid. The talk presents an extension of thin-shell elasticity theory that is applicable to aggregates of *functional biomolecules* at length scales comparable to that of the component molecules themselves. Unlike classical elasticity theory, the stress and strain fields have a network of *mathematical discontinuities* along the interfaces of the proteins, due to the conformational incompatibility of packing proteins as well as to conformational transitions of the proteins. The method is applied to the P-II to EI transition of the protein shell of the virus HK97 driven by hexon skewing. The combination of the intrinsic stresses of icosahedral shells and the conformational pre-stress turns the P-II state into a “critical” state whose shape is independent of the bending and Young’s moduli.

¹In collaboration with Ankush Aggarwal, Department of Aerospace Engineering, UCLA and William Klug, Department of Aerospace Engineering, UCLA.

1:03PM Z46.00004 The Role of Multivalent Counterions in Protein Crystallization¹, FAJUN ZHANG, Institut für Angewandte Physik, Universität Tübingen, Germany — In this talk, I will give an overview of our recent studies on the phase behavior of model globular proteins in solution in the presence of multivalent counterions. We have shown that negatively charged globular proteins at neutral pH in the presence of multivalent counterions undergo a “reentrant condensation (RC)” phase behavior [1,2], i.e. a phase-separated regime occurs in between two critical salt concentrations, $c^* < c^{**}$, giving a metastable liquid-liquid phase separation (LLPS) [3]. This reentrant phase behavior corresponds to an effective charge inversion of proteins as confirmed by zeta-potential measurements and supported by Monte Carlo simulations [1,2]. Crystallization from the condensed regime follows different mechanisms. Near c^* , crystals grow following a classic nucleation and growth mechanism; near c^{**} , the crystallization follows a two-step mechanism, i.e. crystals growth follows a metastable LLPS [3,4]. Nucleation rate is faster from the protein-poor phase than that from the protein-rich phase, which cannot be explained by the recent theories. SAXS measurements demonstrate that protein clusters act as precursors for crystal growth, which reduce the energy barrier of nucleation [4]. X-ray diffraction analyses on the high quality single crystals provide direct evidence of the crystal structure and cation binding sites [3]. The bridging effect of the metal cations explains the cluster formation.

[1] Zhang, F.; et al. *Phys. Rev. Lett.* **2008**, 101, 148101.

[2] Zhang, F.; et al. *Proteins* **2010**, 78, 3450.

[3] Zhang, F.; et al. *J. Appl. Cryst.* **2011**, 44, 755.

[4] Zhang, F.; et al. In preparation.

¹This work is supported by DFG

1:39PM Z46.00005 Self-assembly and Evolution from protein complexes to DNA nanostructures, ARD A. LOUIS, Rudolf Peierls Centre for Theoretical Physics, Oxford, UK — The remarkable ability of biological matter to robustly self-assemble into well defined composite objects excites the imagination, suggesting that these processes could perhaps be emulated through the judicious design of synthetic building blocks. We use statistical mechanics to uncover the design rules for self-assembly into well defined three dimensional composite objects. In Nature, the rules for self-assembly emerge from an evolutionary process. We show how some patterns in protein complexes can be explained by their evolutionary origin [1]. We also introduce a coarse-grained rigid nucleotide model of DNA that reproduces the basic thermodynamics of short strands: duplex hybridization, single-stranded stacking and hairpin formation, and also captures the essential structural properties of DNA: the helical pitch, persistence length and torsional stiffness of double-stranded molecules, as well as the comparative flexibility of unstacked single strands [2]. We apply the model to calculate the detailed free-energy landscape of one full cycle of DNA “tweezers,” a simple machine driven by hybridization and strand displacement. We also study other nanomachines as well as processes such as force-induced melting, cruciform formation and the self-assembly of DNA tetrahedra.

[1] The self-assembly and evolution of homomeric protein complexes Gabriel Villar, et al., *Phys. Rev. Lett.* 102, 118106 (2009)

[2] Structural and thermodynamic properties of a coarse-grained model of DNA, Thomas E. Ouldridge, Ard A. Louis, Jonathan P.K. Doye, *J. Chem. Phys.* 134, 085101 (2011)

Friday, March 2, 2012 11:15AM - 1:51PM –
Session Z47 DPOLY: Self-Assembly and Polymer Composites 160C

11:15AM Z47.00001 Highly piezoelectric Biocompatible and Soft Composite Fibers, ANTAL JAKLI, JASON MORVAN, Kent State University Kent, OH 44242, EBRU BUYUKTANIR, Stark State College, North Canton, OH, 44720, JOHN WEST, Kent State University Kent, OH 44242 — We report the fabrication of highly piezoelectric biocompatible soft fibers containing Barium Titanate (BT) ferroelectric ceramic particles dispersed in electrospun poly lactic acid (PLA). These fibers form mats that have two orders of magnitude larger piezoelectric constant per weight than single crystal barium titanate films. We demonstrate that the observed super-piezoelectricity results from the electrospinning induced polar alignment of the ferroelectric particles and the increased surface area compared to single crystal films. Due to the biocompatibility of PLA that encases the ferroelectric particles, these mats can be applied even in biological applications such as bio-sensors, artificial muscles and energy harvesting devices.

11:27AM Z47.00002 Phase Behavior of Polymer Nanocomposites from Gravity-based Combinatorial Simulations, DONG MENG, SANAT KUMAR, Department of Chemical Engineering, Columbia University — The phase behavior of polymers mixed with nanoparticles, termed nanocomposites, has been of great current interest. Holding the promise of improved engineering properties, the property improvement is critically dependent on the spatial dispersion of nanoparticles, which is controlled by polymer-nanoparticle phase behavior. Enumerating the appropriate phase diagrams, however, still remain outside the realm of most simulation-based methods. The difficulty arises since inserting a large particle into a dense sea of small particles, critically for establishing phase equilibrium, is prohibitively difficult. Here we extend a gravity-based combinatorial method, first devised by Biben et al., and used primarily in the context of pure fluids to circumvent this insertion issue. Our results are validated against available simulations for colloid mixtures, but provide new insight into the phase behavior of polymers and nanoparticles.

11:39AM Z47.00003 Diffusive and re-orientation dynamics in lyotropic gels of self-assembled organic nanotubes, LUTZ WIEGART, Brookhaven National Laboratory, PIERRE WIEGART, CEA-Grenoble, UM5819, INAC-SPrAM, CHIARA CARONNA, SLAC National Accelerator Laboratory — It is known that dispersing lithocholic bile acid (LCA) in aqueous solutions of sodium hydroxide or ammonia leads to the formation of organic nanotubes with well-defined diameters on the nanometer scale. The suspensions appear to be tunable from liquid- to solid-like via the LCA concentration. The length of the tubes is decreasing as a function of temperature, favoring the formation of a phase where the tubes form hexagonally ordered bundles for an appropriate LCA concentration and temperature. In the present study, we have used X-ray Photon Correlation Spectroscopy (XCPS) to probe the diffusive dynamics of the nanotubes in these lyotropic gels under various conditions (concentration, counter ion, temperature). The multispeckle analysis of the coherent scattering pattern reveals domains in the sample with differing diffusive dynamics. The re-orientation process of different domains of nanotube bundles into a preferred parallel alignment has been observed.

11:51AM Z47.00004 Carbon Nanotube Liquid Crystals: Nematic Droplets and Coarsening Dynamics, NATNAEL BEHABTU, Rice University, BOHDAN SENYUK, IVAN SMALYUKH, University of Colorado Boulder, MATTEO PASQUALI, Rice University — On a fundamental basis, carbon nanotubes (CNTs) offer a new model molecule to explore the dynamics and phases of rigid rods and test theories. Their large aspect ratio (100 to 100,000) and persistence length (~ 100 microns) allow exploring the physics of nematic phases with high Frank elastic constant. Moreover, understanding of CNT liquid crystals is key to their rational processing into ordered materials such as fibers. Here we report the formation of elongated nematic droplets of CNTs in chlorosulfonic acid. In nematic droplets, a continuous transition from a homogeneous to bipolar nematic director field is expected theoretically, as a function of droplet volume; yet, experimental determination of such transition has been elusive. We show that CNT nematic droplets display such transition. We study the coarsening dynamics of positive and negative nematic droplets and observe that two or more droplets merge by matching their nematic director. Merging scenarios that lead to defect formation are not observed. Negative tactoids (isotropic phase in liquid crystalline continuum) merge through attractive forces induced by the nematic director distortion with quadrupolar symmetry.

12:03PM Z47.00005 Free volume in a granular nanocomposite, REGHAN J. HILL, AHMAD MOHADDESPOUR, McGill University — Free volume plays a determinative role in the unusual molecular sieving and rheological characteristics of nanocomposites. To help elucidate the nanoparticle influence on polymer-chain packing, we mixed acrylic spheres with aluminum ball-chains and ascertained from measurements of the bulk density the partial molar sphere volume at small but finite sphere volume fractions. This macroscopic mechanical model permits a systematic exploration of how the chain length, sphere size, and mixture composition influence free volume. We show that the nanoparticle radius to the chain loop size is the primary dimensionless parameter that bridges the solvent and continuum scaling regimes. In the intermediate regime, where the inclusion and polymer nanoscales are comparable, the primary sphere-chain interaction increases free volume—up to twice the intrinsic inclusion volume per particle—and the primary sphere-sphere interaction decreases free volume. Comparisons will be made with data gleaned from PALS and the bulk density of molecular nanocomposites reported in the literature.

12:15PM Z47.00006 Molecular packing in bone collagen fibrils prior to mineralization, BENJAMIN HSIAO¹, Stony Brook University, HONG-WEN ZHOU², Stony Brook University, CHRISTIAN BURGER³, BENJAMIN CHU⁴, Stony Brook University, MELVIN J. GLIMCHER⁵, Harvard Medical School — The three-dimensional packing of collagen molecules in bone collagen fibrils has been largely unknown because even in moderately mineralized bone tissues, the organic matrix structure is severely perturbed by the deposition of mineral crystals. During the past decades, the structure of tendon collagen (e.g. rat tail) — a tissue that cannot mineralize in vivo, has been assumed to be representative for bone collagen fibrils. Small-angle X-ray diffraction analysis of the native, uncalcified intramuscular fish bone has revealed a new molecular packing scheme, significantly different from the quasi-hexagonal arrangement often found in tendons. The deduced structure in bone collagen fibrils indicates the presence of spatially discrete microfibrils, and an arrangement of intrafibrillar space to form “channels”, which could accommodate crystals with dimensions typically found in bone apatite.

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12:27PM Z47.00007 Understanding the self-assembly of meso-tetra(4-sulfonatophenyl)porphyrin (H_2TPPS^{4-}) in aqueous solutions¹, JAVORIS HOLLINGSWORTH, ALLISON RICHARD, GRACA VICENTE, PAUL RUSSO, Louisiana State University — The aggregation of meso-tetra(4-sulfonatophenyl)porphyrin (H_2TPPS^{4-}) in phosphate solutions was investigated as a function of pH, concentration, time, ionic strength, and solution preparation (either from dilution of a freshly prepared 2 mM stock or by direct preparation of μM solution concentrations) using a combination of complementary analytical techniques. UV-Vis and fluorescence spectroscopy indicated the formation of staggered, side-by-side (J-type) assemblies. Their size and self-associative behavior was determined using analytical ultracentrifugation and small angle X-ray scattering. Our results indicate that in neutral and basic solutions of H_2TPPS^{4-} , porphyrin dimers and trimers are formed at μM concentrations and in the absence of NaCl to screen any ionic interactions. At these low concentrations and pH 4, the protonated H_4TPPS^{2-} species self-assembles leading to the formation of particularly stable aggregates bearing 25 ± 3 macrocycles. At higher concentrations, these structures further organize or re-organize into tubular, rod-like shapes of various lengths which were imaged by cryogenic and freeze-fracture transmission electron microscopy. Micron-scale fibrillar aggregates were obtained even at μM concentrations at pH 4 when prepared from dilution of a 2 mM stock solution and/or upon addition of NaCl.

¹This research was partially funded by NIH R01 CA098902 and by NSF DMR-1005707.

12:39PM Z47.00008 Self-Assembly of Polystyrene Tethered Hydrophilic POSS/C60 Nanoparticles, XINFEI YU, STEPHEN Z.D. CHENG, Department of Polymer Science, The University of Akron — Self-assembly of nanobuilding block provides unique opportunities to arrange nanoparticles into larger, functional ensembles. Anisotropy or symmetry breaking will lead to the formation of specific hierarchical structures with novel properties. Polymer tethered particle is one of the approaches to break the symmetry of nanobuilding blocks, which are promise to become the elementary building blocks for self-assembled materials. Shape and interactions are two important factors to determine the self-assembly of these molecules. Although a few examples have been reported during the last decade, little is known about ordered self-assembly structures from these anisotropic building blocks in bulk or solution by experiments. To solve this problem, hydrophilic POSS and C60 have been designed and synthesized, to which hydrophobic polystyrene tail(s) was tethered with controlled topology. The designed molecules could form micelles and colloidal particles in solutions. The effects of PS tail length, solvent properties, and molecular topology on self-assembly morphologies have been studied. The designed molecules could form ordered nanophase separation structures in bulk state with the feature sizes of sub-22 nm, which has great potential applications in advanced lithography technologies.

12:51PM Z47.00009 Self-Assembly of Narrowly Dispersed Brush Diblock Copolymers with Domain Spacing more than 100 nm¹, WEIYIN GU, University of Massachusetts Amherst, BENJAMIN SVEINBJORNSSON, California Institute of Technology, SUNG WOO HONG, University of Massachusetts Amherst, ROBERT GRUBBS, California Institute of Technology, THOMAS RUSSELL, University of Massachusetts Amherst — Self-assembled structures of high molecular weight (MW), narrow molecular weight distribution brush block copolymers containing poly(lactic acid) (PLA) and polystyrene (PS) side chains with similar MWs were studied in both the melt and thin films. The polynorbornene-backbone-based brush diblock copolymers containing approximately equal volume fractions of each block self-assembled into highly ordered lamellae with domain spacing over 100 nm, as revealed by SAXS, GISAXS and AFM. The domain size increased approximately linearly with backbone length, which indicated an extended conformation of the backbone in the ordered state. The length of side chains also played a significant role in terms of controlling the domain size. As the degree of polymerization (DP) increased, the symmetric brush diblock copolymers with longer side chains tended to form larger lamellar microdomains in comparison to those that have the same DP but shorter side chains.

¹Funding: NSF-MRESC, DOE

1:03PM Z47.00010 Non-Classical Ordering of Sphere Forming SISO Tetrablock Terpolymers

JINGWEN ZHANG, University of Minnesota, SCOTT SIDES, Tech-X Research Corporation, FRANK BATES, University of Minnesota — ABAC tetrablock terpolymers represent the simplest symmetry breaking multiblock extension of ABC triblocks. The model system poly(styrene-*b*-isoprene-*b*-styrene-*b*-ethylene oxide) (SISO) tetrablock terpolymers were synthesized in relatively monodisperse form and the resulting morphologies were characterized by small-angle X-ray scattering, transmission electron microscopy, differential scanning calorimetry and dynamic mechanical spectroscopy. Two non-classical sphere-based ordered phases have been established in these single component materials with P_6/mmm (simple hexagonal) and P_{42}/mnm (tetragonal sigma phase) symmetry. A third state, tentatively associated with quasicrystalline order, has been identified at temperatures between the hexagonal and sigma phases, which occur at low temperatures, and prior to disordering, respectively. This unusual set of morphologies will be discussed in the context of segregation under the constraints associated with the tetrablock molecular architecture. Self-consistent mean-field theoretical calculations, obtained using the PolySwift++ software package, provide valuable insights into the molecular configurations associated with these morphologies.

1:15PM Z47.00011 Tear rotation in reinforced natural rubber

PAUL SOTTA, BRICE GABRIELLE, ARNAUD VIEYRES, LPMA CNRS/Rhodia, LOIC VANEL, University of Lyon, DIDIER LONG, LPMA CNRS/Rhodia, OLIVIER SANSEAU, Rhodia, PIERRE-ANTOINE ALBOUY, LPS CNRS/Universite Paris-Sud — We analyze the impact of tear rotation, that is, an abrupt instability in the direction of propagation of a notch, on the tensile strength of natural rubber elastomers reinforced with carbon black or precipitated silica, in single edge notched samples stretched at constant velocity. As a consequence of tear rotation, the energy at break increases by a factor of 6 to 8 in some cases. We show how the tensile strength of a test sample is related to the presence of tear rotations and analyze semi-quantitatively this increase in tensile strength, based on energetic arguments, without entering into a detailed description of the elastic strain field in the vicinity of the tear tip. The proposed interpretation is based on the idea that tear rotations create a macroscopic tip radius, which relaxes the local strain (or stress) at the tear tip. Materials reinforced with carbon black or precipitated silica aggregates show similar behavior. The relation to strain-induced crystallization is discussed.

1:27PM Z47.00012 Quantification of Folding in Sheet-like Nanostructures

DURGESH RAI, GREGORY BEAUCAGE, RAMANTH RAMACHANDRAN, SIDDHARTH PRADHAN, University of Cincinnati — Two-dimensional nanostructures are of interest to a wide range of scientists from biologists interested in membranes to polymer scientists producing graphene reinforced nanocomposites. Considering two-dimensional structures as a class of nanomaterials, we could use the sheet thickness and lateral size as structural description. In addition to these parameters, two-dimensional structures are, at times, capable of folding or crumpling, largely depending on the interfacial chemistry and to some extent on thermodynamics. We have studied this crumpling behavior using small-angle neutron and x-ray scattering in a range of nano-materials, specifically, membrane bilayers, graphene oxide, as well as exfoliated nano-sheets of molybdenum sulfide, boron nitride, and tungsten sulfide. A new parameterization of crumpling in these two-dimensional nanostructures will be described with indications of how this quantification can lead to general categories of crumpling behavior that differ in the systems mentioned above. (A helpful discussion with Fyl Pincus assisted with this work.)

1:39PM Z47.00013 Rheology of cube shaped particles in a suspension

RAJESH MALLAVAJULA, DONALD KOCH, LYNDEN ARCHER, Cornell University — The rheological properties of suspensions of Brownian cube-shaped particles are interesting because of the greater increase in the translational freedom caused by layering relative to suspensions of Brownian spheres. Theoretical solutions for a simple shear flow around an isolated cube were obtained using the geometric properties of cubes. Since stress-strain relationship is anisotropic, the suspension viscosity in the limit of zero shear rate can be obtained from the orientational average of the stresslet acting on the cube. The value of intrinsic viscosity was found to be 3.1. Brownian dynamics simulations were carried out with the obtained anisotropic stress relationship to understand hydrodynamic interactions between cubes at low to moderate volume fractions and lubrication hydrodynamic interactions at higher volume fractions. Interesting transitions are observed in rheological properties as the volume fraction of particles in suspension rises above a critical value substantially lower than the minimum close-packing. We have also synthesized model cube-shaped particles with two different chemistries and sizes: Iron oxide, Fe_3O_4 , nanocubes (20nm and 100nm) and hollow Manganese Carbonate ($MnCO_3$) microcubes (1-2microns). $MnCO_3$ microspheres were also synthesized to compare their properties with the cubic particle suspensions. At low particle volume fractions, the experimentally determined intrinsic viscosity for the suspension of cubic particles is in excellent accord with expectations from theory. The talk will also compare results of rheological properties of spheres and cubes for both high and low volume fractions over a range of Peclet numbers.

Friday, March 2, 2012 11:15AM - 1:51PM –

Session Z48 DPOLY DBIO: Focus Session: Statistical Physics of Active Systems Away from Detailed Balance; Motors, Swimmers and All That 161

11:15AM Z48.00001 Mechanical manipulation and bifurcation dynamics of stereociliary bundles

SEUNG JI, LEA FREDRICKSON-HEMSING, ROBIJN BRUINSMA, DOLORES BOZOVIC, UCLA — We propose a numerical model for the mechanical response of hair cells of the inner ear. These mechanically sensitive cells have been described previously using systems of nonlinear differential equations, that captured the main features of the experimental phenomena. Here we extend the study to include the effects of static and time-dependent forcing, and show it to induce transitions across different types of bifurcations. We compare the theory to the experimental measurements of the phase-locked response of spontaneously oscillating hair cells of the bullfrog sacculus, under varying mechanical deflections. For a static deflection, when adaptation phenomena play an important role, the offset generates a critical point where the frequency but not the amplitude vanishes, as opposed to the expected Hopf bifurcation where the amplitude vanishes. On the other hand, for a periodic deflection, mode-locking of the spontaneous oscillations to the drive period can proceed via different types of bifurcations, depending on the degree of detuning. We will present a simple dynamic systems framework that captures the main features of the experimentally observed behavior in the form of an Arnold Tongue.

11:27AM Z48.00002 Towards an active hydrodynamic theory of the metaphase spindle

JAN BRUGUES, DANIEL NEEDLEMAN, Harvard University — The spindle is a dynamic steady-state structure composed of microtubules and a wide range of factors which control microtubule nucleation, growth, and motion. While many of the individual components of the spindle have been studied in detail, it is still unclear how these molecular constituents self-organize into this structure. Here I describe how we are using spatio-temporal correlations of microtubule density and orientation to formulate a continuum coarse grained theory for the spindle. Our results suggest that microtubule turnover plays a crucial role in stabilizing the giant density fluctuations predicted by traditional active hydrodynamic theories.

11:39AM Z48.00003 A phase transition between collective and individual dynamics in suspension of swimming bacteria¹

ANDREY SOKOLOV, IGOR ARONSON, Argonne National Laboratory — We present the experimental study of the onset of collective behavior in suspension of swimming bacteria *Bacillus Subtilis* in a liquid film. The system behavior is analyzed as the average swimming speed is varied in a wide range while the concentration of bacteria is constant. The average swimming speed was controlled by adjusting the concentration of dissolved oxygen in a fluid with bacteria. We obtained phase diagrams for the transition of the system between the state of collective swimming and the disordered state at different conditions.

¹This work was supported by the US DOE, Office of Basic Sciences, contract DEAC02-06CH11357

11:51AM Z48.00004 Chemotaxis of Phoretic Swimmers, SUROPRIYA SAHA, SRIRAM RAMASWAMY, Indian Institute of Science, Bangalore, RAMIN GLOESTANIAN, Rudolf Peierls Centre for Theoretical Physics, University of Oxford — An artificial phoretic swimmer in a uniform bath of reactant propels itself in a direction dictated by the polarity of the enzymatic and mobility patterning on its surface. We have shown that a polar active particle of this type can also orient itself along an imposed gradient of reactant concentration. This amounts to a theoretical demonstration of a phoretic analogue of chemotaxis, that is, the ability of a self-propelled particle to align with respect to, and hence to move up or down, a chemical gradient. The nature of the chemotaxis depends on the shape of the particle, on the distribution of enzymatic sites on its surface, and on the surface mobility. We have also considered the type of motion that arises when the orientation time of the particle becomes comparable to the diffusion time of the cloud of reaction products around it. Lastly, we consider motion arising from the interaction of two or more such chemotactic particles.

12:03PM Z48.00005 Active viscosity of E-Coli suspensions¹, ERIC CLEMENT, JEREMIE GACHELIN, GASTON MINO, HELENE BERTHET, ANKE LINDNER, ANNIE ROUSSELET, PMMH-ESPCI - University Pierre et Marie Curie — Active suspension is the name borne by fluids laden with self-swimming entities such as bacteria, algae or artificial swimmers. Such fluids display emergent constitutive properties differing strongly from those of passive suspensions. Here, we present a recent work, where we measure the viscosity of a wild type E-Coli suspension in the dilute and semi-dilute limits. To this purpose, we use micro-fluidic device build as a Y shape micro-fluidic channel. On one side of the arm, the active suspension is injected and on the other arm, the suspending fluid is injected at the same flow rate. From the position of the interface between the pure fluid and the suspension, we extract the suspension relative viscosity. Varying bacteria density and flow rate, we show a regime specific to active fluids, where the relative viscosity is lower than the viscosity of the suspending viscous fluid. We discuss our results in the perspective of recent theoretical and experimental works.

¹Supported by the CNRS-UMR7636, the PGDG foundation and the SESAME Ile-de-France research program

12:15PM Z48.00006 Molecular Dynamics Study of Self-propelled Droplets on Solid Substrates, MURAT MÜLAYIM, MARCUS MÜLLER, Georg-August Universität — We study, by molecular simulation, the statics and dynamics of chemically driven polymer droplets on regularly and finely corrugated substrates. Droplets are driven by a self-induced wettability gradient, which is formed under the droplet by changing the strength of the polymer-substrate interaction when the polymer get into contact with a reactive substrate with a pre-defined probability. The effect of reaction rate on droplet profile, slip and motion are investigated in the quasi steady-state. Moreover wetting properties of heterogeneous, partially reacted, systems are studied and a connection to experiments in the literature and thin film theoretical results on driven droplets are drawn, via exploring velocity profiles and dissipation mechanisms in the system.

12:27PM Z48.00007 Self-assembled structures in immiscible systems of active, switchable nanocolloids¹, ANTONIO OSORIO-VIVANCO, University of Michigan, IGAL SZLEIFER, Northwestern University, SHARON GLOTZER, University of Michigan — We consider the synthesis and fabrication of active building blocks that can dynamically switch between two or more states and assemble into novel structures. We present novel steady-state structures predicted by computer simulation to assemble in systems of switchable, immiscible building blocks. We discuss the dynamics that stabilize these structures, explore approaches to analyze the dissipative nature of the system, and provide a mapping to experimental colloidal systems where these concepts could be implemented.

¹ Non-Equilibrium Energy Research Center (NERC), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0000989

12:39PM Z48.00008 Collective motion in active solids and active crystals¹, CRISTIAN HUEPE, Unaffiliated, ELISEO FERRANTE, ALI EMRE TURGUT, IRIDIA, CoDe, Université Libre de Bruxelles — We introduce a minimal model for self-propelled particles with strong attraction-repulsion interactions, but no explicit alignment rules, that displays collective polar or rotational motion. We describe a novel elasticity-based mechanism responsible for such collective motion and compute analytically its required conditions in the continuous elastic sheet approximation. By studying the mechanism's dynamics numerically and analytically, we show that it supports collective motion even for finite noise levels if the coupling between individual self-propulsion and elastic modes transfers energy towards larger and larger wavelengths. We hypothesize that this elasticity-based mechanism could provide an alternative explanation for collective motion in some biological groups without explicit alignment interactions, given their natural cohesion.

¹Work partially supported by the National Science Foundation under Grant No. PHY-0848755

12:51PM Z48.00009 Statistics and dynamics in an optical vortex¹, Yael Roichman, Yulia Sokolov, DEREK FRYDEL, Tel Aviv University, DAVID GRIER, New York University, HAIM DIAMANT, Tel Aviv University — When two identical particles are driven along a straight line by an identical force there are no attractions forces between them. Surprisingly, when the same two particles are driven along a ring of light, with identical force, they attract and form a pair. The pairing mechanism is a pure non-equilibrium phenomena and is a result of symmetry breaking due to the path's curvature. We use experiment, simulation and theory to demonstrate and explain this effect. We show that dynamic limit-cycles and structure emerge due to this pseudo-potential in many particle systems, and demonstrate how they depend on temperature and trapping stiffness.

¹This study was supported by the Israel Science Foundation through Grants Numbers 1271/08, 588/06, and 8/10.

1:03PM Z48.00010 Induced Motion by Asymmetric Enzymatic Degradation of Hydrogels, JENNIFER HOU, ADAM COHEN, Harvard University — Biological hydrogels are continuously turned over through secretion and degradation. This non-equilibrium flux is critical to understanding cellular and molecular transport through biogels such as mucus and the extracellular matrix. Gel-digesting enzymes can drastically change the physical and chemical properties of the hydrogel environment. We report that a spatial gradient in the degradation of two gel/enzyme systems—gelatin/trypsin and hyaluronan/hyaluronidase—leads to directional motion of particles embedded in the gel in the direction of higher enzyme concentration. We study the rate at which the degradation front propagates through the gel and the ensuing velocity of the embedded particles, as functions of enzyme and gel concentrations. We propose that asymmetric degradation leads to asymmetric swelling, which transports particles up the enzyme concentration gradient.

1:15PM Z48.00011 Possible mechanisms for initiating macroscopic left-right asymmetry in developing organisms¹, CHRISTOPHER L. HENLEY, RICKY CHACHRA, JIMMY X. SHEN, Cornell Univ. — Systematic left-right (L/R) asymmetry in development –i.e. body axes satisfying a “right-hand rule” – emerges at the organism level out of the microscopic handedness of biological molecules, not by the usual pattern-forming mechanisms of reactions (including regulation) plus diffusion, but rather (at the cell level) from the cytoskeleton and molecular motors – usually in collective two-dimensional states associated with the cell membrane ². I outline possible scenarios we are simulating for (i) snails and C. elegans, from a chiral shearing tendency in the actomyosin layer and/or (ii) for plant cells, from a precession of the nematic order direction in the microtubule array.

¹Supported by DOE

²C. L. Henley, Landau 2008 conference (arxiv:0811.0055)

1:27PM Z48.00012 Activation of nanoscale allosteric protein domain motion revealed by neutron spin echo spectroscopy¹, ZIMEI BU, City College of New York, BELA FARAGO, Institut Laue Langevin, DAVID CALLAWAY, City College of New York — NHERF1 is a multi-domain scaffolding protein that assembles the signaling complexes, and regulates the cell surface expression and endocytic recycling of a variety of membrane proteins. The ability of the two PDZ domains in NHERF1 to assemble protein complexes is allosterically modulated by a membrane-cytoskeleton linker protein ezrin, whose binding site is located as far as 110 angstroms away from the PDZ domains. Here, using neutron spin echo (NSE) spectroscopy, selective deuterium labeling, and theoretical analyses, we reveal the activation of interdomain motion in NHERF1 on nanometer length scales and on sub-microsecond time scales upon forming a complex with ezrin. We show that a much simplified coarse-grained model is sufficient to describe inter-domain motion of a multi-domain protein or protein complex. We expect that future NSE experiments will benefit by exploiting our approach of selective deuteration to resolve the specific domain motions of interest from a plethora of global translational and rotational motions. The results demonstrate that propagation of allosteric signals to distal sites involves the activation of long-range coupled domain motions on submicrosecond time scales, and that these coupled motions can be distinguished and characterized by NSE.

¹NIH 5R01HL086496

1:39PM Z48.00013 Effector CD8⁺ T cells migrate via chemokine-enhanced generalized Lévy walks, EDWARD BANIGAN, Physics & Astronomy, University of Pennsylvania, TAJIE HARRIS, DAVID CHRISTIAN, Pathobiology, University of Pennsylvania, ANDREA LIU, Physics & Astronomy, University of Pennsylvania, CHRISTOPHER HUNTER, Pathobiology, University of Pennsylvania — Chemokines play a central role in regulating processes essential to the immune function of T cells, such as their migration within lymphoid tissues and targeting of pathogens in sites of inflammation. In order to understand the role of the chemokine CXCL10 during chronic infection by the parasite *T. gondii*, we analyze tracks of migrating CD8⁺ T cells in brain tissue. Surprisingly, we find that T cell motility is not described by a Brownian walk, but instead is consistent with a generalized Lévy walk consisting of Lévy-distributed runs alternating with pauses of Lévy-distributed durations. According to our model, this enables T cells to find rare targets more than an order of magnitude more efficiently than Brownian random walkers. The chemokine CXCL10 increases the migration speed without changing the character of the walk statistics. Thus, CD8⁺ T cells use an efficient search strategy to facilitate an effective immune response, and CXCL10 aids them in shortening the average time to find rare targets.

Friday, March 2, 2012 11:15AM - 2:15PM –
Session Z50 DPOLY DFD: Focus Session: Micro and Nano Fluidics IV: Emulsions and Complex Fluids 162B

11:15AM Z50.00001 Active Emulsions: Synchronization of Chemical Oscillators, SETH FRADEN, Brandeis University — We explore the dynamical behavior of emulsions consisting of nanoliter volume droplets of the oscillatory Belousov-Zhabotinsky (BZ) reaction separated by a continuous oil phase. Some of the aqueous BZ reactants partition into the oil leading to chemical coupling of the drops. We use microfluidics to vary the size, composition and topology of the drops in 1D and 2D. Addition of a light sensitive catalyst to the drops and illumination with a computer projector allows each drop to be individually perturbed. A variety of synchronous regimes are found that systematically vary with the coupling strength and whether coupling is dominated by activatory or inhibitory species. In 1D we observe in- and anti-phase oscillations, stationary Turing patterns in which drops stop oscillating, but form spatially periodic patterns of drops in the oxidized and reduced states, and more complex combinations of stationary and oscillatory drops. In 2D, the attractors are more complex and vary with network topology and coupling strength. For hexagonal lattices as a function of increasing coupling strength we observe right and left handed rotating oscillations, mixed oscillatory and Turing states and finally full Turing states. Reaction – diffusion models based on a simplified description of the BZ chemistry and diffusion of messenger species reproduce a number of the experimental results. For a range of parameters, a simplified phase oscillator model provides an intuitive understanding of the complex synchronization patterns.

“Coupled oscillations in a 1D emulsion of Belousov–Zhabotinsky droplets,” Jorge Delgado, Ning Li, Marcin Leda, Hector O. Gonzalez-Ochoa, Seth Fraden and Irving R. Epstein, *Soft Matter*, 7, 3155 (2011).

11:51AM Z50.00002 Double Emulsion Templated Celloidosomes¹, LAURA R. ARRIAGA, Department of Physics and Division of Engineering and Applied Science, Harvard University, Cambridge, MA 02138, SAMANTHA M. MARQUEZ, Maggie L. Walker Governor's School, 1000N. Lombardy St. Richmond, VA 23220, SHIN-HYUN KIM, CONNIE CHANG, JIM WILKING, Department of Physics and Division of Engineering and Applied Science, Harvard University, Cambridge, MA 02138, FRANCISCO MONROY, Department of Physical Chemistry, Complutense University, 28040 Madrid, Spain, MANUEL MARQUEZ, YNano LLC 14148 Riverdowns S. Dr. Midlothian, VA 23113, DAVID A. WEITZ, Department of Physics and Division of Engineering and Applied Science, Harvard University, Cambridge, MA 02138 — We present a novel approach for fabricating celloidosomes®, which represent a hollow and spherical three-dimensional self-assembly of living cells encapsulating an aqueous core. Glass- capillary microfluidics is used to generate monodisperse water-in-oil-in-water double emulsion templates using lipids as stabilizers. Such templates allow for obtaining single but also double concentric celloidosomes. In addition, after a solvent removal step the double emulsion templates turn into monodisperse lipid vesicles, whose membrane spontaneously phase separates when choosing the adequate lipid composition, providing the adequate scaffold for fabricating Janus-celloidosomes. These structures may find applications in the development of bioreactors in which the synergistic effects of two different types of cells selectively adsorbed on one of the vesicle hemispheres may be exploited.

¹Laura R. Arriaga would like to thank Real Colegio Complutense for financial support

12:03PM Z50.00003 Viscoelastic Flow Instabilities of Worm-like Micellar Solutions in Microfluidic Devices, THOMAS OBER, GARETH MCKINLEY, Massachusetts Institute of Technology — Worm-like micellar (WLM) fluids are a unique class of complex fluids whose large deformation rate rheology is not fully understood. By combining mechanical pressure measurements, μ -PIV and spatially-resolved measurements of flow-induced birefringence, we study the behavior of WLM solutions undergoing large deformation rates in microfluidic rectilinear and converging geometries, whose small characteristic dimensions facilitate experiments at high elasticity number (i.e. low inertia). In our experiments, we observe the extensional flow of a shear-banding WLM fluid in a planar hyperbolic contraction. We classify the flow regimes and observe the onset of spatio-temporally unsteady flow often referred to as “elastic turbulence.” We use pressure drop measurements to calculate the apparent extensional viscosity of both Newtonian fluids and WLM fluids. We also investigate the onset of elastically driven instabilities in flows nominally without streamwise curvature in a high aspect ratio straight channel. These latter experiments are aimed at determining if elastically-driven turbulence in dilute polymer solutions can be initiated and sustained in pressure-driven rectilinear flows.

12:15PM Z50.00004 Elastic instability in straight channels, ANNIE COLIN, HUGUES BODIGUEL, JULIEN BEAUMONT, University Bordeaux 1 — Polymer solutions exhibit purely elastic flow instabilities even in the absence of inertia. The almost ubiquitous ingredient of such an elastic instability is the curvature of streamlines: polymers that have been extended along curved streamlines are taken by fluctuations across shear rate gradient in the unperturbed state which, in turn, couples the hoop stresses acting along the curved streamlines to the radial and axial flows and amplifies the perturbation. It has been tacitly assumed for over 30 years that in line with this instability scenario, visco-elastic parallel shear flows are stable, since the streamlines are straight. Recently, Saarloos and coworkers [1] derived a general instability criterion, which shows that these flows invariably exhibit a nonlinear instability. At this stage only a few studies support and validate this analysis [2]. In this work, we take advantage of microfluidic devices and study the flow of highly elastic polymers and surfactant solutions in a straight microchannel located after a constriction. The velocity of the solution is measured using Particle Imaging Velocimetry. The amplitude of the perturbation is controlled by the shape of the constriction. Using such devices, we present a comprehensive flow diagram in the parameter plane amplitude of the perturbation, Weissenberg number. 1/ Bernard Meulenbroek at all J. Non-Newtonian Fluid Mech. 116 (2004) 235–268 2/ Daniel Bonn et al Phys Rev E 84, 045301(R) (2011)

12:27PM Z50.00005 Microfluidic Fabrication of Functional Capsules with ultra-thin membranes¹, SHIN-HYUN KIM, ALIREZA ABBASPOURRAD, DAVID WEITZ, Harvard University — We have developed a new emulsification technique to produce monodisperse double-emulsion drops with an ultra-thin middle layer through a one-step emulsification. A biphasic flow, consisting of sheath of one fluid flowing along the capillary wall and surrounding a second fluid flowing through center of the capillary, is created in a form of either a jet or drops, which is emulsified into double-emulsion drops with ultra-thin middle layer. The ultra-thin middle phases provide stability to the double-emulsion drops by putting the fluid in the middle phase in the lubrication regime. We have employed such stable double-emulsion drops to make functional microcapsules using evaporation-induced consolidation. Simplest form is microcapsules with homogenous membrane. Using biodegradable polymers such as PLA or PLGA as a membrane material, we can achieve a long-term release of various bioactives from the capsules as the membrane degrades by hydrolysis. Heterogeneous membrane can also be prepared by using polymer blends. For example, a polymer blend of PMMA and PLA with small interaction parameter makes heterogeneous structure at nanoscale, while a polymer blend of PS and PLA with large interaction parameter makes their phase separation at one micrometer scale.

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12:39PM Z50.00006 Coupled oscillations in a 1D emulsion of Belousov–Zhabotinsky droplets¹, NING LI, Brandeis University, JORGE DELGADO, University of Guanajuato, HECTOR GONZALEZ OCHOA, San Luis Potosi Institute of Scientific Research and Technology (IPICYT), MARCIN LEDA, Institute of Physical Chemistry (Polish Academy of Science), SETH FRADEN, IRVING EPSTEIN, Brandeis University, BRANDEIS UNIVERSITY TEAM — We experimentally and computationally study the dynamics of interacting oscillating Belousov–Zhabotinsky (BZ) droplets of 100 micron diameter separated by perfluorinated oil and arranged in a one-dimensional array. A microfluidic chip is used for mixing the BZ reactants, forming monodisperse droplets by flow-focusing and directing them into a hydrophobized 100 micron diameter capillary. In order to make quantitative comparison with theory, we use photosensitive Ru(bipy)₃ catalyzed BZ droplets and set both boundary and initial conditions of arrays of small numbers of oscillating BZ droplets with a programmable illumination source. The coupling strength is a function of malonic acid concentration and varying coupling strength leads to the generation of different dynamical attractors. In many cases, simulations agree well with experiments.

¹Funded by MRSEC.

12:51PM Z50.00007 Double emulsion templated monodisperse phospholipid liposomes incorporating Doxorubicin hydrochloride, MINGTAN HAI, University of Science and Technology Beijing/Harvard University, DAVID WEITZ, Harvard University — We present a novel approach for fabricating monodisperse phospholipid liposomes incorporating water soluble anticancer drug Doxorubicin hydrochloride using controlled w/o/w double emulsions as templates. Glass-capillary microfluidics is used to generate monodisperse w/o/w double emulsion templates and double emulsion droplet size is from 20 to 100 μm according to different flow rates. We show that the high uniformity in size and shape of the templates are maintained in the final phospholipid liposomes after a solvent removal step by Nikon eclipse microscopy. The lipid bilayers encapsulating anticancer drug inside is retained after the emulsion drops are converted to vesicles. The liposomes vesicles are promising water soluble anticancer drug delivery vehicles.

1:03PM Z50.00008 Drops of Yield-Stress Liquid Impacting a Solid Surface, QIN XU, HEINRICH JAEGER, James Frank Institute and Department of Physics, The University of Chicago — We use high-speed video to investigate the drop impact process for yield-stress fluids under different initial conditions. Unlike Newtonian fluids, the impact dynamics of yield-stress liquids are greatly affected by their viscoelasticity, which can be attributed to either a surface stress or bulk material properties. To explore these two different mechanisms, we perform impact experiments for two model fluids: liquid metals and particle suspensions, which both exhibit significant yield-stress in rheology. By controlling surface oxidation (for liquid metals) and packing density (for suspensions), we quantitatively vary the yield-stress within several orders of magnitude. In this way, we draw a direct comparison between the two fluids at various impact velocities to clarify the role of different sources of yield stress. Also, we build up an approach to bridge impact dynamics with rheological measurements.

1:15PM Z50.00009 Oscillatory shear of non-colloidal fiber suspensions, ALEXANDRE FRANCESCHINI, EMMANOUELA FILIPPIDI, NYU, Dept Phys, Ctr Soft Matter Res, New York, NY 10003 USA, ELIZABETH GUAZZELLI, Aix Marseille Univ U1, IUSTI, CNRS, UMR Polytech Marseille 6595, F-13453 Marseille 13, France, DAVID PINE, NYU, Dept Phys, Ctr Soft Matter Res, New York, NY 10003 USA — Concentrated suspensions of non-colloidal fibers under slow periodic strain undergo a phase transition from an absorbing state to an active fluctuating state. Fiber trajectories are reversible in the absorbing state and irreversible in the fluctuating state. The activity, measured by the translational diffusivity between successive periods, vanishes in the absorbing state but reaches a finite value in the fluctuating state. We show that the transition is controlled by a collision cross-section, which is a function of the strain amplitude, concentration and fiber orientation. Over the course of an experiment, the activity drives the orientation toward the vorticity, subsequently reducing the cross section. We evaluate the influence of the control parameter decay on the phase transition and then focus on the fluctuating state dynamics.

1:27PM Z50.00010 Dynamics in Semidilute Rod Suspensions, PRAMUKTA KUMAR, DAN BLAIR, JEFFREY URBACH, Department of Physics, Georgetown University — While shear-thinning in semidilute suspensions of rod-like particles has been widely observed, the underlying mechanisms are often unclear. We have developed a model system of fluorescent SU-8 rods suspended in a Glycerol/Ethylene-Glycol solution. This model system exhibits an order of magnitude difference in apparent viscosity at low shear rates as compared to high shear rates while showing no discernible difference in structure. Using a coupled confocal microscope and rheometer instrument along with fiber identification and particle tracking routines, we directly image and quantify the 3D structure and dynamics of our model system under shear flow in order to determine how particle interactions could be generating the observed shear thinning. In particular we look at how interactions modify Jeffery's orbits in semidilute suspensions as compared to the motion of an isolated rod or ellipsoid.

1:39PM Z50.00011 The field effect on local temperature distribution in natural convection in a magnetic fluid , JUN HUANG, WEILI LUO, University of Central Florida — Previously, we have reported the magnetic field effect on the flow front of natural convection in magnetic fluids. In this work we present the local temperature distribution as a function of applied field, from which flow patterns are constructed. We will also report, and discuss the possible mechanism for, a crossover field, above which the field dependence diminishes.

1:51PM Z50.00012 Mixing dynamics of slurry in rotating drum , KIWING TO¹, Institute of Physics, Academia Sinica, CHUN CHUNG LIAO², SHU-SAN HSIAU³, Department of Mechanical Engineering, National Central University — We study the effects of interstitial fluid viscosity on the rates of dynamical processes in a thin rotating drum half-filled with monodisperse glass beads. The rotating speed is fixed at the rolling regime such that a continuously flowing layer of beads persists at the free surface. While the characteristic speed of a bead in the flowing layer decreases with the fluid viscosity, the mixing rate of the beads is found to increase with the fluid viscosity. These findings are consistent to a simple model related to the thickness of the flowing layer.

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2:03PM Z50.00013 Bubble production using a Non-Newtonian fluid in microfluidic flow focusing device , YI-LIN WANG, National Taiwan University of Science and Technology, THOMAS WARD, CHRISTINE GRANT, North Carolina State University — We experimentally study the production of micrometer-sized bubbles using microfluidic technology and a flow-focusing geometry. Bubbles are produced by using a mixture containing aqueous polyacrylamide of concentrations ranging from 0.01-0.10% by weight and several solution also containing a sodium-lauryl-sulfate (SLS) surfactant at concentrations ranging 0.01-0.1% by weight. The fluids are driven by controlling the static pressure above a hydrostatic head of the liquid while the disperse phase fluid static pressure is held constant (air). In the absence of surfactant the bubble production is discontinuous. The addition of surfactant stabilizes the bubble production. In each type of experiment, the bubble length ℓ , velocity U and production frequency ω are measured and compared as a function of the inlet pressure ratio. The bubbles exhibit a contraction in their downstream length as a function of the polymer concentration which is investigated.